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Convergence of split-step generalized-Laguerre–Fourier–Hermite methods for Gross–Pitaevskii equations with rotation term

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Abstract A convergence analysis for time-splitting generalized-Laguerre–Fourier–Hermite pseudo-spectral methods applied to time-dependent Gross–Pitaevskii equations with rotation term is given. The space discretization combines the generalized-Laguerre–Fourier spectral method with respect to the (x, y)-variables and the Hermite spectral method with respect to the z-direction. For the time integration exponential operator splitting methods are studied. Under suitable regularity requirements on the problem data spectral accuracy of the spatial discretization and the nonstiff convergence order for the time integrator is retained. Essential ingredients are a general functional analytic framework of abstract nonlinear evolution equations and fractional power spaces defined by the principal linear part, Sobolev-type inequalities in curved rectangles, and results on the asymptotical distribution of the nodes and weights associated with Gauß–Laguerre quadrature. The theoretical convergence estimate is confirmed by a numerical example.

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1 Introduction

Scope of applications. The realization of dilute gaseous Bose–Einstein condensation in physical experiments has received great attention among physicists to date. Current research activities aim for a better understanding of the creation and evolution of quantized vortices in rotating Bose–Einstein condensates. The extensive experimental work is supplemented by mathematical investigations, see for instance [7,8] and references therein.

Time-dependent Gross–Pitaevskii equation with rotation term. At temperatures significantly below the critical temperature of the condensate, the time evolution of a rotating condensate is mathematically described by a nonlinear Schrödinger equation for the macroscopic wave function $\psi : \mathbb{R}^3 \times [0,T] \to \mathbb{C} : (\mathbf{x},t) = (x,y,z,t) \mapsto \psi(\mathbf{x},t)$, the time-dependent Gross–Pitaevskii equation with additional rotation term

$$\mathrm{i}\,\partial_t \psi(\mathbf{x},t) = \big(- \tfrac{1}{2} \Delta + V_{\mathrm{ext}}(\mathbf{x}) - \Omega L_z + \beta\,|\psi(\mathbf{x},t)|^2 \big)\,\psi(\mathbf{x},t), \tag{1a}$$

subject to asymptotic boundary conditions and an initial condition. Here, $V_{\mathrm{ext}} : \mathbb{R}^3 \to \mathbb{R}$ denotes an external real-valued potential, which we assume to comprise a scaled harmonic potential that is symmetric with respect to the (x,y)-components and an additional sufficiently regular potential $V : \mathbb{R}^3 \to \mathbb{R}$, and $\beta \in \mathbb{R}$ the interaction constant. The rotation term involves the angular momentum rotation speed $\Omega \in \mathbb{R}$ and the angular momentum operator

$$L_z = -\,\mathrm{i}\big(x\,\partial_y - y\,\partial_x\big). \tag{1b}$$

For our purposes it is useful to employ the following formulation of (1a) as abstract evolution equation

$$\mathrm{i}\,\tfrac{\mathrm{d}}{\mathrm{d}t} u(t) = A u(t) + B[u(t)]\,u(t), \qquad 0 \le t \le T, \tag{1c}$$

where the linear differential operator A is given by

$$(Au)(\mathbf{x}) = \big(- \tfrac{1}{2} \Delta + \tfrac{1}{2}\,\gamma\,(x^2+y^2) + \tfrac{1}{2}\,\gamma_z\,z^2 - \Omega L_z \big)\,u(\mathbf{x}) \tag{1d}$$

with weights $\gamma, \gamma_z > 0$ and B denotes a nonlinear multiplication operator

$$B = B[u] = V + \beta\,|u|^2, \tag{1e}$$

acting on a function $v : \mathbb{R}^3 \to \mathbb{C}$ as

$$(B[u]v)(\mathbf{x}) = V(\mathbf{x})\,v(\mathbf{x}) + \beta\,|u(\mathbf{x})|^2\,v(\mathbf{x}). \tag{1f}$$

A discussion of the physical background of this model and numerical investigation of its solution behavior is found for instance in [3], see also references given therein. The favourable behavior of higher-order time-splitting pseudo-spectral methods in accuracy, efficiency, and the conservation of physically relevant quantities is confirmed by a variety of contributions; to mention a few we refer to the works [3,4,6]. As detailed below, for our purposes it is useful to first study the Gross–Pitaevskii equation in two space dimensions, where $\mathbf{x} = (x, y)$ and (1d) is replaced by

$$(Au)(\mathbf{x}) = \big(- \tfrac{1}{2} \Delta + \tfrac{1}{2} \gamma \, (x^2 + y^2) - \Omega L_z \big) \, u(\mathbf{x}). \tag{1g}$$

Convergence analysis for full discretizations. In this paper our main objective is to provide a convergence analysis for time-splitting generalized-Laguerre–Fourier–Hermite pseudo-spectral methods applied to Gross–Pitaevskii equations with rotation term in order to justify the use of this class of numerical methods for practical applications and to identify the regularity requirements on the data of the problem. The space discretization relies on a combination of the generalized-Laguerre–Fourier spectral method with respect to the (x, y)-variables and the Hermite spectral method with respect to the z-direction, and the time integration is realized by exponential operator splitting methods. Our approach extends the works [9,15] and the recent contributions [12, 20]. In the seminal work [15] the stability and error behavior of the second-order Strang splitting method for nonlinear Schrödinger equations such as the cubic Schrödinger equation is analyzed, and a convergence analysis for full discretizations of the Gross–Pitaevskii equation (without rotation term) based on the Hermite pseudo-spectral method and the Strang splitting method is given in [9]. The error behavior of high-order splitting methods applied to nonlinear evolutionary Schrödinger equations has been studied in [12] for semi-discretizations in time. Our approach is closely related to [20], where a convergence analysis for high-order time-splitting pseudo-spectral methods (Fourier, Sine, Hermite) applied to the Gross–Pitaevskii equation is given. However, the complexity of the spectral discretization considered in this work implies a considerable increase of technicalities. For this reason, we focus on the case of two space dimensions as this constitutes the main challenge and briefly comment on the extension to three space dimensions based on Hermite basis functions for the z-variable. Moreover, for the sake of simplicity, we include a detailed analysis for the Strang splitting method and indicate the generalization to high-order splitting methods, since this is then in the lines of [12,20].

Outline. The present manuscript has the following structure. In Section 2, we collect prerequisites related to the spatial discretization by the generalized-Laguerre–Fourier pseudo-spectral method. In particular, this includes fundamental results on scaled generalized-Laguerre functions such as relations for partial derivatives of the basis functions involving four basis functions with neighboring indices (Lemma 1), Sobolev-type inequalities on curved rectangles (Lemma 5), the asymptotical distribution of the Gauß–Laguerre quadrature nodes and weights, and bounds for the spectral interpolant (Lemma 7).

A general functional analytic framework [20] exposes the similarities between different pseudo-spectral methods. Section 3 is devoted to the derivation of the convergence result for the Strang-splitting generalized-Laguerre–Fourier pseudo-spectral method applied to the time-dependent Gross–Pitaevskii equations with rotation term. The theoretical error estimate is finally illustrated by a numerical example in Section 4.

2 Fundamental preliminaries

In this section, we deduce basic auxiliary results that are related to the generalized-Laguerre–Fourier–Hermite pseudo-spectral method for the spatial discretization of Gross–Pitaevskii equations with rotation term. Henceforth, we employ standard notations and results for Lebesgue and Sobolev spaces, see also [2]. For notational convenience, we do not distinguish between the spatial variables and the associated multiplication operators; for instance, we write xf for the function $x \mapsto xf(x,y)$.

2.1 Scaled generalized-Laguerre functions

Generalized-Laguerre polynomials. The generalized-Laguerre polynomials $(k, m = 0, 1, 2, \dots)$

$$L_k^m(r) = \tfrac{1}{k!}\, r^{-m}\, \mathrm{e}^{r}\, \tfrac{\mathrm{d}^k}{\mathrm{d}r^k}\big(\mathrm{e}^{-r}\, r^{k+m}\big) \tag{2a}$$

obey the differential equation $(k, m = 0, 1, 2, \dots)$

$$\big(r\, \tfrac{\mathrm{d}^2}{\mathrm{d}r^2} + (m+1-r)\, \tfrac{\mathrm{d}}{\mathrm{d}r}\big)\, L_k^m(r) + k L_k^m(r) = 0$$

and the orthogonality relations $(k, l, m = 0, 1, 2, \dots)$

$$\int_0^\infty r^m\, \mathrm{e}^{-r}\, L_k^m(r)\, L_l^m(r)\, \mathrm{d}r = C_k^m\, \delta_{kl}, \qquad C_k^m = \prod_{j=1}^{m} (k+j), \tag{2b}$$

cf. for example [1,17] or [19, Section 7.1]. Furthermore, they satisfy the relations $(k = 1, 2, \dots,\ m = 0, 1, 2, \dots)$

$$L_k^m(r) = L_k^{m+1}(r) - L_{k-1}^{m+1}(r), \tag{2c}$$

$$\tfrac{\mathrm{d}}{\mathrm{d}r} L_k^m(r) = -\, L_{k-1}^{m+1}(r), \tag{2d}$$

and $(k = 0, 1, 2, \dots,\ m = 1, 2, \dots)$

$$r L_k^m(r) = -\,(k+1) L_{k+1}^{m-1}(r) + (k+m) L_k^{m-1}(r), \tag{2e}$$

$$m L_k^m(r) = r L_k^{m+1}(r) + (k+1) L_{k+1}^{m-1}(r). \tag{2f}$$

Scaled generalized-Laguerre and related functions. Following [3], the scaled generalized-Laguerre functions involving a positive weight $\gamma > 0$ are given by $(k, m = 0, 1, 2, \dots)$

$$\widetilde{L}_{km}^{\gamma}(r) = \frac{1}{\sqrt{\pi C_k^m}}\, \gamma^{(m+1)/2}\, r^m\, \mathrm{e}^{-\gamma r^2/2}\, L_k^m(\gamma r^2). \tag{3}$$

The related complex-valued functions $\mathcal{L}_{km}^{\gamma} : \mathbb{R}^2 \to \mathbb{C}$ are defined in terms of polar coordinates

$$\mathcal{L}_{km}^{\gamma}(r\cos\vartheta, r\sin\vartheta) = \widetilde{L}_{k,|m|}^{\gamma}(r)\,\mathrm{e}^{im\vartheta}, \quad (k,m) \in \mathcal{M}, \tag{4a}$$

where the set of valid indices is introduced for convenience

$$\mathcal{M} = \{(k,m) : k = 0, 1, 2, \dots,\ m = 0, \pm 1, \pm 2, \dots\}.$$

Clearly, in Cartesian coordinates it follows

$$\mathcal{L}_{km}^{\gamma}(x,y) = \widetilde{L}_{k,|m|}^{\gamma}\big(\sqrt{x^2+y^2}\big)\left(\frac{x + \mathrm{i}\,y}{\sqrt{x^2+y^2}}\right)^m, \quad (k,m) \in \mathcal{M}. \tag{4b}$$

Pointwise multiplication and partial derivatives. The following auxiliary result is needed in order to establish relations between the norm in Sobolev and fractional power spaces. We note that the amount of technicalities in the proof is significantly reduced by the consideration of $\mathcal{L}_{km}^{\gamma} : \mathbb{R} \to \mathbb{C}$ as a complex function $\mathcal{L}_{km}^{\gamma} : \mathbb{C} \to \mathbb{C}$.

Lemma 1 *The following identities are valid for all* $(k,m) \in \mathcal{M}$ *where* $\mathcal{L}_{-1,m\pm 1}^{\gamma} = 0$*:*

$$x\,\mathcal{L}_{km}^{\gamma} = \begin{cases} -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m+1}^{\gamma} + \frac{\sqrt{k+m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^{\gamma} \\ \quad + \frac{\sqrt{k+m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^{\gamma} - \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m-1}^{\gamma}, & m > 0, \\ -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,+1}^{\gamma} + \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,-1}^{\gamma} \\ \quad + \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,+1}^{\gamma} - \frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,-1}^{\gamma}, & m = 0, \\ -\frac{\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m-1}^{\gamma} + \frac{\sqrt{k-m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^{\gamma} \\ \quad + \frac{\sqrt{k-m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^{\gamma} - \frac{\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m+1}^{\gamma}, & m < 0, \end{cases} \tag{5a}$$

$$y\,\mathcal{L}_{km}^{\gamma} = \begin{cases} +\frac{\mathrm{i}\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m+1}^{\gamma} + \frac{\mathrm{i}\sqrt{k+m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^{\gamma} \\ \quad - \frac{\mathrm{i}\sqrt{k+m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^{\gamma} - \frac{\mathrm{i}\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m-1}^{\gamma}, & m > 0, \\ -\frac{\mathrm{i}\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,+1}^{\gamma} + \frac{\mathrm{i}\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,-1}^{\gamma} \\ \quad - \frac{\mathrm{i}\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,+1}^{\gamma} + \frac{\mathrm{i}\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,-1}^{\gamma}, & m = 0, \\ -\frac{\mathrm{i}\sqrt{k}}{2\sqrt{\gamma}}\mathcal{L}_{k-1,m-1}^{\gamma} - \frac{\mathrm{i}\sqrt{k-m}}{2\sqrt{\gamma}}\mathcal{L}_{k,m+1}^{\gamma} \\ \quad + \frac{\mathrm{i}\sqrt{k-m+1}}{2\sqrt{\gamma}}\mathcal{L}_{k,m-1}^{\gamma} + \frac{\mathrm{i}\sqrt{k+1}}{2\sqrt{\gamma}}\mathcal{L}_{k+1,m+1}^{\gamma}, & m < 0, \end{cases} \tag{5b}$$

$$\partial_x \mathcal{L}^\gamma_{km} = \begin{cases} -\frac{\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,m+1} + \frac{\sqrt{\gamma(k+m)}}{2}\mathcal{L}^\gamma_{k,m-1} \\ \quad -\frac{\sqrt{\gamma(k+m+1)}}{2}\mathcal{L}^\gamma_{k,m+1} + \frac{\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k+1,m-1}, & m>0, \\ -\frac{\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,+1} - \frac{\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k,-1} \\ \quad -\frac{\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k,+1} - \frac{\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,-1}, & m=0, \\ -\frac{\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,m-1} + \frac{\sqrt{\gamma(k-m)}}{2}\mathcal{L}^\gamma_{k,m+1} \\ \quad -\frac{\sqrt{\gamma(k-m+1)}}{2}\mathcal{L}^\gamma_{k,m-1} + \frac{\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k+1,m+1}, & m<0, \end{cases} \tag{5c}$$

$$\partial_y \mathcal{L}^\gamma_{km} = \begin{cases} \frac{\mathrm{i}\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,m+1} + \frac{\mathrm{i}\sqrt{\gamma(k+m)}}{2}\mathcal{L}^\gamma_{k,m-1} \\ \quad +\frac{\mathrm{i}\sqrt{\gamma(k+m+1)}}{2}\mathcal{L}^\gamma_{k,m+1} + \frac{\mathrm{i}\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k+1,m-1}, & m>0, \\ \frac{\mathrm{i}\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,+1} - \frac{\mathrm{i}\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k,-1} \\ \quad +\frac{\mathrm{i}\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k,+1} - \frac{\mathrm{i}\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,-1}, & m=0, \\ -\frac{\mathrm{i}\sqrt{\gamma k}}{2}\mathcal{L}^\gamma_{k-1,m-1} - \frac{\mathrm{i}\sqrt{\gamma(k-m)}}{2}\mathcal{L}^\gamma_{k,m+1} \\ \quad -\frac{\mathrm{i}\sqrt{\gamma(k-m+1)}}{2}\mathcal{L}^\gamma_{k,m-1} - \frac{\mathrm{i}\sqrt{\gamma(k+1)}}{2}\mathcal{L}^\gamma_{k+1,m+1}, & m<0. \end{cases} \tag{5d}$$

Proof We consider the complex functions $(k, m = 0, 1, 2, \dots)$

$$f^\gamma_{km}(z) = z^m\, \mathrm{e}^{-\gamma|z|^2/2}\, L^m_k(\gamma|z|^2).$$

With $z = x + \mathrm{i}\, y = r\mathrm{e}^{\mathrm{i}\vartheta}$ it holds

$$\mathcal{L}^\gamma_{km}(x,y) = \begin{cases} \frac{1}{\sqrt{\pi C^m_k}}\, \gamma^{(m+1)/2}\, f^\gamma_{km}(z), & m \ge 0, \\ \frac{1}{\sqrt{\pi C^{|m|}_k}}\, \gamma^{(|m|+1)/2}\, \bar{f}^\gamma_{km}(z), & m<0, \end{cases}$$

where $\bar{f}^\gamma_{km}(z) = \bar{z}^m \mathrm{e}^{-\gamma|z|^2/2} L^m_k(\gamma|z|^2)$ is the complex conjugate of $f^\gamma_{km}(z)$.

