Lecture on

Time-Splitting Spectral Methods for Nonlinear Schrödinger Equations

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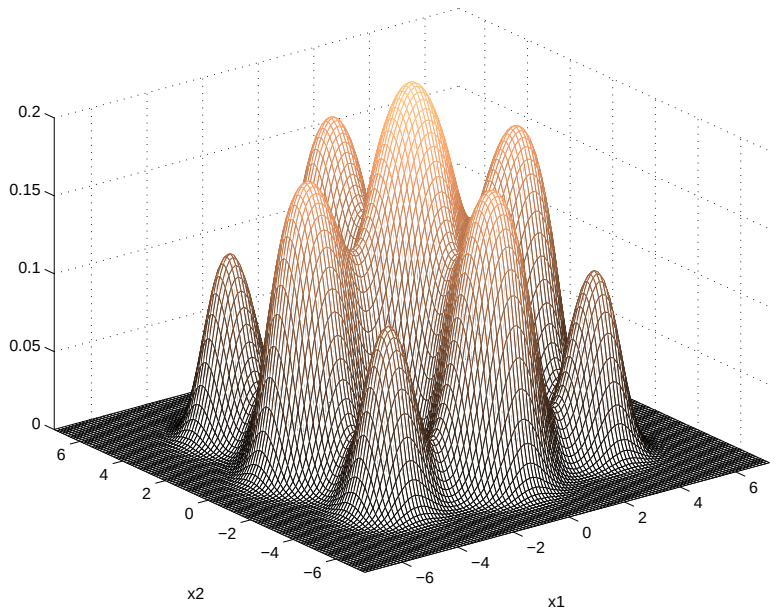

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Summary

In this lecture, I address the issue of efficient numerical methods for the time integration of nonlinear Schrödinger equations. As model problems, I consider systems of coupled Gross–Pitaevskii equations that arise in quantum physics for the description of multi-component Bose–Einstein condensates. My concern is to study the quantitative and qualitative behaviour of high-accuracy space and time discretisations that rely on time-splitting Fourier and Hermite spectral methods. In particular, this includes a stability and convergence analysis of high-order exponential operator splitting methods for evolutionary Schrödinger equations. Numerical examples illustrate the theoretical results.

Contents

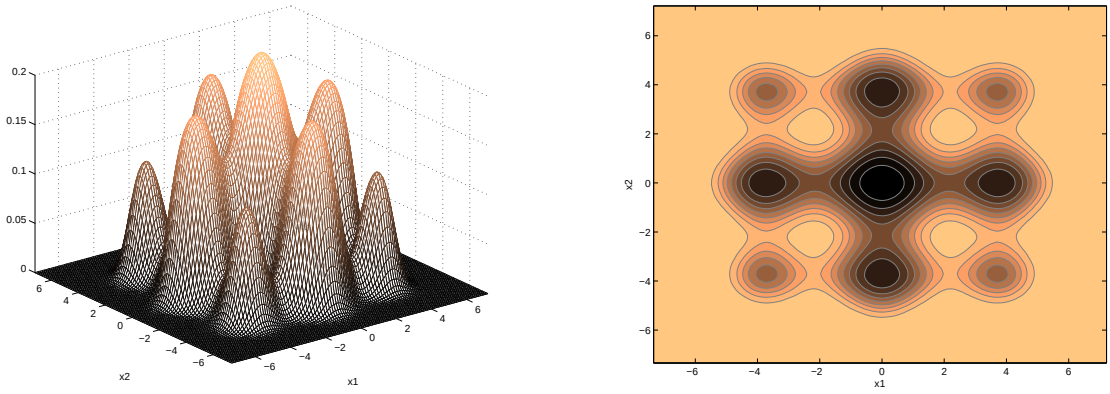

Figure 1.: Ground state solution of the Gross–Pitaevskii equation (1) with $\kappa = 25$ and $\vartheta = 400$.

Preface

The actual research activities on efficient space and time discretisations for time-independent as well as time-dependent nonlinear Schrödinger equations is reflected in various contributions [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 16, 18, 22, 23, 24, 26, 27, 28, 31, 33, 38, 42, 43, 45, 48, 49]. The present manuscript shall provide an introduction to advanced integration methods for nonlinear Schrödinger equations that rely on high-order time-splitting Hermite and Fourier spectral methods.

Part I is dedicated to exponential operator splitting methods [11, 30, 32, 34, 35, 41, 50] for ordinary differential equations. In particular, a result on the convergence behaviour of splitting methods is deduced. To avoid technicalities, the focus is on a splitting scheme involving two compositions applied to non-stiff linear differential equations. Extensions to splitting methods of arbitrarily high order and nonlinear evolutionary problems of parabolic or Schrödinger type, respectively, are indicated, see also [10, 17, 19, 20, 21, 25, 26, 31, 33, 36, 37, 44]. In Part II, Fourier and Hermite spectral methods and their numerical realisations are discussed, see [12, 46]. Part III is concerned with high-order time-splitting Fourier and Hermite pseudo-spectral methods for the space and time discretisation of Gross–Pitaevskii systems [29, 39] that arise in the description of multi-component Bose–Einstein condensates. In an appendix, the works [13, 14, 36, 44] are included.

As an illustration, the ground state of the two-dimensional Gross–Pitaevskii equation

$$\begin{aligned} \mathrm{i}\,\partial_t \psi(\xi,t) &= \Big(-\tfrac{1}{2}\Delta + U(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2\Big)\,\psi(\xi,t)\,, \qquad \xi\in\mathbb{R}^2\,, \quad t\geq 0\,, \\ \big\|\psi(\cdot,0)\big\|_{L^2} &= 1\,, \qquad U(\xi) = U(\xi_1,\xi_2) = \tfrac{1}{2}\sum_{i=1}^{2}\Big(\xi_i^2 + \kappa\sin^2\big(\tfrac{\pi}{4}\,\xi_i\big)\Big)\,, \end{aligned} \tag{1}$$

describing a Bose-Einstein condensate in a lattice under an external harmonic potential is displayed in Figure 1. The ground state solution is computed by means of the imaginary time method; hereby, the space and time discretisation relies on the Fourier spectral method with 256 basis functions in each space direction and a linearly implicit Euler method with constant time step 10^{-3}. A MATLAB code for the ground state computation and the time evolution of Gross–Pitaevskii systems in one, two, and three space dimensions is available on request.

Part I.

Exponential operator splitting methods

Situation. Let $X = \mathbb{R}^d$. We consider the following initial value problem for $y : [t_0, T] \to X$ involving a nonlinear autonomous differential equation

$$y'(t) = F\big(y(t)\big), \quad t_0 \le t \le T, \qquad y(t_0) \text{ given}. \tag{0.2}$$

Assumption. Throughout, we suppose the function $F : D \subset X \to X$ defining the right-hand side of the differential equation in (0.2) to be sufficiently often differentiable with bounded derivatives. For simplicity, we further assume $D = X$.

Generalisation. It is straightforward to extend our considerations to the case where the Euclidian space $X = \mathbb{R}^d$ is replaced with a Banach space $\big(X, \|\cdot\|_X\big)$.

Exact solution. For the following, it is useful to introduce the exact solution operator E_F associated with the initial value problem (0.2) through

$$y(t_0 + \tau) = E_F\big(\tau, t_0, y(t_0)\big), \qquad 0 \le \tau \le T - t_0. \tag{0.3a}$$

A standard existence and uniqueness result for (0.2) implies the identity

$$E_F\big(\sigma + \tau, t_0, y(t_0)\big) = E_F\big(\tau, t_0 + \sigma, y(t_0 + \sigma)\big), \qquad 0 \le \sigma + \tau \le T - t_0. \tag{0.3b}$$

Numerical approximation. For an initial approximation $y_0 \approx y(t_0)$ and a time grid with associated time stepsizes

$$t_0 < t_1 < \cdots < t_N = T, \qquad h_{n-1} = t_n - t_{n-1}, \quad 1 \le n \le N,$$

numerical approximations y_n to the exact solution values at time t_n are determined through a reccurrence relation of the form

$$y_n = \Phi_F(h_{n-1}, t_{n-1}, y_{n-1}), \quad 1 \le n \le N, \qquad y_0 \text{ given};$$

this is in accordance with the identity

$$y(t_n) = E_F\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big), \quad 1 \le n \le N, \qquad y(t_0) \text{ given},$$

see also (0.3). A numerical method is said to be consistent of order p iff the local error fulfills

$$d_n = \Phi_F\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big) - E_F\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big) = \mathcal{O}\big(h_{n-1}^{p+1}\big), \tag{0.4}$$

provided that the exact solution of (0.2) and the nonlinear function F defining the differential equation are sufficiently regular. It suffices to specify the first step of the numerical scheme

$$y_1 = \Phi_F(h, t_0, y_0) \;\approx\; y(t_1) = E_F\big(h, t_0, y(t_0)\big), \qquad h = h_0.$$

1. Linear problems

Situation. Let $X = \mathbb{R}^d$. Henceforth, we consider the following initial value problem for a function $y : [t_0, T] \to X$ involving a linear differential equation of the form

$$y'(t) = A\,y(t) + B\,y(t)\,, \quad t_0 \le t \le T\,, \qquad y(t_0) \text{ given}\,. \tag{1.1}$$

Generalisation. It is straightforward to extend our considerations to the case where the Euclidian space $X = \mathbb{R}^d$ is replaced with a Banach space $\big(X, \|\cdot\|_X\big)$.

Assumption. We suppose the matrices $A, B \in \mathbb{R}^{d\times d}$ or linear operators $A, B : X \to X$, respectively, to be bounded, that is, there exist (moderate) constants $C_A, C_B \ge 0$ such that

$$\big\|A\big\|_{X\leftarrow X} \le C_A\,, \qquad \big\|B\big\|_{X\leftarrow X} \le C_B\,; \tag{1.2}$$

we tacitly assume $C_A, C_B \ge 1$. Consequently, also $A + B$ is bounded

$$\big\|A + B\big\|_{X\leftarrow X} \le C_A + C_B\,.$$

In general, the linear operators A and B do not commute, that is, it holds $AB \ne BA$.

Exact solution. In the present situation, the exact solution of the initial value problem (1.1) is given by

$$y(t_0 + \tau) = \mathrm{e}^{\tau\,(A+B)}\,y(t_0)\,, \qquad 0 \le \tau \le T - t_0\,.$$

Here, for any matrix $L \in \mathbb{R}^{d\times d}$ or bounded linear operator $L : X \to X$, respectively, the exponential function is well defined through

$$\mathrm{e}^{\tau L} = \sum_{j=0}^{\infty} \tfrac{1}{j!}\,\tau^j L^j\,, \quad \tau \in \mathbb{R}\,. \tag{1.3}$$

Noting that the exact solution operator E_{A+B} is linear with respect to the initial value, we write $E_{A+B}(\tau)\,y(t_0) = E_{A+B}\big(\tau, t_0, y(t_0)\big)$ for short, that is, we have

$$y(t_0 + \tau) = E_{A+B}(\tau)\,y(t_0) = \mathrm{e}^{\tau\,(A+B)}\,y(t_0)\,, \qquad 0 \le \tau \le T - t_0\,. \tag{1.4}$$

Numerical approximation. In regard to relation (1.4), we require the numerical solution operator Φ_{A+B} to be linear with respect to the initial value

$$y_1 = \Phi_{A+B}(h)\, y_0 \;\approx\; y(t_1) = E_{A+B}(h)\, y(t_0)\,, \qquad h = h_0\,.$$

1.1. Splitting methods

Approach. Exponential operator splitting methods rely on a decomposition of the right-hand side of the differential equation in (1.1) into two (or more) parts and the presumption that the initial value problems

$$\begin{aligned} z'(t) &= A\, z(t)\,, \quad t_0 \le t \le T\,, \qquad z(t_0) \text{ given}\,, \\ \widetilde{z}'(t) &= B\, \widetilde{z}(t)\,, \quad t_0 \le t \le T\,, \qquad \widetilde{z}(t_0) \text{ given}\,, \end{aligned} \tag{1.5}$$

are solvable numerically in an accurate and efficient manner. The (approximate) solutions of the initial value problems (1.5) are then composed in a suitable way; this yields an approximation $\Phi_{A+B} \approx E_{A+B}$ to the exact solution operator. For simplicity and in view of Gross–Pitaevskii systems, we may assume that the exact solutions of (1.5)

$$\begin{aligned} z(t_0+\tau) &= E_A(\tau)\, z(t_0) = \mathrm{e}^{\tau A}\, z(t_0)\,, \qquad 0 \le \tau \le T - t_0\,, \\ \widetilde{z}(t_0+\tau) &= E_B(\tau)\, \widetilde{z}(t_0) = \mathrm{e}^{\tau B}\, \widetilde{z}(t_0)\,, \qquad 0 \le \tau \le T - t_0\,, \end{aligned}$$

are available.

General form of splitting methods. Any exponential operator splitting method involving several compositions can be cast into the following form

$$y_1 = \Phi_{A+B}(h)\, y_0 = \prod_{i=1}^{s} E_B(b_i h)\, E_A(a_i h)\, y_0 = \prod_{i=1}^{s} \mathrm{e}^{b_i h B}\, \mathrm{e}^{a_i h A}\, y_0\,, \qquad h = h_0\,, \tag{1.6}$$

yielding an approximation to the exact solution value

$$y(t_1) = E_{A+B}(h)\, y(t_0) = \mathrm{e}^{h(A+B)}\, y(t_0)\,, \qquad h = h_0\,.$$

In (1.6), the product is defined downwards, i.e., for linear operators $(L_i)_{j \le i \le k}$ we set

$$\prod_{i=j}^{k} L_i = L_k \cdots L_{j+1}\, L_j\,, \quad j \le k\,, \qquad \prod_{i=j}^{k} L_i = I\,, \quad j > k\,.$$

Example (Lie–Trotter splitting method). The Lie–Trotter splitting method for (1.1) can be cast into the general form (1.6) with

$$s = 1\,, \quad a_1 = 1\,, \quad b_1 = 1\,, \qquad \text{or} \qquad s = 2\,, \quad a_1 = 0\,, \quad a_2 = 1 \quad b_1 = 1\,, \quad b_2 = 0\,, \tag{1.7a}$$

method		order	#comp.
McLachlan	McLachlan [30, V.3.1, (3.3), pp. 138–139]	$p=2$	$s=3$
Strang	Strang (1.8)	$p=2$	$s=2$
BM4-1	Blanes & Moan [11, Table 2, PRKS_6]	$p=4$	$s=7$
BM4-2	Blanes & Moan [11, Table 3, SRKN_6^b]	$p=4$	$s=7$
M4	McLachlan [30, V.3.1, (3.6), pp. 140]	$p=4$	$s=6$
S4	Suzuki [30, II.4, (4.5), pp. 41]	$p=4$	$s=6$
Y4	Yoshida [30, II.4, (4.4), pp. 40]	$p=4$	$s=4$
BM6-1	Blanes & Moan [11, Table 2, PRKS_{10}]	$p=6$	$s=11$
BM6-2	Blanes & Moan [11, Table 3, SRKN_{11}^b]	$p=6$	$s=12$
BM6-3	Blanes & Moan [11, Table 3, SRKN_{14}^a]	$p=6$	$s=15$
KL6	Kahan & Li [30, V.3.2, (3.12), pp. 144]	$p=6$	$s=10$
S6	Suzuki [30, II.4, (4.5), pp. 41]	$p=6$	$s=26$
Y6	Yoshida [30, V.3.2, (3.11), pp. 144]	$p=6$	$s=8$

Table 1.: Exponential operator splitting methods of order p involving s compositions.

respectively, that is, the first numerical solution value is given by

$$y_1 = \mathrm{e}^{hB}\,\mathrm{e}^{hA}\,y_0\,, \qquad \text{or} \qquad y_1 = \mathrm{e}^{hA}\,\mathrm{e}^{hB}\,y_0\,, \tag{1.7b}$$

respectively. In Section 1.2 it is verified that the Lie–Trotter splitting method is of (classical) order one.

Example (Strang splitting method). The symmetric Lie–Trotter splitting method or Strang splitting method [40, 47] can be cast into the general form (1.6) with

$$s=2\,,\ a_1=a_2=\tfrac{1}{2}\,,\ b_1=1\,,\ b_2=0\,, \qquad \text{or} \qquad s=2\,,\ a_1=0\,,\ a_2=1\,,\ b_1=b_2=\tfrac{1}{2}\,, \tag{1.8a}$$

respectively, that is, the first numerical solution value is given by

$$y_1 = \mathrm{e}^{\frac{1}{2}hA}\,\mathrm{e}^{hB}\,\mathrm{e}^{\frac{1}{2}hA}\,y_0\,, \qquad \text{or} \qquad y_1 = \mathrm{e}^{\frac{1}{2}hB}\,\mathrm{e}^{hA}\,\mathrm{e}^{\frac{1}{2}hB}\,y_0\,, \tag{1.8b}$$

respectively. The computational effort of the Strang splitting method is essentially that of the Lie–Trotter splitting method. In Section 1.2 it is verified that the Strang splitting method is of (classical) order two.

Higher order splitting methods. Exponential operator splitting methods of order four and six are given in [11, 30], e.g., see also Table 1.

1.2. Convergence analysis

Objective. In the following, we are concerned with deducing an estimate for the global error $y_N - y(T)$ of an exponential operator splitting method (1.6) when applied to the initial value problem (1.1); to this purpose, we follow a standard approach based on a *Lady Windermere's Fan* argument.

Local error and order. In the present situation, the local error equals

$$d_n = D(h_{n-1})\, y(t_{n-1}) = \big(\Phi_{A+B}(h_{n-1}) - E_{A+B}(h_{n-1})\big)\, y(t_{n-1}), \qquad 1 \le n \le N,$$

see also (0.4). Therefore, the numerical method (1.6) is consistent of order p, see also (0.4), whenever the defect operator D fulfills

$$D(h) = \mathcal{O}\big(h^{p+1}\big). \tag{1.9}$$

Lady Windermere's Fan. In order to relate the global and the local error, we employ the telescopic identity

$$y_N - y(t_N) = \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\,\big(y_0 - y(t_0)\big) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\, d_n. \tag{1.10}$$

In Sections 1.2.1 and 1.2.2, we are concerned with deriving a bound for the splitting operator Φ_{A+B} and a suitable expansion of the defect operator D.

Explanation. The validity of relation (1.10) is verified by a short calculation

$$\begin{aligned}
&\prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\,\big(y_0 - y(t_0)\big) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\, d_n \\
&\quad= \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\,\big(y_0 - y(t_0)\big) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\,\big(\Phi_{A+B}(h_{n-1}) - E_{A+B}(h_{n-1})\big)\, y(t_{n-1}) \\
&\quad= \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\, y_0 - \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\, y(t_0) \\
&\qquad + \sum_{n=1}^{N} \prod_{j=n-1}^{N-1} \Phi_{A+B}(h_j)\, y(t_{n-1}) - \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\, y(t_n) \\
&\quad= y_N - \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\, y(t_0) + \sum_{n=0}^{N-1} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\, y(t_n) - \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\, y(t_n) \\
&\quad= y_N - \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\, y(t_0) + \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\, y(t_0) - y(t_N) \\
&\quad= y_N - y(t_N).
\end{aligned}$$

1.2.1. Stability

Assumption. In order to prove the desired stability result for exponential operator splitting methods, we employ the bounds

$$\left\| \mathrm{e}^{\tau A} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_A |\tau|}, \quad \left\| \mathrm{e}^{\tau B} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_B |\tau|}, \qquad \tau \in \mathbb{R}, \tag{1.11}$$

involving certain positive constants $M_A, M_B \geq 0$.

Remark. In the present situation, for bounded linear operators $A, B : X \to X$ relation (1.11) holds with $M_A = C_A$ and $M_B = C_B$, see (1.2). Namely, a straightforward estimation of the exponential series (1.3) yields

$$\left\| \mathrm{e}^{\tau L} \right\|_{X \leftarrow X} \leq \mathrm{e}^{\|L\|_{X \leftarrow X} |\tau|}, \qquad \tau \in \mathbb{R}.$$

Stability result. Under assumption (1.11), the estimate

$$\left\| \Phi_{A+B}(h_j) \right\|_{X \leftarrow X} \leq \prod_{i=1}^{s} \left\| \mathrm{e}^{b_i h_j B} \right\|_{X \leftarrow X} \left\| \mathrm{e}^{a_i h_j A} \right\|_{X \leftarrow X} \leq \mathrm{e}^{C_\Phi h_j},$$

follows, see also (1.6), which further implies the stability bound

$$\left\| \prod_{j=k}^{m-1} \Phi_{A+B}(h_j) \right\|_{X \leftarrow X} \leq \mathrm{e}^{C_\Phi (t_m - t_k)}, \quad C_\Phi = M_A \sum_{i=1}^{s} |a_i| + M_B \sum_{i=1}^{s} |b_i|, \qquad m > k \geq 0. \tag{1.12}$$

Extension (Evolutionary Schrï¿½dinger equations). The above stability estimate (1.12) can also be established in the context of abstract evolution problems. For instance, for evolutionary Schrï¿½dinger equations of the form (1.1), we require that the unbounded linear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$ generate $\mathscr{C}_0$-groups $\left(\mathrm{e}^{\tau A}\right)_{\tau \in \mathbb{R}}$ and $\left(\mathrm{e}^{\tau B}\right)_{\tau \in \mathbb{R}}$ such that

$$\left\| \mathrm{e}^{\tau A} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_A |\tau|}, \quad \left\| \mathrm{e}^{\tau B} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_B |\tau|}, \qquad \tau \in \mathbb{R}.$$

In this case, exponential operator splitting methods that involve negative coefficients are permitted.

Extension (Parabolic evolution equations) . For evolution equations (1.1) of parabolic type, we require the unbounded linear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$ to generate $\mathscr{C}_0$-semigroups $\left(\mathrm{e}^{\tau A}\right)_{\tau \geq 0}$ and $\left(\mathrm{e}^{\tau B}\right)_{\tau \geq 0}$ such that

$$\left\| \mathrm{e}^{\tau A} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_A \tau}, \quad \left\| \mathrm{e}^{\tau B} \right\|_{X \leftarrow X} \leq \mathrm{e}^{M_B \tau}, \qquad \tau \geq 0.$$

In this case, exponential operator splitting methods that involve complex coefficients with positive real part are permitted.

1.2.2. Local error expansion

Situation. For the following, to avoid technicalities, we consider exponential operator splitting methods (1.6) that involve two compositions only

$$y_1 = \mathrm{e}^{b_2 hB}\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA}\,y_0\,, \qquad h = h_0\,. \tag{1.13}$$

Method examples that can be cast into this form are the Lie–Trotter splitting method (1.7) and the Strang splitting method (1.8).

Objective. We are concerned with deducing a suitable expansion of the defect operator

$$D(h) = \Phi_{A+B}(h) - E_{A+B}(h) = \mathrm{e}^{b_2 hB}\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} - \mathrm{e}^{h(A+B)}\,, \tag{1.14}$$

with respect to h, see also (1.4) and (1.6).