Using (2c) we obtain

$$\begin{aligned} z f^\gamma_{km}(z) &= \mathrm{e}^{-\gamma|z|^2/2}\left(z^{m+1} L^m_k(\gamma|z|^2)\right) \\ &= \mathrm{e}^{-\gamma|z|^2/2}\left(z^{m+1} L^{m+1}_k(\gamma|z|^2) - z^{m+1} L^{m+1}_{k-1}(\gamma|z|^2)\right) \\ &= f^\gamma_{k,m+1}(z) - f^\gamma_{k-1,m+1}(z), \end{aligned} \tag{6a}$$

and, using (2e),

$$\begin{aligned} \bar{z} f^\gamma_{km}(z) &= \tfrac{1}{\gamma}\, \mathrm{e}^{-\gamma|z|^2/2}\left(\gamma|z|^2 z^{m-1} L^m_k(\gamma|z|^2)\right) \\ &= \mathrm{e}^{-\gamma|z|^2/2}\left(-\tfrac{k+1}{\gamma}\, z^{m-1}\, L^{m-1}_{k+1}(\gamma|z|^2) + \tfrac{k+m}{\gamma}\, z^{m-1}\, L^{m-1}_k(\gamma|z|^2)\right) \\ &= -\tfrac{k+1}{\gamma}\, f^\gamma_{k+1,m-1}(z) + \tfrac{k+m}{\gamma}\, f^\gamma_{k,m-1}(z). \end{aligned} \tag{6b}$$

With $x = \frac{1}{2}(z + \bar{z})$ and $y = -\frac{1}{2}\mathrm{i}(z - \bar{z})$ the relations (5a) and (5b) follow from (6a) and (6b) in the case $m \geq 1$. The cases $m = 0$ and $m < 0$ are proven similarly.

In order to prove (5c) and (5d) we consider the differential operators

$$\partial_z = \tfrac{1}{2}(\partial_x - \mathrm{i}\,\partial_y), \quad \partial_{\bar{z}} = \tfrac{1}{2}(\partial_x + \mathrm{i}\,\partial_y).$$

These can be applied as if z and $\bar{z}$ were independent variables, see [18, Section 1.4]. Using the product rule for the differential operator ∂_z and the equation (2d) for the derivative of the Laguerre polynomial L_k^m we obtain

$$\begin{aligned}\partial_z f_{km}^\gamma(z) &= \partial_z\left(z^m \mathrm{e}^{-\gamma z\bar{z}/2} L_k^m(\gamma z\bar{z})\right)\\ &= \mathrm{e}^{-\gamma|z|^2/2}\big(m z^{m-1} L_k^m(\gamma|z|^2) - \tfrac{\gamma}{2} z\bar{z} z^{m-1} L_k^m(\gamma|z|^2)\\ &\qquad\qquad - \gamma z\bar{z} z^{m-1} L_{k-1}^{m+1}(\gamma|z|^2)\big).\end{aligned}$$

Here we substitute (2f) to obtain

$$m z^{m-1} L_k^m(\gamma|z|^2) = \gamma z\bar{z} z^{m-1} L_k^{m+1}(\gamma|z|^2) + (k+1) z^{m-1} L_{k+1}^{m-1}(\gamma|z|^2),$$

and further

$$\begin{aligned}\partial_z f_{km}^\gamma(z) = \mathrm{e}^{-\gamma|z|^2/2}\Big(&\gamma z\bar{z} z^{m-1}\big(L_k^{m+1}(\gamma|z|^2) - L_{k-1}^{m+1}(\gamma|z|^2) - \tfrac{1}{2} L_k^m(\gamma|z|^2)\big)\\ &+ (k+1) z^{m-1} L_{k+1}^{m-1}(\gamma|z|^2)\Big),\end{aligned}$$

where we first apply (2c) and then substitute (2e),

$$\tfrac{\gamma}{2} z\bar{z} z^{m-1} L_k^m(\gamma|z|^2) = -\tfrac{k+1}{2} z^{m-1} L_{k+1}^{m-1}(\gamma|z|^2) + \tfrac{k+m}{2} z^{m-1} L_k^{m-1}(\gamma|z|^2),$$

to obtain

$$\begin{aligned}\partial_z f_{km}^\gamma(z) &= \mathrm{e}^{-\gamma|z|^2/2}\big(\tfrac{\gamma}{2} z\bar{z} z^{m-1} L_k^m(\gamma|z|^2) + (k+1) z^{m-1} L_{k+1}^{m-1}(\gamma|z|^2)\big)\\ &= \mathrm{e}^{-\gamma|z|^2/2}\big(\tfrac{k+1}{2} z^{m-1} L_{k+1}^{m-1}(\gamma|z|^2) + \tfrac{k+m}{2} z^{m-1} L_k^{m-1}(\gamma|z|^2)\big)\\ &= \tfrac{k+1}{2} f_{k+1,m-1}^\gamma(z) + \tfrac{k+m}{2} f_{k,m-1}^\gamma(z). \qquad (6c)\end{aligned}$$

Using the product rule for the differential operator $\partial_{\bar{z}}$ together with equation (2d), and then (2c) we have

$$\begin{aligned}\partial_{\bar{z}} f_{km}^\gamma(z) &= \partial_{\bar{z}}\left(z^m \mathrm{e}^{-\gamma z\bar{z}/2} L_k^m(\gamma z\bar{z})\right)\\ &= \mathrm{e}^{-\gamma|z|^2/2}\big(-\tfrac{\gamma}{2} z^{m+1} L_k^m(\gamma|z|^2) - \gamma z^{m+1} L_{k-1}^{m+1}(\gamma|z|^2)\big)\\ &= \mathrm{e}^{-\gamma|z|^2/2}\big(-\tfrac{\gamma}{2} z^{m+1} L_k^{m+1}(\gamma|z|^2) - \tfrac{\gamma}{2} z^{m+1} L_{k-1}^{m+1}(\gamma|z|^2)\big)\\ &= -\tfrac{\gamma}{2} f_{k-1,m+1}^\gamma(z) - \tfrac{\gamma}{2} f_{k,m+1}^\gamma(z). \qquad (6d)\end{aligned}$$

With $\partial_x = \partial_z + \partial_{\bar{z}}$ and $\partial_y = \mathrm{i}(\partial_z - \partial_{\bar{z}})$ the relations (5c) and (5d) follow from (6c) and (6d) in the case $m \geq 1$. Again, the cases $m = 0$ and $m < 0$ are shown similarly. □

2.2 Functional analytic framework

Complete orthonormal system. The considered time-splitting generalized-Laguerre–Fourier pseudo-spectral method for the discretization of the two-dimensional Gross–Pitaevskii equation (1) relies on the fact that the eigenfunctions $(\mathcal{L}^{\gamma}_{km})_{(k,m)\in\mathcal{M}}$ associated with the densely defined self-adjoint operator $A : D(A) \subset L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$ form a complete orthonormal system of the Lebesgue space $L^2(\mathbb{R}^2)$, see [3] for further details and recall (4a). That is, the eigenvalue relation

$$\begin{aligned} A\,\mathcal{L}^{\gamma}_{km} &= \big(-\tfrac{1}{2}\Delta + \tfrac{1}{2}\,\gamma\,(x^2+y^2) - \Omega L_z\big)\,\mathcal{L}^{\gamma}_{km} = \lambda_{km}\,\mathcal{L}^{\gamma}_{km}, \\ \lambda_{km} &= \gamma\,(2k+|m|+1) - m\Omega\,, \qquad (k,m)\in\mathcal{M}, \end{aligned} \tag{7a}$$

the orthogonality relation

$$\begin{aligned} \langle \mathcal{L}^{\gamma}_{km}, \mathcal{L}^{\gamma}_{k'm'}\rangle_{L^2(\mathbb{R}^2)} &= \int_{\mathbb{R}^2} \overline{\mathcal{L}^{\gamma}_{km}(x,y)}\,\mathcal{L}^{\gamma}_{k',m'}(x,y)\,\mathrm{d}x\,\mathrm{d}y \\ &= \int_0^{2\pi}\int_0^{\infty} r\,\widetilde{L}^{\gamma}_{k,|m|}(r)\,\widetilde{L}^{\gamma}_{k',|m'|}(r)\,\mathrm{e}^{i(m'-m)\vartheta}\,\mathrm{d}r\,\mathrm{d}\vartheta \\ &= \delta_{kk'}\delta_{mm'}, \qquad (k,m),\,(k',m')\in\mathcal{M}, \end{aligned} \tag{7b}$$

and for any $u \in L^2(\mathbb{R}^2)$ the spectral representation

$$u = \sum_{(k,m)\in\mathcal{M}} c_{km}(u)\,\mathcal{L}^{\gamma}_{km}, \qquad c_{km}(u) = \langle \mathcal{L}^{\gamma}_{km}, u\rangle_{L^2(\mathbb{R}^2)}\,, \quad (k,m)\in\mathcal{M},$$

are valid. Furthermore, by Parseval's identity, for $u \in L^2(\mathbb{R}^2)$ it follows

$$\|u\|^2_{L^2(\mathbb{R}^2)} = \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2.$$

Fractional power spaces. Throughout, we employ the assumption

$$|\Omega| < \gamma, \tag{8}$$

which implies that all eigenvalues are positive and thus the linear operator A is positive-definite. Consequently, for arbitrary exponents $\alpha \in \mathbb{R}$ the fractional powers $A^{\alpha} : X_{\alpha} = D(A^{\alpha}) \subset L^2(\mathbb{R}^2) \to L^2(\mathbb{R}^2)$, defined by

$$\begin{aligned} A^{\alpha}u &= \sum_{(k,m)\in\mathcal{M}} c_{km}(u)\,\lambda^{\alpha}_{km}\,\mathcal{L}^{\gamma}_{km}, \\ \|u\|^2_{X_\alpha} = \|A^{\alpha}u\|^2_{L^2(\mathbb{R}^2)} &= \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2\,\lambda^{2\alpha}_{km}, \\ X_{\alpha} &= \big\{u \in L^2(\mathbb{R}^2) : \|u\|_{X_\alpha} < \infty\big\}\,, \end{aligned}$$

are again linear, self-adjoint, and positive-definite operators. The spaces X_α are called fractional power spaces associated with the operator A; in particular, it holds $X_0 = L^2(\mathbb{R}^2)$ and $X_1 = D(A)$.

2.3 Estimates in fractional power spaces

In this section, we derive estimates for products of functions in fractional power spaces. A first auxiliary result relates estimates with respect to Sobolev-norms to estimates in fractional power spaces.

Lemma 2 *For any $\alpha \geq 0$ it holds*

$$\|x\, u\|_{X_\alpha} + \|y\, u\|_{X_\alpha} + \|\partial_x u\|_{X_\alpha} + \|\partial_y u\|_{X_\alpha} \leq \mathcal{C}\, \|u\|_{X_{\alpha+\frac{1}{2}}}, \quad u \in X_{\alpha+\frac{1}{2}},$$

with a constant $\mathcal{C}$ that is independent of u.

Proof From equations (5a) and (5d) it follows that $F\mathcal{L}^\gamma_{km}$, $F \in \{x, y, \partial_x, \partial_y\}$, can be represented in the form

$$F\mathcal{L}^\gamma_{km} = \sum_{(k',m')\in\mathcal{M}} a^{km}_{k'm'}\, \mathcal{L}^\gamma_{k'm'} = \sum_{\substack{k'=k-1,k,k+1\\ m'=m\pm1}} a^{km}_{k'm'}\, \mathcal{L}^\gamma_{k'm'},$$

where for given $(k,m) \in \mathcal{M}$, $a^{km}_{k'm'} \neq 0$ only holds for $k' \in \{k-1, k, k+1\}$ and $m' \in \{m-1, m+1\}$. Conversely, for given $(k',m') \in \mathcal{M}$, $a^{km}_{k'm'} \neq 0$ only holds for $k \in \{k'-1, k', k'+1\}$ and $m \in \{m'-1, m'+1\}$. Therefore,

$$\begin{aligned}
A^\alpha F u &= A^\alpha \sum_{(k,m)\in\mathcal{M}} c_{km}(u)\, F\, \mathcal{L}^\gamma_{km} \\
&= A^\alpha \sum_{(k,m)\in\mathcal{M}} c_{km}(u) \sum_{\substack{k'=k-1,k,k+1\\ m'=m\pm1}} a^{km}_{k'm'}\, \mathcal{L}^\gamma_{k'm'} \\
&= \sum_{(k',m')\in\mathcal{M}} \sum_{\substack{k=k'-1,k',k'+1\\ m=m'\pm1}} c_{km}(u)\, a^{km}_{k'm'}\, \lambda^\alpha_{k'm'}\, \mathcal{L}^\gamma_{k'm'}.
\end{aligned}$$

From the explicitly given values of $a^{km}_{k'm'}$ in (5a) and (5d) and the estimate

$$\begin{aligned}
\lambda_{km} &= \gamma(2k + |m| + 1) - \Omega m \geq \gamma\,(2k+1) + (\gamma - |\Omega|)\,|m| \\
&\geq (\gamma - |\Omega|)\,(k + |m| + 1)
\end{aligned} \tag{9a}$$

we obtain

$$|a^{km}_{k'm'}|^2 \leq \tfrac{1}{4}\,\gamma^{\pm1}\,(k + |m| + 1) \leq \tfrac{1}{4}\,\frac{\gamma^{\pm1}}{\gamma - |\Omega|}\,\lambda_{km} \leq \mathcal{C}\,\lambda_{km},$$

where $\gamma^{\pm1} = \gamma^{+1}$ for $F \in \{\partial_x, \partial_y\}$ and $\gamma^{\pm1} = \gamma^{-1}$ for $F \in \{x, y\}$; recall $|\Omega| < \gamma$. Using

$$|z_1 + \cdots + z_N|^2 \leq N\,(|z_1|^2 + \cdots + |z_N|^2), \quad z_1, \ldots, z_N \in \mathbb{C}, \tag{9b}$$

which follows easily from the arithmetic-geometric mean inequality,[1] we obtain

$$\begin{aligned}\|A^\alpha F u\|_{X_0}^2 &= \sum_{(k',m')\in\mathcal{M}} \lambda_{k'm'}^{2\alpha} \Big| \sum_{\substack{k=k'-1,k',k'+1\\ m=m'\pm 1}} c_{km}(u)\, a_{k'm'}^{km} \Big|^2 \\ &\le \mathcal{C} \sum_{(k',m')\in\mathcal{M}} \lambda_{k'm'}^{2\alpha} \sum_{\substack{k=k'-1,k',k'+1\\ m=m'\pm 1}} |c_{km}(u)|^2\, \lambda_{km} \\ &= \mathcal{C} \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2\, \lambda_{km} \sum_{\substack{k'=k-1,k,k+1\\ m'=m\pm 1}} \lambda_{k'm'}^{2\alpha},\end{aligned}$$

where in the last step we changed the order of summation. Now it is easily seen that $\lambda_{k'm'} \le \mathcal{C}\lambda_{km}$ holds for all $k' \in \{k-1,k,k+1\}$ and $m' \in \{m-1,m+1\}$. Therefore, finally, the stated result

$$\begin{aligned}\|Fu\|_{X_\alpha}^2 = \|A^\alpha F u\|_{X_0}^2 &\le \mathcal{C} \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2\, \lambda_{km}^{2\alpha+1} \\ &= \mathcal{C}\, \|A^{\alpha+\frac{1}{2}} u\|_{X_0}^2 = \mathcal{C}\, \|u\|_{X_{\alpha+\frac{1}{2}}}^2\end{aligned}$$

is obtained. □

The following estimates result from the application of a Sobolev imbedding theorem [5] and Lemma 2. Within our general analytic framework its proof is independent of the considered spectral space discretisation, see [20] for details of the proof.

Lemma 3 *For any* $\alpha \ge 1$ *it holds*

$$\|u\|_{L^\infty(\mathbb{R}^2)} \le \mathcal{C}\, \|u\|_{H^2(\mathbb{R}^2)} \le \mathcal{C}\, \|u\|_{X_\alpha}, \qquad u \in X_\alpha, \tag{10a}$$

$$\|u\, v\|_{X_0} \le \mathcal{C}\, \|u\|_{X_0}\, \|v\|_{X_\alpha}, \qquad u \in X_0, \quad v \in X_\alpha. \tag{10b}$$

For any $\alpha \in \mathbb{N}$ *with* $\alpha \ge 1$ *it holds*

$$\|u\, v\|_{X_\alpha} \le \mathcal{C}\, \|u\|_{X_\alpha} \|v\|_{X_\alpha}, \qquad u, v \in X_\alpha. \tag{10c}$$

[1] From

$$\begin{aligned}\Re(z_n\, \bar z_m) &= \Re\big((x_n + \mathrm{i} y_n)\,(x_m - \mathrm{i} y_m)\big) = x_n\, x_m + y_n\, y_m \le \sqrt{x_n^2\, x_m^2} + \sqrt{y_n^2\, y_m^2} \\ &\le \tfrac{1}{2}\,(x_n^2 + x_m^2 + y_n^2 + y_m^2) = \tfrac{1}{2}\,(|z_n|^2 + |z_m|^2)\end{aligned}$$

it follows

$$\Big|\sum_{n=1}^N z_n\Big|^2 = \sum_{n=1}^N |z_n|^2 + 2 \sum_{n\ne m} \Re(z_n\, z_m) \le N \sum_{n=1}^N |z_n|^2.$$

2.4 Sobolev-type inequalities

In this section, we derive Sobolev-type inequalities, which hold on finite subsets of the line and the plane, respectively. We note that the constants appearing in the bounds could be given explicitly in all cases.

Lemma 4 *(i) For any $u \in H^1(a,b)$ with $a < b$ it holds*

$$\begin{aligned}\max_{x\in[a,b]} |u(x)| &\le \tfrac{1}{b-a} \int_a^b |u(x)|\, \mathrm{d}x + \int_a^b |\tfrac{\mathrm{d}}{\mathrm{d}x} u(x)|\, \mathrm{d}x \\ &= \tfrac{1}{b-a} \|u\|_{L^1(a,b)} + \|\tfrac{\mathrm{d}}{\mathrm{d}x} u\|_{L^1(a,b)} \qquad (11a)\\ &\le \tfrac{1}{\sqrt{b-a}} \|u\|_{L^2(a,b)} + \sqrt{b-a}\, \|\tfrac{\mathrm{d}}{\mathrm{d}x} u\|_{L^2(a,b)}. \qquad (11b)\end{aligned}$$

(ii) Let $\Omega = (a,b) \times (c,d)$ with $a < b$ and $c < d$. For any $u \in H^2(\Omega_1)$ with $\Omega_1 \supset \overline{\Omega}$ a bounded Lipschitz domain it holds

$$\begin{aligned}&\max_{(x,y)\in\overline{\Omega}} |u(x,y)| \\ &\quad\le \tfrac{1}{(b-a)(d-c)} \|u\|_{L^1(\Omega)} + \tfrac{1}{d-c} \|\partial_x u\|_{L^1(\Omega)} + \tfrac{1}{b-a} \|\partial_y u\|_{L^1(\Omega)} \\ &\qquad + 2\, \|\partial_{xy} u\|_{L^1(\Omega)} \qquad (11c)\\ &\quad\le \tfrac{1}{\sqrt{(b-a)(d-c)}} \|u\|_{L^2(\Omega)} + \tfrac{\sqrt{b-a}}{\sqrt{d-c}} \|\partial_x u\|_{L^2(\Omega)} \\ &\qquad + \tfrac{\sqrt{d-c}}{\sqrt{b-a}} \|\partial_y u\|_{L^2(\Omega)} + 2\sqrt{(b-a)(d-c)}\, \|\partial_{xy} u\|_{L^2(\Omega)}. \qquad (11d)\end{aligned}$$

Proof (i) This result is also given in [19]. Since the proof of (ii) proceeds similarly, however, we also give a proof for (i). For any $u \in H^1(a,b)$ it holds $u \in C[a,b]$ by the Sobolev imbedding theorem[2] and thus there exists $x_* \in [a,b]$ with $|u(x_*)| = \min_{x\in[a,b]} |u(x)|$. Clearly, the minimum is not greater than the mean value

$$|u(x_*)| \le \tfrac{1}{b-a} \int_a^b |u(x)| \mathrm{d}x = \tfrac{1}{b-a} \|u\|_{L^1(a,b)}.$$

Together with

$$|u(x)| - |u(x_*)| \le |u(x) - u(x_*)| \le \int_a^b |\tfrac{\mathrm{d}}{\mathrm{d}x} u(x)|\, \mathrm{d}x = \|\tfrac{\mathrm{d}}{\mathrm{d}x} u\|_{L^1(a,b)}$$

this implies (11a), and (11b) follows by Schwarz's inequality.

(ii) For any $u \in H^2(\Omega_1)$ it follows $u \in C(\Omega_1)$ by the Sobolev imbedding theorem. For fixed $y_1, y_2 \in [c,d]$ the function

$$v(x) = \int_{y_1}^{y_2} \partial_y u(x,y)\, \mathrm{d}y$$

[2] In 1D this is easy to prove: For any $x_1, x_2 \in [a,b]$ it holds

$$|u(x_1) - u(x_2)| \le \int_{x_1}^{x_2} |\tfrac{\mathrm{d}}{\mathrm{d}x} u(x)|\, \mathrm{d}x \le \sqrt{|x_2 - x_1|}\, \|\tfrac{\mathrm{d}}{\mathrm{d}x} u\|_{L^2(a,b)}.$$

is in $H^1(a,b)$, so by (11a)

$$
\begin{aligned}
|u(x_1,y_1) - u(x_1,y_2)| &= |v(x_1)| \le \max_{x\in[a,b]} |v(x)| \\
&\le \tfrac{1}{b-a} \int_a^b |v(x)| \,\mathrm{d}x + \int_a^b |\partial_x v(x)| \,\mathrm{d}x \\
&\le \tfrac{1}{b-a} \int_a^b \int_c^d |\partial_y u(x,y)| \,\mathrm{d}y\,\mathrm{d}x + \int_a^b \int_c^d |\partial_{xy} u(x,y)| \,\mathrm{d}y\,\mathrm{d}x \\
&= \tfrac{1}{b-a} \|\partial_y u\|_{L^1(\Omega)} + \|\partial_{xy} u\|_{L^1(\Omega)}.
\end{aligned}
$$

Note that the final estimate does not depend on y_1, y_2. Similarly, it follows

$$
|u(x_1,y_2) - u(x_2,y_2)| \le \tfrac{1}{d-c} \|\partial_x u\|_{L^1(\Omega)} + \|\partial_{xy} u\|_{L^1(\Omega)},
$$

and thus

$$
\begin{aligned}
|u(x_1,y_1) - u(x_2,y_2)| &\le |u(x_1,y_1) - u(x_1,y_2)| + |u(x_1,y_2) - u(x_2,y_2)| \\
&\le \tfrac{1}{d-c} \|\partial_x u\|_{L^1(\Omega)} + \tfrac{1}{b-a} \|\partial_y u\|_{L^1(\Omega)} + 2 \|\partial_{xy} u\|_{L^1(\Omega)} \qquad (12)
\end{aligned}
$$

for $(x_1,y_1),(x_2,y_2) \in \overline{\Omega}$. Applying the above estimate with $(x_2,y_2) = (x_*,y_*)$ for which $|u(x_*,y_*)| = \min\{|u(x,y)| : (x,y) \in \overline{\Omega}\}$ we obtain (11c) using the fact that the mean value $\frac{1}{(b-a)(d-c)} \|u\|_{L^1(\Omega)}$ is not less than the minimum, similarly as in part (i). Finally, (11d) follows by Schwarz's inequality. □

The following result provides an estimate for the maximum of a function on a curved rectangle

$$
R = \{(x,y) = (r\cos\vartheta, r\sin\vartheta) :\ r \in (r_A, r_B), \vartheta \in (\vartheta_A, \vartheta_B)\}, \qquad (13)
$$

where $0 < r_A < r_B$, $\vartheta_A < \vartheta_B$, and $\vartheta_B - \vartheta_A \le 2\pi$.

Lemma 5 *For any $u \in H^2(\mathbb{R}^2)$ the estimate*

$$
\begin{aligned}
\max_{(x,y)\in\overline{R}} |u(x,y)| \le c_0 \|u\|_{L^2(R)} &\\
+ (c_{11} + c_{12} + c_{13}) \left(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\right) & \qquad (14a) \\
+ c_2 \left(\|\partial_x^2 u\|_{L^2(R)} + \|\partial_y^2 u\|_{L^2(R)} + \|\partial_{xy} u\|_{L^2(R)}\right), &
\end{aligned}
$$

is valid on a curved rectangle of the form (13) *with constants*

$$
c_0 = \tfrac{1}{\sqrt{\mathrm{Vol} R}} = \frac{1}{\sqrt{\frac{1}{2}(r_B^2 - r_A^2)(\vartheta_B - \vartheta_A)}}, \qquad (14b)
$$

$$
c_{11} = \tfrac{1}{\sqrt{\vartheta_B - \vartheta_A}} \sqrt{\log \tfrac{r_B}{r_A}} \le \tfrac{1}{\sqrt{\vartheta_B - \vartheta_A}} \sqrt{\tfrac{r_B^2 - r_A^2}{2 r_A^2}}, \qquad (14c)
$$

$$
c_{12} = \sqrt{\tfrac{(\vartheta_B - \vartheta_A)\,(r_A + r_B)}{2(r_B - r_A)}}, \qquad (14d)
$$

$$
c_{13} = 2\sqrt{(\vartheta_B - \vartheta_A) \log \tfrac{r_B}{r_A}} \le 2\sqrt{\vartheta_B - \vartheta_A} \sqrt{\tfrac{r_B^2 - r_A^2}{2 r_A^2}}, \qquad (14e)
$$

$$
c_2 = 2\sqrt{\mathrm{Vol} R} = \sqrt{2\,(r_B^2 - r_A^2)\,(\vartheta_B - \vartheta_A)}. \qquad (14f)
$$

Proof We set
$$\widetilde{R} = \{(r, \vartheta) : \; r \in (r_A, r_B), \vartheta \in (\vartheta_A, \vartheta_B)\}$$
and for some bounded Lipschitz domain $\widetilde{R}_1 \supseteq \widetilde{R}$ define a function $\widetilde{u}$ on $\widetilde{R}_1$ by
$$\widetilde{u}(r, \vartheta) = u(r \cos \vartheta, r \sin \vartheta), \quad (r, \vartheta) \in \widetilde{R}_1.$$
Then $\widetilde{u} \in H^2(\widetilde{R}_1)$ and thus by equation (12) it follows
$$\begin{aligned} &|u(x_1, y_1) - u(x_2, y_2)| \\ &\quad \le \tfrac{1}{(\vartheta_B - \vartheta_A)} \|\partial_r \widetilde{u}\|_{L^1(\widetilde{R})} + \tfrac{1}{(r_B - r_A)} \|\partial_\vartheta \widetilde{u}\|_{L^1(\widetilde{R})} + 2 \|\partial_{r\vartheta} \widetilde{u}\|_{L^1(\widetilde{R})} \end{aligned} \tag{15a}$$
for all $(x_1, y_1), (x_2, y_2) \in \overline{R}$.

From $|\partial_r \widetilde{u}| = |\cos\vartheta \partial_x u + \sin\vartheta \partial_y u| \le |\partial_x u| + |\partial_y u|$ it follows using Schwarz's inequality
$$\begin{aligned} \|\partial_r \widetilde{u}\|_{L^1(\widetilde{R})} &= \int_{\vartheta_A}^{\vartheta_B} \int_{r_A}^{r_B} |\partial_r \widetilde{u}| \, \mathrm{d}r \, \mathrm{d}\vartheta = \int_R \tfrac{1}{r} |\partial_r \widetilde{u}| \, \mathrm{d}x \mathrm{d}y \\ &\le \int_R \tfrac{1}{r} |\partial_x u| \, \mathrm{d}x \mathrm{d}y + \int_R \tfrac{1}{r} |\partial_y u| \, \mathrm{d}x \, \mathrm{d}y \\ &\le \sqrt{\int_R \tfrac{1}{r^2} \, \mathrm{d}x \, \mathrm{d}y} \, \big(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\big) \\ &= \sqrt{\int_{\vartheta_A}^{\vartheta_B} \int_{r_A}^{r_B} \tfrac{1}{r} \, \mathrm{d}r \, \mathrm{d}\vartheta} \, \big(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\big) \\ &= \sqrt{(\vartheta_B - \vartheta_A) \log \tfrac{r_B}{r_A}} \, \big(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\big) . \end{aligned} \tag{15b}$$
Similarly, from
$$|\partial_\vartheta \widetilde{u}| = |-r \sin\vartheta \, \partial_x u + r \cos\vartheta \, \partial_y u| \le r \, |\partial_x u| + r \, |\partial_y u|$$
it follows
$$\begin{aligned} \|\partial_\vartheta \widetilde{u}\|_{L^1(\widetilde{R})} &= \int_{\vartheta_A}^{\vartheta_B} \int_{r_A}^{r_B} |\partial_\vartheta \widetilde{u}| \, \mathrm{d}r \, \mathrm{d}\vartheta = \int_R \tfrac{1}{r} |\partial_\vartheta \widetilde{u}| \, \mathrm{d}x \, \mathrm{d}y \\ &\le \int_R |\partial_x u| \, \mathrm{d}x \, \mathrm{d}y + \int_R |\partial_y u| \, \mathrm{d}x \, \mathrm{d}y \\ &\le \sqrt{\int_R 1 \, \mathrm{d}x \, \mathrm{d}y} \, \big(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\big) \\ &= \sqrt{\tfrac{1}{2} (\vartheta_B - \vartheta_A) (r_B^2 - r_A^2)} \, \big(\|\partial_x u\|_{L^2(R)} + \|\partial_y u\|_{L^2(R)}\big) \end{aligned} \tag{15c}$$
and, using
$$\begin{aligned} |\partial_{r\vartheta} \widetilde{u}| = \big| &- \sin\vartheta \, \partial_x u + \cos\vartheta \, \partial_y u - r \cos\vartheta \sin\vartheta \, \partial_x^2 u \\ &+ r \cos\vartheta \sin\vartheta \, \partial_y^2 u + r \, (\cos^2\vartheta - \sin^2\vartheta) \, \partial_{xy} u \big| \\ \le |\partial_x u| &+ |\partial_y u| + r \, |\partial_x^2 u| + r \, |\partial_y^2 u| + r \, |\partial_{xy} u|, \end{aligned}$$

we obtain

$$\|\partial_{r\vartheta}\widetilde{u}\|_{L^1(\widetilde{R})} \le \sqrt{(\vartheta_B-\vartheta_A)\log\tfrac{r_B}{r_A}}\,\big(\|\partial_x u\|_{L^2(R)}+\|\partial_y u\|_{L^2(R)}\big) \qquad (15d)$$
$$+\sqrt{\tfrac12\,(\vartheta_B-\vartheta_A)\,(r_B^2-r_A^2)}\,\big(\|\partial_x^2 u\|_{L^2(R)}+\|\partial_y^2 u\|_{L^2(R)}+\|\partial_{xy} u\|_{L^2(R)}\big)\,.$$

Substituting (15b), (15c), and (15d) in (15a) we obtain

$$|u(x_1,y_1)-u(x_2,y_2)| \le (c_{11}+c_{12}+c_{13})\,\big(\|\partial_x u\|_{L^2(R)}+\|\partial_y u\|_{L^2(R)}\big)$$
$$+c_2\,\big(\|\partial_x^2 u\|_{L^2(R)}+\|\partial_y^2 u\|_{L^2(R)}+\|\partial_{xy} u\|_{L^2(R)}\big)$$

for all $(x_1,y_1),(x_2,y_2)\in\overline{R}$. Applying this estimate with $(x_2,y_2)=(x_*,y_*)$ for which $|u(x_*,y_*)|=\min\{|u(x,y)|:(x,y)\in\overline{R}\}$ we obtain (14a) using the fact that the mean value $\frac{1}{\mathrm{Vol}R}\|u\|_{L^1(R)}\le\frac{1}{\sqrt{\mathrm{Vol}R}}\|u\|_{L^2(R)}$ is not less than the minimum.

The inequalities in (14c) and (14e) follow by the mean value theorem

$$\log\tfrac{r_B}{r_A}=\tfrac12\,(\log r_B^2-\log r_A^2)\le\tfrac12\,\tfrac{r_B^2-r_A^2}{r_A^2}.$$

Altogether, this yields the stated estimates. □

2.5 Estimates in a discrete L^2-norm related to Gauß–Laguerre quadrature

In the following, we deduce a bound with respect to a discrete L^2-norm involving Gauß–Laguerre quadrature nodes and weights, needed for the estimation of the generalized-Laguerre–Fourier spectral interpolant. For this purpose, we first discuss the asymptotical distribution of the Gauß–Laguerre quadrature nodes and weights.

Gauß–Laguerre quadrature nodes and weights. We recall the definition (2a) of the generalized-Laguerre polynomials. The zeros of the (standard) Laguerre polynomial $L_N = L_N^0$ and the corresponding weights associated with the Gauß–Laguerre quadrature formula of order $2N$ are denoted by

$$\varrho_{0N}<\varrho_{1N}<\cdots<\varrho_{N-2,N}<\varrho_{N-1,N},\quad \omega_{jN}=\frac{\varrho_{jN}}{(N+1)^2\,(L_{N+1}(\omega_{jN}^0))^2}.$$

The smallest zero satisfies the relation

$$\mathcal{C}_1\,N^{-1}\le\varrho_{0N}\le\mathcal{C}_2\,N^{-1} \qquad (16a)$$

with constants $\mathcal{C}_1,\mathcal{C}_2>0$ independent of N, cf. [13, Theorem 1.4 (1.22)], and the largest zero satisfies the bound

$$\varrho_{N-1,N}\le 4N, \qquad (16b)$$

cf. for example [17, §18.16.13]. Following [13, eq. (1.18)] we define the function

$$\varphi_N(r)=\frac{\sqrt{r+4N^{-1}}\,(8N-r)}{N\sqrt{4N+4N^{1/3}-r}},\quad r\in[0,4N].$$

Then, for $N \geq N_0$ the quadrature weights satisfy the relation

$$\mathcal{C}_1\, \varphi_N(\varrho_{jN}) \leq \omega_{jN}\, \mathrm{e}^{\varrho_{jN}} \leq \mathcal{C}_2\, \varphi_N(\varrho_{jN}), \quad j = 0, \ldots, N-1, \tag{17a}$$

with constants $\mathcal{C}_1, \mathcal{C}_2$ independent of N and j, cf. [13, Theorem 1.3 (1.19)]. Furthermore, for $N \geq 1$ it holds

$$\mathcal{C}_1 \varphi_N(\varrho_{jN}) \leq \varrho_{jN} - \varrho_{j-1,N} \leq \mathcal{C}_2\, \varphi_N(\varrho_{jN}), \quad j = 1, \ldots, N-1, \tag{17b}$$

with constants $\mathcal{C}_1, \mathcal{C}_2$ independent of N and j, cf. [14, Theorem 1.4]. By elementary calculus it follows that $\varphi_N(r)$ has no local extremum in $(0, 4N)$ for all $N \geq 2$. Hence, the minimum and maximum are attained at $r = 0$ and $r = 4N$, respectively,

$$\varphi_N(r) \geq \varphi_N(0) = \frac{8}{\sqrt{N^2 + N^{4/3}}} \geq 4\sqrt{2}\, N^{-1}, \quad r \in [0, 4N], \tag{18a}$$

$$\varphi_N(r) \leq \varphi_N(4N) = 4\, \frac{\sqrt{N + N^{-1}}}{N^{1/6}} \leq 4\sqrt{2}\, N^{1/3}, \quad r \in [0, 4N]. \tag{18b}$$

Moreover, due to the fact that the function $r \mapsto \frac{(8N-r)^2}{4N+4N^{1/3}-r}$ has no local maximum in $(0, 4N)$ and thus attains its maximum at one of the boundary points $r = 0$ or $r = 4N$, the estimate

$$\begin{aligned} \tfrac{1}{r}\, \varphi_N(r)^2 &= \frac{(1 + \frac{4N^{-1}}{r})\, (8N - r)^2}{N^2\, (4N + 4N^{1/3} - r)} \\ &\leq \mathcal{C}\, \frac{(8N - r)^2}{N^2 (4N + 4N^{1/3} - r)} \leq \mathcal{C}\, N^{-1/3}, \qquad \mathcal{C}N^{-1} \leq r \leq 4N, \end{aligned} \tag{19}$$

is valid. Also, by means of (16a) it follows

$$\varphi_N(\varrho_{0N}) \leq \frac{8N\sqrt{(\mathcal{C}_2 + 4)\, N^{-1}}}{N\, \sqrt{4N + 4N^{1/3} - \mathcal{C}_2 N^{-1}}} \leq \mathcal{C}\, \frac{N^{-1/2}}{N^{1/2}} = \mathcal{C}N^{-1}. \tag{20}$$

Discrete L^2-norm. Following [3, eq. (2.29)], we introduce scaled Gauß–Laguerre nodes and weights

$$r_{jN} = \sqrt{\tfrac{\varrho_{jN}}{\gamma}}, \quad w_{jN} = \tfrac{1}{\gamma}\, \pi\, \omega_{jN}\, \mathrm{e}^{\varrho_{jN}}, \quad j = 0, 2, \ldots, N-1, \tag{21}$$

and for even integer $M > 0$ we consider the equidistant nodes

$$\vartheta_{sM} = \tfrac{2\pi s}{M}, \quad s = 0, \ldots, M-1,$$

associated with the trapezoidal rule. For functions $u \in H^2(\mathbb{R}^2) \subset C(\mathbb{R}^2)$ we define a discrete L^2-norm through

$$\|u\|_{NM}^2 = \tfrac{1}{M} \sum_{j=0}^{N-1} \sum_{s=0}^{M-1} w_{jN}\, |u(r_{jN} \cos\vartheta_{sM}, r_{jN} \sin\vartheta_{sM})|^2. \tag{22}$$

The following result relates discrete L^2-norms to L^2-norms and Sobolev-seminorms.