Approach. We employ the power series expansion (1.3) for the matrix exponential; more precisely, performing a stepwise Taylor series expansion of $\mathrm{e}^{\tau L}$, we obtain

$$\begin{aligned}
\mathrm{e}^{\tau L} &= I + \mathrm{e}^{\sigma\tau L}\Big|_{\sigma=0}^{1} \\
&= I + \tau L \int_0^1 \mathrm{e}^{\sigma\tau L}\,\mathrm{d}\sigma \\
&= I + \tau L + \tau^2 L^2 \int_0^1 (1-\sigma)\,\mathrm{e}^{\sigma\tau L}\,\mathrm{d}\sigma \\
&= I + \tau L + \tfrac{1}{2}\tau^2 L^2 + \tau^3 L^3 \int_0^1 \tfrac{1}{2}(1-\sigma)^2\,\mathrm{e}^{\sigma\tau L}\,\mathrm{d}\sigma\,, \qquad \tau \geq 0\,.
\end{aligned}$$

With the help of the bounds (1.2) and (1.11), we thus have

$$\begin{aligned}
\mathrm{e}^{\tau L} &= I + \mathscr{O}(\tau, C_L, M_L) \\
&= I + \tau L + \mathscr{O}\big(\tau^2, C_L^2, M_L\big) \\
&= I + \tau L + \tfrac{1}{2}\tau^2 L^2 + \mathscr{O}\big(\tau^3, C_L^3, M_L\big)\,, \qquad \tau \geq 0\,.
\end{aligned} \tag{1.15}$$

Expansion (Exact solution operator). By means of (1.15), we obtain the following expansion of the exact solution operator

$$\begin{aligned}
E_{A+B}(h) &= \mathrm{e}^{h(A+B)} \\
&= I + h(A+B) + \tfrac{1}{2}h^2\big(A^2 + AB + BA + B^2\big) + \mathscr{O}\big(h^3, C_{A+B}^3, M_{A+B}\big)\,;
\end{aligned} \tag{1.16}$$

here, we assume that the following estimate is valid

$$\big\|\mathrm{e}^{\tau(A+B)}\big\|_{X\leftarrow X} \leq \mathrm{e}^{M_{A+B}|\tau|}\,, \qquad \tau \in \mathbb{R}\,.$$

Expansion (Splitting operator). By means of relation (1.15), we next employ a stepwise expansion of the splitting operator

$$\begin{aligned}
\Phi_{A+B}(h) &= \mathrm{e}^{b_2 hB}\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} \\
&= \big(I + b_2 hB + \tfrac{1}{2}\,b_2^2 h^2 B^2\big)\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + \mathscr{O}\big(h^3, C_B^3, M_A, M_B\big) \\
&= \mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + b_2 hB\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + \tfrac{1}{2}\,b_2^2 h^2 B^2\,\mathrm{e}^{a_2 hA}\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} \\
&\quad + \mathscr{O}\big(h^3, C_B^3, M_A, M_B\big) \\
&= \big(I + a_2 hA + \tfrac{1}{2}\,a_2^2 h^2 A^2\big)\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + b_2 hB\,\big(I + a_2 hA\big)\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} \\
&\quad + \tfrac{1}{2}\,b_2^2 h^2 B^2\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big) \\
&= \mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + h\,\big(a_2 A + b_2 B\big)\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} \\
&\quad + h^2\,\big(\tfrac{1}{2}\,a_2^2 A^2 + a_2\,b_2 B\,A + \tfrac{1}{2}\,b_2^2 B^2\big)\,\mathrm{e}^{b_1 hB}\,\mathrm{e}^{a_1 hA} + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big)
\end{aligned}$$

and, furthermore, we have

$$\begin{aligned}
\Phi_{A+B}(h) &= \big(I + b_1 hB + \tfrac{1}{2}\,b_1^2 h^2 B^2\big)\,\mathrm{e}^{a_1 hA} + h\,\big(a_2 A + b_2 B\big)\,\big(I + b_1 hB\big)\,\mathrm{e}^{a_1 hA} \\
&\quad + h^2\,\big(\tfrac{1}{2}\,a_2^2 A^2 + a_2\,b_2 B\,A + \tfrac{1}{2}\,b_2^2 B^2\big)\,\mathrm{e}^{a_1 hA} + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big) \\
&= \mathrm{e}^{a_1 hA} + h\,\big(a_2 A + (b_1 + b_2) B\big)\,\mathrm{e}^{a_1 hA} \\
&\quad + h^2\,\big(\tfrac{1}{2}\,a_2^2 A^2 + a_2 b_1\,A B + a_2\,b_2 B\,A + \tfrac{1}{2}\,(b_1 + b_2)^2 B^2\big)\,\mathrm{e}^{a_1 hA} \\
&\quad + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big) \\
&= I + a_1 hA + \tfrac{1}{2}\,a_1^2 h^2 A^2 + h\,\big(a_2 A + (b_1 + b_2) B\big)\,\big(I + a_1 hA\big) \\
&\quad + h^2\,\big(\tfrac{1}{2}\,a_2^2 A^2 + a_2 b_1\,A B + a_2\,b_2 B\,A + \tfrac{1}{2}\,(b_1 + b_2)^2 B^2\big) \\
&\quad + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big).
\end{aligned}$$

This finally yields the following expansion

$$\begin{aligned}
\Phi_{A+B}(h) = I &+ h\,\big((a_1 + a_2) A + (b_1 + b_2) B\big) \\
&+ h^2\,\big(\tfrac{1}{2}\,(a_1 + a_2)^2 A^2 + a_2 b_1\,A B + \big(a_1 (b_1 + b_2) + a_2\,b_2\big) B\,A \\
&\quad + \tfrac{1}{2}\,(b_1 + b_2)^2 B^2\big) + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B\big).
\end{aligned} \tag{1.17}$$

Expansion (Defect operator). Altogether, the above relations (1.16) and (1.17) imply the following expansion of the defect operator $D = \Phi_{A+B} - E_{A+B}$ with respect to h

$$\begin{aligned}
D(h) = h &\big((a_1 + a_2 - 1) A + (b_1 + b_2 - 1) B\big) \\
&+ h^2 \Big(\tfrac{1}{2}\,\big((a_1 + a_2)^2 - 1\big) A^2 + \big(a_2 b_1 - \tfrac{1}{2}\big) A\,B + \big(a_1 (b_1 + b_2) + a_2\,b_2 - \tfrac{1}{2}\big) B\,A \\
&\quad + \tfrac{1}{2}\,\big((b_1 + b_2)^2 - 1\big) B^2\Big) + \mathscr{O}\big(h^3, C_A^3, C_B^3, M_A, M_B, M_{A+B}\big).
\end{aligned} \tag{1.18}$$

Order conditions. Employing the above expansion (1.18) of the defect operator D and requiring (1.9) to be valid with $p = 1$ for arbitrary matrices or bounded linear operators A and B, respectively, the (classical) first order conditions

$$a_1 + a_2 = 1\,, \qquad b_1 + b_2 = 1\,, \tag{1.19a}$$

follow. For (classical) order two, that is, setting $p = 2$, the additional conditions are $a_2 b_1 = \frac{1}{2}$ and $a_1 + a_2\, b_2 = \frac{1}{2}$, or, equivalently,

$$(1 - a_1)\, b_1 = \tfrac{1}{2}\,. \tag{1.19b}$$

Obviously, the Lie–Trotter splitting method (1.7) has (classical) order one; the second-order Strang splitting method (1.8) is retained from the order conditions (1.19) under the symmetry requirement $b_2 = 0$ and $a_1 = a_2$ or $a_1 = 0$ and $b_1 = b_2$, respectively.

Local error estimate. The above consideration imply the local error estimate

$$\big\| D(h) \big\|_{X \leftarrow X} \le C\, h^{p+1} \tag{1.20}$$

with constant C depending on $C_A^{p+1}, C_B^{p+1}, M_A, M_B, M_{A+B}$, and further on the method coefficients. In particular, the above bound holds true with $p = 1$ for the Lie–Trotter splitting method (1.7) and with $p = 2$ for the Strang splitting method (1.8).

1.2.3. Convergence result

Convergence estimate. Assume that the exponential operator splitting method (1.6) applied to the linear problem (1.1) fulfills the (classical) order conditions for order $p \ge 1$. Then, the following global error estimate

$$\big\| y_N - y(t_N) \big\|_X \le C \left(\big\| y_0 - y(t_0) \big\|_X + \sum_{n=0}^{N-1} h_n^{p+1} \right)$$

holds with constant C depending in particular on $C_A, C_B, M_{A+B}, M_A, M_B, T$, and $y(t_0)$. Namely, estimating the global error relation (1.10) by means of the stability bound (1.12) and the local error estimate (1.20), the desired result follows. Especially, for constant stepsizes, that is, it holds $h_n = h$ for $0 \le n \le N-1$, the expected convergence bound

$$\big\| y_n - y(t_n) \big\|_X \le C \left(\big\| y_0 - y(0) \big\|_X + h^p \right), \qquad 0 \le n \le N\,,$$

follows.

2. Alternative local error expansions

Situation. As before, we focus on exponential operator splitting methods (1.6) for linear initial value problems of the form (1.1) that involve two compositions only, see (1.13).

Objective. Regarding possible extensions of the convergence analysis given in Section 1.2 to evolutionary Schrï¿½dinger equations or parabolic evolution equations, respectively, we next investigate alternative approaches for deducing a suitable expansion of the defect operator (1.14) with respect to h.

Notation. For matrices $L_1, L_2 \in \mathbb{R}^{d\times d}$ or bounded linear operators $L_1, L_2 : X \to X$, respectively, the iterated commutators are defined by

$$\mathrm{ad}_{L_1}^{j+1}(L_2) = \big[L_1, \mathrm{ad}_{L_1}^{j}(L_2)\big] = L_1\,\mathrm{ad}_{L_1}^{j}(L_2) - \mathrm{ad}_{L_1}^{j}(L_2)L_1\,, \qquad j \geq 0\,, \tag{2.1}$$

where $\mathrm{ad}_{L_1}^{0}(L_2) = L_2$, see [30]. Note that for the first commutator $\mathrm{ad}_{L_1}(L_2) = L_1L_2 - L_2L_1$ it follows $\mathrm{ad}_{L_1}(L_1) = 0$ and $\mathrm{ad}_{L_2}(L_1) = -\mathrm{ad}_{L_1}(L_2)$.

2.1. Baker–Campbell–Hausdorff formula

Approach. The Baker–Campbell–Hausdorff formula considerably facilitates the expansion of compositions involving the matrix exponential, see for example [30]. However, as for the power series expansion (1.3), it is not evident to extend this approach to evolutionary equations (1.1) with unbounded linear operators A and B; in particular, it is difficult to obtain error estimates that are optimal with respect to the regularity properties of the exact solution.

2.1.1. Derivation of the Baker–Campbell–Hausdorff formula

Objective. The objective is to determine a time-dependent linear operator $\Omega(t) : X \to X$, $t \geq 0$, such that the identity

$$\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1} = \mathrm{e}^{\Omega(t)}\,, \qquad t \geq 0\,, \tag{2.2}$$

holds for (non-commuting) bounded linear operators $L_1, L_2 : X \to X$. More precisely, the aim is to calculate the time-independent linear operators $\Omega_j : X \to X$ arising in the expansion of $\Omega(t)$

$$\Omega(t) = \sum_{j=0}^{\infty} t^j\,\Omega_j\,. \tag{2.3}$$

The derivation of the Baker–Campbell–Hausdorff formula relies on the following auxiliary results.

Notation. The (analytic) exponential functions $\varphi_0, \varphi_1 : \mathbb{C} \to \mathbb{C}$ are given by

$$\varphi_0(z) = \sum_{j=0}^{\infty} \tfrac{1}{j!}\, z^j = \mathrm{e}^z\,, \qquad z \in \mathbb{C}\,,$$

$$\varphi_1(z) = \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\, z^j = \begin{cases} \frac{\mathrm{e}^z - 1}{z}\,, & 0 \neq z \in \mathbb{C}\,, \\ 1\,, & z = 0\,. \end{cases}$$

Furthermore, we introduce the complex function $\psi_1 : \{z \in \mathbb{C} : |z| < \pi\} \to \mathbb{C}$, defined by

$$\psi_1(z) = \sum_{j=0}^{\infty} \tfrac{1}{j!}\, \beta_j\, z^j\,,$$

with Bernoulli numbers $\beta_0 = 1$, $\beta_1 = -\frac{1}{2}$, etc. Note that $\varphi_1(z)\,\psi_1(z) = 1 = \psi_1(z)\,\varphi_1(z)$ for all $z \in \mathbb{C}$ with $|z| < \pi$.

Fréchet derivative. A function $f : X \to Y$ between Banach spaces $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ is called Fréchet differentiable at $x \in X$ with Fréchet derivative $f'(x) = L$ if there exists a bounded linear operator $L = L(x) : X \to Y$ such that

$$f(x+z) - f(x) = Lz + o(\|z\|_X)\,.$$

Auxiliary relation. The Fréchet derivative of Ω^k, $k \geq 0$, with $\Omega : X \to X$ a bounded linear operator, can be rewritten as

$$\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\, \Omega^k = \sum_{j=0}^{k-1} \binom{k}{j+1}\, \mathrm{ad}_{\Omega}^{j}(\cdot)\, \Omega^{k-(j+1)}\,, \qquad k \geq 0\,.$$

Clearly, the above identity holds for the trivial cases

$$k = 0: \quad \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\, I = 0\,, \qquad k = 1: \quad \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\, \Omega = I\,.$$

Furthermore, by means of the product rule and the relation

$$\Omega X = \Omega\, X \mp X \Omega = X\Omega + \mathrm{ad}_{\Omega}(X)\,,$$

we have

$$k = 2: \quad \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\, \Omega^2 = \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\, \Omega\,\Omega = (\cdot)\,\Omega + \Omega\,(\cdot) = 2\,(\cdot)\,\Omega + \mathrm{ad}_{\Omega}(\cdot)\,,$$

as well as

$$\begin{aligned} k=3: \quad \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega^3 &= \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega\,\Omega^2 \\ &= (\cdot)\,\Omega^2 + \Omega\left(2\,(\cdot)\,\Omega + \mathrm{ad}_\Omega(\cdot)\right) \\ &= (\cdot)\,\Omega^2 + 2 \underbrace{\Omega\,(\cdot)}_{=(\cdot)\,\Omega+\mathrm{ad}_\Omega(\cdot)} \Omega + \underbrace{\Omega\,\mathrm{ad}_\Omega(\cdot)}_{\mathrm{ad}_\Omega(\cdot)\,\Omega+\mathrm{ad}_\Omega^2(\cdot)} \\ &= 3\,(\cdot)\,\Omega^2 + 3\,\mathrm{ad}_\Omega(\cdot)\,\Omega + \mathrm{ad}_\Omega^2(\cdot)\,. \end{aligned}$$

In general, proceeding by induction and using that

$$\binom{k}{j} + \binom{k}{j+1} = \binom{k+1}{j+1},$$

we obtain

$$\begin{aligned} k \to k+1: \quad \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega^{k+1} &= \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega\,\Omega^k \\ &= (\cdot)\,\Omega^k + \Omega \sum_{j=0}^{k-1} \tbinom{k}{j+1}\,\mathrm{ad}_\Omega^j(\cdot)\,\Omega^{k-(j+1)} \\ &= (\cdot)\,\Omega^k + \sum_{j=0}^{k-1} \tbinom{k}{j+1} \underbrace{\Omega\,\mathrm{ad}_\Omega^j(\cdot)}_{=\mathrm{ad}_\Omega^j(\cdot)\,\Omega+\mathrm{ad}_\Omega^{j+1}(\cdot)} \Omega^{k-(j+1)} \\ &= (k+1)\,(\cdot)\,\Omega^k + \sum_{j=1}^{k-1} \left(\tbinom{k}{j+1} + \tbinom{k}{j}\right) \mathrm{ad}_\Omega^j(\cdot)\,\Omega^{k+1-(j+1)} + \mathrm{ad}_\Omega^k(\cdot) \\ &= \sum_{j=0}^{k} \tbinom{k+1}{j+1}\,\mathrm{ad}_\Omega^j(\cdot)\,\Omega^{k+1-(j+1)}\,. \end{aligned}$$

Derivative of exponential. For a bounded linear operator $\Omega : X \to X$, the first derivative of e^Ω with respect to Ω is given by

$$\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\mathrm{e}^\Omega = \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\,\mathrm{ad}_\Omega^j(\cdot)\,\mathrm{e}^\Omega = \left(\varphi_1(\mathrm{ad}_\Omega)\right)(\cdot)\,\mathrm{e}^\Omega\,.$$

Namely, employing the exponential series and the previously deduced identity for $\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega^k$ and exchanging the order of summation, it follows

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\mathrm{e}^\Omega &= \sum_{k=0}^{\infty} \tfrac{1}{k!}\,\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\Omega^k \\ &= \sum_{k=0}^{\infty} \tfrac{1}{k!} \sum_{j=0}^{k-1} \tbinom{k}{j+1}\,\mathrm{ad}_\Omega^j(\cdot)\,\Omega^{k-(j+1)} \end{aligned}$$

and furthermore

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}\Omega}\,\mathrm{e}^{\Omega} &= \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\,\mathrm{ad}_{\Omega}^{j}(\cdot) \sum_{k=j+1}^{\infty} \tfrac{1}{(k-j-1)!}\,\Omega^{k-j-1} \\ &= \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\,\mathrm{ad}_{\Omega}^{j}(\cdot) \sum_{\ell=0}^{\infty} \tfrac{1}{\ell!}\,\Omega^{\ell} \\ &= \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\,\mathrm{ad}_{\Omega}^{j}(\cdot)\,\mathrm{e}^{\Omega}.\end{aligned}$$

As a consequence, taking the first time derivative of $\mathrm{e}^{\Omega(t)}$ yields

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{\Omega(t)} = \sum_{j=0}^{\infty} \tfrac{1}{(j+1)!}\,\mathrm{ad}_{\Omega(t)}^{j}\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t)\big)\,\mathrm{e}^{\Omega(t)} = \big(\varphi_1(\mathrm{ad}_{\Omega(t)})\big)\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t)\big)\,\mathrm{e}^{\Omega(t)}, \qquad t \geq 0. \tag{2.4}$$

Initial value problem. On the one hand, in regard to (2.2), it follows

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{\Omega(t)} = \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1} = L_2\,\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1} + \mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1}L_1 = L_2\,\mathrm{e}^{\Omega(t)} + \mathrm{e}^{\Omega(t)}L_1, \qquad t \geq 0.$$

With the help of the above relation (2.4) we thus have

$$L_2\,\mathrm{e}^{\Omega(t)} + \mathrm{e}^{\Omega(t)}L_1 = \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{\Omega(t)} = \big(\varphi_1(\mathrm{ad}_{\Omega(t)})\big)\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t)\big)\,\mathrm{e}^{\Omega(t)}, \qquad t \geq 0,$$

Furthermore, by a multiplication from the right with $\mathrm{e}^{-\Omega(t)}$, making use of the fact that

$$\mathrm{e}^{K} L\,\mathrm{e}^{-K} = \sum_{j=0}^{\infty} \tfrac{1}{j!}\,\mathrm{ad}_{K}^{j}(L) = \big(\varphi_0(\mathrm{ad}_K)\big)(L),$$

we obtain the identity

$$L_2 + \big(\varphi_0(\mathrm{ad}_{\Omega(t)})\big)(L_1) = \big(\varphi_1(\mathrm{ad}_{\Omega(t)})\big)\big(\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t)\big), \qquad t \geq 0.$$

Applying $\psi_1(\mathrm{ad}_{\Omega(t)})$, the inverse of $\big(\varphi_1(\mathrm{ad}_{\Omega(t)})\big)$ (under certain restrictions on the norm of $\Omega(t)$), and noting that $\varphi_0(z) = 1 + z\,\varphi_1(z)$ for $z \in \mathbb{C}$, yields

$$\begin{aligned}\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t) &= \big(\psi_1(\mathrm{ad}_{\Omega(t)})\big)\Big(L_2 + \big(\varphi_0(\mathrm{ad}_{\Omega(t)})\big)(L_1)\Big) \\ &= \big(\psi_1(\mathrm{ad}_{\Omega(t)})\big)\Big(L_1 + L_2 + \big(\mathrm{ad}_{\Omega(t)}\varphi_1(\mathrm{ad}_{\Omega(t)})\big)(L_1)\Big) \\ &= \big(\psi_1(\mathrm{ad}_{\Omega(t)})\big)\,(L_1 + L_2) + \mathrm{ad}_{\Omega(t)}(L_1) \\ &= \mathrm{ad}_{\Omega(t)}(L_1) + \beta_0\,(L_1 + L_2) + \beta_1\,\mathrm{ad}_{\Omega(t)}(L_1 + L_2) + \sum_{j=2}^{\infty} \tfrac{1}{j!}\,\beta_j\,\mathrm{ad}_{\Omega(t)}^{j}(L_1 + L_2) \\ &= L_1 + L_2 + \tfrac{1}{2}\,\mathrm{ad}_{\Omega(t)}(L_1 - L_2) + \sum_{j=2}^{\infty} \tfrac{1}{j!}\,\beta_j\,\mathrm{ad}_{\Omega(t)}^{j}(L_1 + L_2), \qquad t \geq 0.\end{aligned}$$

Altogether, the initial value problem

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\Omega(t) = L_1 + L_2 + \tfrac{1}{2}\,\mathrm{ad}_{\Omega(t)}(L_1 - L_2) + \sum_{j=2}^{\infty} \tfrac{1}{j!}\,\beta_j\,\mathrm{ad}^j_{\Omega(t)}(L_1 + L_2)\,, \quad t \geq 0\,, \qquad \Omega(0) = 0\,.$$

results, see also (2.2).

Successive solution. Inserting relation (2.3) into the above initial value problem for $\Omega(t)$, comparing like powers of t, the linear operators Ω_j can be computed. In particular, noting that $\Omega_0 = \Omega(0) = 0$ due to (2.2), and, for instance

$$\mathrm{ad}^2_{\Omega(t)}(L_1 + L_2) = \Big[\, t\,\Omega_1 + \mathcal{O}\big(t^2\big), \big[\, t\,\Omega_1 + \mathcal{O}\big(t^2\big), L_1 + L_2\big]\Big] = \mathcal{O}\big(t^2\big)\,,$$

this procedure yields

$$\begin{aligned}\Omega_1 + 2\,t\,\Omega_2 + \mathcal{O}\big(t^2\big) &= \tfrac{\mathrm{d}}{\mathrm{d}t}\left(t\,\Omega_1 + t^2\Omega_2 + \mathcal{O}\big(t^3\big)\right) \\ &= L_1 + L_2 + t\,\tfrac{1}{2}\,\mathrm{ad}_{\Omega_1}(L_1 - L_2) + \mathcal{O}\big(t^2\big)\,, \qquad t \geq 0\,,\end{aligned}$$

We conclude $\Omega_1 = L_1 + L_2$ and $\Omega_2 = \frac{1}{4}\,\mathrm{ad}_{\Omega_1}(L_1 - L_2) = \frac{1}{4}\,\big[L_1 + L_2, L_1 - L_2\big] = -\frac{1}{2}\,\mathrm{ad}_{L_1}(L_2)$, whence

$$\Omega_0 = 0\,, \quad \Omega_1 = L_1 + L_2\,, \quad \Omega_2 = -\tfrac{1}{2}\,\mathrm{ad}_{L_1}(L_2)\,.$$

2.1.2. Local error expansion

Baker–Campbell–Hausdorff formula. The Baker–Campbell–Hausdorff formula implies the expansion

$$\mathrm{e}^{h\,L_2}\,\mathrm{e}^{h\,L_1} = \mathrm{e}^{h\,L}\,, \qquad L = L_1 + L_2 - \tfrac{1}{2}\,h\,\mathrm{ad}_{L_1}(L_2) + \mathcal{O}\big(h^2\big)\,. \tag{2.5}$$

Local error expansion. An application of the above relation (2.5) to (1.13) yields

$$\mathrm{e}^{b_i\,h\,B}\,\mathrm{e}^{a_i\,h\,A} = \mathrm{e}^{h\,L_i}\,, \qquad L_i = a_i\,A + b_i\,B - \tfrac{1}{2}\,h\,a_i\,b_i\,\mathrm{ad}_A(B) + \mathcal{O}\big(h^2\big)\,, \qquad i = 1,2\,;$$

moreover, we obtain the identity

$$\begin{aligned}\Phi_{A+B}(h) &= \mathrm{e}^{b_2\,h\,B}\,\mathrm{e}^{a_2\,h\,A}\,\mathrm{e}^{b_1\,h\,B}\,\mathrm{e}^{a_1\,h\,A} = \mathrm{e}^{h\,L_2}\,\mathrm{e}^{h\,L_1} = \mathrm{e}^{h\,L}\,, \\ L &= (a_1 + a_2)\,A + (b_1 + b_2)\,B - \tfrac{1}{2}\,h\,\big(a_1(b_1 + b_2) + a_2(b_2 - b_1)\big)\,\mathrm{ad}_A(B) + \mathcal{O}\big(h^2\big)\,.\end{aligned}$$

As a consequence, the requirement

$$D(h) = \Phi_{A+B}(h) - E_{A+B}(h) = \mathrm{e}^{h\,L} - \mathrm{e}^{h\,(A+B)} = \mathcal{O}\big(h^{p+1}\big)$$

implies $L - (A + B) = \mathcal{O}\big(h^p\big)$, that is, we have

$$(a_1 + a_2 - 1)\,A + (b_1 + b_2 - 1)\,B - \tfrac{1}{2}\,h\,\big(a_1(b_1 + b_2) + a_2(b_2 - b_1)\big)\,\mathrm{ad}_A(B) = \mathcal{O}\big(h^p\big)\,.$$

In particular, for $p = 1$ or $p = 2$, respectively, we retain the first and second order conditions (1.19).