Lemma 6 *For any $u \in H^2(\mathbb{R}^2)$ the bound*

$$\|u\|_{NM} \leq \mathcal{C} \Big(\|u\|_{L^2(\mathbb{R}^2)} + \big(N^{-1/6} + M^{-1} N^{1/2}\big) |u|_{H^1(\mathbb{R}^2)} + \big(M^{-1} N^{1/3} + N^{-1/2}\big) |u|_{H^2(\mathbb{R}^2)} \Big) \quad (23a)$$

$$\leq \mathcal{C} \Big(\|u\|_{L^2(\mathbb{R}^2)} + M^{-1/6} |u|_{H^1(\mathbb{R}^2)} + M^{-1/2} |u|_{H^2(\mathbb{R}^2)} \Big) \quad (23b)$$

is valid, where in the second estimate N is chosen proportional to M.

Proof We first estimate the summands in (22) by ($j = 1, \dots, N-1,\ s = 0, \dots, M-1$)

$$\tfrac{1}{M}\, w_{jN}\, |u(r_{jN} \cos\vartheta_{sM}, r_{jN} \sin\vartheta_{sM})|^2 \leq \tfrac{1}{M}\, w_{jN} \max_{(x,y) \in \overline{R}_{js}^{NM}} |u(x,y)|^2, \quad (24)$$

where R_{js}^{NM} denotes the curved rectangle

$$R_{js}^{NM} = \{(x,y) = (r\cos\vartheta, r\sin\vartheta) : r \in (r_{j-1,N}, r_{jN}), \vartheta \in (\vartheta_{sM}, \vartheta_{s+1,M})\}.$$

The remaining summands for $j = 0$, $s = 0, \dots, M-1$ will be treated separately. We apply Lemma 5 and the above estimates (16a) and (16b) as well as (17a)–(18b), which in terms of the scaled quadrature nodes and weights (21) yields

$$\mathcal{C}_1\, N^{-1} \leq r_{jN}^2 \leq \mathcal{C}_2\, N, \quad j = 0, \dots, N-1, \quad (25a)$$

$$\mathcal{C}_3\, N^{-1} \leq \mathcal{C}_4\, w_{jN} \leq \mathcal{C}_5\, (r_{jN}^2 - r_{j-1,N}^2) \leq \mathcal{C}_6\, w_{jN} \leq \mathcal{C}_7\, N^{1/3}, \quad j = 1, \dots, N-1, \quad (25b)$$

with constants $\mathcal{C}_1, \dots, \mathcal{C}_7$ independent of N. Furthermore, it holds

$$w_{jN}\, \frac{r_{jN}^2 - r_{j-1,N}^2}{r_{j-1,N}^2} \leq \mathcal{C}\, \frac{\varphi_N(\varrho_{jN})}{\varrho_{j-1,N}} \leq \mathcal{C}\, \frac{\varphi_N(\varrho_{j-1,N})}{\varrho_{j-1,N}} \leq \mathcal{C}_8\, N^{-1/3}, \quad j = 1, \dots, N-1, \quad (25c)$$

where we applied the estimate $\varphi_N(\varrho_{jN}) \leq \mathcal{C} \varphi_N(\varrho_{j-1,N})$ which follows from [13, eq. (7.14) in the proof of Theorem 7.3(c)] and then (19). We need the following estimates involving the expressions (14b)–(14f). By (25b) and (25c) it follows

$$\tfrac{1}{M}\, w_{jN}\, c_0^2 \leq \mathcal{C}\, \frac{1}{(\vartheta_{s+1,M} - \vartheta_{sM})M}\, \frac{w_{jN}}{r_{jN}^2 - r_{j-1,N}^2} \leq \mathcal{C},$$

$$\tfrac{1}{M}\, w_{jN}\, c_{11}^2 \leq \mathcal{C}\, \frac{1}{(\vartheta_{s+1,M} - \vartheta_{sM})M}\, w_{jN}\, \frac{r_{jN}^2 - r_{j-1,N}^2}{r_{j-1,N}^2} \leq \mathcal{C}\, N^{-1/3},$$

$$\tfrac{1}{M}\, w_{jN}\, c_{13}^2 \leq \mathcal{C}\, \tfrac{1}{M}\, (\vartheta_{s+1,M} - \vartheta_{sM})\, w_{jN}\, \frac{r_{jN}^2 - r_{j-1,N}^2}{r_{j-1,N}^2} \leq \mathcal{C}\, M^{-2}\, N^{-1/3},$$

and by (25b) and then (25a) we obtain

$$\begin{aligned}\tfrac{1}{M}\, w_{jN}\, c_{12}^2 &\leq \mathcal{C}\, \tfrac{1}{M}\, (\vartheta_{s+1,M} - \vartheta_{sM})\, w_{jN}\, \frac{r_{j-1,N} + r_{jN}}{r_{jN} - r_{j-1,N}} \\ &\leq \mathcal{C}\, M^{-2}\, (r_{j,N}^2 - r_{j-1,N}^2)\, \frac{r_{j-1,N} + r_{jN}}{r_{jN} - r_{j-1,N}} \\ &= \mathcal{C}\, M^{-2}\, (r_{j-1,N} + r_{jN})^2 \leq \mathcal{C}\, M^{-2}\, N.\end{aligned}$$

Finally, by (25b) we have

$$\tfrac{1}{M}\, w_{jN}\, c_2^2 \leq \mathcal{C}\, \tfrac{1}{M}\, (\vartheta_{s+1,M} - \vartheta_{sM})\, w_{jN}\, (r_{jN}^2 - r_{j-1,N}^2) \leq \mathcal{C}\, M^{-2}\, N^{2/3}.$$

Using these estimates together with (9b) in (24) and (14a), summing up, and applying the following relation for disjoint domains Ω_1, Ω_2,

$$\|u\|_{L^2(\Omega_1)}^2 + \|u\|_{L^2(\Omega_2)}^2 = \int_{\Omega_1} |u|^2 + \int_{\Omega_2} |u|^2 = \int_{\Omega_1 \cup \Omega_2} |u|^2 = \|u\|_{L^2(\Omega_1 \cup \Omega_2)}^2,$$

we obtain the estimate

$$\begin{aligned}&\tfrac{1}{M} \sum_{j=1}^{N-1} \sum_{s=0}^{M-1} w_{jN}\, |u(r_{jN} \cos \vartheta_{sM}, r_{jN} \sin \vartheta_{sM})|^2 \\ &\leq \mathcal{C}\, \big(\|u\|_{L^2(\mathbb{R}^2)}^2 + (N^{-1/3} + M^{-2} N)\, |u|_{H^1(\mathbb{R}^2)}^2 + M^{-2}\, N^{2/3}\, |u|_{H^2(\mathbb{R}^2)} \big). \quad (26a)\end{aligned}$$

The remaining summands for $j = 0$, $s = 0, \dots, M-1$ are easily estimated by using (17a) together with (20) and the Sobolev inequality,

$$\tfrac{1}{M}\, w_1 \sum_{s=0}^{M-1} |u(r_1 \cos \vartheta_s, r_1 \sin \vartheta_s)|^2 \leq w_1\, \|u\|_{L^\infty(\mathbb{R}^2)} \leq \mathcal{C}\, N^{-1}\, \|u\|_{H^2(\mathbb{R}^2)}. \quad (26b)$$

Finally, the relations (26a) and (26b) imply (23a). □

2.6 Estimates for generalized-Laguerre–Fourier spectral interpolants

In the following, we state an estimate for the generalized-Laguerre–Fourier spectral interpolant. Together with Lemma 6 this fundamental result is needed in order to deduce a stability bound for the fully discrete evolution operator.

Orthogonal projection and spectral interpolant. For even integer $M \geq 2$ and integer $K \geq 1$ we define the subspace

$$\begin{aligned}X_{KM} &= \operatorname{span}\{\mathcal{L}_{km}^\gamma : (k,m) \in \mathcal{M}_{km}\}, \\ \mathcal{M}_{KM} &= \big\{(k,m) \in \mathcal{M} : k = 0, \dots, K-1, m = -\tfrac{M}{2}, \dots, \tfrac{M}{2} - 1\big\}.\end{aligned}$$

The orthogonal projection $\mathcal{P}_{KM}: \ X_0 = L^2(\mathbb{R}^2) \to X_{KN}$ is given by

$$\mathcal{P}_{KM}(u) = \sum_{(k,m)\in\mathcal{M}_{KM}} c_{km}(u)\,\mathcal{L}^{\gamma}_{km},$$

$$\begin{aligned} c_{km}(u) &= \langle \mathcal{L}^{\gamma}_{km}, u\rangle_{L^2(\mathbb{R}^2)} \\ &= \int_0^{2\pi}\int_0^{\infty} r\,\widetilde{L}^{\gamma}_{k,|m|}(r)\,\mathrm{e}^{-\mathrm{i}m\vartheta}\,u(r\cos\vartheta, r\sin\vartheta)\,\mathrm{d}r\,\mathrm{d}\vartheta. \end{aligned} \tag{27}$$

For $N = K + \frac{M}{2}$ we denote by

$$r_j = r_{j,K+\frac{M}{2}}, \quad w_{j,K+\frac{M}{2}}, \qquad j = 0,\dots,K+\tfrac{M}{2}-1,$$

scaled Gauß–Laguerre nodes and weights, cf. (21), and further set

$$\vartheta_s = \vartheta_{sM} = \tfrac{2\pi s}{M}, \quad s = 0,\dots,M-1.$$

According to [3], in (27) we substitute $r = \sqrt{\varrho/\gamma}$, approximate the inner integral by the Gauß–Laguerre quadrature formula, and the outer integral by the trapezoidal rule to obtain the spectral *interpolant*

$$\mathcal{Q}_{KM}\,u = \sum_{(k,m)\in\mathcal{M}_{KM}} \widetilde{c}_{km}(u)\,\mathcal{L}^{\gamma}_{km}, \tag{28a}$$

where we employ the abbreviations

$$\begin{aligned} \mathcal{K}_{KM} &= \left\{(j,s) : j = 0,\dots,K+\tfrac{M}{2}-1, s = 0,\dots,M-1\right\}, \\ x_{js} &= r_j\cos\vartheta_s, \quad y_{js} = r_j\sin\vartheta_s, \qquad (j,s)\in\mathcal{K}_{KM}, \\ \widetilde{c}_{km}(u) &= \tfrac{1}{M}\sum_{(j,s)\in\mathcal{K}_{KM}} w_j\,\overline{\mathcal{L}^{\gamma}_{km}(x_{js},y_{js})}\,u(x_{js},y_{js}), \quad (k,m)\in\mathcal{M}_{KM}. \end{aligned} \tag{28b}$$

Evidently, the spectral interpolant is well-defined for any function $u \in C(\mathbb{R}^2)$ and in particular for $u \in X_\alpha$ with $\alpha \geq 1$, see also Lemma 3. We point out that the interpolation property at the quadrature nodes only holds approximately

$$u(x_{js},y_{js}) \approx (\mathcal{Q}_{KM}u)(x_{js},y_{js}), \quad (j,s)\in\mathcal{K}_{KM},$$

since the number of interpolation points $\#\mathcal{K}_{KM} = (K+\frac{M}{2})\,M$ exceeds the number of basis functions $\#\mathcal{M}_{KM} = KM$. However, choosing $N = K + \frac{M}{2}$ (and not merely $N = K$) Gauß–Laguerre quadrature nodes is needed in order to ensure exact quadrature.

Basic relations for spectral interpolants. Basic relations and a first estimate for the generalized-Laguerre–Fourier spectral interpolant is provided by the following result.

Lemma 7 *(i) The spectral basis functions satisfy the following discrete orthogonality relation for all $(k,m),(k',m') \in \mathcal{M}_{KM}$:*

$$\tfrac{1}{M} \sum_{(j,s)\in\mathcal{K}_{KM}} w_j \, \overline{\mathcal{L}^{\gamma}_{km}(x_{js},y_{js})} \, \mathcal{L}^{\gamma}_{k'm'}(x_{js},y_{js}) = \delta_{kk'}\delta_{mm'}. \tag{29a}$$

(ii) For any $u \in X_0 = L^2(\mathbb{R}^2)$ it holds

$$\mathcal{Q}_{KM}\,\mathcal{P}_{KM}\,u = \mathcal{P}_{KM}\,u. \tag{29b}$$

(iii) For any $u \in C(\mathbb{R}^2)$ and in particular for any $u \in X_\alpha$ with $\alpha \geq 1$ the following bound is valid:

$$\|\mathcal{Q}_{KM}u\|_{L^2(\mathbb{R}^2)} = \|\mathcal{Q}_{KM}u\|_{K+\frac{M}{2},M} \leq \|u\|_{K+\frac{M}{2},M}. \tag{29c}$$

Proof (i) In the following, we denote by $\varrho_j = \varrho_{j,K+\frac{M}{2}}$, $\omega_j = \omega_{j,K+\frac{M}{2}}$, $j = 0,\dots,K+\frac{M}{2}-1$, the zeros of the (standard) Laguerre polynomial $L^0_{K+N/2}(r) = L_{K+N/2}(r)$ and the corresponding weights associated with Gauß–Laguerre quadrature. Using the definition (21) of the scaled Gauß–Laguerre points and weights $r_j = r_{j,K+\frac{M}{2}}$, $w_j = w_{j,K+\frac{M}{2}}$, the definition (3) of the scaled generalized-Laguerre functions $\widetilde{L}^{\gamma}_{km}(r)$, the exactness property of Gauß–Laguerre quadrature, and the orthogonality relations (2b) for the generalized-Laguerre polynomials $L^m_k(r)$ we obtain ($k,k' = 0,\dots,K-1$, $m = 0,\dots,\frac{M}{2}$)

$$\begin{aligned}
\sum_{j=0}^{K+\frac{M}{2}-1} w_j\, \widetilde{L}^{\gamma}_{km}(r_j)\, \widetilde{L}^{\gamma}_{k'm}(r_j) &= \tfrac{\pi}{\gamma} \sum_{j=0}^{K+\frac{M}{2}-1} \omega_j\, \mathrm{e}^{\varrho_j}\, L^{\gamma}_{km}\big(\sqrt{\tfrac{\varrho_j}{\gamma}}\big) \widetilde{L}^{\gamma}_{k'm}\big(\sqrt{\tfrac{\varrho_j}{\gamma}}\big) \\
&= \tfrac{1}{\sqrt{C^m_k C^m_{k'}}} \sum_{j=0}^{K+\frac{M}{2}-1} \omega_j\, \varrho_j^m\, L^m_k(\varrho_j)\, L^m_{k'}(\varrho_j) \\
&= \tfrac{1}{\sqrt{C^m_k C^m_{k'}}} \int_0^\infty r^m\, \mathrm{e}^{-r}\, L^m_k(r)\, L^m_{k'}(r) = \delta_{kk'}.
\end{aligned}$$

Together with the corresponding discrete orthogonality relations for the Fourier spectral method

$$\tfrac{1}{M} \sum_{s=0}^{M-1} \mathrm{e}^{-\mathrm{i}m\vartheta_s}\, \mathrm{e}^{\mathrm{i}m'\vartheta_s} = \delta_{mm'}, \quad m,m' = -\tfrac{M}{2},\dots,\tfrac{M}{2}-1,$$

and the definition (4a) of the spectral basis functions this yields (29a).