2.1.3. Construction of a fourth-order splitting scheme

Situation. Consider a linear differential equation of the form

$$y'(t) = A\,y(t) + B\,y(t)\,, \qquad t \geq 0\,. \tag{2.6}$$

For the numerical solution of (2.6), apply a splitting method involving s stages

$$\Phi_{A+B}(t) = \prod_{i=1}^{s} \mathrm{e}^{tB_i}\,\mathrm{e}^{tA_i} \quad \approx \quad E_{A+B}(t) = \mathrm{e}^{t(A+B)}\,, \qquad t \geq 0\,,$$

where $A_i = a_i A$ and $B_i = b_i B$ for $1 \leq i \leq s$.

Adjoint method. The adjoint method of a splitting method for (2.6) is given by

$$\Phi^*_{A+B}(t) = \Phi^{-1}_{A+B}(-t) = \left(\mathrm{e}^{-tB_s}\,\mathrm{e}^{-tA_s}\cdots\mathrm{e}^{-tB_1}\,\mathrm{e}^{-tA_1}\right)^{-1} = \mathrm{e}^{tA_1}\,\mathrm{e}^{tB_1}\cdots\mathrm{e}^{tA_s}\,\mathrm{e}^{tB_s}\,, \qquad t \geq 0\,;$$

namely, using for instance that for $E_B(t)E_A(t) = \mathrm{e}^{tB}\,\mathrm{e}^{tA}$ it follows $(E_B\,E_A)^{-1}(t) = \mathrm{e}^{-tA}\,\mathrm{e}^{-tB}$ and $(E_B\,E_A)^{-1}(-t) = \mathrm{e}^{tA}\,\mathrm{e}^{tB}$. Provided that the underlying method satisfies the local error relation

$$D_{A+B}(t) = \Phi_{A+B}(t) - E_{A+B}(t) = t^{p+1}C_{A+B} + \mathscr{O}\left(t^{p+2}\right), \qquad t \geq 0\,,$$

the adjoint splitting method fulfills

$$D^*_{A+B}(t) = \Phi^*_{A+B}(t) - E_{A+B}(t) = (-1)^p\,t^{p+1}C_{A+B} + \mathscr{O}\left(t^{p+2}\right), \qquad t \geq 0\,.$$

Namely, noting that $E^{-1}_{A+B}(t) = \mathrm{e}^{-t(A+B)} = E_{A+B}(-t)$ and further

$$\begin{aligned} -\,D_{A+B}(-t)\,E_{A+B}(t) &= \left(E_{A+B}(-t) - \Phi_{A+B}(-t)\right)\,E_{A+B}(t) \\ &= I - \Phi_{A+B}(-t)E_{A+B}(t) \\ &= \Phi_{A+B}(-t)\left(\Phi^*_{A+B}(t) - E_{A+B}(t)\right) \\ &= \Phi_{A+B}(-t)\,D^*_{A+B}(t)\,, \qquad t \geq 0\,, \end{aligned}$$

due to the fact that $E_{A+B}(t) = I + \mathscr{O}(t)$ as well as $\Phi^*_{A+B}(t) = I + \mathscr{O}(t)$, the relation

$$\begin{aligned} D^*_{A+B}(t) &= -\,\Phi^*_{A+B}(t)\,D_{A+B}(-t)\,E_{A+B}(t) \\ &= -\,\Phi^*_{A+B}(t)\left((-t)^{p+1}C_{A+B} + \mathscr{O}\left(t^{p+2}\right)\right)E_{A+B}(t) \\ &= (-1)^p\,t^{p+1}C_{A+B} + \mathscr{O}\left(t^{p+2}\right), \qquad t \geq 0\,. \end{aligned}$$

Symmetry. A method is called symmetric if $\Phi^*_{A+B} = \Phi_{A+B}$ for $t \geq 0$, that is, it holds

$$\Phi^*_{A+B}(t) = \mathrm{e}^{tA_1}\,\mathrm{e}^{tB_1}\cdots\mathrm{e}^{tA_s}\,\mathrm{e}^{tB_s} = \mathrm{e}^{tB_s}\,\mathrm{e}^{tA_s}\cdots\mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1} = \Phi_{A+B}(t)\,, \qquad t \geq 0\,.$$

The above considerations imply $C_{A+B} = (-1)^p C_{A+B}$, that is, the order of a symmetric splitting method is even.

Objective. Construct splitting methods of order $p = 4$ and $p = 3$, respectively, involving $s = 4$ stages. For this purpose, employ the BCH formula to rewrite the splitting operator as

$$\Phi_{A+B}(t) = \underbrace{\mathrm{e}^{tB_4}\,\mathrm{e}^{tA_4}}_{=\mathrm{e}^{tL_4}}\,\underbrace{\mathrm{e}^{tB_3}\,\mathrm{e}^{tA_3}}_{=\mathrm{e}^{tL_3}}\,\underbrace{\mathrm{e}^{tB_2}\,\mathrm{e}^{tA_2}}_{=\mathrm{e}^{tL_2}}\,\underbrace{\mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1}}_{=\mathrm{e}^{tL_1}} = \underbrace{\mathrm{e}^{tL_4}\,\mathrm{e}^{tL_3}}_{=\mathrm{e}^{tK_2}}\,\underbrace{\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1}}_{=\mathrm{e}^{tK_1}} = \underbrace{\mathrm{e}^{tK_2}\,\mathrm{e}^{tK_1}}_{=\mathrm{e}^{tM}} = \mathrm{e}^{tM}\,, \qquad t \geq 0\,,$$

and deduce the order conditions from the requirement

$$\Phi_{A+B}(t) - E_{A+B}(t) = \mathrm{e}^{tM} - \mathrm{e}^{t(A+B)} = \mathcal{O}\big(t^{p+1}\big)\,, \qquad t \geq 0\,,$$

which is equivalent to the relation

$$M - (A+B) = \mathcal{O}\big(t^{p}\big)\,, \qquad t \geq 0\,,$$

as seen from a taylor series expansion of the exponential.

BCH formula. The BCH formula yields the representation

$$\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1} = \mathrm{e}^{\Omega(t)}\,, \qquad \Omega(t) = \sum_{i=1}^{\infty} t^i\,\Omega_i\,, \qquad t \geq 0\,.$$

In particular, the relation

$$\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1} = \mathrm{e}^{tL}\,, \quad L = \sum_{j=1}^{4} t^{j-1}\Omega_j + \mathcal{O}\big(t^4\big) = \Omega_1 + t\,\Omega_2 + t^2\Omega_3 + t^3\Omega_4 + \mathcal{O}\big(t^4\big)\,, \qquad t \geq 0\,,$$

$$\Omega_1 = L_1 + L_2\,, \qquad \Omega_2 = -\tfrac{1}{2}\,[L_1, L_2]\,,$$

$$\Omega_3 = \tfrac{1}{12}\Big(\big[L_1,[L_1,L_2]\big] + \big[L_2,[L_2,L_1]\big]\Big)\,, \quad \Omega_4 = \tfrac{1}{24}\,\big[L_2,\big[L_1,[L_1,L_2]\big]\big]\,,$$

follows.

BCH formula – Extension. In case that

$$L_i = \sum_{j=1}^{4} t^{j-1}\Omega_j^{(L_i)} + \mathcal{O}\big(t^4\big) = \Omega_1^{(L_i)} + t\,\Omega_2^{(L_i)} + t^2\Omega_3^{(L_i)} + t^3\Omega_4^{(L_i)} + \mathcal{O}\big(t^4\big)\,, \qquad t \geq 0\,,$$

the following expansion results

$$\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1}=\mathrm{e}^{tL},\qquad L=\sum_{j=1}^{4}t^{j-1}\Omega_j+\mathscr{O}\big(t^4\big)=\Omega_1+t\,\Omega_2+t^2\Omega_3+t^3\Omega_4+\mathscr{O}\big(t^4\big),\qquad t\geq 0,$$

$$\Omega_1=\Omega_1^{(L_1)}+\Omega_1^{(L_2)},\qquad \Omega_2=\Omega_2^{(L_1)}+\Omega_2^{(L_2)}-\tfrac{1}{2}\,[\Omega_1^{(L_1)},\Omega_1^{(L_2)}]\,,$$

$$\Omega_3=\Omega_3^{(L_1)}+\Omega_3^{(L_2)}-\tfrac{1}{2}\big([\Omega_1^{(L_1)},\Omega_2^{(L_2)}]+[\Omega_2^{(L_1)},\Omega_1^{(L_2)}]\big)+\tfrac{1}{12}\big(\big[\Omega_1^{(L_1)},[\Omega_1^{(L_1)},\Omega_1^{(L_2)}]\big]+\big[\Omega_1^{(L_2)},[\Omega_1^{(L_2)},\Omega_1^{(L_1)}]\big]\big),$$

$$\begin{aligned}\Omega_4=\Omega_4^{(L_1)}+\Omega_4^{(L_2)}&-\tfrac{1}{2}\big([\Omega_1^{(L_1)},\Omega_3^{(L_2)}]+[\Omega_2^{(L_1)},\Omega_2^{(L_2)}]+[\Omega_3^{(L_1)},\Omega_1^{(L_2)}]\big)\\&+\tfrac{1}{12}\big(\big[\Omega_1^{(L_1)},[\Omega_1^{(L_1)},\Omega_2^{(L_2)}]\big]+\big[\Omega_1^{(L_2)},[\Omega_1^{(L_2)},\Omega_2^{(L_1)}]\big]+\big[\Omega_1^{(L_1)},[\Omega_2^{(L_1)},\Omega_1^{(L_2)}]\big]\\&+\big[\Omega_1^{(L_2)},[\Omega_2^{(L_2)},\Omega_1^{(L_1)}]\big]+\big[\Omega_2^{(L_1)},[\Omega_1^{(L_1)},\Omega_1^{(L_2)}]\big]+\big[\Omega_2^{(L_2)},[\Omega_1^{(L_2)},\Omega_1^{(L_1)}]\big]\big)\\&+\tfrac{1}{24}\big[\Omega_1^{(L_2)},\big[\Omega_1^{(L_1)},[\Omega_1^{(L_1)},\Omega_1^{(L_2)}]\big]\big]\,.\end{aligned}$$

Namely, an application of the BCH formula yields

$$\mathrm{e}^{tL_2}\,\mathrm{e}^{tL_1}=\mathrm{e}^{tL},\quad L=\widetilde{\Omega}_1+t\,\widetilde{\Omega}_2+t^2\widetilde{\Omega}_3+t^3\widetilde{\Omega}_4+\mathscr{O}\big(t^4\big),\qquad t\geq 0,$$

$$\widetilde{\Omega}_1=L_1+L_2\,,\qquad \widetilde{\Omega}_2=-\tfrac{1}{2}\,[L_1,L_2]\,,$$

$$\widetilde{\Omega}_3=\tfrac{1}{12}\Big(\big[L_1,[L_1,L_2]\big]+\big[L_2,[L_2,L_1]\big]\Big),\quad \widetilde{\Omega}_4=\tfrac{1}{24}\big[L_2,\big[L_1,[L_1,L_2]\big]\big]\,.$$

Inserting the above representations for L_1 and L_2 gives

$$\widetilde{\Omega}_1=\sum_{j=1}^{4}t^{j-1}\Big(\Omega_j^{(L_1)}+\Omega_j^{(L_2)}\Big)+\mathscr{O}\big(t^4\big),$$

$$\widetilde{\Omega}_2=-\tfrac{1}{2}\sum_{j_1=1}^{4}\sum_{j_2=1}^{4}t^{j_1+j_2-2}[\Omega_{j_1}^{(L_1)},\Omega_{j_2}^{(L_2)}]+\mathscr{O}\big(t^4\big),$$

$$\widetilde{\Omega}_3=\tfrac{1}{12}\sum_{j_1=1}^{4}\sum_{j_2=1}^{4}\sum_{j_3=1}^{4}t^{j_1+j_2+j_3-3}\Big(\big[\Omega_{j_1}^{(L_1)},[\Omega_{j_2}^{(L_1)},\Omega_{j_3}^{(L_2)}]\big]+\big[\Omega_{j_1}^{(L_2)},[\Omega_{j_2}^{(L_2)},\Omega_{j_3}^{(L_1)}]\big]\Big)+\mathscr{O}\big(t^4\big),$$

$$\widetilde{\Omega}_4=\tfrac{1}{24}\sum_{j_1=1}^{4}\sum_{j_2=1}^{4}\sum_{j_3=1}^{4}\sum_{j_4=1}^{4}t^{j_1+j_2+j_3+j_4-4}\big[\Omega_{j_1}^{(L_2)},\big[\Omega_{j_2}^{(L_1)},[\Omega_{j_3}^{(L_1)},\Omega_{j_4}^{(L_2)}]\big]\big]+\mathscr{O}\big(t^4\big).$$

As a consequence, we obtain

$$
\begin{aligned}
L = \sum_{j=1}^{4} t^{j-1}\Big(\Omega_j^{(L_1)} + \Omega_j^{(L_2)}\Big) - \tfrac{1}{2}\sum_{j_1,j_2=1}^{4} t^{j_1+j_2-1}[\Omega_{j_1}^{(L_1)}, \Omega_{j_2}^{(L_2)}] \\
+ \tfrac{1}{12}\sum_{j_1,j_2,j_3=1}^{4} t^{j_1+j_2+j_3-1}\Big(\big[\Omega_{j_1}^{(L_1)}, [\Omega_{j_2}^{(L_1)}, \Omega_{j_3}^{(L_2)}]\big] + \big[\Omega_{j_1}^{(L_2)}, [\Omega_{j_2}^{(L_2)}, \Omega_{j_3}^{(L_1)}]\big]\Big) \\
+ \tfrac{1}{24}\sum_{j_1,j_2,j_3,j_4=1}^{4} t^{j_1+j_2+j_3+j_4-1}\big[\Omega_{j_1}^{(L_2)}, \big[\Omega_{j_2}^{(L_1)}, [\Omega_{j_3}^{(L_1)}, \Omega_{j_4}^{(L_2)}]\big]\big] \\
+ \mathcal{O}\big(t^4\big).
\end{aligned}
$$

Taking into account the indices

$$
\begin{gathered}
j = 1,2,3, \\
(j_1, j_2) = (1,1),(1,2),(2,1),(1,3),(2,2),(3,1), \\
(j_1, j_2, j_3) = (1,1,1),(1,1,2),(1,2,1),(2,1,1), \\
(j_1, j_2, j_3, j_4) = (1,1,1,1)\,,
\end{gathered}
$$

we further have

$$
\begin{aligned}
L = \Big(\Omega_1^{(L_1)} + \Omega_1^{(L_2)}\Big) \\
+ t\Big(\Omega_2^{(L_1)} + \Omega_2^{(L_2)} - \tfrac{1}{2}\,[\Omega_1^{(L_1)}, \Omega_1^{(L_2)}]\Big) \\
+ t^2\Big(\Omega_3^{(L_1)} + \Omega_3^{(L_2)} - \tfrac{1}{2}\big([\Omega_1^{(L_1)}, \Omega_2^{(L_2)}] + [\Omega_2^{(L_1)}, \Omega_1^{(L_2)}]\big) \\
+ \tfrac{1}{12}\big(\big[\Omega_1^{(L_1)}, [\Omega_1^{(L_1)}, \Omega_1^{(L_2)}]\big] + \big[\Omega_1^{(L_2)}, [\Omega_1^{(L_2)}, \Omega_1^{(L_1)}]\big]\big)\Big) \\
+ t^3\Big(\Omega_4^{(L_1)} + \Omega_4^{(L_2)} - \tfrac{1}{2}\big([\Omega_1^{(L_1)}, \Omega_3^{(L_2)}] + [\Omega_2^{(L_1)}, \Omega_2^{(L_2)}] + [\Omega_3^{(L_1)}, \Omega_1^{(L_2)}]\big) \\
+ \tfrac{1}{12}\big(\big[\Omega_1^{(L_1)}, [\Omega_1^{(L_1)}, \Omega_2^{(L_2)}]\big] + \big[\Omega_1^{(L_2)}, [\Omega_1^{(L_2)}, \Omega_2^{(L_1)}]\big] + \big[\Omega_1^{(L_1)}, [\Omega_2^{(L_1)}, \Omega_1^{(L_2)}]\big] \\
+ \big[\Omega_1^{(L_2)}, [\Omega_2^{(L_2)}, \Omega_1^{(L_1)}]\big] + \big[\Omega_2^{(L_1)}, [\Omega_1^{(L_1)}, \Omega_1^{(L_2)}]\big] + \big[\Omega_2^{(L_2)}, [\Omega_1^{(L_2)}, \Omega_1^{(L_1)}]\big]\big) \\
+ \tfrac{1}{24}\big[\Omega_1^{(L_2)}, \big[\Omega_1^{(L_1)}, [\Omega_1^{(L_1)}, \Omega_1^{(L_2)}]\big]\big]\Big) \\
+ \mathcal{O}\big(t^4\big), \qquad t \geq 0\,.
\end{aligned}
$$

Construction. The construction of a fourth-order splitting method relies on the following approach.

- Employ symmetry of splitting method

$$
\begin{aligned}
\Phi_{A+B}(t) &= \mathrm{e}^{tB_4}\,\mathrm{e}^{tA_4}\,\mathrm{e}^{tB_3}\,\mathrm{e}^{tA_3}\,\mathrm{e}^{tB_2}\,\mathrm{e}^{tA_2}\,\mathrm{e}^{tB_1}\,\mathrm{e}^{tA_1} \\
&= \Phi_{A+B}^{*}(t) = \mathrm{e}^{tA_1}\,\mathrm{e}^{tB_1}\,\mathrm{e}^{tA_2}\,\mathrm{e}^{tB_2}\,\mathrm{e}^{tA_3}\,\mathrm{e}^{tB_3}\,\mathrm{e}^{tA_4}\,\mathrm{e}^{tB_4}\,, \qquad t \geq 0\,,
\end{aligned}
$$

that is, employ for instance the symmetry requirements

$$a_1 = 0\,, \quad a_4 = a_2\,, \quad b_4 = b_1\,, \quad b_3 = b_2\,.$$

- Deduce third-order conditions.
- Solve third-order conditions (real/complex case).

2.2. Quadrature formulas

Approach. In the following, we present an approach that is more involved than the Baker–Campbell–Hausdorff formula but well suited for an extension to linear and nonlinear evolutionary equations, see [26, 31, 33, 36, 44]. The basic idea is to expand the exact solution operator by means of the variation-of-constants formula and to deduce a similar expansion of the splitting operator by employing the standard exponential power series for terms of the form $\mathrm{e}^{b_i h B}$; the expansion of the splitting operator is then considered as a quadrature formula approximation of a multiple integral.

Variation-of-constants formula. The exact solution of the initial value problem (1.1) can also be represented by means of the variation-of-constants formula

$$y(t_0+\tau) = \Big(\mathrm{e}^{\tau A} + \int_0^\tau \mathrm{e}^{(\tau-\sigma)A}\, B\, \mathrm{e}^{\sigma(A+B)}\,\mathrm{d}\sigma\Big)\, y(t_0)\,, \qquad 0 \le \tau \le T - t_0\,;$$

we thus obtain the following representation of the exact solution operator

$$E_{A+B}(\tau) = \mathrm{e}^{\tau A} + \int_0^\tau \mathrm{e}^{(\tau-\sigma)A}\, B\, \mathrm{e}^{\sigma(A+B)}\,\mathrm{d}\sigma\,, \tag{2.7}$$

see also (1.4).