(ii) It remains to show that for a function of the form

$$u = \sum_{(k,m)\in\mathcal{M}_{KM}} c_{km}(u)\, \mathcal{L}^{\gamma}_{km}$$

it holds $\widetilde{c}_{km}(u) = c_{km}(u)$, see (28b). Due to linearity it is sufficient to consider $u = \mathcal{L}^\gamma_{k'm'}$ for $(k', m') \in \mathcal{M}_{KM}$. Then by (28b) (29a), (7b), and (27) we obtain

$$\widetilde{c}_{km}(\mathcal{L}^\gamma_{k'm'}) = \delta_{kk'}\delta_{mm'} = \langle \mathcal{L}^\gamma_{km}, \mathcal{L}^\gamma_{k'm'}\rangle_{L^2(\mathbb{R}^2)} = c_{km}(\mathcal{L}^\gamma_{km})$$

for $(k, m), (k', m') \in \mathcal{M}_{KM}$.

(iii) For a given function $u \in C(\mathbb{R}^2)$ we collect the values of u at the interpolation points in a column vector with indices (j, s) occurring in the order $(0, 0), \ldots, (K + \frac{M}{2} - 1, 0), (0, 1), \ldots, (K + \frac{M}{2} - 1, M - 1)$,

$$\mathbf{u} = (\ldots, u(x_{js}, y_{js}), \ldots)^T \in \mathbb{R}^{(K+\frac{M}{2})M}, \hat{\mathbf{u}} = (\ldots, \widetilde{c}_{km}(u), \ldots)^T \in \mathbb{R}^{KM},$$

and in a similar manner the Fourier coefficients (28b) in the order $(0, 0), \ldots, (K - 1, 0), (0, 1), \ldots, (K - 1, M - 1)$. Then the transformation to *frequency space* (28b) can be written in the compact form

$$\begin{aligned}\hat{\mathbf{u}} &= L^\dagger W \mathbf{u},\\ W &= \tfrac{1}{M}\operatorname{diag}(\ldots, w_0, \ldots, w_{K+\frac{M}{2}-1}, \ldots) \in \mathbb{R}^{(K+\frac{M}{2})M\times(K+\frac{M}{2})M},\\ L &= \big(\mathcal{L}^\gamma_{km}(x_{js}, y_{js})\big) \in \mathbb{R}^{KM\times(K+\frac{M}{2})M},\end{aligned}$$

where the sequence $w_0, \ldots, w_{K+\frac{M}{2}-1}$ occurs M times, and with indices (j, s) indexing columns, and indices (k, m) indexing rows in the same orders as in the vectors $\mathbf{u}$ and $\hat{\mathbf{u}}$, respectively; $L^\dagger$ denotes the conjugate transpose of the matrix L. In compact matrix notation, the discrete orthogonality relation (29a) becomes

$$L^\dagger W L = I. \tag{30}$$

As transformation to *physical space*, that is, evaluation of a spectral interpolant at the interpolation points, corresponds to the mapping $\hat{\mathbf{u}} \mapsto L\hat{\mathbf{u}}$, the vector comprising the values of the spectral interpolant (28a) at the interpolation points is given by

$$\mathcal{Q}\,\mathbf{u} = L\hat{\mathbf{u}} = LL^\dagger W\mathbf{u} = (\ldots, \mathcal{Q}_{KM}u(x_{js}, y_{js}), \ldots)^T \in \mathbb{R}^{(K+\frac{M}{2})M}.$$

Moreover, the discrete L^2-norm of u equals

$$\|u\|^2_{K+\frac{M}{2},M} = \mathbf{u}^\dagger W\mathbf{u},$$

recall also (22), and thus by Parseval's identity and and (30) it follows

$$\begin{aligned}\|\mathcal{Q}_{KM}u\|^2_{L^2(\mathbb{R}^2)} &= \sum_{(k,m)\in\mathcal{M}_{KM}} |\widetilde{c}_{km}(u)|^2 = \hat{\mathbf{u}}^\dagger\hat{\mathbf{u}} = \mathbf{u}^\dagger WLL^\dagger W\mathbf{u}\\ &= \mathbf{u}^\dagger WLL^\dagger WLL^\dagger W\mathbf{u} = \|\mathcal{Q}_{KM}u\|^2_{K+\frac{M}{2},M}.\end{aligned} \tag{31}$$

Applying (31) and the identity $WLL^{\dagger}W(I-LL^{\dagger}W)=0$ resulting from (30), we finally obtain

$$\begin{aligned}\|u\|^2_{K+\frac{M}{2},M} &= \|\mathcal{Q}_{KM}u + (\mathrm{Id}-\mathcal{Q}_{KM})u\|^2_{K+\frac{M}{2},M}\\ &= \mathbf{u}^{\dagger}\big(LL^{\dagger}W + (I-LL^{\dagger}W)\big)^{\dagger}W\big((LL^{\dagger}W + (I-LL^{\dagger}W)\big)\mathbf{u}\\ &= \|\mathcal{Q}_{KM}u\|^2_{K+\frac{M}{2},M} + \|(\mathrm{Id}-\mathcal{Q}_{KM})u\|^2_{K+\frac{M}{2},M}\\ &\qquad +2\,\Re\big(\mathbf{u}^{\dagger}WLL^{\dagger}W(I-LL^{\dagger}W)\mathbf{u}\big)\\ &\geq \|\mathcal{Q}_{KM}u\|^2_{K+\frac{M}{2},M} = \|\mathcal{Q}_{KM}u\|^2_{L^2(\mathbb{R}^2)},\end{aligned}$$

which yields the stated bound (29c). □

Estimates for spectral interpolants in fractional power spaces. The following result provides estimates for the generalized-Laguerre–Fourier spectral interpolant in fractional power spaces.

Lemma 8 *(i) For all $u,v\in X_\alpha$ with $\alpha\geq 1$ it holds*

$$\|\mathcal{Q}_{KM}u\|_{X_\alpha} \leq \lambda_{\max}^{\alpha}\,\|\mathcal{Q}_{KM}u\|_{X_0}, \tag{32a}$$

$$\|\mathcal{Q}_{KM}(uv)\|_{X_0} \leq \|u\|_{L^\infty(\mathcal{K}_{KM})}\|v\|_{K+\frac{M}{2},M} \leq \mathcal{C}\,\|u\|_{X_\alpha}\|v\|_{K+\frac{M}{2},M}, \tag{32b}$$

where $\|u\|_{L^\infty(\mathcal{K}_{KM})} = \max\{|u(x_{js},y_{js})| : (j,s)\in\mathcal{K}_{KM}\}$ *and*

$$\lambda_{\max} = \max_{(k,m)\in\mathcal{M}_{KM}}\lambda_{km} \leq \max_{(k,m)\in\mathcal{M}_{KM}}\gamma\,(2k+2m+1) \leq \mathcal{C}\,(K+M)$$

denotes the maximum eigenvalue in the index set $\mathcal{M}_{KM}$.

(ii) Provided that K is proportional to M, for any $u\in X_\alpha$ with $\alpha\geq 1$ and for $0\leq\zeta\leq\alpha$ the estimates

$$\begin{aligned}\|\mathcal{Q}_{KM}u\|_{X_0} &\leq \|u\|_{K+\frac{M}{2},M} &(32c)\\ &\leq \mathcal{C}\big(\|u\|_{X_0} + M^{-1/6}\,\|u\|_{X_{1/2}} + M^{-1/2}\,\|u\|_{X_1}\big) \leq \mathcal{C}\,\|u\|_{X_\alpha},\\ \|(\mathcal{Q}_{KM}-\mathrm{Id})\,u\|_{X_\zeta} &\leq \mathcal{C}\,\lambda_{\max}^{-(\alpha-\zeta)}\,\big(1+\lambda_{\max}^{1/2}\,M^{-1/6} + \lambda_{\max}\,M^{-1/2}\big)\,\|u\|_{X_\alpha} &(32d)\\ &\leq \mathcal{C}\,M^{-(\alpha-\zeta-1/2)}\,\|u\|_{X_\alpha}, &(32e)\end{aligned}$$

are valid.

Proof We recall the general assumption (8) on the angular momentum rotation speed.

(i) The first statement follows from the relation

$$\|\mathcal{Q}_{KM}u\|_{X_\alpha} = \Big\|\sum_{(k,m)\in\mathcal{M}_{KM}}\widetilde{c}_{km}(u)\,\lambda_{km}^{\alpha}\,\mathcal{L}_{km}^{\gamma}\Big\|_{X_0} \leq \lambda_{\max}^{\alpha}\,\|\mathcal{Q}_{KM}u\|_{X_0},$$

as well as

$$
\begin{aligned}
\|\mathcal{Q}_{KM}(uv)\|_{X_0}^2 &= \|\mathcal{Q}_{KM}(uv)\|_{K+\frac{M}{2},M}^2 \\
&= \tfrac{1}{M} \sum_{(j,s)\in\mathcal{K}_{K,M}} w_j\, |u(x_{js},y_{js})|^2\, |v(x_{js},y_{js})|^2 \\
&\leq \|u\|_{L^\infty(\mathcal{K}_{KM})}^2\, \|v\|_{K+\frac{M}{2}}^2 \leq \mathcal{C}\, \|u\|_{X_\alpha}^2 \|v\|_{K+\frac{M}{2},M}^2,
\end{aligned}
$$

where for the last inequality we used Lemma 3 (10a).

(ii) Relation (32c) follows easily from (23b), (29c), and (10a). For $u \in X_\alpha$ with $\alpha \geq 1$ and for $0 \leq \zeta \leq \alpha$, due to

$$
A^\zeta\,(\mathcal{P}_{KM} - \mathrm{Id})\, u = - \sum_{(k,m)\in\mathcal{M}\setminus\mathcal{M}_{KM}} c_{km}(u)\, \lambda_{km}^\zeta\, \mathcal{L}_{km}^\gamma,
$$

we obtain the estimate

$$
\begin{aligned}
\|A^\zeta(\mathcal{P}_{KM} - \mathrm{Id})\, u\|_{X_0}^2 &= \sum_{(k,m)\in\mathcal{M}\setminus\mathcal{M}_{KM}} |c_{km}(u)|^2 \lambda_{km}^{2\zeta} \\
&\leq \lambda_{\max}^{-2(\alpha-\zeta)} \sum_{(k,m)\in\mathcal{M}\setminus\mathcal{M}_{KM}} |c_{km}(u)|^2\, \lambda_{km}^{2\alpha} \\
&\leq \lambda_{\max}^{-2(\alpha-\zeta)} \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2\, \lambda_{km}^{2\alpha} = \lambda_{\max}^{-2(\alpha-\zeta)}\, \|u\|_{X_\alpha}^2
\end{aligned}
$$

Using the identity (cf. (29b))

$$
\mathcal{Q}_{KM} - \mathrm{Id} = (\mathcal{Q}_{KM} - \mathcal{P}_{KM}) + (\mathcal{P}_{KM} - \mathrm{Id}) = \mathcal{Q}_{KM}\,(\mathrm{Id} - \mathcal{P}_{KM}) + (\mathcal{P}_{KM} - \mathrm{Id}),
$$

and previous statements of this lemma, we obtain (32d),

$$
\begin{aligned}
\|(\mathcal{Q}_{KM} - \mathrm{Id})\, u\|_{X_\zeta} &\leq \|\mathcal{Q}_{KM}(\mathrm{Id} - \mathcal{P}_{KM})\, u\|_{X_\zeta} + \|(\mathcal{P}_{KM} - \mathrm{Id})\, u\|_{X_\zeta} \\
&\leq \lambda_{\max}^\zeta\, \|\mathcal{Q}_{KM}(\mathrm{Id} - \mathcal{P}_{KM})\, u\|_{X_0} + \lambda_{\max}^{-(\alpha-\zeta)}\, \|u\|_{X_\alpha} \\
&\leq \mathcal{C}\, \lambda_{\max}^\zeta\, \big(\|(\mathrm{Id} - \mathcal{P}_{KM})\, u\|_{X_0} + M^{-1/6}\, \|(\mathrm{Id} - \mathcal{P}_{KM})\, u\|_{X_{1/2}} \\
&\quad + M^{-1/2}\, \|(\mathrm{Id} - \mathcal{P}_{KM})\, u\|_{X_1}\big) + \lambda_{\max}^{-(\alpha-\zeta)}\, \|u\|_{X_\alpha} \\
&\leq \mathcal{C}\, \lambda_{\max}^{-(\alpha-\zeta)}\, \big(1 + \lambda_{\max}^{1/2} M^{-1/6} + \lambda_{\max} M^{-1/2}\big) \|u\|_{X_\alpha},
\end{aligned}
$$

from which (32e) follows using that $\lambda_{\max} \leq \mathcal{C}\, M$ if K is proportional to M. □

3 Convergence analysis

This section is devoted to the derivation of a convergence result for full discretizations of Gross–Pitaevskii equations with rotation term (1) by time-splitting generalized-Fourier–Laguerre–Hermite pseudo-spectral methods. As an illustration of the global error estimate for the fully discrete solution, stated in Section 3.1, a numerical example for a two-dimensional problem is given in Section 4 below.

Our approach in the lines of [9, 15, 20] in particular utilises the stability and error analysis for semi-discretizations in time given therein. In the derivation of the convergence result, to reduce the amount of technicalities and to keep the manuscript at a reasonable length, we restrict ourselves to the second-order Strang splitting method. However, it is clear that the result extends to higher-order splittings by using the preliminary results from the previous sections. Moreover, in Section 3.2 we do not specify the local error expansion for the Strang splitting found in literature [15]. We meanwhile focus on the case of two space dimensions and indicate the extension to the three-dimensional case in Section 3.4.

Full discretization (Strang). For integer $K \geq 1$, even integer $M \geq 2$, and a time-step $\Delta t > 0$ the Strang time-splitting generalized-Fourier–Laguerre–Hermite pseudo-spectral method yields numerical approximations u^n_{KM} to the exact solution values at times $t_n = n\,\Delta t$ through the recurrence relation

$$\begin{aligned} u^{n+1}_{KM} &= \mathcal{F}_{KM}(\Delta t)\, u^n_{KM} \\ &= \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\Delta t B[\mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM} u^n_{KM}]}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, u^n_{KM}, \end{aligned} \tag{33a}$$

see Section 2.6 and in particular (28a) for the definition of the spectral interpolation operator.

Semi-discretization in time (Strang). For our error analysis of full discretizations it is useful to introduce the approximation values obtained from a Strang splitting semi-discretization in time

$$u^{n+1} = \mathcal{S}(\Delta t)\, u^n = \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathrm{e}^{-\mathrm{i}\Delta t B[e^{-i\frac{\Delta t}{2}A} u^n]}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, u^n, \tag{33b}$$

which will be studied in Section 3.2.

3.1 Main result

Global error estimate. A standard idea in the derivation of a global error bound for the fully discrete solution is to interpose the time-discrete solution to obtain the estimate

$$\|u^n_{KM} - u(t_n)\|_{X_0} \leq \|u^n_{KM} - u^n\|_{X_0} + \|u^n - u(t_n)\|_{X_0},$$

by the triangle inequality. A bound for the contribution of the semi-discretization in time (33b) is provided by Theorem 2, see Section 3.2. The difference $u^n_{KM} - u^n$ is rewritten by means of a telescopic identity

$$\begin{aligned} u^n_{KM} - u^n &= (\mathcal{Q}_{KM} - \mathrm{Id})\, u^n + u^n_{KM} - \mathcal{Q}_{KM}\, u^n \\ &= (\mathcal{Q}_{KM} - \mathrm{Id})\, u^n + \mathcal{F}_{KM}(\Delta t)^n\, u^0 - \mathcal{Q}_{KM}\, u^n \\ &= (\mathcal{Q}_{KM} - \mathrm{Id})\, u^n \\ &\quad + \sum_{j=0}^{n-1} \mathcal{F}_{KM}(\Delta t)^{n-j-1}\, \big(\mathcal{F}_{KM}(\Delta t)\, u^j - \mathcal{Q}_{KM}\, \mathcal{S}(\Delta t)\, u^j\big) \end{aligned} \tag{34}$$

and estimated with the help of the auxiliary results given in Section 3.3 for the Strang splitting method. Altogether, we are able to establish the following convergence result, where $p = 2$ for the second-order Strang splitting method. The generalization to higher-order time-splitting methods follows the arguments detailed in [20] for space discretzations based on the Fourier, Sine, and Hermite pseudo-spectral methods, respectively. In order to simultaneously capture the cases of two and three space dimensions, we suppose the additional space discretization parameters K, L to be proportional to M and write $u_M^n = u_{KM}^n$ or $u_M^n = u_{KLM}^n$, respectively, for short, see also Section 3.4.

Theorem 1 *Assume that the potential V and the values of the exact solution to the Gross–Pitaevskii equation* (1) *remain bounded in the fractional power space X_p, where $p \geq 1$ denotes the nonstiff order of the considered time-splitting method. Then the global error estimate*

$$\left\| u_M^n - u(t_n) \right\|_{X_0} \leq \mathcal{C} \left((\Delta t)^p + M^{-q} \right), \qquad 0 \leq t_n \leq T,$$

is valid with constant $\mathcal{C}$ depending in particular on the upper bounds for $\|V\|_{X_p}$ and $\max\{\|u(t)\|_{X_p} : 0 \leq t \leq T\}$. In two space dimensions, that is, for the generalized-Laguerre–Fourier pseudo-spectral method it holds $q = p - \frac{3}{2} = p - \frac{9}{6}$, and in three space dimensions, that is, for the generalized-Laguerre–Fourier–Hermite pseudo-spectral method it follows $q = p - \frac{11}{6}$.

Remark We note that the corresponding result for the Hermite pseudo-spectral method involves the exponents $q = p - \frac{5}{3} = p - \frac{10}{6}$ in two space dimensions and $q = p - 2$ in three space dimensions, see [20].

3.2 Semi-discretization in time

In order to establish a convergence estimate for the Strang time-splitting method applied to (1), we pursue the standard approach of combining stability bounds and local error estimates. We note that our approach is general and permits to cover different spectral methods; the particular choice of the specific spectral method enters in the definition of the operators A, B and the auxiliary results deduced in Section 2.

3.2.1 Stability

Estimates for the evolution operator associated with B. Bounds for the action of the operator B and the associated evolution operator in fractional power spaces are provided by the following result. By means of the auxiliary estimates results deduced in Section 2 the corresponding results given in [20] carry over literally, see also [9, 15]; however, for the sake of completeness and for the convenience of the reader we include the proof of Lemma 9 below.

Lemma 9 *Let $\alpha \in \mathbb{N}$ with $\alpha \geq 1$ and set $\zeta = 0$ or $\zeta = \alpha$, respectively. Then for $u \in X_\alpha$ and $v \in X_\zeta$ the bounds*

$$\|B[u]\,v\|_{X_\zeta} \leq \mathcal{C}\,(\|V\|_{X_\alpha} + |\beta|\,\|u\|^2_{X_\alpha})\,\|v\|_{X_\zeta}, \tag{35a}$$
$$\|\mathrm{e}^{-\mathrm{i}tB[u]}\,v\|_{X_\zeta} \leq \mathrm{e}^{\mathcal{C}\,(\|V\|_{X_\alpha}+|\beta|\|u\|^2_{X_\alpha})t}\,\|v\|_{X_\zeta}, \tag{35b}$$

are valid. Furthermore, for $u, v, w \in X_\alpha$ it holds

$$\|(B[u] - B[v])\,w\|_{X_\zeta} \leq \mathcal{C}\,|\beta|\,(\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\,\|w\|_{X_\alpha}\,\|u - v\|_{X_\zeta}. \tag{35c}$$

Proof By Lemma 3 and relations (10b), (10c) we obtain (35a),

$$\|B[u]\,v\|_{X_\zeta} \leq \mathcal{C}\,\|B[u]\|_{X_\alpha}\|v\|_{X_\zeta} \leq \mathcal{C}\,(\|V\|_{X_\alpha} + |\beta|\,\|u\|^2_{X_\alpha})\,\|v\|_{X_\zeta}.$$

Similarly, rewriting the difference as

$$(B[u] - B[v])\,w = \beta\,(u\overline{u} - v\overline{v})\,w = \beta\big((u - v)\,\overline{u} + \overline{(u - v)}\,v\big)\,w$$

the bound (35c) follows. As $\widetilde{v}(t) = \mathrm{e}^{-\mathrm{i}tB[u]}\,v$ is the solution of the initial value problem

$$\mathrm{i}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\widetilde{v}(t) = B[u]\,\widetilde{v}(t), \quad \widetilde{v}(0) = v,$$

integration and an application of (35a) yields

$$\begin{aligned}\|\widetilde{v}(t)\|_{X_\zeta} &= \Big\|v - \mathrm{i}\int_0^t B[u]\,\widetilde{v}(\tau)\,\mathrm{d}\tau\Big\|_{X_\zeta}\\ &\leq \|v\|_{X_\zeta} + \mathcal{C}\,(\|V\|_{X_\alpha} + |\beta|\,\|u\|^2_{X_\alpha})\int_0^t \|\widetilde{v}(\tau)\|_{X_\zeta}\mathrm{d}\tau.\end{aligned}$$

A Gronwall-type inequality finally implies the stated bound (35b). □

Stability bound for the Strang semi-discretization in time. As before, for the sake of completeness we recapitulate arguments given in [9,15,20] to obtain a stability bound for the Strang semi-discretization in time; we note that the latter contribution also covers the case of high-order time-spitting methods.

Lemma 10 *For any $u, v \in X_\alpha$ with $\alpha \geq 1$ and for $\zeta = 0$ or $\zeta = \alpha$, respectively, it holds*

$$\|\mathcal{S}(t)\,u - \mathcal{S}(t)\,v\|_{X_\zeta} \leq \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2|\beta|)t}\,\|u - v\|_{X_\zeta},$$

where $\mathcal{C}_V$ denotes an upper bound for $\|V\|_{X_\alpha}$, $\mathcal{C}_\alpha$ denotes an upper bound for $\|u\|_{X_\alpha}$ and $\|v\|_{X_\alpha}$, and where $\mathcal{C}$ depends on α, additionally to its dependence on γ and Ω.

Proof For any $\alpha \geq 0$ Parseval's identity implies

$$\begin{aligned}\|\mathrm{e}^{-\mathrm{i}tA}\, u\|_{X_\alpha}^2 &= \Big\| \sum_{(k,m)\in\mathcal{M}} c_{km}(u)\, \lambda_{km}^{\alpha}\, \mathrm{e}^{-\mathrm{i}t\lambda_{km}}\, \mathcal{L}_{km}^{\gamma} \Big\|_{X_0}^2 \\ &= \sum_{(k,m)\in\mathcal{M}} |c_{km}(u)|^2\, \lambda_{km}^{2\alpha} = \|u\|_{X_\alpha}^2 .\end{aligned}$$

Thus, the application of the linear operator $\mathrm{e}^{-\mathrm{i}tA}$ in $\mathcal{S}(t)$ preserves the X_α norm. Hence, it only remains to show that for $\zeta = 0$ and $\zeta = \alpha$, respectively, it holds

$$\|\widetilde{u}(t) - \widetilde{v}(t)\|_{X_\zeta} \leq \|\mathrm{e}^{-\mathrm{i}tB[u]}\, u - \mathrm{e}^{-\mathrm{i}tB[v]}\, v\|_{X_\zeta} \leq \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)t}\, \|u - v\|_{X_\zeta}. \quad (36)$$

Here, with a slight mabuse of notation, we denote by $\widetilde{u}(t) = \mathrm{e}^{-\mathrm{i}tB[u]}\, u$ and $\widetilde{v}(t) = \mathrm{e}^{-\mathrm{i}tB[v]}\, v$ the solutions to the initial value problems

$$\mathrm{i}\, \tfrac{\mathrm{d}}{\mathrm{d}t} \widetilde{u}(t) = B[u]\, \widetilde{u}(t), \quad \widetilde{u}(0) = u, \qquad \mathrm{i}\, \tfrac{\mathrm{d}}{\mathrm{d}t} \widetilde{v}(t) = B[v]\, \widetilde{v}(t), \quad \widetilde{v}(0) = v.$$

Evidently, the difference satisfies

$$\begin{aligned}\mathrm{i}\, \tfrac{\mathrm{d}}{\mathrm{d}t} (\widetilde{u} - \widetilde{v})(t) &= B[u]\, \widetilde{u}(t) - B[v]\, \widetilde{v}(t) \\ &= B[u]\, (\widetilde{u}(t) - \widetilde{v}(t)) + (B[u] - B[v])\, \widetilde{v}(t), \\ (\widetilde{u} - \widetilde{v})(0) &= u - v.\end{aligned}$$

Hence, an application of the variation-of-constants formula yields

$$(\widetilde{u} - \widetilde{v})(t) = \mathrm{e}^{-\mathrm{i}tB[u]}\, (u - v) + \int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\, (B[u] - B[v])\, \mathrm{e}^{-\mathrm{i}\tau B[v]}\, v\, \mathrm{d}\tau. \quad (37)$$

Using Lemma 9 (35b)-(35c) and then (35b) we obtain the following bound for the integral

$$\begin{aligned}&\Big\| \int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\, (B[u] - B[v])\, \mathrm{e}^{-\mathrm{i}\tau B[v]}\, v\, \mathrm{d}\tau \Big\|_{X_\zeta} \\ &\quad \leq \int_0^t \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta| \|u\|_{X_\alpha}^2)(t-\tau)}\, \big\|(B[u] - B[v])\, \mathrm{e}^{-\mathrm{i}\tau B[v]}\, v\big\|_{X_\zeta}\, \mathrm{d}\tau \\ &\quad \leq \mathcal{C}\, |\beta|\, (\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\, \|u - v\|_{X_\zeta} \\ &\qquad \times \int_0^t \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta| \|u\|_{X_\alpha}^2)(t-\tau)}\, \big\|\mathrm{e}^{-\mathrm{i}\tau B[v]}\, v\big\|_{X_\alpha}\, \mathrm{d}\tau \\ &\quad \leq \mathcal{C}\, |\beta|\, (\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\, \|u - v\|_{X_\zeta}\, \|v\|_{X_\alpha} \\ &\qquad \times \int_0^t \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta| \|u\|_{X_\alpha}^2)(t-\tau+\tau)}\, \mathrm{d}\tau \\ &\quad = \mathcal{C}\, |\beta|\, (\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\, \|v\|_{X_\alpha}\, t\, \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta| \|u\|_{X_\alpha}^2)t}\, \|u - v\|_{X_\zeta}.\end{aligned}$$

Together with the estimate (35b) of the first term,

$$\|\mathrm{e}^{-\mathrm{i}tB[u]}\, (u - v)\|_{X_\zeta} \leq \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta| \|u\|_{X_\alpha}^2)t}\, \|u - v\|_{X_\zeta}$$

and $1 + x \le \mathrm{e}^x$ for $x \ge 0$ this gives

$$\begin{aligned}\|\widetilde{u}(t) - \widetilde{v}(t)\|_{X_\varsigma} &\le (1 + \mathcal{C}\,|\beta|\,(\|u\|_{X_\alpha} + \|v\|_{X_\alpha})\,\|v\|_{X_\alpha} t) \\ &\qquad\qquad \times \mathrm{e}^{\mathcal{C}(\|V\|_{X_\alpha} + |\beta|\|u\|^2_{X_\alpha})t}\,\|u - v\|_{X_\varsigma} \\ &\le \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)t}\,\|u - v\|_{X_\varsigma},\end{aligned}$$

which proves (36) and thus the statement of the lemma. □

3.2.2 Local error

Commutator bounds. Essential ingredients in local error estimates for time-splitting methds are bounds for iterated Lie-commutators. The following result provides estimates for the first and second iterated Lie-commutators needed in connection with the second-order Strang splitting. We note that in its proof the iterated commutators are expressed in terms of the linear operator A and the potential V and that the specific form of A is not exploited; in the case of a nonlinear operator B defining the problem this simplification is useful, however, in the linear case, in order to obtain bounds which are optimal with respect to the required regularity properties of u, the cancellation of terms has to be taken into account. Following [20] an analogous result for higher iterated Lie commutators arising in the local error analysis of higher-order time-splitting methods applied to (1) can be obtained.

Lemma 11 *Let* $\hat{A}(u) = -\,\mathrm{i}Au$ *and* $\hat{B}(u) = -\,\mathrm{i}B[u]\,u = -\,\mathrm{i}\,(V + \beta\,|u|^2)\,u$. *Then for* $u \in X_{\alpha+1}$ *with integer exponent* $\alpha \ge 1$ *the bounds*

$$\|[\hat{A}, \hat{B}](u)\|_{X_\alpha} \le \mathcal{C}\,\big(|\beta|\,\|u\|^3_{X_{\alpha+1}} + \|V\|_{X_{\alpha+1}}\|u\|_{X_{\alpha+1}}\big), \qquad (38a)$$

$$\|[\hat{A}, [\hat{A}, \hat{B}]](u)\|_{X_0} \le \mathcal{C}\,\big(|\beta|\,\|u\|^3_{X_{\alpha+1}} + \|V\|_{X_{\alpha+1}}\|u\|_{X_{\alpha+1}}\big), \qquad (38b)$$

are valid with constant $\mathcal{C} > 0$ *depending on* α, *additionally to its dependence on* γ *and* Ω.

Proof The Fréchet derivatives of $\hat{A}$ and $\hat{B}$ are given by

$$\hat{A}'(u)\,v = -\mathrm{i}Av, \quad \hat{B}'(u)\,v = -\mathrm{i}\,(V\,v + 2\,\beta\,|u|^2\,v + \beta\,u^2\,v),$$

respectively, so that

$$\begin{aligned}[\hat{A}, \hat{B}](u) &= \hat{A}'(u)\,\hat{B}(u) - \hat{B}'(u)\,\hat{A}(u) \\ &= -A\,(V\,u + \beta\,|u|^2\,u) + V A\,u + 2\,\beta\,|u|^2\,Au - \beta\,u^2\,\overline{Au} \\ &= -[A, V]\,u - \beta\,\big(A\,(|u|^2 u) - 2\,|u|^2 Au + u^2\,\overline{Au}\big).\end{aligned}$$

Applying the definition of the norm in the fractional power space X_α and Lemma 3 (10c) it follows

$$\begin{aligned}\big\|A\,(|u|^2 u) - 2\,|u|^2 Au + u^2\,\overline{Au}\big\|_{X_\alpha} &\le \mathcal{C}\,\|u\|^3_{X_{\alpha+1}}, \\ \|[A, V]\,u\|_{X_\alpha} &\le \mathcal{C}\,\|V\|_{X_{\alpha+1}}\|u\|_{X_{\alpha+1}},\end{aligned}$$

which proves (38a). As by assumption $\alpha \geq 1$, the first term in

$$[\hat{A}, [\hat{A}, \hat{B}]](u) = \hat{A}'(u)([\hat{A}, \hat{B}](u)) - [\hat{A}, \hat{B}]'(u)(\hat{A}u)$$

is estimated by means of (38a),

$$\|\hat{A}'(u)([\hat{A}, \hat{B}](u))\|_{X_0} = \|[\hat{A}, \hat{B}](u)\|_{X_1} \leq \|[\hat{A}, \hat{B}](u)\|_{X_\alpha},$$

which is compatible with (38b). In order to estimate the second term we determine the Fréchet derivative of $[\hat{A}, \hat{B}](u)$ as

$$\begin{aligned}[\hat{A}, \hat{B}]'(u)\, v = &- [A, V]\, v - \beta \big(A\,(2\,|u|^2 v + u^2 \bar{v}) \\ &-2\,u\,\bar{v}\,Au - 2\,\bar{u}\,v\,Au - 2\,|u|^2 Av + u^2\,\overline{Av} + 2\,u\,v\,\overline{Au}\big),\end{aligned}$$

and thus

$$\begin{aligned}[\hat{A}, \hat{B}]'(u)(\hat{A}u) = &\,\mathrm{i}\,[A, V]\,Au + \mathrm{i}\,\beta \big(A\,(2\,|u|^2\,Au - u^2\,\overline{Au}) \\ &+2\,u\,|Au|^2 - 2\,\bar{u}\,(Au)^2 - 2\,|u|^2\,A^2 u - u^2\,\overline{A^2 u} + 2\,u\,|Au|^2\big).\end{aligned}$$

Using Lemma 3 (10c) the X_0-norm of the terms in parentheses can be estimated by $\mathcal{C}\,\|u\|_{X_2}^3 \leq \mathcal{C}\,\|u\|_{X_{\alpha+1}}^3$, and similarly

$$\|[A, V]\,u\|_{X_0} \leq \mathcal{C}\,\|V\|_{X_2}\,\|u\|_{X_2} \leq \mathcal{C}\,\|V\|_{X_{\alpha+1}}\|u\|_{X_{\alpha+1}}.$$

Altogether we obtain the estimate (38b). □

Local error estimate. By means of the local error expansion for the Strang-splitting method deduced in [15] and the Lie-commutator bounds provided by Lemma 11, it is straightforward to obtain the following local error bound with $p = 2$. We omit the specification of the local error expansion deduced in [15] and refer to [20] for a generalization to high-order splitting methods.

Lemma 12 *Let $u(\Delta t)$ denote the exact solution to the evolution equation* (1c) *at time Δt with initial value u_0. For a splitting method of nonstiff order $p \geq 1$, the local error estimates*

$$\begin{aligned}\|\mathcal{S}(\Delta t)\,u_0 - u(\Delta t)\|_{X_1} &\leq \mathcal{C}\,(\Delta t)^p, \\ \|\mathcal{S}(\Delta t)\,u_0 - u(\Delta t)\|_{X_0} &\leq \mathcal{C}\,(\Delta t)^{p+1},\end{aligned}$$

are valid with constant $\mathcal{C} > 0$ depending in particular on upper bounds for $\|u_0\|_{X_p}$ and $\|V\|_{X_p}$.

3.2.3 Global error

Global error estimate. A standard approach based on a telescopic identity yields an estimate of the global error in terms of stability bounds and local error estimates as provided by Lemmas 10 and 12. We omit a detailed proof and refer to [15] for the case of the Strang splitting method, where $p = 2$. The generalization to high-order splitting methods is given in [20]; the error analysis shows that the nonstiff order of convergence is retained under suitable regularity requirements on the exact solution. For simplicity, we henceforth assume that the starting value u_0 coincides with the exact initial value $u(0)$.

Theorem 2 *For a splitting method of nonstiff order $p \geq 1$ the global error estimate*

$$\big\|u_n - u(t_n)\big\|_{X_0} \leq \mathcal{C}\,(\Delta t)^p, \qquad 0 \leq t_n \leq T,$$

is valid with constant $\mathcal{C} > 0$ depending in particular on upper bounds for $\max\{\|u(t)\|_{X_p} : 0 \leq t \leq T\}$ and $\|V\|_{X_p}$.

3.3 Full discretization

In this section, we deduce stability estimates and bounds for the defect that are needed for the estimation of (34).