Expansion (Exact solution). A repeated application of the above relation (2.7) yields

$$\begin{aligned}
E_{A+B}(h) &= \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A}\, B\, \mathrm{e}^{\sigma_1(A+B)}\,\mathrm{d}\sigma_1 \\
&= \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A}\, B \Big(\mathrm{e}^{\sigma_1 A} + \int_0^{\sigma_1} \mathrm{e}^{(\sigma_1-\sigma_2)A}\, B\, \mathrm{e}^{\sigma_2(A+B)}\,\mathrm{d}\sigma_2\Big)\,\mathrm{d}\sigma_1 \\
&= \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A}\, B\, \mathrm{e}^{\sigma_1 A}\,\mathrm{d}\sigma_1 + \int_0^h \int_0^{\sigma_1} \mathrm{e}^{(h-\sigma_1)A}\, B\, \mathrm{e}^{(\sigma_1-\sigma_2)A}\, B\, \mathrm{e}^{\sigma_2(A+B)}\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1 \\
&= \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A}\, B\, \mathrm{e}^{\sigma_1 A}\,\mathrm{d}\sigma_1 \\
&\qquad + \int_0^h \int_0^{\sigma_1} \mathrm{e}^{(h-\sigma_1)A}\, B\, \mathrm{e}^{(\sigma_1-\sigma_2)A}\, B \Big(\mathrm{e}^{\sigma_2 A} + \int_0^{\sigma_2} \mathrm{e}^{(\sigma_2-\sigma_3)A}\, B\, \mathrm{e}^{\sigma_3(A+B)}\,\mathrm{d}\sigma_3\Big)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,,
\end{aligned}$$

and, moreover, we have

$$E_{A+B}(h) = \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A} B\, \mathrm{e}^{\sigma_1 A}\, \mathrm{d}\sigma_1 + \int_0^h \int_0^{\sigma_1} \mathrm{e}^{(h-\sigma_1)A} B\, \mathrm{e}^{(\sigma_1-\sigma_2)A} B\, \mathrm{e}^{\sigma_2 A}\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1 + \int_0^h \int_0^{\sigma_1} \int_0^{\sigma_2} \mathrm{e}^{(h-\sigma_1)A} B\, \mathrm{e}^{(\sigma_1-\sigma_2)A} B\, \mathrm{e}^{(\sigma_2-\sigma_3)A} B\, \mathrm{e}^{\sigma_3(A+B)}\, \mathrm{d}\sigma_3\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1 .$$

We thus obtain the following expansion of the exact solution operator with respect to $h = h_0$

$$E_{A+B}(h) = \mathrm{e}^{hA} + \int_0^h \mathrm{e}^{(h-\sigma_1)A} B\, \mathrm{e}^{\sigma_1 A}\, \mathrm{d}\sigma_1 + \int_0^h \int_0^{\sigma_1} \mathrm{e}^{(h-\sigma_1)A} B\, \mathrm{e}^{(\sigma_1-\sigma_2)A} B\, \mathrm{e}^{\sigma_2 A}\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1 + \mathscr{O}\big(h^3, C_B^3, M_A, M_{A+B}\big).$$

Expansion of exponential. Regarding a stepwise expansion of the splitting operator, it is convenient to employ the following stepwise expansion of the exponential function; to capture the remainder, we introduce the complex functions $\varphi_j : \mathbb{C} \to \mathbb{C} : z \mapsto \varphi_j(z)$, $j \geq 0$, defined through

$$\varphi_0(z) = \mathrm{e}^z, \qquad \varphi_j(z) = \tfrac{1}{(j-1)!} \int_0^1 \sigma^{j-1}\, \mathrm{e}^{(1-\sigma)z}\, \mathrm{d}\sigma, \quad j \geq 1, \qquad z \in \mathbb{C}.$$

Relation (1.11) for the exponential implies the bound

$$\big\| \varphi_j(\tau B) \big\|_{X \leftarrow X} \leq \tfrac{1}{j!}\, \mathrm{e}^{M_B |\tau|}, \qquad j \geq 0, \quad \tau \in \mathbb{R}. \tag{2.8}$$

By a partial integration, it is seen that the φ-functions fulfill the recurrence relation

$$\varphi_j(z) = \tfrac{1}{j!} + z\, \varphi_{j+1}(z), \qquad j \geq 0, \quad z \in \mathbb{C}. \tag{2.9}$$

For instance, we obtain the following expansion

$$\mathrm{e}^z = 1 + z\, \varphi_1(z) = 1 + z + z^2\, \varphi_2(z) = 1 + z + \tfrac{1}{2} z^2 + z^3\, \varphi_3(z),$$

which correspond to a standard Taylor series expansion

$$\mathrm{e}^z = 1 + z \int_0^1 \mathrm{e}^{\sigma z}\, \mathrm{d}\sigma = 1 + z + z^2 \int_0^1 (1-\sigma)\, \mathrm{e}^{\sigma z}\, \mathrm{d}\sigma = 1 + z + \tfrac{1}{2} z^2 + z^3 \int_0^1 \tfrac{1}{2} (1-\sigma)^2\, \mathrm{e}^{\sigma z}\, \mathrm{d}\sigma .$$

Expansion (Splitting operator). As a first step, we expand the splitting operator $\Phi_{A+B}(h)$ by means of the identity $\mathrm{e}^{\tau B} = I + \tau B\, \varphi_1(\tau B)$, see also (2.9); more precisely, replacing $\mathrm{e}^{b_i hB}\, \mathrm{e}^{a_i hA}$ with $\mathrm{e}^{a_i hA} + b_i hB\, \varphi_1(b_i hB)\, \mathrm{e}^{a_i hA}$, $i = 1, 2$, we obtain

$$\begin{aligned} \Phi_{A+B}(h) &= \mathrm{e}^{b_2 hB}\, \mathrm{e}^{a_2 hA}\, \mathrm{e}^{b_1 hB}\, \mathrm{e}^{a_1 hA} \\ &= \mathrm{e}^{(a_1+a_2)hA} + h\big(b_1 \mathrm{e}^{a_2 hA} B\, \varphi_1(b_1 hB)\, \mathrm{e}^{a_1 hA} + b_2 B\, \varphi_1(b_2 hB)\, \mathrm{e}^{(a_1+a_2)hA}\big) \\ &\quad + h^2 b_1 b_2 B\, \varphi_1(b_2 hB)\, \mathrm{e}^{a_2 hA} B\, \varphi_1(b_1 hB)\, \mathrm{e}^{a_1 hA}. \end{aligned}$$

In order to discover the similarities between the expansion of the exact solution operator and the expansion of the splitting operator, we henceforth denote

$$c_1 = a_1\,, \qquad c_2 = a_1 + a_2\,,$$

and further require the order condition $c_2 = a_1 + a_2 = 1$ to be fulfilled. Consequently, it follows

$$\begin{aligned}\Phi_{A+B}(h) = \mathrm{e}^{hA} &+ h\big(b_1 \mathrm{e}^{(1-c_1)hA} B\,\varphi_1(b_1 hB)\,\mathrm{e}^{c_1 hA} + b_2 B\,\varphi_1(b_2 hB)\,\mathrm{e}^{hA}\big)\\ &+ h^2 b_1 b_2 B\,\varphi_1(b_2 hB)\,\mathrm{e}^{(1-c_1)hA} B\,\varphi_1(b_1 hB)\,\mathrm{e}^{c_1 hA}.\end{aligned}$$

Inserting the identity $\varphi_1(\tau B) = I + \tau B\,\varphi_2(\tau B)$, we further obtain

$$\begin{aligned}\Phi_{A+B}(h) &= \mathrm{e}^{hA} + h\big(b_1 \mathrm{e}^{(1-c_1)hA} B\big(I + b_1 hB\,\varphi_2(b_1 hB)\big)\mathrm{e}^{c_1 hA} + b_2 B\big(I + b_2 hB\,\varphi_2(b_2 hB)\big)\mathrm{e}^{hA}\big)\\ &\quad + h^2 b_1 b_2 B\big(I + b_2 hB\,\varphi_2(b_2 hB)\big)\mathrm{e}^{(1-c_1)hA} B\,\varphi_1(b_1 hB)\,\mathrm{e}^{c_1 hA}\\ &= \mathrm{e}^{hA} + h\big(b_1 \mathrm{e}^{(1-c_1)hA} B\,\mathrm{e}^{c_1 hA} + b_2 B\,\mathrm{e}^{hA}\big) + h^2\big(b_1^2\,\mathrm{e}^{(1-c_1)hA} B^2 \varphi_2(b_1 hB)\,\mathrm{e}^{c_1 hA}\\ &\quad + b_1 b_2 B\,\mathrm{e}^{(1-c_1)hA} B\,\varphi_1(b_1 hB)\,\mathrm{e}^{c_1 hA} + b_2^2 B^2 \varphi_2(b_2 hB)\,\mathrm{e}^{hA}\big) + \mathcal{O}\big(h^3, C_B^3, M_A, M_B\big)\,,\end{aligned}$$

see also (2.9) and (2.8). We finally expand all terms involving h^2 by means of the recurrence relation (2.9); in particular, inserting the identity $\varphi_2(\tau B) = \frac{1}{2}\,I + \tau B\,\varphi_3(\tau B)$, it follows

$$\begin{aligned}\Phi_{A+B}(h) = \mathrm{e}^{hA} &+ h\big(b_1 \mathrm{e}^{(1-c_1)hA} B\,\mathrm{e}^{c_1 hA} + b_2 B\,\mathrm{e}^{hA}\big)\\ &+ h^2\big(\tfrac{1}{2}\,b_1^2\,\mathrm{e}^{(1-c_1)hA} B^2 \mathrm{e}^{c_1 hA} + b_1 b_2 B\,\mathrm{e}^{(1-c_1)hA} B\,\mathrm{e}^{c_1 hA} + \tfrac{1}{2}\,b_2^2 B^2\,\mathrm{e}^{hA}\big)\\ &+ \mathcal{O}\big(h^3, C_B^3, M_A, M_B\big)\,.\end{aligned}$$

Expansion (Defect operator). Altogether, the above expansions yield the following relation for the defect operator $D = \Phi_{A+B} - E_{A+B}$

$$\begin{aligned}D(h) &= Q_1 - I_1 + Q_2 - I_2 + \mathcal{O}\big(h^3, C_B^3, M_A, M_B, M_{A+B}\big)\,,\\ Q_1 &= h\big(b_1 \mathrm{e}^{(1-c_1)hA} B\,\mathrm{e}^{c_1 hA} + b_2 B\,\mathrm{e}^{hA}\big)\,, \qquad I_1 = \int_0^h \mathrm{e}^{(h-\sigma_1)A} B\,\mathrm{e}^{\sigma_1 A}\,\mathrm{d}\sigma_1\,,\\ Q_2 &= h^2\big(\tfrac{1}{2}\,b_1^2\,\mathrm{e}^{(1-c_1)hA} B^2 \mathrm{e}^{c_1 hA} + b_1 b_2 B\,\mathrm{e}^{(1-c_1)hA} B\,\mathrm{e}^{c_1 hA} + \tfrac{1}{2}\,b_2^2 B^2\,\mathrm{e}^{hA}\big)\,,\\ I_2 &= \int_0^h \int_0^{\sigma_1} \mathrm{e}^{(h-\sigma_1)A} B\,\mathrm{e}^{(\sigma_1-\sigma_2)A} B\,\mathrm{e}^{\sigma_2 A}\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,.\end{aligned}$$

We next relate Q_1 and Q_2 to the integrals I_1 and I_2. More precisely, we consider Q_1 as an approximation to the single integral I_1

$$\begin{aligned}g(\sigma_1) &= \mathrm{e}^{(h-\sigma_1)A} B\,\mathrm{e}^{\sigma_1 A}\,, \qquad 0 \le \sigma_1 \le h\,,\\ Q_1 &= h\big(b_1\,g(c_1 h) + b_2\,g(c_2 h)\big)\,, \qquad I_1 = \int_0^h g(\sigma_1)\,\mathrm{d}\sigma_1\,,\end{aligned}$$

resulting from the application of a quadrature formula with weights and nodes $(b_i, c_i)_{i=1}^2$, where $s = 2$. A standard Taylor series expansion of the integrand g about zero yields

$$g'(\sigma_1) = -\operatorname{e}^{(h-\sigma_1)A} \operatorname{ad}_A(B) \operatorname{e}^{\sigma_1 A}, \quad g''(\sigma_1) = \operatorname{e}^{(h-\sigma_1)A} \operatorname{ad}_A^2(B) \operatorname{e}^{\sigma_1 A}, \qquad 0 \le \sigma_1 \le h,$$
$$Q_1 = h\,(b_1 + b_2)\, g(0) + h^2\,(b_1 c_1 + b_2 c_2)\, g'(0) + \mathcal{O}\big(h^3, g''\big),$$
$$I_1 = h\, g(0) + \tfrac{1}{2} h^2\, g'(0) + \mathcal{O}\big(h^3, g''\big).$$

In a similar manner, we interprete Q_2 as quadrature formula approximation to the double integral I_2

$$G(\sigma_1, \sigma_2) = \operatorname{e}^{(h-\sigma_1)A} B \operatorname{e}^{(\sigma_1-\sigma_2)A} B \operatorname{e}^{\sigma_2 A}, \qquad 0 \le \sigma_2 \le \sigma_1 \le h,$$
$$Q_2 = h^2\big(\tfrac{1}{2} b_1^2\, G(c_1 h, c_1 h) + b_1 b_2\, G(c_2 h, c_1 h) + \tfrac{1}{2} b_2^2\, G(c_2 h, c_2 h)\big),$$
$$I_2 = \int_0^h \int_0^{\sigma_1} G(\sigma_1, \sigma_2)\, \mathrm{d}\sigma_2 \mathrm{d}\sigma_1.$$

Here, by a Taylor series expansion of the function G, it follows

$$G'(\sigma_1, \sigma_2) = -\operatorname{e}^{(h-\sigma_1)A}\big(\operatorname{ad}_A(B) \operatorname{e}^{(\sigma_1-\sigma_2)A} B, B \operatorname{e}^{(\sigma_1-\sigma_2)A} \operatorname{ad}_A(B)\big) \operatorname{e}^{\sigma_2 A}, \qquad 0 \le \sigma_2 \le \sigma_1 \le h,$$
$$Q_2 = \tfrac{1}{2} h^2 (b_1 + b_2)^2\, G(0,0) + \mathcal{O}\big(h^3, G'\big), \qquad I_2 = \tfrac{1}{2} h^2\, G(0,0) + \mathcal{O}\big(h^3, G'\big),$$

with G' denoting the Jacobian of G. Provided that the bound

$$\big\|\operatorname{ad}_A(B)\big\|_{X \leftarrow X} + \big\|\operatorname{ad}_A^2(B)\big\|_{X \leftarrow X} \le C_{\mathrm{ad}}$$

holds with some constant $C_{\mathrm{ad}} > 0$, see also (2.1) for the definition of the iterated commutators, we finally have

$$\begin{aligned} D(h) &= h\,(b_1 + b_2 - 1)\, g(0) + h^2 \Big(\big(b_1 c_1 + b_2 c_2 - \tfrac{1}{2}\big)\, g'(0) + \tfrac{1}{2}\big((b_1 + b_2)^2 - 1\big)\, G(0,0)\Big) \\ &\quad + \mathcal{O}\big(h^3, C_B^3, M_A, M_B, M_{A+B}, C_{\mathrm{ad}}\big) \\ &= h\,(b_1 + b_2 - 1)\operatorname{e}^{hA} B - h^2 \Big(\big(b_1 c_1 + b_2 c_2 - \tfrac{1}{2}\big)\operatorname{e}^{hA} \operatorname{ad}_A(B) + \tfrac{1}{2}\big((b_1 + b_2)^2 - 1\big)\operatorname{e}^{hA} B^2\Big) \\ &\quad + \mathcal{O}\big(h^3, C_B^3, M_A, M_B, M_{A+B}, C_{\mathrm{ad}}\big). \end{aligned}$$

Note that the remainder does *not* depend on the quantity C_A. As before, the requirement $D(h) = \mathcal{O}\big(h^{p+1}\big)$ for $p = 1$ or $p = 2$, respectively, yields the first and second order conditions (1.19).

2.3. Differential equations

Approach. Another approach that is particularly suited for evolutionary equations involving critical parameters relies on the deduction of a differential equation for the splitting operator, see also [20, 21]. As the general approach involves several rather technical arguments, we restrict ourselves to the consideration of the Strang splitting method.

Integral relation for defect operator. We consider the second-order Strang splitting method involving two compositions

$$S = S_2\, S_1\,, \qquad S_i(t) = \mathrm{e}^{tB_i}\, \mathrm{e}^{tA_i}\,, \qquad t \geq 0\,,$$

where $A_i = a_i\, A$ and $B_i = b_i B$ for $i = 1,2$. In particular, the method coefficients fulfill the first order conditions $a_1 + a_1 = 1 = b_1 + b_2$. Using that $S_i' = S_i\, A_i + B_i\, S_i$, we determine the first time derivative

$$S' = \big(S_2\, A_2 + B_2\, S_2\big)\, S_1 + S_2\, \big(S_1\, A_1 + B_1\, S_1\big)$$

and obtain the following initial value problem for the splitting operator

$$S'(t) = (A+B)\, S(t) + R(t)\,, \quad t \geq 0\,, \qquad S(0) = I\,.$$

On the other hand the corresponding initial value problem for the evolution operator is as follows

$$E'(t) = (A+B)\, E(t)\,, \quad t \geq 0\,, \qquad E(0) = I\,.$$

Thus, by the variation-of-constants formula, the defect operator $D = S - E$ fulfills the relation

$$D(t) = \int_0^t E(t-\tau)\, R(\tau)\, \mathrm{d}\tau\,, \quad t \geq 0\,,$$
$$R = \big(S_2\, A_2 + B_2\, S_2\big)\, S_1 + S_2\, \big(S_1\, A_1 + B_1\, S_1\big) - (A+B)S\,.$$

Remainder. We next rewrite the remaining term by using that $A_1 + A_2 = A$ and $B_1 + B_2 = B$ as well as

$$\big[S_2\, S_1, A_1\big] = S_2\, \big[S_1, A_1\big] + \big[S_2, A_1\big]\, S_1\,.$$

We obtain the relation

$$\begin{aligned} R &= S_2\, A_2\, S_1 + S_2\, \big(S_1\, A_1 + B_1\, S_1\big) - \big(A_1 + A_2 + B_1\big) S_2\, S_1 \\ &= \big[S_2, A_2 + B_1\big]\, S_1 + S_2\, \big[S_1, A_1\big] + \big[S_2, A_1\big]\, S_1 \\ &= \big[S_2, A\big]\, S_1 + b_1\, \big[S_2, B\big]\, S_1 + a_1\, S_2\, \big[S_1, A\big]\,. \end{aligned}$$

This further implies the identity $R = R_1 + R_2$ with

$$R_1(t) = a_1\, S_2(t)\, \big[\mathrm{e}^{tB_1}, A\big]\, \mathrm{e}^{tA_1}\,, \qquad R_2(t) = \Big(\big[\mathrm{e}^{tB_2}, A\big]\, \mathrm{e}^{tA_2} + b_1\, \mathrm{e}^{tB_2}\, \big[\mathrm{e}^{tA_2}, B\big]\Big)\, S_1(t)\,.$$

We aim at a suitable representation of the remainder such that $R = S_2\, \mathscr{T}\, S_1$, that is, it holds $R_1 = S_2\, \mathscr{T}_1\, S_1$ and $R_2 = S_2\, \big(\mathscr{T}_{21} + \mathscr{T}_{22}\big)\, S_1$ with

$$a_1 \big[\mathrm{e}^{tB_1}, A\big] = \mathscr{T}_1(t)\, \mathrm{e}^{tB_1}\,, \qquad \big[\mathrm{e}^{tB_2}, A\big]\, \mathrm{e}^{tA_2} = S_2(t)\, \mathscr{T}_{21}(t)\,, \quad b_1 \big[\mathrm{e}^{tA_2}, B\big] = \mathrm{e}^{tA_2}\, \mathscr{T}_{22}(t)\,.$$

For this purpose, we consider a single term of the form

$$r(t) = \big[\mathrm{e}^{tK}, L\big] = \mathrm{e}^{tK} L - L\, \mathrm{e}^{tK}\,.$$

Determining the first time derivative

$$r'(t) = K\,\mathrm{e}^{tK}L - LK\,\mathrm{e}^{tK} = K\left(\mathrm{e}^{tK}L - L\mathrm{e}^{tK}\right) + \left(KL - LK\right)\mathrm{e}^{tK},$$

we obtain following initial value problem

$$r'(t) = K\,r(t) + \big[K,L\big]\,\mathrm{e}^{tK}, \quad t \geq 0, \qquad r(0) = 0.$$

Another application of the variation-of-constants formula yields

$$\big[\mathrm{e}^{tK},L\big] = \int_0^t \mathrm{e}^{\tau K}\big[K,L\big]\,\mathrm{e}^{-\tau K}\,\mathrm{d}\tau\;\mathrm{e}^{tK} = \mathrm{e}^{tK}\int_0^t \mathrm{e}^{-\tau K}\big[K,L\big]\,\mathrm{e}^{\tau K}\,\mathrm{d}\tau, \qquad t \geq 0.$$

Applying the above relation and using that $\big[K,L\big] = -\big[L,K\big]$ yields

$$\mathscr{T}_1(t)\,\mathrm{e}^{tB_1} = a_1\big[\mathrm{e}^{tB_1},A\big] = a_1\int_0^t \mathrm{e}^{\tau B_1}\big[B_1,A\big]\,\mathrm{e}^{-\tau B_1}\,\mathrm{d}\tau\;\mathrm{e}^{tB_1},$$
$$\mathrm{e}^{tA_2}\,\mathscr{T}_{22}(t) = b_1\big[\mathrm{e}^{tA_2},B\big] = b_1\mathrm{e}^{tA_2}\int_0^t \mathrm{e}^{-\tau A_2}\big[A_2,B\big]\,\mathrm{e}^{\tau A_2}\,\mathrm{d}\tau.$$

Furthermore, we have

$$\begin{aligned}
S_2(t)\,\mathscr{T}_{21}(t) &= \big[\mathrm{e}^{tB_2},A\big]\,\mathrm{e}^{tA_2} = \mathrm{e}^{tB_2}\int_0^t \mathrm{e}^{-\tau B_2}\big[B_2,A\big]\,\mathrm{e}^{\tau B_2}\,\mathrm{d}\tau\,\mathrm{e}^{tA_2}\\
&= S_2(t)\int_0^t \mathrm{e}^{-\tau B_2}\big[B_2,A\big]\,\mathrm{e}^{\tau B_2}\,\mathrm{d}\tau - \mathrm{e}^{tB_2}\Big[\mathrm{e}^{tA_2},\int_0^t \mathrm{e}^{-\tau B_2}\big[B_2,A\big]\,\mathrm{e}^{\tau B_2}\,\mathrm{d}\tau\Big]\\
&= S_2(t)\left(\int_0^t \mathrm{e}^{-\tau B_2}\big[B_2,A\big]\,\mathrm{e}^{\tau B_2}\,\mathrm{d}\tau - \int_0^t\int_0^t \mathrm{e}^{-\tau A_2}\big[A_2,\mathrm{e}^{-\sigma B_2}\big[B_2,A\big]\,\mathrm{e}^{\sigma B_2}\big]\,\mathrm{e}^{\tau A_2}\,\mathrm{d}\sigma\,\mathrm{d}\tau\right).
\end{aligned}$$

Taylor series expansion. From the above considerations, we obtain the representation of the defect operator

$$D(t) = \int_0^t E(t-\tau)\,S_2(\tau)\,\mathscr{T}(\tau)\,S_1(\tau)\,\mathrm{d}\tau,$$
$$\mathscr{T}(\tau) = \int_0^\tau g(\tau_1)\,\mathrm{d}\tau_1 + \int_0^\tau\int_0^\tau G(\tau_1,\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1,$$

involving the functions $g:[0,T]\to X$ and $G:[0,T]\times[0,T]\to X$, defined by

$$g(\tau_1) = -\,a_1\,b_1\,\mathrm{e}^{\tau_1 B_1}\big[A,B\big]\,\mathrm{e}^{-\tau_1 B_1} - b_2\,\mathrm{e}^{-\tau_1 B_2}\big[A,B\big]\,\mathrm{e}^{\tau_1 B_2} + a_2\,b_1\,\mathrm{e}^{-\tau_1 A_2}\big[A,B\big]\,\mathrm{e}^{\tau_1 A_2},$$
$$G(\tau_1,\tau_2) = a_2\,b_2\,\mathrm{e}^{-\tau_1 A_2}\big[A,\mathrm{e}^{-\tau_2 B_2}\big[A,B\big]\,\mathrm{e}^{\tau_2 B_2}\big]\,\mathrm{e}^{\tau_1 A_2}.$$

We next employ the Taylor series expansion

$$g(\tau_1) = g(0) + \tau_1\int_0^1 g'(\zeta\tau_1)\,\mathrm{d}\zeta,$$

where

$$g(0) = \big((a_2 - a_1)\, b_1 - b_2\big)\,\big[A,B\big]\,,$$
$$g'(\tau_1) = -\,a_1\, b_1^2\, \mathrm{e}^{\tau_1 B_1}\big[B,[A,B]\big]\,\mathrm{e}^{-\tau_1 B_1} + b_2^2\, \mathrm{e}^{-\tau_1 B_2}\big[B,[A,B]\big]\,\mathrm{e}^{\tau_1 B_2} - a_2^2\, b_1\, \mathrm{e}^{-\tau_1 A_2}\big[A,[A,B]\big]\,\mathrm{e}^{\tau_1 A_2}\,.$$

Recall that the first order conditions $a_1 + a_1 = 1$ and $b_1 + b_2 = 1$ are fulfilled. Thus, provided that the second order condition $(1 - a_1)\, b_1 = \frac{1}{2}$ is satisfied, it follows $g(0) = 0$.

Integral relation for defect operator. In particular, we finally obtain the following integral representation for the defect operator associated with the Strang splitting method

$$\begin{aligned} D(t) = &\int_0^t\!\!\int_0^\tau\!\!\int_0^1 \tau_1\, E(t-\tau)\, S_2(\tau)\, g'(\zeta\tau_1)\, S_1(\tau)\,\mathrm{d}\zeta\,\mathrm{d}\tau_1\,\mathrm{d}\tau \\ &+ \int_0^t\!\!\int_0^\tau\!\!\int_0^\tau E(t-\tau)\, S_2(\tau)\, G(\tau_1,\tau_2)\, S_1(\tau)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,\mathrm{d}\tau\,, \end{aligned}$$

$$g'(\tau_1) = -\,a_1\, b_1^2\, \mathrm{e}^{\tau_1 B_1}\big[B,[A,B]\big]\,\mathrm{e}^{-\tau_1 B_1} + b_2^2\, \mathrm{e}^{-\tau_1 B_2}\big[B,[A,B]\big]\,\mathrm{e}^{\tau_1 B_2} - a_2^2\, b_1\, \mathrm{e}^{-\tau_1 A_2}\big[A,[A,B]\big]\,\mathrm{e}^{\tau_1 A_2}\,,$$
$$G(\tau_1,\tau_2) = a_2\, b_2\, \mathrm{e}^{-\tau_1 A_2}\big[A,\mathrm{e}^{-\tau_2 B_2}\big[A,B\big]\,\mathrm{e}^{\tau_2 B_2}\big]\,\mathrm{e}^{\tau_1 A_2}\,.$$

Clearly, the above identity implies $D(h) = \mathscr{O}(h^3)$.

3. Nonlinear problems

Situation. Let $X = \mathbb{R}^d$. Henceforth, we consider the following initial value problem for $y : [t_0, T] \to X$ involving a nonlinear differential equation of the form

$$y'(t) = A\big(y(t)\big) + B\big(y(t)\big), \quad t_0 \le t \le T, \qquad y(t_0) \text{ given}. \tag{3.1}$$

Generalisation. It is straightforward to extend our considerations to the case where the Euclidian space $X = \mathbb{R}^d$ is replaced with a Banach space $(X, \|\cdot\|_X)$.

Assumption. We suppose the functions $A : X \to X$ and $B : X \to X$ to be sufficiently often differentiable with bounded derivatives.

Exact solution. The exact solution of the initial value problem (3.1) is (formally) given by the nonlinear exact solution operator E_{A+B}, that is, it holds

$$y(t_0 + \tau) = E_{A+B}\big(\tau, t_0, y(t_0)\big), \qquad 0 \le \tau \le T - t_0, \tag{3.2a}$$

see also (0.3). Employing the compact, formally linear notation of Lie-derivatives, we have

$$y(t_0 + \tau) = \mathrm{e}^{\tau D_{A+B}} y(t_0), \qquad 0 \le \tau \le T - t_0, \tag{3.2b}$$

see Section 3.1.

Numerical approximation. In accordance with the above relation for the exact solution, the numerical approximation at time t_1 is given by

$$y_1 = \Phi_{A+B}(h, t_0, y_0) \;\approx\; y(t_1) = E_{A+B}\big(h, t_0, y(t_0)\big), \qquad h = h_0,$$

with numerical solution operator Φ_{A+B}.

3.1. Calculus of Lie derivatives

Approach. A most useful tool in the statement and the theoretical error analysis of high-order exponential operator splitting methods for nonlinear evolution equations is the formal calculus of Lie derivatives, which is suggestive of the less involved linear case, see also [30]. In the following, we review basic definitions and results needed in the derivation of our local

error expansion; we note that the calculus of Lie derivatives is used as a formal means under the tacit requirement that the arising (unbounded) operators and compositions thereof are well-defined on suitably chosen domains and time intervals.

Evolution operator and Lie derivative. We consider an initial value problem of the form

$$u'(t) = F\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) = u_0, \tag{3.3}$$

where the unbounded nonlinear operator $F : D(F) \subset X \to X$ is defined on a non-empty subset of the underlying Banach space $(X, \|\cdot\|_X)$. Formally, the exact solution of the evolutionary problem (3.3) is given by

$$u(t) = E_F(t, u_0), \qquad 0 \le t \le T, \tag{3.4a}$$

with the evolution operator E_F depending on the actual time and the initial value; as we restrict ourselves to an autonomous differential equation, we may omit the dependence on the initial time. Furthermore, it is most helpful to employ the formal notation

$$u(t) = \mathrm{e}^{tD_F} u_0, \qquad 0 \le t \le T. \tag{3.4b}$$

More precisely, the evolution operator $(\mathrm{e}^{tD_F})_{0\le t\le T}$ and the Lie derivative D_F associated with F are given through the relations

$$\mathrm{e}^{tD_F} G\, u_0 = G\big(E_F(t, u_0)\big), \quad 0 \le t \le T, \qquad D_F\, G\, u_0 = G'(u_0)\, F(u_0), \tag{3.4c}$$

for any (unbounded) nonlinear operator $G : D(G) \subset X \to X$ (with suitable domain); if $G = I$ is the identity operator, we write $\mathrm{e}^{tD_F} u_0 = E_F(t, u_0)$ and $D_F\, u_0 = F(u_0)$ for short. Using that $E_F(0, u_0) = u_0$ as well as $\frac{\mathrm{d}}{\mathrm{d}t} E_F(t, u_0) = F\big(E_F(t, u_0)\big)$, an application of the chain rule yields

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, \mathrm{e}^{tD_F} G\, u_0 = \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, G\big(E_F(t, u_0)\big) = G'\big(E_F(t, u_0)\big)\, F\big(E_F(t, u_0)\big)\big|_{t=0} = G'(u_0)\, F(u_0) = D_F\, G\, u_0;$$

thus, in accordance with the identity $L = \frac{\mathrm{d}}{\mathrm{d}t}|_{t=0}\, \mathrm{e}^{tL}$, which holds true for instance for any bounded linear operator $L : X \to X$ with the exponential function defined by the power series $\mathrm{e}^{tL} = \sum_{j=0}^{\infty} \frac{1}{j!}\, t^j\, L^j$, we may also set

$$D_F = \tfrac{\mathrm{d}}{\mathrm{d}t}\big|_{t=0}\, \mathrm{e}^{tD_F}. \tag{3.4d}$$

Then, the defining relation for the Lie derivative is a consequence of the first relation in (3.4c).

Basic manipulation rules. The evolution operator forms a local one-parameter group

$$\mathrm{e}^{(t+s)D_F} = \mathrm{e}^{tD_F}\, \mathrm{e}^{sD_F} = \mathrm{e}^{sD_F}\, \mathrm{e}^{tD_F}, \quad 0 \le t + s \le T, \qquad \mathrm{e}^{tD_F}\big|_{t=0} = I, \tag{3.5a}$$

since $E_F(t + s, u_0) = E_F\big(s, E_F(t, u_0)\big)$ by the local existence and uniqueness of the solution and consequently $\mathrm{e}^{(t+s)D_F} G\, u_0 = G\big(E_F(t + s, u_0)\big) = G\big(E_F\big(s, E_F(t, u_0)\big)\big) = \mathrm{e}^{tD_F}\, \mathrm{e}^{sD_F} G\, u_0$; in the

context of parabolic evolution equations, the above relation is restricted to positive times $0 \le t, s \le t+s \le T$. In regard to the general scheme of an exponential operator splitting method, it should also be noted that the composition of evolution operators acts in reversed order, i.e., it holds

$$\mathrm{e}^{tD_{F_1}}\,\mathrm{e}^{sD_{F_2}}\,G\,u_0 = G\Big(E_{F_2}\big(s, E_{F_1}(t,u_0)\big)\Big), \qquad 0 \le t+s \le T\,. \tag{3.5b}$$

Moreover, the following linearity and scaling relations are valid

$$\begin{gathered}
D_{F_1+F_2} = D_{F_1} + D_{F_2}\,, \qquad D_{cF} = c\,D_F\,, \\
D_F\,(G_1+G_2) = D_F\,G_1 + D_F\,G_2\,, \qquad D_F\,(c\,G) = c\,D_F\,G\,, \\
\mathrm{e}^{tD_F}(G_1+G_2) = \mathrm{e}^{tD_F}G_1 + \mathrm{e}^{tD_F}G_2\,, \quad \mathrm{e}^{tD_F}(c\,G) = c\,\mathrm{e}^{tD_F}G\,, \qquad 0 \le t \le T\,, \\
\mathrm{e}^{tD_{cF}} = \mathrm{e}^{ctD_F}\,, \qquad 0 \le t \le T\,,
\end{gathered} \tag{3.5c}$$

for any complex scalar c, due to the fact that the evolution operator associated with an autonomous problem satisfies $E_{cF}(t,u_0) = E_F(ct,u_0)$ and thus

$$\mathrm{e}^{tD_{cF}}G\,u_0 = G\big(E_{cF}(t,u_0)\big) = G\big(E_F(ct,u_0)\big) = \mathrm{e}^{ctD_F}G\,u_0\,.$$

In order to show (3.5c), we calculate

$$\begin{gathered}
D_{cF}\,G\,u_0 = c\,G'(u_0)\,F(u_0) = c\,D_F\,G\,u_0\,, \qquad D_F\,(c\,G)\,u_0 = c\,G'(u_0)\,F(u_0) = c\,D_F\,G\,u_0\,, \\
D_{F_1+F_2}\,G\,u_0 = G'(u_0)\,\big(F_1(u_0)+F_2(u_0)\big) = G'(u_0)\,F_1(u_0) + G'(u_0)\,F_2(u_0) = D_{F_1}\,G\,u_0 + D_{F_2}\,G\,u_0\,, \\
D_F(G_1+G_2)\,u_0 = \big(G_1'(u_0)+G_2'(u_0)\big)\,F(u_0) = G_1'(u_0)\,F(u_0) + G_2'(u_0)\,F(u_0) = D_F\,G_1\,u_0 + D_F\,G_2\,u_0\,, \\
\mathrm{e}^{tD_F}(G_1+G_2)\,u_0 = G_1\big(E_F(t,u_0)\big) + G_2\big(E_F(t,u_0)\big) = \mathrm{e}^{tD_F}G_1\,u_0 + \mathrm{e}^{tD_F}G_2\,u_0\,, \qquad 0 \le t \le T\,, \\
\mathrm{e}^{tD_F}(c\,G)\,u_0 = c\,G\big(E_F(t,u_0)\big) = c\,\mathrm{e}^{tD_F}G\,u_0\,, \qquad 0 \le t \le T\,.
\end{gathered}$$

But, in general, $\mathrm{e}^{tD_F}G\,u_0$ and $D_F\,G\,u_0$ are nonlinear with respect to u_0.

Derivatives. Besides, we employ the formal relation

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{tD_F} = D_F\,\mathrm{e}^{tD_F} = \mathrm{e}^{tD_F}D_F\,, \qquad 0 \le t \le T\,, \tag{3.5d}$$

which allows to rewrite the initial value problem (3.3) as

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{e}^{tD_F}u_0 = D_F\,\mathrm{e}^{tD_F}u_0 = \mathrm{e}^{tD_F}D_F\,u_0\,, \quad 0 \le t \le T\,, \qquad \mathrm{e}^{tD_F}\big|_{t=0}\,u_0 = u_0\,. \tag{3.5e}$$

The above identity is verified by the following calculation

$$\begin{aligned}
D_F\,\mathrm{e}^{tD_F}G\,u_0 &= G'\big(E_F(t,u_0)\big)\,\partial_2 E_F(t,u_0)\,F(u_0) = G'\big(E_F(t,u_0)\big)\,\tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,E_F\big(t,E_F(s,u_0)\big) \\
&= G'\big(E_F(t,u_0)\big)\,\tfrac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\,E_F(t+s,u_0) = G'\big(E_F(t,u_0)\big)\,F\big(E_F(t,u_0)\big) \\
&= \mathrm{e}^{tD_F}D_F\,G\,u_0\,, \qquad 0 \le t \le T\,,
\end{aligned}$$

or, in brief, $D_F\,\mathrm{e}^{\,tD_F} = \frac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\mathrm{e}^{\,sD_F}\mathrm{e}^{\,tD_F} = \frac{\mathrm{d}}{\mathrm{d}s}\big|_{s=0}\mathrm{e}^{\,(t+s)D_F} = \mathrm{e}^{\,tD_F}\,D_F$. Here, we denote by $\partial_2 E_F$ the derivative of the evolution operator with respect to the initial value; we recall that E_F and $\partial_2 E_F$ solve the initial value problems

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}t}\,E_F(t,u_0) &= F\big(E_F(t,u_0)\big)\,, \quad 0\le t\le T\,, \qquad E_F(t,u_0)\big|_{t=0} = u_0\,,\\ \tfrac{\mathrm{d}}{\mathrm{d}t}\,\partial_2 E_F(t,u_0) &= F'\big(E_F(t,u_0)\big)\,\partial_2 E_F(t,u_0)\,, \quad 0\le t\le T\,, \qquad \partial_2 E_F(t,u_0)\big|_{t=0} = I\,. \end{aligned} \tag{3.5f}$$

To justify manipulations below, we further note that the identity

$$\mathrm{e}^{\,tD_F} = I + \mathrm{e}^{\tau D_F}\big|_{\tau=0}^{t} = I + \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}\tau}\,\mathrm{e}^{\tau D_F}\,\mathrm{d}\tau = I + \int_0^t \mathrm{e}^{\tau D_F} D_F\,\mathrm{d}\tau\,, \qquad 0\le t\le T\,, \tag{3.5g}$$

which is justified by the above considerations, implies the formal expansion

$$\mathrm{e}^{\,tD_F} = \sum_{j=0}^{k-1} \tfrac{1}{j!}\,t^j D_F^j + \int_{T_k} \mathrm{e}^{\tau_k D_F} D_F^k\,\mathrm{d}\tau\,, \qquad 0\le t\le T\,, \quad k\ge 1\,, \tag{3.5h}$$

where we denote $T_k = \big\{\tau = (\tau_1,\tau_2,\dots,\tau_k)\in\mathbb{R}^k : 0\le\tau_k\le\cdots\le\tau_1\le\tau_0 = t\big\}$ and, as common usage, set $D_F^0 = I$. For the stepwise expansion of the splitting operator, it is useful to employ the formal recurrence relation

$$\varphi_j(tD_F) = \tfrac{1}{j!}\,I + \varphi_{j+1}(tD_F)\;tD_F\,, \qquad j\ge 0\,, \tag{3.5i}$$

with $\varphi_0(tD_F) = \mathrm{e}^{\,tD_F}$; in particular, for $j=0$ we retain (3.5g).

Iterated Lie commutators. The Lie commutator of two nonlinear operators is given by

$$\mathrm{ad}_F(G)\,v = \big[F,G\big](v) = F'(v)\,G(v) - G'(v)\,F(v)\,;$$

in particular, whenever F and G are linear, the above relation reduces to $\mathrm{ad}_F(G) = FG - GF$ since $F'(v) = F$ as well as $G'(v) = G$. In accordance with the above definition, we further set

$$\mathrm{ad}_{D_F}(D_G)\,v = \big[D_F, D_G\big]\,v = D_F\,D_G\,v - D_G\,D_F\,v\,, \tag{3.5j}$$

whence $\mathrm{ad}_{D_F}(D_G) = -\mathrm{ad}_F(G)$. Moreover, higher iterated Lie commutators are defined by induction

$$\mathrm{ad}^0_{D_F}(D_G) = D_G, \qquad \mathrm{ad}^j_{D_F}(D_G) = \big[D_F, \mathrm{ad}_{D_F^{j-1}}(D_G)\big], \quad j\ge 1\,; \tag{3.5k}$$

they naturally arise in the local error expansion based on quadrature formulas.

Nonlinear variation-of-constants formula (Grï¿½bner–Alekseev formula). An essential tool in the derivation of the local error representation for high-order splitting methods is the nonlinear variation-of-constants formula. This result states that the solutions of the initial value

problems

$$u'(t) = F\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) = u_0,$$
$$u'(t) = F\big(u(t)\big) + R\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) = u_0,$$

are related through the nonlinear variation-of-constants formula

$$E_{F+R}(t, u_0) = E_F(t, u_0) + \int_0^t \partial_2 E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\, R\big(E_{F+R}(\tau, u_0)\big)\, \mathrm{d}\tau, \qquad 0 \le t \le T,$$

which in formal notation takes the form

$$\mathrm{e}^{\,tD_{F+R}}\, u_0 = \mathrm{e}^{\,tD_F}\, u_0 + \int_0^t \mathrm{e}^{\tau D_{F+R}}\, D_R\, \mathrm{e}^{(t-\tau)D_F}\, u_0\, \mathrm{d}\tau, \qquad 0 \le t \le T. \tag{3.6}$$

Proof. With the help of basic definitions and manipulation rules, see (3.5), we obtain

$$\begin{aligned}
\tfrac{\mathrm{d}}{\mathrm{d}\tau}\, \mathrm{e}^{\tau D_{F+R}}\, \mathrm{e}^{(t-\tau)D_F}\, G\, u_0 &= \tfrac{\mathrm{d}}{\mathrm{d}\tau}\, G\big(E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\big) \\
&= G'\big(E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\big)\Big(- F\big(E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\big) \\
&\qquad + \partial_2 E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\, \big(F\big(E_{F+R}(\tau, u_0)\big) + R\big(E_{F+R}(\tau, u_0)\big)\big)\Big) \\
&= G'\big(E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\big)\, \partial_2 E_F\big(t-\tau, E_{F+R}(\tau, u_0)\big)\, R\big(E_{F+R}(\tau, u_0)\big) \\
&= \mathrm{e}^{\tau D_{F+R}}\, D_R\, \mathrm{e}^{(t-\tau)D_F}\, G\, u_0,
\end{aligned}$$

which is in accordance with the formal calculation

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}\, \mathrm{e}^{\tau D_{F+R}}\, \mathrm{e}^{(t-\tau)D_F} = \mathrm{e}^{\tau D_{F+R}}\big(D_{F+R} - D_F\big)\, \mathrm{e}^{(t-\tau)D_F} = \mathrm{e}^{\tau D_{F+R}}\, D_R\, \mathrm{e}^{(t-\tau)D_F}.$$

As a consequence, using that

$$\begin{aligned}
\mathrm{e}^{\,tD_{F+R}}\, G\, u_0 - \mathrm{e}^{\,tD_F}\, G\, u_0 &= \mathrm{e}^{\tau D_{F+R}}\, \mathrm{e}^{(t-\tau)D_F}\, G\, u_0\big|_{\tau=0}^{t} \\
&= \int_0^t \tfrac{\mathrm{d}}{\mathrm{d}\tau}\, \mathrm{e}^{\tau D_{F+R}}\, \mathrm{e}^{(t-\tau)D_F}\, G\, u_0\, \mathrm{d}\tau \\
&= \int_0^t \mathrm{e}^{\tau D_{F+R}}\, D_R\, \mathrm{e}^{(t-\tau)D_F}\, G\, u_0\, \mathrm{d}\tau, \qquad 0 \le t \le T,
\end{aligned} \tag{3.7}$$

the desired result follows when setting $G = I$.

3.2. Splitting methods

Approach. Exponential operator splitting methods rely on a decomposition of the right-hand side of the differential equation (3.1) into two (or more) parts and the presumption that the

initial value problems

$$\begin{aligned} z'(t) &= A\big(z(t)\big), \quad t_0 \le t \le T, \qquad z(t_0) \text{ given}, \\ \widetilde{z}'(t) &= B\big(\widetilde{z}(t)\big), \quad t_0 \le t \le T, \qquad \widetilde{z}(t_0) \text{ given}, \end{aligned} \tag{3.8}$$

are solvable numerically in an accurate and efficient manner. The (approximate) solutions of the initial value problems (3.8) are then composed in a suitable way; this yields an approximation $\Phi_{A+B} \approx E_{A+B}$ to the exact solution operator. For simplicity and in view of Gross–Pitaevskii systems, we may assume that the exact solutions of (1.5)

$$\begin{aligned} z(t_0+\tau) &= E_A\big(\tau, t_0, z(t_0)\big), \qquad 0 \le \tau \le T - t_0, \\ \widetilde{z}(t_0+\tau) &= E_B\big(\tau, t_0, \widetilde{z}(t_0)\big), \qquad 0 \le \tau \le T - t_0, \end{aligned}$$

are available.

General form of splitting method. Any exponential operator splitting method involving several compositions can be cast into the following form

$$\begin{gathered} \tau_0 = t_0, \qquad Y_0 = y_0, \\ Y_i = E_B\big(b_i h, \tau_{i-1} + a_i h, E_A\big(a_i h, \tau_{i-1}, Y_{i-1}\big)\big), \quad \tau_i = \tau_{i-1} + (a_i + b_i)h, \qquad 1 \le i \le s, \\ y_1 = Y_s, \end{gathered} \tag{3.9a}$$

yielding an approximation to the exact solution value

$$y(t_1) = E_{A+B}\big(h, t_0, y(t_0)\big), \qquad h = h_0.$$

Employing the compact notation of Lie-derivative, we have

$$y_1 = \Phi_{A+B}(h, t_0, y_0) = \prod_{i=1}^{s} \mathrm{e}^{a_{s+1-i} h D_A} \, \mathrm{e}^{b_{s+1-i} h D_B} \, y_0, \qquad h = h_0; \tag{3.9b}$$

as before, the product is defined downwards. In comparison with (1.6), the order of the compositions is reversed.

Explanation. Recall that by definition (3.4c) it holds $\mathrm{e}^{\tau D_F} G\, y(t_0) = G\big(E_F\big(\tau, t_0, y(t_0)\big)\big)$. Consequently, setting $G = \mathrm{e}^{b_i h D_B}$, i.e., $G\big(z(\tau)\big) = E_B\big(b_i h, \tau, z(\tau)\big)$, it follows

$$\mathrm{e}^{a_i h D_A} \, \mathrm{e}^{b_i h D_B} \, Y_{i-1} = G\big(E_A(a_i h, \tau_{i-1}, Y_{i-1})\big) = E_B\big(b_i h, \tau_{i-1} + a_i h, E_A(a_i h, \tau_{i-1}, Y_{i-1})\big) = Y_i.$$

By repetition we obtain (3.9b).

Examples. The first-order Lie–Trotter splitting method (1.7) and the second-order Strang splitting method (1.8) can be cast into the general form (3.9). As well, methods of higher order are included, see also Table 1.

3.3. Convergence analysis

Objective. In the following, we are concerned with deducing an estimate for the global error $y_N - y(T)$ of an exponential operator splitting method (3.9) when applied to the initial value problem (3.1) To this purpose, as in the linear case, we follow a standard approach based on a *Lady Windermere's Fan* argument.

Local error and order. In the present situation, the local error equals

$$\begin{aligned} d_n &= D\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big) \\ &= \Phi_{A+B}\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big) - E_{A+B}\big(h_{n-1}, t_{n-1}, y(t_{n-1})\big), \qquad 1 \le n \le N, \end{aligned}$$

see also (0.4). Thus, the numerical method (3.9) is consistent of order p iff

$$d_n = \mathcal{O}\big(h_{n-1}^{p+1}\big).$$

Again, it suffices to consider the case $n = 1$.

Lady Windermere's Fan. For nonlinear differential equations, similarly as in the linear case, the global error fulfills the telescopic identity

$$y_N - y(t_N) = \prod_{j=0}^{N-1} \Phi_{A+B}(h_j)\,\big(y_0 - y(t_0)\big) + \sum_{n=1}^{N} \prod_{j=n}^{N-1} \Phi_{A+B}(h_j)\,d_n, \tag{3.10}$$

see also (1.10); here, we employ the short notation

$$\prod_{j=k}^{m-1} \Phi_{A+B}(h_j)\,z(t_k) = \Phi_{A+B}\Big(h_{m-1}, t_{m-1}, \Phi_{A+B}\big(\ldots, \Phi_{A+B}\big(h_k, t_k, z(t_k)\big)\big)\Big), \qquad m > k \ge 0.$$

In Section 3.3.1, we are concerned with extending the local error expansion of Section 1.2.2 to nonlinear problems.

3.3.1. Local error expansion

Situation. For the following, to avoid technicalities, we consider exponential operator splitting methods (3.9) that involve two compositions only

$$y_1 = \Phi_{A+B}\big(h, t_0, y(t_0)\big) = \mathrm{e}^{a_1 h D_A}\,\mathrm{e}^{b_1 h D_B}\,\mathrm{e}^{a_2 h D_A}\,\mathrm{e}^{b_2 h D_B}\,y_0, \qquad h = h_0.$$

Method examples that can be cast into this form are the Lie–Trotter splitting method (1.7) and the Strang splitting method (1.8).