3.3.1 Stability

Estimates for the evolution operator associated with B. A first stability result for the composition of the spectral interpolation operator and the evolution operator associated with B is provided by the following result.

Lemma 13 *For all $u, v \in X_\alpha$ with $\alpha \in \mathbb{N}$ such that $\alpha \geq 1$ the estimate*

$$\big\|\mathcal{Q}_{KM}\left(\mathrm{e}^{-\mathrm{i}tB[u]}\,u - \mathrm{e}^{-\mathrm{i}tB[v]}\,v\right)\big\|_{X_0} \leq \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2|\beta|)t}\,\|u - v\|_{K+\frac{M}{2},M} \tag{39a}$$

is valid with $\mathcal{C}_\alpha$ and $\mathcal{C}_V$ denoting upper bounds for $\|u\|_{X_\alpha}$, $\|v\|_{X_\alpha}$, and $\|V\|_{X_\alpha}$, respectively. In particular, if $u, v \in X_{KM}$, that is, $\mathcal{P}_{KM}\,u = \mathcal{Q}_{KM}\,u = u$ and $\mathcal{P}_{KM}\,v = \mathcal{Q}_{KM}\,v = v$, the relation

$$\big\|\mathcal{Q}_{KM}\left(\mathrm{e}^{-\mathrm{i}tB[u]}\,u - \mathrm{e}^{-\mathrm{i}tB[v]}\,v\right)\big\|_{X_0} \leq \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2|\beta|)t}\,\|u - v\|_{X_0} \tag{39b}$$

follows.

Proof For simplicity, we assume $V = 0$ and refer to [20] for the case $V \neq 0$. Let $\widetilde{u}(t) = \mathrm{e}^{-\mathrm{i}tB[u]}\,u$ and $\widetilde{v}(t) = \mathrm{e}^{-\mathrm{i}tB[v]}\,v$ be defined as in the proof of Lemma 10. From (37) we obtain

$$\begin{aligned}\|\mathcal{Q}_{KM}\,(\widetilde{u}(t) - \widetilde{v}(t))\|_{X_0} &\leq \|\mathcal{Q}_{KM}\,\mathrm{e}^{-\mathrm{i}tB[u]}\,(u-v)\|_{X_0}\\ &\quad+ \Big\|\mathcal{Q}_{KM}\int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\,(B[u] - B[v])\,\mathrm{e}^{-\mathrm{i}\tau B[v]}\,v\,\mathrm{d}\tau\Big\|_{X_0}.\end{aligned}$$

Here we estimate the two terms on the right separately. Using Lemma 7 (29c) and the definition of the norm $\|\cdot\|_{K+\frac{M}{2},M}$ we obtain

$$\begin{aligned}
\|\mathcal{Q}_{KM}\,\mathrm{e}^{-\mathrm{i}tB[u]}\,(u-v)\|_{X_0}^2 &\leq \|\mathrm{e}^{-\mathrm{i}tB[u]}\,(u-v)\|_{K+\frac{M}{2},M}^2 \\
&= \tfrac{1}{M}\sum_{(j,s)\in\mathcal{K}_{KM}} w_j\,\big|\mathrm{e}^{-\mathrm{i}tB[u](x_{js},y_{js})}\big|^2 |\,(u-v)(x_{js},y_{js})|^2 \\
&= \tfrac{1}{M}\sum_{(j,s)\in\mathcal{K}_{KM}} w_j\,|(u-v)(x_{js},y_{js})|^2 = \|u-v\|_{K+\frac{M}{2},M}^2.
\end{aligned}$$

Similarly, it follows

$$\begin{aligned}
&\Big\|\mathcal{Q}_{KM}\int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\,(B[u]-B[v])\,\mathrm{e}^{-\mathrm{i}\tau B[v]}\,v\;\mathrm{d}\tau\Big\|_{X_0} \\
&\quad\leq \Big\|\int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\,(B[u]-B[v])\,\mathrm{e}^{-\mathrm{i}\tau B[v]}\,v\;\mathrm{d}\tau\Big\|_{K+\frac{M}{2},M} \\
&\quad\leq \int_0^t \big\|\mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}\,(B[u]-B[v])\,\mathrm{e}^{-\mathrm{i}\tau B[v]}\,v\big\|_{K+\frac{M}{2},M}\;\mathrm{d}\tau \\
&\quad= \int_0^t \big\|(B[u]-B[v])\,v\big\|_{K+\frac{M}{2},M}\mathrm{d}\tau \\
&\quad= |\beta|\,t\,\big\|\big((u-v)\,\bar{u}+(\overline{u-v})\,v\big)\,v\big\|_{K+\frac{M}{2},M} \\
&\quad\leq |\beta|\,t\,\big(\|u\|_{L^\infty(\mathcal{K}_{KM})}+\|v\|_{L^\infty(\mathcal{K}_{KM})}\big)\,\|v\|_{L^\infty(\mathcal{K}_{KM})}\,\|u-v\|_{K+\frac{M}{2},M} \\
&\quad\leq \mathcal{C}\,|\beta|\,t\,\big(\|u\|_{X_\alpha}+\|v\|_{X_\alpha}\big)\,\|v\|_{X_\alpha}\,\|u-v\|_{K+\frac{M}{2},M} \\
&\quad\leq \mathcal{C}\,\mathcal{C}_\alpha^2\,|\beta|\,t\,\|u-v\|_{K+\frac{M}{2},M},
\end{aligned} \tag{40}$$

where the norm $\|\cdot\|_{L^\infty(\mathcal{K}_{KM})}$ is defined in Lemma 8, and the inequality $\|u\|_{L^\infty(\mathcal{K}_{KM})} \leq \|u\|_{X_\alpha}$ follows from Lemma 3 (10a). Altogether, using $1+x\leq \mathrm{e}^x$ this proves (39a). For $u,v\in X_{KM}$ the stated relation (39b) then follows from Lemma 7 (29c). □

Stability of the discrete evolution operator. An analogous stability bound to Lemma 10 is provided by the following auxiliary result. The statement follows at once from Lemma 13 (39b), noting that the evolution operator $\mathrm{e}^{-\mathrm{i}tA}$ preserves the X_0-norm and that $\mathrm{e}^{-\mathrm{i}tA}u\in X_{KM}$ for any $u\in X_{KM}$.

Lemma 14 *For all $u,v\in X_{KM}$ the estimate*

$$\|\mathcal{F}_{KM}(t)\,u-\mathcal{F}_{KM}(t)\,v\|_{X_0}\leq \mathrm{e}^{\mathcal{C}(\mathcal{C}_V+\mathcal{C}_\alpha^2|\beta|)t}\,\|u-v\|_{X_0} \tag{41}$$

is valid with $\mathcal{C}_\alpha$ and $\mathcal{C}_V$ depending on upper bounds for $\|u\|_{X_\alpha}$, $\|v\|_{X_\alpha}$, and $\|V\|_{X_\alpha}$, respectively, where $\alpha\in\mathbb{N}$ such that $\alpha\geq 1$.

3.3.2 Local error

Estimate for the defect. A bound for the difference $\mathcal{F}_{KM}(\varDelta t)\,u - \mathcal{Q}_{KM}\,\mathcal{S}(\varDelta t)\,u$ is given in Lemma 18. Several auxiliary estimates are provided by the following results. We recall the assumption that the integers K, M are proportional.

Lemma 15 *For any $u \in X_\alpha$ with $\alpha \geq 1$ it holds*

$$\|\mathcal{Q}_{KM}\,\mathrm{e}^{-\mathrm{i}tA}\,(\mathcal{Q}_{KM} - \mathrm{Id})\,u\|_{X_0} \leq \mathcal{C}\,t\,M^{-(\alpha-3/2)}\,\|u\|_{X_\alpha}. \tag{42}$$

Proof Let $v(t) = \mathcal{Q}_{KM}\,\mathrm{e}^{-\mathrm{i}tA}\,\mathcal{Q}_{KM}\,u = \mathrm{e}^{-\mathrm{i}tA}\,\mathcal{Q}_{KM}\,u$ and $w(t) = \mathrm{e}^{-\mathrm{i}tA}\,u$. Then $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}v(t) = Av(t)$ and

$$\mathrm{i}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{Q}_{KM}\,w(t)\big) = \mathcal{Q}_{KM}Aw(t) = A\mathcal{Q}_{KM}\,w(t) - [A, \mathcal{Q}_{KM}]\,w(t)$$

such that $\eta(t) = \mathcal{Q}_{KM}\,\mathrm{e}^{-\mathrm{i}tA}\,(\mathcal{Q}_{KM} - \mathrm{Id})\,u = v(t) - \mathcal{Q}_{KM}\,w(t)$ is the solution of

$$\mathrm{i}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\eta(t) = A\eta(t) + [A, \mathcal{Q}_{KM}]\,w(t), \quad \eta(0) = v(0) - \mathcal{Q}_{KM}\,w(0) = 0.$$

By the variation of constants formula it holds

$$\eta(t) = \int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)A}\,[A, \mathcal{Q}_{KM}]\,w(\tau)\,\mathrm{d}\tau = \int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)A}\,[A, \mathcal{Q}_{KM}]\,\mathrm{e}^{-\mathrm{i}\tau A}\,u\,\mathrm{d}\tau.$$

From Lemma 8 (32e) we obtain

$$\begin{aligned}\|[A, \mathcal{Q}_{KM}]\,u\|_{X_0} &= \|A\mathcal{Q}_{KM}\,u - Au + Au - \mathcal{Q}_{KM}\,Au\|_{X_0}\\ &\leq \|A\,(\mathcal{Q}_{KM} - \mathrm{Id})\,u\|_{X_0} + \|(\mathcal{Q}_{KM} - \mathrm{Id})\,Au\|_{X_0}\\ &\leq \mathcal{C}\,M^{-(\alpha-3/2)}\,\|u\|_{X_\alpha}\end{aligned}$$

for $u \in X_\alpha$, and hence

$$\|\eta(t)\|_{X_0} \leq \int_0^t \|[A, \mathcal{Q}_{KM}]\,\mathrm{e}^{-\mathrm{i}\tau A}\,u\|_{X_0}\,\mathrm{d}\tau \leq \mathcal{C}\,t\,M^{-(\alpha-3/2)}\,\|u\|_{X_\alpha},$$

which yields the stated result. □

Lemma 16 *For any $u \in X_\alpha$ with $\alpha \in \mathbb{N}$ such that $\alpha \geq 1$ the estimate*

$$\begin{aligned}&\|(\mathrm{Id} - \mathcal{Q}_{KM})\,\mathrm{e}^{-\mathrm{i}tB[\mathcal{Q}_{KM}u]}\,\mathcal{Q}_{KM}\,u\|_{X_0}\\ &\qquad \leq \mathcal{C}\,\mathcal{C}_\alpha\,(\mathcal{C}_V + \mathcal{C}_\alpha^2\,|\beta|)\,\mathrm{e}^{\mathcal{C}(\mathcal{C}_V+\mathcal{C}_\alpha^2|\beta|)t}\,t\,M^{-(\alpha-1/2)}\end{aligned} \tag{43}$$

holds, where $\mathcal{C}_\alpha$ denotes an upper bound for $\|\mathcal{Q}_{KM}u\|_{X_\alpha}$ and $\mathcal{C}_V$ denotes an upper bound for $\|V\|_{X_\alpha}$.

Proof Set $v = \mathcal{Q}_{KM} u$. By Lemma 8 (32e) it holds

$$\begin{aligned}\|(\mathrm{Id} - \mathcal{Q}_{KM})\, \mathrm{e}^{-\mathrm{i}tB[u]}\, v\|_{X_0} &= \|(\mathrm{Id} - \mathcal{Q}_{KM})\, (\mathrm{e}^{-\mathrm{i}tB[v]} - \mathrm{Id})\, v\|_{X_0} \\ &\leq \mathcal{C}\, M^{-(\alpha-1/2)}\, \|(\mathrm{e}^{-\mathrm{i}tB[v]} - \mathrm{Id})\, v\|_{X_\alpha} \\ &= \mathcal{C}\, M^{-(\alpha-1/2)}\, \|\eta(t)\|_{X_\alpha},\end{aligned}$$

where $\eta(t) = (\mathrm{e}^{-\mathrm{i}tB[v]} - \mathrm{Id})\, v$ is the solution to the initial value problem

$$\mathrm{i}\, \tfrac{\mathrm{d}}{\mathrm{d}t} \eta(t) = B[v]\, \eta(t) + B[v]\, v, \quad \eta(0) = 0.$$

By the variation-of-constants formula, it follows

$$\eta(t) = \int_0^t \mathrm{e}^{\mathrm{i}(t-\tau)B[v]}\, B[v]\, v\, \mathrm{d}\tau = \int_0^t B[v]\, \mathrm{e}^{\mathrm{i}(t-\tau)B[v]}\, v\, \mathrm{d}\tau,$$

so that by Lemma 9 (35a)–(35b) we have

$$\begin{aligned}\|\eta(t)\|_{X_\alpha} &\leq \mathcal{C}\, (\mathcal{C}_V + \mathcal{C}_\alpha^2\, |\beta|) \int_0^t \mathrm{e}^{\mathcal{C}\, (\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)\tau}\, \|v\|_{X_\alpha}\, \mathrm{d}\tau \\ &\leq \mathcal{C}\, \mathcal{C}_\alpha\, (\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)\, \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)t}\, t,\end{aligned}$$

from which (43) follows. □

Lemma 17 *For $u \in X_\alpha$ with $\alpha \in \mathbb{N}$ such that $\alpha \geq 1$ it holds*

$$\begin{aligned}&\left\| \mathcal{Q}_{KM} \left(\mathrm{e}^{-\mathrm{i}tB[u]}\, u - \mathrm{e}^{-\mathrm{i}tB[\mathcal{Q}_{KM} u]}\, \mathcal{Q}_{KM}\, u \right) \right\|_{X_0} \\ &\qquad \leq \mathcal{C}\, \mathcal{C}_\alpha\, (\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)\, \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)t}\, t\, M^{-(\alpha-3/2)}, \qquad (44)\end{aligned}$$

where $\mathcal{C}_\alpha$ denotes an upper bound for $\|u\|_{X_\alpha}$ as well as $\|\mathcal{Q}_{KM} u\|_{X_\alpha}$ and $\mathcal{C}_V$ denotes an upper bound for $\|V\|_{X_\alpha}$.

Proof In the following, we set $v(t) = \mathrm{e}^{-\mathrm{i}tB[u]}\, u$, $w(t) = \mathrm{e}^{-\mathrm{i}tB[\mathcal{Q}_{KM} u]}\, \mathcal{Q}_{KM}\, u$, and $\eta(t) = \mathcal{Q}_{KM}\, (v(t) - w(t))$. Then $\eta(t)$ is the solution of the initial value problem

$$\begin{aligned}\mathrm{i}\, \tfrac{\mathrm{d}}{\mathrm{d}t} \eta(t) &= B[u]\, \eta(t) - [B[u], \mathcal{Q}_{KM}]\, v(t) + (B[u]\, \mathcal{Q}_{KM} - \mathcal{Q}_{KM}\, B[\mathcal{Q}_{KM} u])\, w(t) \\ &= B[u]\, \eta(t) - [B[u], \mathcal{Q}_{KM}]\, (v(t) - w(t)) \\ &\qquad + \mathcal{Q}_{KM}\, (B[u] - B[\mathcal{Q}_{KM} u])\, w(t)\end{aligned}$$

with initial value $\eta(0) = 0$. By the variation-of-constants formula,

$$\begin{aligned}\eta(t) = \int_0^t \mathrm{e}^{-\mathrm{i}(t-\tau)B[u]} \big(&-[B[u], \mathcal{Q}_{KM}]\, (v(\tau) - w(\tau)) \\ &+ \mathcal{Q}_{KM}\, (B[u] - B[\mathcal{Q}_{KM} u])\, w(\tau) \big)\, \mathrm{d}\tau.\end{aligned}$$

Noting that $\eta(t) = \mathcal{Q}_{KM}\,\eta(t)$ and using Lemma 7 (29c) and the fact that the operator $\mathrm{e}^{-\mathrm{i}(t-\tau)B[u]}$ is unitary with respect to the norm $\|\cdot\|_{K+\frac{M}{2},M}$ it follows

$$\begin{aligned}\|\eta(t)\|_{X_0} \le \int_0^t \|[B[u], \mathcal{Q}_{KM}]\,(v(\tau) - w(\tau))\|_{K+\frac{M}{2},M}\,\mathrm{d}\tau \\ + \int_0^t \|(B[u] - B[\mathcal{Q}_{KM}u])\,w(\tau)\|_{K+\frac{M}{2},M}\,\mathrm{d}\tau. \qquad (45)\end{aligned}$$

As in the proof of Lemma 13 (see formula (40)) for the second integral in (45) we obtain

$$\begin{aligned}&\int_0^t \|(B[u] - B[\mathcal{Q}_{KM}u])\,\mathrm{e}^{-\mathrm{i}\tau B[\mathcal{Q}_{KM}u]}\,\mathcal{Q}_{KM}\,u\|_{K+\frac{M}{2},M}\,\mathrm{d}\tau \\ &\quad\le \mathcal{C}\,\mathcal{C}_\alpha^2\,|\beta|\,t\|(\mathcal{Q}_{KM} - \mathrm{Id})\,u\|_{K+\frac{M}{2},M} \\ &\quad\le \mathcal{C}\,\mathcal{C}_\alpha^3\,|\beta|\,t\,M^{-(\alpha-3/2)} \le \mathcal{C}\,\mathcal{C}_\alpha\,(\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)\,\mathrm{e}^{\mathcal{C}(\mathcal{C}_V+|\beta|\mathcal{C}_\alpha^2)t}\,t\,M^{-(\alpha-3/2)},\end{aligned}$$

where we used

$$\|(\mathcal{Q}_{KM} - \mathrm{Id})\,u\|_{K+\frac{M}{2},M} \le \mathcal{C}\,\|(\mathcal{Q}_{KM} - \mathrm{Id})\,u\|_{X_\alpha} \le \mathcal{C}\,M^{-(\alpha-3/2)}\,\|u\|_{X_\alpha}, \quad (46)$$

which follows from Lemma 8, eqs. (32c), (32e).