Objective. We are concerned with deducing a suitable expansion of the defect

$$\begin{aligned} d_1 &= \Phi_{A+B}\big(h, t_0, y(t_0)\big) - E_{A+B}\big(h, t_0, y(t_0)\big) \\ &= \mathrm{e}^{a_1 h D_A}\, \mathrm{e}^{b_1 h D_B}\, \mathrm{e}^{a_2 h D_A}\, \mathrm{e}^{b_2 h D_B}\, y(t_0) - \mathrm{e}^{h D_{A+B}}\, y(t_0)\,, \qquad h = h_0\,, \end{aligned}$$

with respect to h, see also (3.2) and (3.9).

Approach. For the solution of an initial value problem of the form (0.2), we employ a Taylor series expansion and further express the arising derivatives of y by means of the function F defining the right-hand side of the differential equation; more precisely, using that $y' = F(y)$ and thus by the chain rule $y'' = F'(y)\, y' = F'(y)\, F(y)$, we obtain

$$\begin{aligned} E_F\big(\tau, t_0, y(t_0)\big) &= y(t_0) + \tau\, y'(t_0) + \tfrac{1}{2}\tau^2\, y''(t_0) + \mathscr{O}\big(\tau^3\big) \\ &= y(t_0) + \tau\, F\big(y(t_0)\big) + \tfrac{1}{2}\tau^2\, F'\big(y(t_0)\big)\, F\big(y(t_0)\big) + \mathscr{O}\big(\tau^3\big)\,, \qquad \tau \geq 0\,, \end{aligned} \tag{3.11}$$

with remainder depending on y'''.

Remark. The above relation (3.11) corresponds to the formal expansion

$$\begin{aligned} \mathrm{e}^{\tau D_F}\, y(t_0) &= \Big(I + \tau D_F + \tfrac{1}{2}\tau^2 D_F^2 + \mathscr{O}\big(\tau^3\big)\Big)\, y(t_0)\,, \\ &= y(t_0) + \tau D_F\, y(t_0) + \tfrac{1}{2}\tau^2 D_F^2\, y(t_0) + \mathscr{O}\big(\tau^3\big)\,. \end{aligned}$$

Namely, applying definition (3.4c), it follows

$$\begin{aligned} G(z) = D_F\, z = F(z)\,, \qquad G'(z) = F'(z)\,, \\ H(z) = D_F^2\, z = \big(D_F\, G\big)(z) = G'(z)\, F(z) = F'(z)\, F(z)\,. \end{aligned}$$

Expansion (Exact solution). Expanding the exact solution value by means of (3.11), yields

$$\begin{aligned} E_{A+B}\big(h, t_0, y(t_0)\big) &= y(t_0) + h\,\Big(A\big(y(t_0)\big) + B\big(y(t_0)\big)\Big) \\ &\qquad + \tfrac{1}{2}\, h^2\,\Big(A'\big(y(t_0)\big) + B'\big(y(t_0)\big)\Big)\Big(A\big(y(t_0)\big) + B\big(y(t_0)\big)\Big) + \mathscr{O}\big(h^3\big) \\ &= y(t_0) + h\,\Big(A\big(y(t_0)\big) + B\big(y(t_0)\big)\Big) \\ &\qquad + \tfrac{1}{2}\, h^2\,\Big(A'\big(y(t_0)\big)A\big(y(t_0)\big) + A'\big(y(t_0)\big)B\big(y(t_0)\big) + B'\big(y(t_0)\big)A\big(y(t_0)\big) \\ &\qquad\quad + B'\big(y(t_0)\big)B\big(y(t_0)\big)\Big) + \mathscr{O}\big(h^3\big)\,, \end{aligned}$$

which corresponds to the formal expansion

$$\mathrm{e}^{h D_{A+B}}\, y(t_0) = y(t_0) + h\, D_{A+B} y(t_0) + \tfrac{1}{2}\, h^2 D_{A+B}^2 y(t_0) + \mathscr{O}\big(h^3\big)\,.$$

Expansion (Splitting solution, single composition). We first consider a single composition

$$\mathrm{e}^{a_i h D_A}\, \mathrm{e}^{b_i h D_B}\, z(\tau) = E_B\big(b_i h, \widetilde{\tau}, \widetilde{z}(\tau)\big), \qquad \widetilde{\tau} = \tau + a_i h, \quad \widetilde{z}(\widetilde{\tau}) = E_A\big(a_i h, \tau, z(\tau)\big).$$

The above relation (3.11) implies

$$\begin{aligned} E_B\big(b_i h, \widetilde{\tau}, \widetilde{z}(\widetilde{\tau})\big) &= \widetilde{z}(\widetilde{\tau}) + \mathscr{O}(h) \\ &= \widetilde{z}(\widetilde{\tau}) + b_i h\, B\big(\widetilde{z}(\widetilde{\tau})\big) + \mathscr{O}\big(h^2\big) \\ &= \widetilde{z}(\widetilde{\tau}) + b_i h\, B\big(\widetilde{z}(\widetilde{\tau})\big) + \tfrac{1}{2}\, b_i^2 h^2 B'\big(\widetilde{z}(\widetilde{\tau})\big)\, B\big(\widetilde{z}(\widetilde{\tau})\big) + \mathscr{O}\big(h^3\big). \end{aligned}$$

In a similar manner, we have

$$\begin{aligned} \widetilde{z}(\widetilde{\tau}) = E_A\big(a_i h, \tau, z(\tau)\big) &= z(\tau) + \mathscr{O}(h) \\ &= z(\tau) + a_i h\, A\big(z(\tau)\big) + \mathscr{O}\big(h^2\big) \\ &= z(\tau) + a_i h\, A\big(z(\tau)\big) + \tfrac{1}{2}\, a_i^2 h^2 A'\big(z(\tau)\big) A\big(z(\tau)\big) + \mathscr{O}\big(h^3\big). \end{aligned}$$

Consequently, by additional Taylor series expansions, it follows

$$\begin{aligned} B\big(\widetilde{z}(\widetilde{\tau})\big) = B\big(z(\tau)\big) + \mathscr{O}(h) &= B\big(z(\tau)\big) + a_i h\, B'\big(z(\tau)\big)\, A\big(z(\tau)\big) + \mathscr{O}\big(h^2\big), \\ B'\big(\widetilde{z}(\widetilde{\tau})\big) = B'\big(z(\tau)\big) + \mathscr{O}(h), \qquad & B'\big(\widetilde{z}(\widetilde{\tau})\big)\, B\big(\widetilde{z}(\widetilde{\tau})\big) = B'\big(z(\tau)\big)\, B\big(z(\tau)\big) + \mathscr{O}(h), \end{aligned}$$

wherefore we finally obtain

$$\begin{aligned} E_B\big(b_i h, \widetilde{\tau}, \widetilde{z}(\widetilde{\tau})\big) = z(\tau) &+ h\Big(a_i A\big(z(\tau)\big) + b_i B\big(z(\tau)\big)\Big) \\ &+ h^2\Big(\tfrac{1}{2}\, a_i^2 A'\big(z(\tau)\big) A\big(z(\tau)\big) + a_i b_i\, B'\big(z(\tau)\big)\, A\big(z(\tau)\big) + \tfrac{1}{2}\, b_i^2 B'\big(z(\tau)\big)\, B\big(z(\tau)\big)\Big) \\ &+ \mathscr{O}\big(h^3\big). \end{aligned}$$

Note that $D_F(z) = F(z)$, $D_F^2\, z = F'(z)\, F(z)$, and further

$$G(z) = D_B\, z = B(z), \qquad G'(z) = B'(z), \qquad D_A D_B\, z = G'(z)\, A(z) = B'(z)\, A(z);$$

we thus conclude that the formal expansion

$$\begin{aligned} \mathrm{e}^{a_i h D_A}\, \mathrm{e}^{b_i h D_B}\, z(\tau) &= \big(I + a_i h\, D_A + \tfrac{1}{2}\, a_i^2 h^2 D_A^2\big)\big(I + b_i h\, D_B + \tfrac{1}{2}\, b_i^2 h^2 D_B^2\big)\, z(\tau) + \mathscr{O}\big(h^3\big) \\ &= \Big(I + h\big(a_i D_A + b_i D_B\big) + h^2\big(\tfrac{1}{2}\, a_i^2 D_A^2 + a_i b_i D_A D_B + \tfrac{1}{2}\, b_i^2 D_B^2\big)\Big)\, z(\tau) + \mathscr{O}\big(h^3\big) \\ &= z(\tau) + h\big(a_i D_A + b_i D_B\big)\, z(\tau) + h^2\big(\tfrac{1}{2}\, a_i^2 D_A^2 + a_i b_i D_A D_B + \tfrac{1}{2}\, b_i^2 D_B^2\big)\, z(\tau) \\ &\quad + \mathscr{O}\big(h^3\big) \\ &= z(\tau) + h\Big(a_i A\big(z(\tau)\big) + b_i B\big(z(\tau)\big)\Big) \\ &\quad + h^2\Big(\tfrac{1}{2}\, a_i^2 A'\big(z(\tau)\big)\, A\big(z(\tau)\big) + a_i b_i B'\big(z(\tau)\big)\, A\big(z(\tau)\big) + \tfrac{1}{2}\, b_i^2 B'\big(z(\tau)\big)\, B\big(z(\tau)\big)\Big) \\ &\quad + \mathscr{O}\big(h^3\big) \end{aligned}$$

is in accordance with the above relation deduced by Taylor series expansions.

Expansion (Splitting solution). We next apply the previously verified formal expansion to a splitting method involving two compositions; this yields

$$\begin{aligned}
\Phi_{A+B}\big(h,t_0,y(t_0)\big) &= \mathrm{e}^{a_1 h D_A}\,\mathrm{e}^{b_1 h D_B}\,\mathrm{e}^{a_2 h D_A}\,\mathrm{e}^{b_2 h D_B}\,y(t_0)\\
&= \Big(I + h\big(a_1 D_A + b_1 D_B\big) + h^2\big(\tfrac{1}{2}\,a_1^2 D_A^2 + a_1 b_1 D_A D_B + \tfrac{1}{2}\,b_1^2 D_B^2\big)\Big)\\
&\qquad \Big(I + h\big(a_2 D_A + b_2 D_B\big) + h^2\big(\tfrac{1}{2}\,a_2^2 D_A^2 + a_2 b_2 D_A D_B + \tfrac{1}{2}\,b_2^2 D_B^2\big)\Big)\,y(t_0) + \mathscr{O}\big(h^3\big)\\
&= y(t_0) + h\big((a_1+a_2) D_A + (b_1+b_2) D_B\big)\,y(t_0)\\
&\qquad + h^2\Big(\tfrac{1}{2}\big(a_1^2+a_2^2\big) D_A^2 + (a_1 b_1 + a_2 b_2) D_A D_B + \tfrac{1}{2}\big(b_1^2+b_2^2\big) D_B^2\\
&\qquad\qquad + \big(a_1 D_A + b_1 D_B\big)\big(a_2 D_A + b_2 D_B\big)\Big)\,y(t_0) + \mathscr{O}\big(h^3\big)\\
&= y(t_0) + h\big((a_1+a_2) D_A + (b_1+b_2) D_B\big)\,y(t_0)\\
&\qquad + h^2\Big(\tfrac{1}{2}\,(a_1+a_2)^2 D_A^2 + \big(a_1(b_1+b_2) + a_2 b_2\big) D_A D_B + b_1 a_2 D_B D_A\\
&\qquad\qquad + \tfrac{1}{2}\,(b_1+b_2)^2 D_B^2\Big)\,y(t_0) + \mathscr{O}\big(h^3\big)\,.
\end{aligned}$$

Recalling the identities $D_F\,z = F(z)$, $D_F^2\,z = F'(z)\,F(z)$, and $D_F D_G\,z = G'(z)\,F(z)$, we finally have

$$\begin{aligned}
\Phi_{A+B}\big(h,t_0,y(t_0)\big) &= y(t_0) + h\Big((a_1+a_2)\,A\big(y(t_0)\big) + (b_1+b_2)\,B\big(y(t_0)\big)\Big)\\
&\qquad + h^2\Big(\tfrac{1}{2}\,(a_1+a_2)^2\,A'\big(y(t_0)\big)\,A\big(y(t_0)\big) + \tfrac{1}{2}\,(b_1+b_2)^2\,B'\big(y(t_0)\big)\,B\big(y(t_0)\big)\\
&\qquad\quad + b_1 a_2\,A'\big(y(t_0)\big)\,B\big(y(t_0)\big) + \big(a_1(b_1+b_2) + a_2 b_2\big)\,B'\big(y(t_0)\big)\,A\big(y(t_0)\big)\Big)\\
&\qquad\quad + \mathscr{O}\big(h^3\big)\,.
\end{aligned}$$

Expansion (Local error). Altogether, the above expansions of the exact and numerical solution value imply

$$\begin{aligned}
d_1 &= \Phi_{A+B}\big(h,t_0,y(t_0)\big) - E_{A+B}\big(h,t_0,y(t_0)\big)\\
&= h\Big((a_1+a_2-1)\,A\big(y(t_0)\big) + (b_1+b_2-1)\,B\big(y(t_0)\big)\Big)\\
&\qquad + h^2\Big(\tfrac{1}{2}\,\big((a_1+a_2)^2-1\big)\,A'\big(y(t_0)\big)\,A\big(y(t_0)\big) + \tfrac{1}{2}\,\big((b_1+b_2)^2-1\big)\,B'\big(y(t_0)\big)\,B\big(y(t_0)\big)\\
&\qquad\quad + \big(b_1 a_2 - \tfrac{1}{2}\big)\,A'\big(y(t_0)\big)\,B\big(y(t_0)\big) + \big(a_1(b_1+b_2) + a_2 b_2 - \tfrac{1}{2}\big)\,B'\big(y(t_0)\big)\,A\big(y(t_0)\big)\Big)\\
&\qquad\quad + \mathscr{O}\big(h^3\big)\,,
\end{aligned}$$

and, as a consequence, we retain the first and second order conditions (1.19) from requiring $d_1 = \mathscr{O}\big(h^{p+1}\big)$ for $p = 1$ or $p = 2$, respectively.

Part II.

Fourier and Hermite spectral methods

Notation. Henceforth, we let $\mathbb{N} = \{m \in \mathbb{Z} : m \geq 0\}$. Further, we employ the multi-index notation $m = (m_1, \ldots, m_d) \in \mathbb{Z}^d$ and the compact vector notation $x = (x_1, \ldots, x_d) \in \mathbb{R}^d$. We denote by $\partial_{x_i}^k$, $1 \leq i \leq d$, the partial derivatives of order k and by $\Delta = \Delta_x = \partial_{x_1}^2 + \cdots + \partial_{x_d}^2$ the d-dimensional Laplace operator. For a domain $\Omega \subset \mathbb{R}^d$, the Lebesgue space $L^2(\Omega) = L^2(\Omega, \mathbb{C})$ of square integrable complex-valued functions is endowed with standard scalar product $(\cdot \,|\, \cdot)_{L^2}$ and corresponding norm $\|\cdot\|_{L^2}$, defined by

$$\big(f \,\big|\, g\big)_{L^2} = \int_\Omega f(x)\, \overline{g(x)}\, \mathrm{d}x, \quad \big\|f\big\|_{L^2} = \sqrt{\big(f \,\big|\, f\big)_{L^2}}, \qquad f, g \in L^2(\Omega).$$

Objective. We are concerned with the efficient numerical solution of the linear partial differential equation

$$\mathrm{i}\, \partial_t \psi(x,t) = \mathscr{A}(x)\, \psi(x,t), \qquad x \in \Omega, \quad t \geq 0, \tag{3.12}$$

involving a second order differential operator $\mathscr{A}$. Regarding the spatial discretisation of nonlinear Schrödiger equations by Fourier and Hermite spectral methods, we focus on the cases $\mathscr{A} = -\Delta$ and $\mathscr{A} = -\Delta + U_\gamma$, where U_γ denotes a scaled harmonic potential.

Approach. For solving (3.12), we make use of the fact that there exists a family $\big(\mathscr{B}_m\big)_{m \in \mathscr{M}}$ which forms a complete orthonormal system of the function space $L^2(\Omega)$, i.e., for any element $\varphi \in L^2(\Omega)$ the representation

$$\varphi = \sum_{m \in \mathscr{M}} \varphi_m\, \mathscr{B}_m, \qquad \varphi_m = \big(\varphi \,\big|\, \mathscr{B}_m\big)_{L^2},$$

holds. Moreover, the basis functions $\big(\mathscr{B}_m\big)_{m \in \mathscr{M}}$ are eigenfunctions of the linear operator $\mathscr{A}$; more precisely, the eigenvalue relation

$$\mathscr{A}\, \mathscr{B}_m = \lambda_m\, \mathscr{B}_m, \qquad m \in \mathscr{M},$$

is valid with real eigenvalues $(\lambda_m)_{m \in \mathscr{M}}$. The above identity motivates the definition of a linear operator $F(\mathscr{A})$ through

$$F(\mathscr{A})\, \varphi = \sum_{m \in \mathscr{M}} \varphi_m\, F(\mathscr{A})\, \mathscr{B}_m = \sum_{m \in \mathscr{M}} \varphi_m\, F(\lambda_m)\, \mathscr{B}_m;$$

for instance, the linear operator $\mathrm{e}^{c\mathscr{A}}$ is given by

$$\mathrm{e}^{c\mathscr{A}} \varphi = \sum_{m \in \mathscr{M}} \varphi_m\, \mathrm{e}^{c\lambda_m}\, \mathscr{B}_m.$$

By Parseval's identity, provided that the sequence $\big(\varphi_m\, F(\lambda_m)\big)_{m \in \mathscr{M}}$ is square-summable, the above definition is well-defined; in particular, for $c \in \mathrm{i}\mathbb{R}$ it follows

$$\big\|\mathrm{e}^{c\mathscr{A}} \varphi\big\|_{L^2} = \big\|\varphi\big\|_{L^2}, \qquad \varphi \in L^2(\Omega).$$

As a consequence, the solution of (3.12) possesses the following representation

$$\psi(\cdot,t) = \mathrm{e}^{-\mathrm{i}\,t\mathscr{A}}\psi(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_m(0)\,\mathrm{e}^{-\mathrm{i}\,t\lambda_m}\mathscr{B}_m\,, \quad t\geq 0\,, \qquad \psi(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_m(0)\,\mathscr{B}_m\,.$$

For the numerical realisation of the above relation, the infinite sum is truncated and the spectral coefficients $\psi_m(0)$ are approximated by means of a quadrature formula.

4. Fourier spectral method

Objective. In the following, we are concerned with the numerical solution of the linear partial differential equation (3.12) involving the d-dimensional Laplace operator

$$\mathscr{A} = -\Delta$$

on a bounded (symmetric) domain $\Omega = (-a_1, a_1) \times \cdots \times (-a_d, a_d) \subset \mathbb{R}^d$ with $a_i > 0$ (sufficiently large), $1 \le i \le d$; furthermore, we impose periodic boundary conditions. We first restrict ourselves to the case $d = 1$ and then extend our considerations to arbitrary space dimensions.

4.1. Approach in one space dimension

Notation. For $a > 0$ we set $\Omega = (-a, a) \subset \mathbb{R}$ and further $\mathscr{M} = \mathbb{Z}$.

Approach. For the construction of the Fourier basis functions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ and the derivation of basic relations we refer to [46]. Combining the theories of Sobolev spaces and selfadjoint linear operators on Hilbert spaces, it is shown that the linear differential operator $\mathscr{A} = -\partial_x^2$, subject to periodic boundary conditions, is selfadjoint on a suitably chosen domain $D(\mathscr{A}) \subset L^2(\Omega)$. Further, the corresponding eigenfunctions $(\mathscr{F}_m)_{m\in\mathscr{M}}$, which form a complete orthonormal system of the function space $L^2(\Omega)$, and the eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$ are determined.

4.1.1. Basic relations

Fourier basis functions. The Fourier basis functions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ are given by

$$\mathscr{F}_m(x) = \tfrac{1}{\sqrt{2a}}\, \mathrm{e}^{\mathrm{i}\pi m\left(\frac{1}{a}x+1\right)}, \qquad x \in \Omega, \quad m \in \mathscr{M}.$$

In particular, they fulfill the orthonormality relation

$$\left(\mathscr{F}_k \,\middle|\, \mathscr{F}_m\right)_{L^2} = \delta_{km}, \qquad k, m \in \mathscr{M}. \tag{4.1}$$

Fourier series expansion. The family $(\mathscr{F}_m)_{m\in\mathscr{M}}$ is complete in $L^2(\Omega)$, i.e., for any function $\varphi \in L^2(\Omega)$ the representation

$$\varphi = \sum_{m\in\mathscr{M}} \varphi_m \mathscr{F}_m, \qquad \varphi_m = \left(\varphi \,\middle|\, \mathscr{F}_m\right)_{L^2}, \tag{4.2}$$

holds with spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$; the convergence of the infinite sum versus φ is ensured in $L^2(\Omega)$.

Parseval's identity. The above relations (4.1) and (4.2) imply

$$\|\varphi\|_{L^2}^2 = \sum_{m\in\mathscr{M}} |\varphi_m|^2, \qquad \varphi \in L^2(\Omega). \tag{4.3}$$

Eigenvalue relation. The differential operator $\mathscr{A} = -\partial_x^2$ fulfills the following eigenvalue relation with eigenfunctions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ and associated eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$

$$-\partial_x^2 \mathscr{F}_m = \lambda_m \mathscr{F}_m, \quad \lambda_m = \tfrac{1}{a^2}\, m^2\pi^2, \qquad m \in \mathscr{M}. \tag{4.4}$$

Explanations. The orthononality relation (4.1) also follows from a straightforward calculation

$$\big(\mathscr{F}_k \,\big|\, \mathscr{F}_m\big)_{L^2} = \int_{-a}^{a} \mathscr{F}_k(x)\, \overline{\mathscr{F}_m(x)}\, \mathrm{d}x = \tfrac{1}{2a} \int_{-a}^{a} \mathrm{e}^{\mathrm{i}\,\pi(k-m)\left(\frac{1}{a}x+1\right)}\, \mathrm{d}x = \begin{cases} 1, & k = m, \\ 0, & k \neq m, \end{cases} \qquad k, m \in \mathscr{M}.$$

Moreover, in an easy manner, the eigenvalues are obtained by differentiation

$$\partial_x \mathscr{F}_m = \mathrm{i}\,\tfrac{1}{a}\, m\pi\, \mathscr{F}_m, \quad \partial_x^2 \mathscr{F}_m = -\tfrac{1}{a^2}\, m^2\pi^2\, \mathscr{F}_m, \qquad m \in \mathscr{M}.$$

4.1.2. Discretisation

Notations. For an even integer number $M > 0$ we set $\mathscr{M}_M = \big\{m \in \mathbb{Z} : -\tfrac{1}{2}M \le m \le \tfrac{1}{2}M - 1\big\}$ and further $\mathscr{J} = \big\{j \in \mathbb{Z} : 0 \le j \le M-1\big\}$.

Approach. We first consider a real-valued regular periodic function $f : \Omega \to \mathbb{R}$ with continuous extension to $\overline{\Omega}$; in particular, it holds $f(-a) = f(a)$. For the quadrature approximation of the integral

$$\int_\Omega f(x)\, \mathrm{d}x$$

we apply the trapezoidal rule with equidistant nodes and corresponding weights $(x_j, \omega_j)_{j\in\mathscr{J}}$

$$\sum_{j\in\mathscr{J}} \omega_j f(x_j) \approx \int_\Omega f(x)\, \mathrm{d}x, \qquad x_j = -a + \tfrac{2a}{M}\, j, \quad \omega_j = \tfrac{2a}{M}, \quad j \in \mathscr{J}. \tag{4.5}$$

The above quadrature approximation extends to complex-valued function $f : \Omega \to \mathbb{C}$ by considering the real and imaginary part of f.

Approximation of spectral coefficients. Note that

$$\mathscr{F}_m(x_j) = \tfrac{1}{\sqrt{2a}}\, \mathrm{e}^{\mathrm{i}\,2\pi\,\frac{jm}{M}}, \qquad m \in \mathscr{M}_M, \quad j \in \mathscr{J}. \tag{4.6}$$

An application of the trapezoidal rule (4.5) yields

$$\varphi_m = \big(\varphi \,\big|\, \mathscr{F}_m\big)_{L^2} = \int_\Omega \varphi(x)\, \overline{\mathscr{F}_m(x)}\, \mathrm{d}x \approx \tfrac{2a}{M} \sum_{j\in\mathscr{J}} \varphi(x_j)\, \overline{\mathscr{F}_m(x_j)}\,, \qquad m \in \mathscr{M}_M\,,$$

see also (4.2); we thus obtain the following approximations to the Fourier spectral coefficients

$$\varphi_m \approx \tfrac{\sqrt{2a}}{M} \sum_{j\in\mathscr{J}} \varphi(x_j)\, \mathrm{e}^{-\mathrm{i}\,2\pi\,\frac{jm}{M}}\,, \qquad m \in \mathscr{M}_M\,. \tag{4.7}$$

Approximation of function values. On the other hand, from the Fourier spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ approximations to the values of φ at the grid points $(x_j)_{j\in\mathscr{J}}$ are retained through

$$\varphi(x_j) \approx \tfrac{1}{\sqrt{2a}} \sum_{m\in\mathscr{M}_M} \varphi_m\, \mathrm{e}^{\mathrm{i}\,2\pi\,\frac{jm}{M}}\,, \qquad j \in \mathscr{J}\,, \tag{4.8}$$

see also (4.2) and (4.6).

4.1.3. Implementation

Notations. As before, for an even integer $M > 0$ we set $\mathscr{M}_M = \big\{m \in \mathbb{Z} : -\tfrac{1}{2}M \le m \le \tfrac{1}{2}M - 1\big\}$ and further $\mathscr{J} = \big\{j \in \mathbb{Z} : 0 \le j \le M-1\big\}$.

Implementation. The efficient implementation of the Fourier spectral method relies on Fast Fourier Techniques. In the following, we discuss the realisation of the pseudo-spectral transformations (4.7) and (4.8) in MATLAB. For notational simplicity, we do not employ different notations for the exact spectral coefficients and the numerical approximations obtained through (4.7); similarly, we do not distinguish between the function values and the numerical approximations (4.8). Tilded letters correspond to quantities in MATLAB.

Grid points. For the Fourier pseudo-spectral transformations, we employ a collocation at the trapezoidal quadrature nodes

$$\widetilde{x}_{j+1} \mathrel{\widetilde{=}} x_j\,, \qquad j \in \mathscr{J}\,.$$

Real to spectral. For given function values

$$\widetilde{\varphi}_{j+1} \mathrel{\widetilde{=}} \varphi(x_j)\,, \qquad j \in \mathscr{J}\,,$$

approximations to the spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ are computed through (4.7)

$$\begin{aligned}\varphi_m &= \tfrac{\sqrt{2a}}{M}\sum_{j\in\mathscr{J}}\varphi(x_j)\,\mathrm{e}^{-\mathrm{i}\,2\pi\frac{jm}{M}}\\ &= \tfrac{\sqrt{2a}}{M}\sum_{j=1}^{M}\varphi(x_{j-1})\,\mathrm{e}^{-\mathrm{i}\,2\pi\frac{(j-1)m}{M}}\\ &\cong \tfrac{\sqrt{2a}}{M}\sum_{j=1}^{M}\widetilde{\varphi}_j\,\mathrm{e}^{-\mathrm{i}\,2\pi\frac{(j-1)m}{M}}, \qquad m\in\mathscr{M}_M.\end{aligned}$$

Note that the periodicity of the Fourier basis functions and the (tacitly assumed) periodicity of φ implies $\varphi_{m+\ell M}=\varphi_m$ for any $\ell\in\mathbb{Z}$. In MATLAB, an application of the command `fft` results in

$$\texttt{fft}\big(\widetilde{\varphi}_1,\dots,\widetilde{\varphi}_M\big)=\big(\widetilde{\varphi}_1^{(\mathrm{s})},\dots,\widetilde{\varphi}_M^{(\mathrm{s})}\big), \qquad \widetilde{\varphi}_k^{(\mathrm{s})}=\sum_{j=1}^{M}\widetilde{\varphi}_j\,\mathrm{e}^{-\mathrm{i}\,2\pi\frac{(j-1)(k-1)}{M}}, \quad 1\le k\le M.$$

A comparison of the above relations shows that

$$\big(\widetilde{\varphi}_1^{(\mathrm{s})},\dots,\widetilde{\varphi}_M^{(\mathrm{s})}\big)\cong\tfrac{M}{\sqrt{2a}}\big(\varphi_0,\dots,\varphi_{\frac12 M-1},\varphi_{-\frac12 M},\dots,\varphi_{-1}\big).$$

Altogether, with the help of the command `fftshift` which swaps the left and right halves of a vector, we obtain approximations to the spectral coefficients through

$$\begin{aligned}\tfrac{\sqrt{2a}}{M}\,\texttt{fftshift}\,\big(\texttt{fft}\big(\widetilde{\varphi}_1,\dots,\widetilde{\varphi}_M\big)\big) &\cong \tfrac{\sqrt{2a}}{M}\,\texttt{fftshift}\big(\widetilde{\varphi}_1^{(\mathrm{s})},\dots,\widetilde{\varphi}_M^{(\mathrm{s})}\big)\\ &\cong \texttt{fftshift}\big(\varphi_0,\dots,\varphi_{\frac12 M-1},\varphi_{-\frac12 M},\dots,\varphi_{-1}\big)\\ &= \big(\varphi_{-\frac12 M},\dots,\varphi_{-1},\varphi_0,\dots,\varphi_{\frac12 M-1}\big).\end{aligned}$$

Spectral to real. On the other hand, starting with given spectral coefficients

$$\begin{aligned}\big(\varphi_{-\frac12 M},\dots,\varphi_{-1},\varphi_0,\dots,\varphi_{\frac12 M-1}\big) &= \big(\varphi_{\frac12 M},\dots,\varphi_{M-1},\varphi_0,\dots,\varphi_{\frac12 M-1}\big)\\ &\cong \big(\widetilde{\varphi}_{\frac12 M+1}^{(\mathrm{s})},\dots,\widetilde{\varphi}_M^{(\mathrm{s})},\widetilde{\varphi}_1^{(\mathrm{s})},\dots,\widetilde{\varphi}_{\frac12 M}^{(\mathrm{s})}\big),\end{aligned}$$

an application of the command `ifft` results in

$$\texttt{ifft}\big(\widetilde{\varphi}_1^{(\mathrm{s})},\dots,\widetilde{\varphi}_M^{(\mathrm{s})}\big)=\big(\widetilde{\varphi}_1,\dots,\widetilde{\varphi}_M\big), \qquad \widetilde{\varphi}_k=\tfrac1M\sum_{j=1}^{M}\widetilde{\varphi}_j^{(\mathrm{s})}\,\mathrm{e}^{\mathrm{i}\,2\pi\frac{(j-1)(k-1)}{M}}, \qquad 1\le k\le M.$$

Moreover, making use of the fact that

$$\tfrac{M}{\sqrt{2a}}\,\widetilde{\varphi}_k=\tfrac{1}{\sqrt{2a}}\sum_{j=1}^{M}\widetilde{\varphi}_j^{(\mathrm{s})}\,\mathrm{e}^{\mathrm{i}\,2\pi\frac{(j-1)(k-1)}{M}}$$

and thus

$$\begin{aligned}\tfrac{M}{\sqrt{2a}}\,\widetilde{\varphi}_k &\mathrel{\widehat{=}} \tfrac{1}{\sqrt{2a}}\sum_{j=1}^{M}\varphi_{j-1}\,\mathrm{e}^{\mathrm{i}\,2\pi\,\frac{(j-1)(k-1)}{M}}\\ &= \tfrac{1}{\sqrt{2a}}\sum_{j\in\mathscr{J}}\varphi_j\,\mathrm{e}^{\mathrm{i}\,2\pi\,\frac{j(k-1)}{M}}\\ &= \tfrac{1}{\sqrt{2a}}\sum_{m\in\mathscr{M}_M}\varphi_m\,\mathrm{e}^{\mathrm{i}\,2\pi\,\frac{m(k-1)}{M}}\\ &\mathrel{\widehat{=}} \varphi(x_{k-1}), \qquad 1\le k\le M,\end{aligned}$$

and that the command `ifftshift` swaps the left and right halves of a vector, approximations to the function values are obtained through

$$\begin{aligned}&\tfrac{M}{\sqrt{2a}}\,\texttt{ifft}\left(\texttt{ifftshift}\left(\varphi_{-\frac{1}{2}M},\dots,\varphi_{-1},\varphi_0,\dots,\varphi_{\frac{1}{2}M-1}\right)\right.\\ &\quad\mathrel{\widehat{=}} \tfrac{M}{\sqrt{2a}}\,\texttt{ifft}\left(\texttt{ifftshift}\left(\widetilde{\varphi}^{(\mathrm{s})}_{\frac{1}{2}M+1},\dots,\widetilde{\varphi}^{(\mathrm{s})}_{M},\widetilde{\varphi}^{(\mathrm{s})}_{1},\dots,\widetilde{\varphi}^{(\mathrm{s})}_{\frac{1}{2}M}\right)\right.\\ &\quad= \tfrac{M}{\sqrt{2a}}\,\texttt{ifft}\left(\widetilde{\varphi}^{(\mathrm{s})}_{1},\dots,\widetilde{\varphi}^{(\mathrm{s})}_{M}\right)\\ &\quad= \tfrac{M}{\sqrt{2a}}\left(\widetilde{\varphi}_1,\dots,\widetilde{\varphi}_M\right)\\ &\quad\mathrel{\widehat{=}} \left(\varphi(x_0),\dots,\varphi_{M-1}(x_{M-1})\right).\end{aligned}$$

4.2. Approach in several space dimensions

Notation. For $a_i>0$, $1\le i\le d$, we set $\Omega=(-a_1,a_1)\times\cdots\times(-a_d,a_d)\subset\mathbb{R}^d$ and further $\mathscr{M}=\mathbb{Z}^d$.

Approach. The considerations for one space dimensions are extended to the general case.

4.2.1. Basic relations

Fourier basis functions. In d space dimensions, the Fourier basis functions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ are given by

$$\begin{aligned}\mathscr{F}_m(x)&=\mathscr{F}_{m_1}(x_1)\cdots\mathscr{F}_{m_d}(x_d), \qquad x\in\Omega,\quad m\in\mathscr{M},\\ \mathscr{F}_{m_i}(x_i)&=\tfrac{1}{\sqrt{2a_i}}\,\mathrm{e}^{\mathrm{i}\,\pi m_i\left(\frac{1}{a_i}x_i+1\right)}, \qquad 1\le i\le d.\end{aligned}$$

In particular, the orthonormality relation (4.1) holds.

Fourier series expansion. The family $(\mathscr{F}_m)_{m\in\mathscr{M}}$ is complete in $L^2(\Omega)$, i.e., for any function $\varphi\in L^2(\Omega)$ the representation (4.2) holds with spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$.

Parseval's identity. Relations (4.1) and (4.2) imply (4.3).

Eigenvalue relation. The Laplace operator $\mathscr{A}(x) = -\Delta$ fulfills the following eigenvalue relation with eigenfunctions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ and associated eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$

$$-\Delta\mathscr{F}_m = \lambda_m\mathscr{F}_m\,,\quad \lambda_m = \sum_{i=1}^{d}\lambda_{m_i} = \pi^2\sum_{i=1}^{d}\tfrac{1}{a_i^2}\,m_i^2\,,\qquad m\in\mathscr{M}\,. \tag{4.9}$$

Explanation. Due to the fact that

$$-\Delta\mathscr{F}_m = -\mathscr{F}_{m_2}\cdots\mathscr{F}_{m_d}\,\partial_{x_1}^2\mathscr{F}_{m_1} - \cdots - \mathscr{F}_{m_1}\cdots\mathscr{F}_{m_{d-1}}\,\partial_{x_d}^2\mathscr{F}_{m_d} = \big(\lambda_{m_1}+\cdots+\lambda_{m_d}\big)\,\mathscr{F}_m\,,$$

the above relation follows by means of (4.4).

4.2.2. Discretisation

Notations. For $M\in\mathbb{N}^d$ with $M_i > 0$ an even integer number for $1\le i\le d$, we set

$$\mathscr{M}_M = \big\{m\in\mathbb{Z}^d : -\tfrac{1}{2}M_i \le m_i \le \tfrac{1}{2}M_i - 1, 1\le i\le d\big\}\,,$$
$$\mathscr{J} = \big\{j\in\mathbb{Z}^d : 0\le j_i\le M_i - 1, 1\le i\le d\big\}\,.$$

Further, we employ the short notation

$$\mathrm{e}^{c\,\frac{j\cdot m}{M}} = \mathrm{e}^{c\,\sum_{i=1}^{d}\frac{j_i m_i}{M_i}}\,,\qquad c\in\mathbb{C}\,,\quad j\in\mathscr{J}\,,\quad m\in\mathscr{M}_M\,.$$

Approach. We consider a complex-valued regular periodic function $f:\Omega\to\mathbb{C}^d$ with continuous extension to $\overline{\Omega}$, i.e. it holds $f(-a) = f(a)$. For the quadrature approximation of the multiple integral

$$\int_\Omega f(x)\,\mathrm{d}x$$

we apply the trapezoidal rule with equidistant nodes and corresponding weights $(x_j,\omega_j)_{j\in\mathscr{J}}$, which are given by the quadrature nodes and weights of the one-dimensional trapezoidal rule

$$\begin{gathered}\sum_{j\in\mathscr{J}}\omega_j f(x_j)\approx\int_\Omega f(x)\,\mathrm{d}x\,,\qquad x_j = (x_{j_1},\ldots,x_{j_d})\,,\quad \omega_j = \omega_{j_1}\cdots\omega_{j_d}\,,\qquad j\in\mathscr{J}\,,\\ x_{j_i} = -a_i + \tfrac{2a_i}{M_i}\,j_i\,,\quad \omega_{j_i} = \tfrac{2a_i}{M_i}\,,\qquad 1\le j_i\le M_i\,,\quad 1\le i\le d\,.\end{gathered} \tag{4.10}$$

Approximation of spectral coefficients. Note that

$$\mathscr{F}_m(x_j) = \prod_{i=1}^{d}\tfrac{1}{\sqrt{2a_i}}\,\mathrm{e}^{\mathrm{i}\,2\pi\,\frac{j\cdot m}{M}}\,,\qquad m\in\mathscr{M}_M\,,\quad j\in\mathscr{J}\,. \tag{4.11}$$

An application of the trapezoidal rule (4.10) yields the following approximations to the Fourier spectral coefficients

$$\varphi_m \approx \prod_{i=1}^{d} \tfrac{\sqrt{2a_i}}{M_i} \sum_{j \in \mathscr{J}} \varphi(x_j)\, \mathrm{e}^{-\mathrm{i}\, 2\pi\, \frac{j\cdot m}{M}}\,, \qquad m \in \mathscr{M}_M\,, \tag{4.12}$$

see also (4.2).

Approximation of function values. On the other hand, from the Fourier spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ approximations to the values of φ at the grid points $(x_j)_{j\in\mathscr{J}}$ are retained through

$$\varphi(x_j) \approx \prod_{i=1}^{d} \tfrac{1}{\sqrt{2a_i}} \sum_{m \in \mathscr{M}_M} \varphi_m\, \mathrm{e}^{\mathrm{i}\, 2\pi\, \frac{j\cdot m}{M}}\,, \qquad j \in \mathscr{J}\,, \tag{4.13}$$

see also (4.2) and (4.11).

4.2.3. Implementation

Notations. As before, for $M \in \mathbb{N}^d$ with $M_i > 0$ an even integer number for $1 \le i \le d$, we set

$$\mathscr{M}_M = \left\{ m \in \mathbb{Z}^d : -\tfrac{1}{2} M_i \le m_i \le \tfrac{1}{2} M_i - 1, 1 \le i \le d \right\},$$
$$\mathscr{J} = \left\{ j \in \mathbb{Z}^d : 0 \le j_i \le M_i - 1, 1 \le i \le d \right\}.$$

Implementation. It is straightforward to extend the considerations of Section 4.1.3 to several space dimensions; again, the pseudo-spectral transformations (4.12) and (4.13) are realised by Fast Fourier Techniques.

Real to spectral. In several space dimensions, approximations to the spectral coefficients are obtained through

$$\big(\varphi_m\big) \cong \prod_{i=1}^{d} \tfrac{\sqrt{2a_i}}{M_i}\, \texttt{fftshift}\left(\texttt{fftn}\big(\varphi(x_j)\big)\right).$$

Spectral to real. In several space dimensions, approximations to the function values are obtained through

$$\big(\varphi(x_j)\big) \cong \prod_{i=1}^{d} \tfrac{M_i}{\sqrt{2a_i}}\, \texttt{ifftn}\left(\texttt{ifftshift}\big(\varphi_m\big)\right).$$

5. Hermite spectral method

Objective. In the following, we are concerned with the numerical solution of the linear partial differential equation (3.12) involving the second order differential operator

$$\mathscr{A}(x) = -\Delta + U_\gamma(x), \qquad U_\gamma(x) = \sum_{i=1}^{d} \gamma_i^4 x_i^2, \quad \gamma_i > 0, \quad 1 \le i \le d, \tag{5.1}$$

on the unbounded domain $\Omega = \mathbb{R}^d$; furthermore, we impose asymptotic boundary conditions. We first restrict ourselves to the case $d = 1$ and then extend our considerations to arbitrary space dimensions.

5.1. Approach in one space dimension

Notation. We set $\Omega = \mathbb{R}$ and $\mathscr{M} = \mathbb{N}$; further, we denote by $\gamma > 0$ a positive weight.

Approach. As before, we also refer to [46] for the construction of the Hermite basis functions $(\mathscr{H}_m^\gamma)_{m\in\mathscr{M}}$ and the derivation of basic relations. Combining the theories of Sobolev spaces and selfadjoint linear operators on Hilbert spaces, it is shown that the linear differential operator $\mathscr{A}(x) = -\partial_x^2 + \gamma^4 x^2$, subject to asymptotic boundary conditions, is selfadjoint on a suitably chosen domain $D(\mathscr{A}) \subset L^2(\Omega)$. Further, the corresponding eigenfunctions $(\mathscr{H}_m^\gamma)_{m\in\mathscr{M}}$, which form a complete orthonormal system of the function space $L^2(\Omega)$, and the eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$ are determined.

5.1.1. Hermite basis functions

Objective. In the following, we are concerned with constructing the orthonormal Hermite basis functions $\left(\mathscr{H}_m^\gamma\right)_{m\in\mathscr{M}}$ which fulfill the eigenvalue relation

$$\mathscr{A}\,\mathscr{H}_m^\gamma = \lambda_m\,\mathscr{H}_m^\gamma, \quad m \in \mathscr{M}, \tag{5.2}$$

with associated eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$.

Ladder operators. The construction of the Hermite basis functions is based on the approach of ladder operators. The algebraic identity $a^2 - b^2 = (a-b)(a+b)$ motivates the consideration

of the differential operators

$$\mathscr{A}(x) = -\partial_x^2 + \gamma^4 x^2\,, \qquad \mathscr{P}(x) = \partial_x + \gamma^2 x\,, \qquad \mathscr{Q}(x) = -\partial_x + \gamma^2 x\,.$$

Although the operators $\mathscr{P}$ and $\mathscr{Q}$ do not commute, that is, it holds $\mathscr{A} \neq \mathscr{Q}\mathscr{P}$ and $\mathscr{A} \neq \mathscr{P}\mathscr{Q}$, we may take advantage of the fact that the product of $\mathscr{P}$ and $\mathscr{Q}$ is close to $\mathscr{A}$; more precisely, we have

$$\mathscr{Q}\mathscr{P} = \mathscr{A} - \gamma^2 I\,, \qquad \mathscr{P}\mathscr{Q} = \mathscr{A} + \gamma^2 I\,,$$

and, as a consequence, we further obtain

$$\mathscr{P}\mathscr{A} = \big(\mathscr{A} + 2\gamma^2 I\big)\mathscr{P}\,, \qquad \mathscr{Q}\mathscr{A} = \big(\mathscr{A} - 2\gamma^2 I\big)\mathscr{Q}\,.$$

Explanations. For a regular function y, it follows

$$\begin{aligned}
\mathscr{Q}(x)\mathscr{P}(x)\,y(x) &= \big(-\partial_x + \gamma^2 x\big)\big(\partial_x y(x) + \gamma^2 x\, y(x)\big) \\
&= -\partial_x^2 y(x) - \gamma^2\big(y(x) \pm x\,\partial_x y(x)\big) + \gamma^4 x^2 y(x) = \mathscr{A}(x)\,y(x) - \gamma^2 y(x)\,, \\
\mathscr{P}(x)\mathscr{Q}(x)\,y(x) &= \big(\partial_x + \gamma^2 x\big)\big(-\partial_x y(x) + \gamma^2 x\, y(x)\big) \\
&= -\partial_x^2 y(x) + \gamma^2\big(y(x) \pm x\,\partial_x y(x)\big) + \gamma^4 x^2 y(x) = \mathscr{A}(x)\,y(x) + \gamma^2 y(x)\,.
\end{aligned}$$

Hence, using that $\mathscr{A} = \mathscr{Q}\mathscr{P} + \gamma^2 I = \mathscr{P}\mathscr{Q} - \gamma^2 I$ we obtain

$$\begin{aligned}
\mathscr{P}\mathscr{A} &= \mathscr{P}\big(\mathscr{Q}\mathscr{P} + \gamma^2 I\big) = \big(\mathscr{P}\mathscr{Q} + \gamma^2 I\big)\mathscr{P} = \big(\mathscr{A} + 2\gamma^2 I\big)\mathscr{P}\,, \\
\mathscr{Q}\mathscr{A} &= \mathscr{Q}\big(\mathscr{P}\mathscr{Q} - \gamma^2 I\big) = \big(\mathscr{Q}\mathscr{P} - \gamma^2 I\big)\mathscr{Q} = \big(\mathscr{A} - 2\gamma^2 I\big)\mathscr{Q}\,.
\end{aligned}$$

First Hermite basis function. The first Hermite basis function $\mathscr{H}_0^\gamma$ is related to the weight function $w(x) = \mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}$; namely, using that $\mathscr{P}w = 0$ it follows $\mathscr{A}w = \big(\mathscr{Q}\mathscr{P} + \gamma^2 I\big)\,w = \gamma^2 w$. Due to the fact that

$$\|w\|_{L^2}^2 = \int_\Omega \mathrm{e}^{-\gamma^2 x^2}\,\mathrm{d}x = \sqrt{\tfrac{\pi}{\gamma^2}}\,,$$

it is seen that the first normalised Hermite basis function $\mathscr{H}_0^\gamma$ is given by

$$\mathscr{H}_0^\gamma(x) = \sqrt[4]{\frac{\gamma^2}{\pi}}\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\,, \qquad x \in \Omega\,,$$

with associated eigenvalue $\lambda_0 = \gamma^2$.