To estimate the first integral in (45) we first note that for $v \in X_\alpha$ it holds

$$\begin{aligned}\|[B[u], \mathcal{Q}_{KM}]v\|_{K+\frac{M}{2},M} &\le \|B[u]\,(\mathcal{Q}_{KM} - \mathrm{Id})\,v\|_{K+\frac{M}{2},M} \\ &\qquad + \|(\mathcal{Q}_{KM} - \mathrm{Id})\,B[u]\,v\|_{K+\frac{M}{2},M} \\ &\le \mathcal{C}\,(\|V\|_{X_\alpha} + |\beta|\,\|u\|_{X_\alpha}^2)\,\|(\mathcal{Q}_{KM} - \mathrm{Id})\,v\|_{K+\frac{M}{2},M} \\ &\qquad + \mathcal{C}\,M^{-(\alpha-3/2)}\,\|B[u]v\|_{X_\alpha} \\ &\le \mathcal{C}\,M^{-(\alpha-3/2)}\,(\|V\|_{X_\alpha} + |\beta|\,\|u\|_{X_\alpha}^2)\,\|v\|_{X_\alpha} \\ &\le \mathcal{C}\,M^{-(\alpha-3/2)}\,(\mathcal{C}_V + \mathcal{C}_\alpha^2\,|\beta|)\,\|v\|_{X_\alpha},\end{aligned}$$

where in the second line we used Lemma 8 (32b) and (46), and in the third line we used (46) and Lemma 9 (35a). By Lemma 9 (35b),

$$\begin{aligned}\|v(\tau) - w(\tau)\|_{X_\alpha} &\le \|\mathrm{e}^{-\mathrm{i}\tau B[u]}\,u\|_{X_\alpha} + \|\mathrm{e}^{-\mathrm{i}\tau B[\mathcal{Q}_{KM}u]}\,\mathcal{Q}_{KM}\,u\|_{X_\alpha} \\ &\le 2\,\mathcal{C}_\alpha \mathrm{e}^{\mathcal{C}(\mathcal{C}_V+\mathcal{C}_\alpha^2|\beta|)\tau},\end{aligned}$$

so that for the first integral in (45) we obtain

$$\begin{aligned}&\int_0^t \|[B[u], \mathcal{Q}_{KM}]\,(v(\tau) - w(\tau))\|_{K+\frac{M}{2},M}\,\mathrm{d}\tau \\ &\qquad\le \mathcal{C}\,\mathcal{C}_\alpha\,(\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)\,\mathrm{e}^{\mathcal{C}(\mathcal{C}_V+|\beta|\mathcal{C}_\alpha^2)t}\,t\,M^{-(\alpha-3/2)}.\end{aligned}$$

Together with the estimate for the second integral this proves (44). □

Lemma 18 *For $u \in X_\alpha$ with $\alpha \in \mathbb{N}$ such that $\alpha \geq 1$ the estimate*

$$\begin{aligned} &\|\mathcal{F}_{KM}(\Delta t)\, u - \mathcal{Q}_{KM}\, \mathcal{S}(\Delta t)\, u\|_{X_0} \\ &\qquad \leq \mathcal{C}\, \mathcal{C}_\alpha\, (\mathcal{C}_V + \mathcal{C}_\alpha^2 |\beta|)\, \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + \mathcal{C}_\alpha^2|\beta|)\Delta t}\, \Delta t\, M^{-(\alpha-3/2)} \end{aligned} \tag{47}$$

is valid, where $\mathcal{C}_\alpha$ denotes an upper bound for $\|u\|_{X_\alpha}$, $\|\mathcal{Q}_{KM}\, u\|_{X_\alpha}$, as well as $\|\mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, u\|_{X_\alpha}$, and $\mathcal{C}_V$ denotes an upper bound for $\|V\|_{X_\alpha}$.

Proof Set $z_1 = \mathrm{e}^{-\mathrm{i}\Delta t B[z_2]}\, z_2$, $z_2 = \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, z_3$, $z_3 = u$. Then we have

$$\mathcal{F}_{KM}(\Delta t)\, u - \mathcal{Q}_{KM}\, \mathcal{S}(\Delta t)\, u = -\,(Z_1 + Z_2 + Z_3),$$

where

$$\begin{aligned} Z_1 &= \mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, (\mathrm{Id} - \mathcal{Q}_{KM})\, z_1, \\ Z_2 &= \mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, \big(\mathrm{e}^{-\mathrm{i}\Delta t B[z_2]}\, z_2 - \mathrm{e}^{-\mathrm{i}\Delta t B[\mathcal{Q}_{KM} z_2]}\, \mathcal{Q}_{KM}\, z_2\big), \\ Z_3 &= \mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, \big(\mathrm{e}^{-\mathrm{i}\Delta t B[\mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, z_3]}\, \mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, z_3 \\ &\qquad\qquad - \mathrm{e}^{-\mathrm{i}\Delta t B[\mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\mathcal{Q}_{KM} z_3]}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, z_3\big). \end{aligned}$$

We estimate Z_1, Z_2, and Z_3 separately. First, by applying Lemma 15 and then Lemma 9 (35c) and the fact that $\mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}$ is unitary with respect to the norm $\|\cdot\|_{X_\alpha}$ we obtain

$$\|Z_1\|_{X_0} \leq \mathcal{C}\, \Delta t\, M^{-(\alpha-3/2)} \|z_1\|_{X_\alpha} \leq \mathcal{C}\, \mathcal{C}_\alpha\, \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)\Delta t}\, \Delta t\, M^{-(\alpha-3/2)}.$$

Second, by noting $\|\mathcal{Q}_{KM}\mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\mathcal{Q}_{KM} v\|_{X_0} = \|\mathcal{Q}_{KM} v\|_{X_0}$ and applying Lemma 17 we obtain

$$\|Z_2\|_{X_0} \leq \mathcal{C}\, \mathcal{C}_\alpha\, (\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)\, \mathrm{e}^{\mathcal{C}(\mathcal{C}_V + |\beta|\mathcal{C}_\alpha^2)\Delta t}\, \Delta t\, M^{-(\alpha-3/2)}.$$

Here we used $\|z_2\|_{X_\alpha} = \|u\|_{X_\alpha} \leq \mathcal{C}_\alpha$. Finally, again by noting

$$\|\mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, \mathcal{Q}_{KM}\, v\|_{X_0} = \|\mathcal{Q}_{KM}\, v\|_{X_0}$$

and applying first Lemma 13 (39b) and then Lemma 15 we obtain

$$\begin{aligned} \|Z_3\|_{X_0} &\leq \mathrm{e}^{\mathcal{C}\mathcal{C}_\alpha^2|\beta|\Delta t}\, \|\mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, (\mathrm{Id} - \mathcal{Q}_{KM})\, u\|_{X_0} \\ &\leq \mathcal{C}\, \mathcal{C}_\alpha \mathrm{e}^{\mathcal{C}\Delta t|\beta|\mathcal{C}_\alpha^2}\, \Delta t\, M^{-(\alpha-3/2)}. \end{aligned}$$

Note that here in the first step we need that $\mathcal{C}_\alpha$ is a bound for $\|\mathcal{Q}_{KM}\, u\|_{X_\alpha}$ and $\|\mathcal{Q}_{KM}\, \mathrm{e}^{-\mathrm{i}\frac{\Delta t}{2}A}\, u\|_{X_\alpha}$. Altogether, these bounds imply (47). □

3.4 Extension to three space dimensions

In this section, we study the generalized-Laguerre–Fourier–Hermite pseudo-spectral method for the space discretization of the three-dimensional Gross–Pitaevskii equation with rotation term (1). As our error analysis for the two-dimensional case naturally carries over to the case of three space dimensions, we only indicate where definitions and estimates have to be extended with some care.

Basic relations. In the present situation, the discretization of the (x, y)-variables relies on the generalized–Laguerre–Fourier spectral method analyzed before, and the discretization of the z-variable uses scaled Hermite functions involving the Hermite polynomials H_ℓ $(\ell = 0, 1, 2, \dots)$

$$\widetilde{H}_\ell^{\gamma_z}(z) = \tfrac{1}{\sqrt{2^\ell \ell!}} \sqrt[4]{\tfrac{\pi}{\gamma_z}} \, \mathrm{e}^{-\gamma_z z^2/2} \, H_\ell(\sqrt{\gamma_z} z),$$

see also [3] for further details. Hence, the eigenfunctions and associated eigenvalues of the linear operator A defined in (1d) are given by

$$\begin{aligned} \mathcal{B}_{km\ell}^{\gamma,\gamma_z}(x, y, z) &= \mathcal{L}_{km}^{\gamma}(x, y) \, \widetilde{H}_\ell^{\gamma_z}(z), \quad (k, m) \in \mathcal{M}, \quad \ell = 0, 1, 2, \dots, \\ \lambda_{km\ell} &= (2k + |m| + 1) \, \gamma - m \, \Omega + (\ell + \tfrac{1}{2}) \, \gamma_z. \end{aligned}$$

Similarly to before, we assume the discretization parameters K and L to be proportional to M, and introduce the index sets

$$\begin{aligned} \mathcal{M}_{KML} &= \{(k, m, \ell) : (k, m) \in \mathcal{M}_{KM}, \ell = 0, \dots, L - 1\}, \\ \mathcal{K}_{KML} &= \{(r, s, q) : (r, s) \in \mathcal{K}_{KM}, q = 0, \dots, L - 1\}. \end{aligned}$$

Consequently, the maximum eigenvalue in the set $\mathcal{M}_{KML}$ satisfies the relation

$$\lambda_{\max} = \max_{(k,m,\ell) \in \mathcal{M}_{KML}} \lambda_{km\ell} \leq \mathcal{C} \, (K + M + L) \leq \mathcal{C} \, M,$$

see Lemma 8. The spectral interpolant now also involves scaled Gauß–Hermite quadrature nodes and weights

$$\begin{aligned} \mathcal{Q}_{KML}(u) &= \sum_{(k,m,\ell) \in \mathcal{M}_{KML}} \widetilde{c}_{km\ell}(u) \, \mathcal{B}_{km\ell}^{\gamma,\gamma_z}, \\ \widetilde{c}_{km\ell}(u) &= \tfrac{1}{M} \sum_{(r,s,q) \in \mathcal{K}_{KML}} w_r \widetilde{w}_q \, \overline{\mathcal{B}_{km\ell}^{\gamma,\gamma_z}(x_{rs}, y_{rs}, z_q)} \, u(x_{rs}, y_{rs}, z_q). \end{aligned}$$

Error analysis. By means of well-known recurrence relations for scaled Hermite functions, analogous to Lemma 1, arguments in the lines of the proof of Lemma 2 yield the estimate

$$\|z \, u\|_{X_\alpha} + \|\partial_z u\|_{X_\alpha} \leq \mathcal{C} \, \|u\|_{X_{\alpha+1/2}}, \quad u \in X_{\alpha+1/2},$$

see also [9, 20]. In order to extend the estimate (23b) we utilise the bound

$$\sum_{q=0}^{L-1} \widetilde{w}_q \, |v(z_q)|^2 \leq \mathcal{C} \int_{\mathbb{R}} \big(|v(z)|^2 + M^{-1/3} \, |\partial_z v(z)|^2 \big) \, \mathrm{d}z, \qquad v \in H^1(\mathbb{R}),$$

deduced in [10]. As a consequence, we obtain the relation

$$
\begin{aligned}
\|u\|_{NML}^2 &= \tfrac{1}{M} \sum_{q=0}^{L-1} \sum_{r=0}^{N-1} \sum_{s=0}^{M-1} w_r\, \widetilde{w}_q\, |u(x_{rs}, y_{rs}, z_q)|^2 \\
&\leq \mathcal{C} \sum_{q=0}^{L-1} \widetilde{w}_q \int_{\mathbb{R}^2} \Big(|u(x,y,z_q)|^2 + M^{-1/3} \left(|\partial_x u(x,y,z_q)|^2 + |\partial_y u(x,y,z_q)|^2 \right) \\
&\qquad + M^{-1} \left(|\partial_x^2 u(x,y,z_q)|^2 + |\partial_y^2 u(x,y,z_q)|^2 + |\partial_{xy} u(x,y,z_q)|^2 \right) \Big)\, \mathrm{d}(x,y) \\
&\leq \mathcal{C} \int_{\mathbb{R}^3} \Big(|u|^2 + M^{-1/3} \left(|\partial_x u|^2 + |\partial_y u)|^2 \right) \\
&\qquad + M^{-1} \left(|\partial_x^2 u|^2 + |\partial_y^2 u|^2 + |\partial_{xy} u|^2 \right) \Big)\, \mathrm{d}(x,y,z) \\
&\qquad + \mathcal{C}\, M^{-1/3} \int_{\mathbb{R}^3} \Big(|\partial_z u|^2 + M^{-1/3} \left(|\partial_{xz} u|^2 + |\partial_{yz} u|^2 \right) \\
&\qquad + M^{-1} \left(|\partial_{xxz} u|^2 + |\partial_{yyz} u|^2 + |\partial_{xyz} u|^2 \right) \Big)\, \mathrm{d}(x,y,z) \\
&\leq \mathcal{C} \Big(\|u\|_{L^2(\mathbb{R}^3)}^2 + M^{-1/3}\, |u|_{H^1(\mathbb{R}^3)}^2 + M^{-2/3}\, |u|_{H^2(\mathbb{R}^3)}^2 + M^{-4/3}\, |u|_{H^3(\mathbb{R}^3)} \Big),
\end{aligned}
$$

which implies the following analogue to (32e)

$$\|(\mathcal{Q}_{KML} - \mathrm{Id})\, u\|_{X_\zeta} \leq \mathcal{C}\, M^{-(\alpha-\zeta-5/6)}\, \|u\|_{X_\alpha}.$$

As a consequence, in the three-dimensional case the factors $M^{-(\alpha-1/2)}$ and $M^{-(\alpha-3/2)}$ arising in the auxiliary results derived in Section 3.3 have to be replaced by $M^{-(\alpha-5/6)}$ and $M^{-(\alpha-11/6)}$ respectively. Altogether, this proves the statement of Theorem 1.

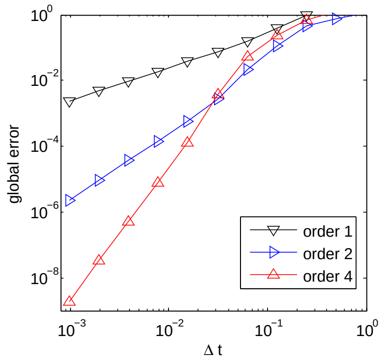
4 Numerical example

In the following we confirm the theoretical global error bound of Theorem 1 by a numerical example. Furthermore we include the reference to a movie, which illustrates the time evolution of the solution to a related problem that was considered in [3, Ex. 1].

Global error bound. We consider the time-dependent Gross–Pitaevskii equation with rotation term (1) in two space dimensions, where we set $\gamma = 0.8$, $\Omega = 0.5$, $V = 0$, and $\beta = 100$, and

$$u(x,y,0) = \tfrac{1}{\sqrt{\pi}}\, \mathrm{e}^{-\frac{1}{2}(x^2+y^2)}\, (x + \mathrm{i}\, y).$$

The problem is discretized in space by the generalized-Laguerre–Fourier pseudo-spectral method. For the time integration we apply splitting methods of (nonstiff) orders $p = 1, 2, 4$, the Lie–Trotter (order 1), Strang (order 2), and Yoshida (order 4) splitting methods, see for instance [11,16]. In Figure 1 (left)



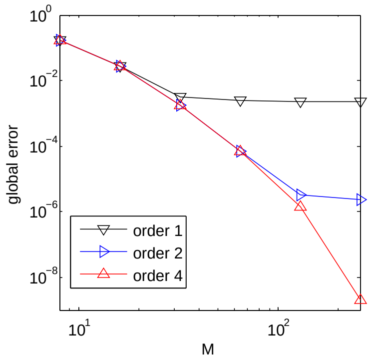


Fig. 1 Global error versus time stepsize Δt (left) and spatial discretization parameter M (right).

we display the global error at time $t = 1$ as a function of the time discretization parameter Δt for fixed spatial discretization parameters $M = 512$ and $K = M + 1$. As expected, for the chosen sufficiently regular initial condition the nonstiff temporal orders are retained. Furthermore, we display the global error in dependence of the space discretization parameter $M = 2^m$ for integer $3 \le m \le 8$, where again $K = M + 1$, with time stepsize fixed to $\Delta t = \frac{1}{1024}$. The numerical results confirm the spectral accuracy in space. We note that the global error is in general dominated by the temporal error; in particular, this behavior is observed for the first-order Lie–Trotter splitting method.

Time evolution. A movie illustrating the evolution of the solution to the specified problem on the time interval $[0, 10]$, but with additional potential

$$V(x, y) = \tfrac{1}{2}\,(\gamma_y^2 - \gamma^2)\, y^2, \qquad \gamma_y = 1.2,$$

is available at

`http://www.othmar-koch.org/fwf-project2011.html`.

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