Preliminaries. We first note that by partial integration the relation

$$\int_\Omega \big(\partial_x \mathscr{H}_m^\gamma(x)\big)^2\,\mathrm{d}x = -\int_\Omega \mathscr{H}_m^\gamma(x)\,\partial_x^2 \mathscr{H}_m^\gamma(x)\,\mathrm{d}x$$

follows. Thus, the eigenvalue relation (5.2) and the normalisation condition $\|\mathscr{H}_m^\gamma\|_{L^2} = 1$ imply

$$\begin{aligned}\int_\Omega \big(\partial_x \mathscr{H}_m^\gamma(x)\big)^2 + \gamma^4 x^2 \big(\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x &= \int_\Omega \mathscr{H}_m^\gamma(x)\,\big(-\partial_x^2 \mathscr{H}_m^\gamma(x) + \gamma^4 x^2 \mathscr{H}_m^\gamma(x)\big)\,\mathrm{d}x \\ &= \int_\Omega \mathscr{H}_m^\gamma(x)\,\mathscr{A}(x)\,\mathscr{H}_m^\gamma(x)\,\mathrm{d}x = \lambda_m \int_\Omega \big(\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x = \lambda_m;\end{aligned}$$

in a similar manner, by partial integration it follows

$$\int_\Omega x\,\mathscr{H}_m^\gamma(x)\,\partial_x \mathscr{H}_m^\gamma(x)\,\mathrm{d}x = -\tfrac{1}{2}.$$

Altogether, we obtain the following identities

$$\begin{aligned}\big\|\mathscr{Q}\mathscr{H}_m^\gamma\big\|_{L^2}^2 &= \int_\Omega \big(-\partial_x \mathscr{H}_m^\gamma(x) + \gamma^2 x\,\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x \\ &= \int_\Omega \big(\partial_x \mathscr{H}_m^\gamma(x)\big)^2 - 2\gamma^2 x\,\mathscr{H}_m^\gamma(x)\,\partial_x \mathscr{H}_m^\gamma(x) + \gamma^4 x^2 \big(\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x = \lambda_m + \gamma^2, \\ \big\|\mathscr{P}\mathscr{H}_m^\gamma\big\|_{L^2}^2 &= \int_\Omega \big(\partial_x \mathscr{H}_m^\gamma(x) + \gamma^2 x\,\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x \\ &= \int_\Omega \big(\partial_x \mathscr{H}_m^\gamma(x)\big)^2 + 2\gamma^2 x\,\mathscr{H}_m^\gamma(x)\,\partial_x \mathscr{H}_m^\gamma(x) + \gamma^4 x^2 \big(\mathscr{H}_m^\gamma(x)\big)^2 \,\mathrm{d}x = \lambda_m - \gamma^2.\end{aligned}$$

Up. We consider the eigenvalue relation (5.2) for the m-th Hermite basis function $\mathscr{H}_m^\gamma$ with corresponding eigenvalue λ_m. Applying the operator $\mathscr{Q}$ and making use of the previously derived relation $\mathscr{Q}\mathscr{A} = \big(\mathscr{A} - 2\gamma^2 I\big)\mathscr{Q}$, we obtain

$$\mathscr{A}\mathscr{Q}\mathscr{H}_m^\gamma = \big(\lambda_m + 2\gamma^2\big)\,\mathscr{Q}\mathscr{H}_m^\gamma;$$

that is, $\mathscr{Q}\mathscr{H}_m^\gamma$ is also an eigenfunction of $\mathscr{A}$ with associated eigenvalue $\lambda_{m+1} = \lambda_m + 2\gamma^2$. Due to the fact that $\lambda_0 = \gamma^2$, it follows

$$\lambda_m = \gamma^2(1+2m), \qquad m \in \mathscr{M}.$$

The above considerations imply $\big\|\mathscr{Q}\mathscr{H}_m^\gamma\big\|_{L^2}^2 = 2\,(m+1)\,\gamma^2$ and thus $\mathscr{H}_{m+1}^\gamma = \frac{1}{\|\mathscr{Q}\mathscr{H}_m^\gamma\|_{L^2}}\,\mathscr{Q}\mathscr{H}_m^\gamma$, i.e.

$$\mathscr{H}_{m+1}^\gamma(x) = \tfrac{1}{\sqrt{2\,(m+1)}\,\gamma}\,\big(-\partial_x \mathscr{H}_m^\gamma(x) + \gamma^2 x\,\mathscr{H}_m^\gamma(x)\big), \qquad x \in \Omega. \tag{5.3}$$

Down. We consider the eigenvalue relation (5.2). Applying the operator $\mathscr{P}$ and employing the relation $\mathscr{P}\mathscr{A} = \big(\mathscr{A} + 2\gamma^2 I\big)\mathscr{P}$, we obtain

$$\mathscr{A}\mathscr{P}\mathscr{H}_m^\gamma = \big(\lambda_m - 2\gamma^2\big)\,\mathscr{P}\mathscr{H}_m^\gamma;$$

that is, $\mathscr{P}\mathscr{H}_m^\gamma$ is also eigenfunction of $\mathscr{A}$ with associated eigenvalue $\lambda_m - 2\gamma^2$. Due to the fact that $\left\|\mathscr{P}\mathscr{H}_m^\gamma\right\|_{L^2}^2 = 2m\gamma^2$ and $\mathscr{H}_{m-1}^\gamma = \frac{1}{\|\mathscr{P}\mathscr{H}_m^\gamma\|_{L^2}}\mathscr{P}\mathscr{H}_m^\gamma$, we thus have

$$\mathscr{H}_{m-1}^\gamma(x) = \tfrac{1}{\sqrt{2m}\,\gamma}\left(\partial_x\mathscr{H}_m^\gamma(x) + \gamma^2 x\,\mathscr{H}_m^\gamma(x)\right), \qquad x\in\Omega. \tag{5.4}$$

Recall that $\mathscr{P}\mathscr{H}_0^\gamma = 0$, i.e. $\mathscr{H}_0^\gamma$ is indeed the first eigenfunction of $\mathscr{A}$.

Recurrence relation. The identities (5.3) and (5.4) yield the recurrence relation

$$\begin{aligned}\mathscr{H}_0^\gamma(x) &= \sqrt[4]{\tfrac{\gamma^2}{\pi}}\,\mathrm{e}^{-\frac{1}{2}\gamma^2x^2}, \qquad \mathscr{H}_1^\gamma(x) = \sqrt[4]{\tfrac{4\gamma^6}{\pi}}\,x\,\mathrm{e}^{-\frac{1}{2}\gamma^2x^2},\\ \mathscr{H}_{m+1}^\gamma(x) &= \tfrac{1}{\sqrt{m+1}}\left(\sqrt{2}\,\gamma x\,\mathscr{H}_m^\gamma(x) - \sqrt{m}\,\mathscr{H}_{m-1}^\gamma(x)\right), \qquad m\geq 1,\quad x\in\Omega.\end{aligned} \tag{5.5}$$

Note that $\mathscr{H}_m^\gamma(x)$ is of the form

$$\mathscr{H}_m^\gamma(x) = H_m^\gamma(x)\,\mathrm{e}^{-\frac{1}{2}\gamma^2x^2}, \qquad x\in\Omega,\quad m\in\mathscr{M},$$

with H_m^γ a polynomial of degree m. Clearly, the Hermite polynomials $\left(H_m^\gamma\right)_{m\in\mathscr{M}}$ also fulfill the recurrence relation in (5.5).

5.1.2. Basic relations

Hermite basis functions. The Hermite basis functions $\left(\mathscr{H}_m^\gamma\right)_{m\in\mathscr{M}}$ are given by

$$\mathscr{H}_m^\gamma(x) = H_m^\gamma(x)\,\mathrm{e}^{-\frac{1}{2}\gamma^2x^2}, \qquad x\in\Omega,\quad m\in\mathscr{M}; \tag{5.6a}$$

here, we denote by H_m^γ the m-th Hermite polynomial which fulfills the recurrence relation

$$\begin{aligned}H_0^\gamma(x) &= \sqrt[4]{\tfrac{\gamma^2}{\pi}}, \qquad H_1^\gamma(x) = \sqrt[4]{\tfrac{4\gamma^6}{\pi}}\,x,\\ H_{m+1}^\gamma(x) &= \tfrac{1}{\sqrt{m+1}}\left(\sqrt{2}\,\gamma x\,H_m^\gamma(x) - \sqrt{m}\,H_{m-1}^\gamma(x)\right), \qquad m\geq 1,\quad x\in\Omega,\end{aligned} \tag{5.6b}$$

see also (5.5). The Hermite basis functions satisfy the orthonormality relation

$$\left(\mathscr{H}_k^\gamma \,\middle|\, \mathscr{H}_m^\gamma\right)_{L^2} = \delta_{km}, \qquad k,m\in\mathscr{M}. \tag{5.7}$$

Hermite series expansion. The family $\left(\mathscr{H}_m^\gamma\right)_{m\in\mathscr{M}}$ is complete in $L^2(\Omega)$, i.e., for any function $\varphi\in L^2(\Omega)$ the representation

$$\varphi = \sum_{m\in\mathscr{M}}\varphi_m\,\mathscr{H}_m^\gamma, \qquad \varphi_m = \left(\varphi \,\middle|\, \mathscr{H}_m^\gamma\right)_{L^2}, \tag{5.8}$$

holds with spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$; the convergence of the infinite series versus φ is ensured in $L^2(\Omega)$.

Parseval's identity. The above relations (5.7) and (5.8) imply (4.3).

Eigenvalue relation. The space dependent differential operator $\mathscr{A}(x) = -\partial_x^2 + \gamma^4 x^2$ fulfills the following eigenvalue relation with eigenfunctions $\big(\mathscr{H}_m^\gamma\big)_{m\in\mathscr{M}}$ and eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$

$$\big(-\partial_x^2 + \gamma^4 x^2\big)\,\mathscr{H}_m^\gamma(x) = \lambda_m\,\mathscr{H}_m^\gamma(x)\,, \quad \lambda_m = \gamma^2(1+2m)\,, \qquad x\in\Omega\,, \quad m\in\mathscr{M}\,.$$

5.1.3. Discretisation

Notations. For a positive integers $M, K > 0$ we set $\mathscr{M}_M = \big\{m\in\mathbb{N} : 0\le m\le M-1\big\}$ and further $\mathscr{J} = \big\{j\in\mathbb{N} : 0\le j\le K-1\big\}$.

Approach. We first consider a real-valued regular function $f:\Omega\to\mathbb{R}$. For the quadrature approximation of an integral of the form

$$\int_\Omega f(x)\,\mathrm{e}^{-\gamma^2x^2}\,\mathrm{d}x$$

we apply the Gauß–Hermite quadrature formula with nodes and weights $(x_j,\omega_j)_{j\in\mathscr{J}}$

$$\sum_{j\in\mathscr{J}} \omega_j f(x_j) \approx \int_\Omega f(x)\,\mathrm{e}^{-\gamma^2x^2}\,\mathrm{d}x\,. \tag{5.9}$$

The above quadrature approximation extends to complex-valued function $f:\Omega\to\mathbb{C}$ by considering the real and imaginary part of f.

Approximation of spectral coefficients. An application of the Gauß–Hermite quadrature formula (5.9) yields

$$\begin{aligned}\varphi_m = \big(\varphi\,\big|\,\mathscr{H}_m^\gamma\big)_{L^2} &= \int_\Omega \varphi(x)\,\mathscr{H}_m^\gamma(x)\,\mathrm{d}x = \int_\Omega \mathrm{e}^{\frac12\gamma^2x^2}\varphi(x)\,H_m^\gamma(x)\,\mathrm{e}^{-\gamma^2x^2}\,\mathrm{d}x\\ &\approx \sum_{j\in\mathscr{J}} \omega_j\,\mathrm{e}^{\frac12\gamma^2x_j^2}\varphi(x_j)\,H_m^\gamma(x_j)\,, \qquad m\in\mathscr{M}_M\,,\end{aligned}$$

see also (5.8); we thus obtain the following approximations to the Hermite spectral coefficients

$$\varphi_m \approx \sum_{j\in\mathscr{J}} \omega_j\,\mathrm{e}^{\frac12\gamma^2x_j^2}\varphi(x_j)\,H_m^\gamma(x_j)\,, \qquad m\in\mathscr{M}_M\,. \tag{5.10}$$

Approximation of function values. On the other hand, from the Hermite spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ approximations to the values of φ at the grid points $(x_j)_{j\in\mathscr{J}}$ are retained through

$$\varphi(x_j) \approx \sum_{m\in\mathscr{M}_M} \varphi_m \, \mathscr{H}_m^\gamma(x_j)\,, \qquad j\in\mathscr{J}\,, \tag{5.11}$$

see also (5.8).

5.1.4. Gauß–Hermite quadrature formula

Order. We recall that a quadrature formula is said to be of order p iff the quadrature approximation yields the exact result for any polynomial f with $\deg f \le p-1$. In particular, the Gauß–Hermite quadrature formula $(x_j,\omega_j)_{j\in\mathscr{J}}$ is said to be of order p iff

$$\sum_{j\in\mathscr{J}} \omega_j f(x_j) = \int_\Omega f(x)\, w(x)\,\mathrm{d}x\,, \qquad \deg f \le p-1\,, \tag{5.12}$$

with weight function $w(x) = \mathrm{e}^{-\gamma^2x^2}$, $x\in\Omega$.

Approach. The construction of the Gauß–Hermite quadrature formula $(x_j,\omega_j)_{j\in\mathscr{J}}$ is in the lines of the construction of the Gauß quadrature formula. For the Gauß–Hermite quadrature formula, the associated orthogonal polynomials are the Hermite polynomials $\big(H_m^\gamma\big)_{m\in\mathbb{N}}$, i.e., it holds

$$\big(w\,H_k^\gamma \,\big|\, H_m^\gamma\big)_{L^2} = \big(\mathscr{H}_k^\gamma \,\big|\, \mathscr{H}_m^\gamma\big)_{L^2} = \delta_{km}\,, \qquad k,m\in\mathbb{N},$$

see also (5.7). The Gauß–Hermite quadrature nodes $(x_j)_{j\in\mathscr{J}}$ are the roots of H_K^γ; the corresponding weights $(\omega_j)_{j\in\mathscr{J}}$ are obtained through the order conditions for order K. By construction, the Gauß–Hermite quadrature formula is of order $2K$.

Computation of quadrature nodes. The Gauß–Hermite quadrature nodes $(x_j)_{j\in\mathscr{J}}$ are computed numerically through the solution of an eigenvalue problem; this approach is closely related to *Sturm's chains*. Namely, we make use of the fact that the characteristic polynomial associated with a symmetric tridiagonal matrix

$$A_m = \begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & & \ddots & \\ & & b_{m-1} & a_m \end{pmatrix} \in \mathbb{R}^{m\times m} \tag{5.13a}$$

fulfills a three-term recurrence relation. More precisely, we consider the polynomial

$$\chi_m : \mathbb{R}\to\mathbb{R} : x \longmapsto \chi(x) = c_m \det(A_m - xI)\,, \qquad m\ge 1\,,$$

with leading coefficient c_m. Expanding the determinant of $A_m - xI$ with respect to the last row and with respect to the last column, respectively, yields

$$\begin{aligned}
\det\big(A_{m+1} - xI\big) &= \det\begin{pmatrix} a_1 - x & b_1 & & & & & \\ b_1 & a_2 - x & b_2 & & & & \\ & & \ddots & & & & \\ & & & \ddots & & & \\ & & & b_{m-2} & a_{m-1} - x & b_{m-1} & \\ & & & & b_{m-1} & a_m - x & b_m \\ & & & & & b_m & a_{m+1} - x \end{pmatrix} \\
&= (a_{m+1} - x)\det\big(A_m - xI\big) - b_m \det\begin{pmatrix} a_1 - x & b_1 & & & \\ & \ddots & & & \\ & b_{m-2} & a_{m-1} - x & & \\ & & b_{m-1} & b_m \end{pmatrix} \\
&= (a_{m+1} - x)\det\big(A_m - xI\big) - b_m^2 \det\big(A_{m-1} - xI\big),
\end{aligned}$$

and, as a consequence, the recurrence relation

$$\begin{aligned}
\chi_0(x) = c_0\,, \qquad \chi_1(x) = c_1\,(a_1 - x)\,, \\
\chi_{m+1}(x) = d_{m+1}\big((a_{m+1} - x)\,\chi_m(x) - d_m\,b_m^2\,\chi_{m-1}(x)\big), \quad m \geq 1\,,
\end{aligned}$$

follows, where $d_m = \frac{c_m}{c_{m-1}}$ for $m \geq 1$. Comparing the above relation with the recurrence relation (5.6b) for the Hermite polynomials, we conclude that $\chi_m = H_m^\gamma$, provided that

$$c_0 = \sqrt[4]{\frac{\gamma^2}{\pi}}\,, \qquad a_m = 0\,, \quad b_m = \tfrac{1}{\gamma}\sqrt{\tfrac{m}{2}}\,, \qquad m \geq 1\,. \tag{5.13b}$$

Thus, the Gauß–Hermite quadrature nodes $(x_j)_{j\in\mathscr{J}}$, that is, the roots of the K-th Hermite polynomial, coincide with the eigenvalues of the associated matrix A_K, see (5.13a). Note that for any x_j, $j \in \mathscr{J}$, the function values $\big(H_0^\gamma(x_j), \ldots, H_{K-1}^\gamma(x_j)\big)^T$ form an eigenvector of A_K with associated eigenvalue x_j.

Computation of quadrature weights. Inserting the Hermite polynomials $\big(H_m^\gamma\big)_{m\in\mathscr{J}}$ into the order conditions (5.12) and applying the orthonormality relation (5.7), yields the following system of linear equations for the Gauß–Hermite quadrature weights $(\omega_j)_{j\in\mathscr{J}}$

$$\begin{gathered}
H\omega = \sqrt[4]{\tfrac{\pi}{\gamma^2}}\,e_1\,, \\
H = \begin{pmatrix} H_0^\gamma(x_0) & \ldots & H_0^\gamma(x_{K-1}) \\ \vdots & & \vdots \\ H_{K-1}^\gamma(x_0) & \ldots & H_{K-1}^\gamma(x_{K-1}) \end{pmatrix}, \qquad \omega = \big(\omega_0, \ldots, \omega_{K-1}\big)^T, \qquad e_1 = \big(1, 0, \ldots, 0\big)^T \in \mathbb{R}^k.
\end{gathered}$$

Recall that the vectors $\big(H_0^\gamma(x_j),\dots,H_{K-1}^\gamma(x_j)\big)^T$, $j\in\mathscr{J}$, form an orthogonal eigenbasis of A_K. Therefore, due to the fact that

$$H^TH = D = \operatorname{diag}\big(d_0,\dots,d_{K-1}\big)\,,\qquad d_j = \sum_{m\in\mathscr{J}}\big(H_m^\gamma(x_j)\big)^2\,,\quad j\in\mathscr{J}\,,$$

$$H^Te_1 = \big(H_0^\gamma(x_0),\dots,H_0^\gamma(x_{K-1})\big)^T = \sqrt[4]{\frac{\gamma^2}{\pi}}\,\big(1,\dots,1\big)^T\,,\qquad D^{-1}\big(1,\dots,1\big)^T = \big(\tfrac{1}{d_0},\dots,\tfrac{1}{d_{K-1}}\big)^T\,,$$

it follows $\omega = \sqrt[4]{\frac{\pi}{\gamma^2}}\,D^{-1}H^Te_1$, that is

$$\omega = \big(\tfrac{1}{d_0},\dots,\tfrac{1}{d_{K-1}}\big)^T\,.$$

Interpolation. The above considerations further imply

$$\sum_{m\in\mathscr{J}} H_m^\gamma(x_j)\,H_m^\gamma(x_k) = \tfrac{1}{\omega_j}\,\delta_{jk}\,,\qquad j,k\in\mathscr{J}\,.$$

As a consequence, for any (regular) function of the form

$$\varphi = \sum_{m\in\mathscr{M}}\varphi_m\,\mathscr{H}_m^\gamma$$

the following interpolatory relation at the quadrature nodes

$$\varphi(x_k) = \sum_{m\in\mathscr{J}}\widetilde{\varphi}_m\,\mathscr{H}_m^\gamma(x_k)\,,\qquad \widetilde{\varphi}_m = \sum_{j\in\mathscr{J}}\omega_j\,\mathrm{e}^{\frac{1}{2}\gamma^2x_j^2}\,\varphi(x_j)\,H_m^\gamma(x_j)\,,\quad m\in\mathscr{J}\,,$$

follows. Namely, a short argument shows that

$$\begin{aligned}\sum_{m\in\mathscr{J}}\widetilde{\varphi}_m\,\mathscr{H}_m^\gamma(x_k) &= \sum_{m\in\mathscr{J}}\sum_{j\in\mathscr{J}}\omega_j\,\mathrm{e}^{\frac{1}{2}\gamma^2(x_j^2-x_k^2)}\,\varphi(x_j)\,H_m^\gamma(x_j)\,H_m^\gamma(x_k)\\ &= \sum_{j\in\mathscr{J}}\omega_j\,\mathrm{e}^{\frac{1}{2}\gamma^2(x_j^2-x_k^2)}\,\varphi(x_j)\sum_{m\in\mathscr{J}}H_m^\gamma(x_j)\,H_m^\gamma(x_k) = \varphi(x_k)\,.\end{aligned}$$

5.1.5. Implementation

Notations. As before, for integers $M,K>0$ we set $\mathscr{M}_M = \big\{m\in\mathbb{N}:0\le m\le M-1\big\}$ as well as $\mathscr{J} = \big\{j\in\mathbb{N}:0\le j\le K-1\big\}$.

Approach. The implementation of the Hermite spectral transformations (5.10) and (5.11) in MATLAB relies on matrix–matrix multiplications. For notational simplicity, we do not employ different notations for the exact spectral coefficients or function values and the numerical approximations.

Preliminaries. Clearly, the multiplication of a full matrix A by a diagonal matrix D yields

$$AD = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} d_1 & & \\ & d_2 & \\ & & d_3 \end{pmatrix} = \begin{pmatrix} d_1 a_{11} & d_2 a_{12} & d_3 a_{13} \\ d_1 a_{21} & d_2 a_{22} & d_3 a_{23} \\ d_1 a_{31} & d_2 a_{32} & d_3 a_{33} \end{pmatrix},$$
$$DA = \begin{pmatrix} d_1 & & \\ & d_2 & \\ & & d_3 \end{pmatrix} \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} d_1 a_{11} & d_1 a_{12} & d_1 a_{13} \\ d_2 a_{21} & d_2 a_{22} & d_2 a_{23} \\ d_3 a_{31} & d_3 a_{32} & d_3 a_{33} \end{pmatrix}.$$

Real to spectral. For given function values $\varphi = \big(\varphi(x_0), \dots, \varphi(x_{K-1})\big)^T$ approximations to the spectral coefficients $\varphi^{(\mathrm{s})} = \big(\varphi_0, \dots, \varphi_{M-1}\big)^T$ are computed through

$$\varphi^{(\mathrm{s})} = \mathscr{T}_{\mathrm{r2s}}\, \varphi\,, \qquad \mathscr{T}_{\mathrm{r2s}} = H\, D_{\mathrm{r2s}}\,,$$
$$H = \begin{pmatrix} H_0^\gamma(x_0) & \dots & H_0^\gamma(x_{K-1}) \\ \vdots & & \vdots \\ H_{M-1}^\gamma(x_0) & \dots & H_{M-1}^\gamma(x_{K-1}) \end{pmatrix}, \quad D_{\mathrm{r2s}} = \begin{pmatrix} \omega_0\, \mathrm{e}^{\frac{1}{2}\gamma^2 x_0^2} & & \\ & \ddots & \\ & & \omega_{K-1}\, \mathrm{e}^{\frac{1}{2}\gamma^2 x_{K-1}^2} \end{pmatrix},$$

see also (5.10).

Spectral to real. On the other hand, for given spectral coefficients $\varphi^{(\mathrm{s})}$ approximations to the function values ψ are computed through

$$\varphi = \mathscr{T}_{\mathrm{s2r}}\, \varphi^{(\mathrm{s})}\,, \qquad \mathscr{T}_{\mathrm{s2r}} = D_{\mathrm{s2r}}\, H^T\,,$$
$$D_{\mathrm{s2r}} = \begin{pmatrix} \mathrm{e}^{-\frac{1}{2}\gamma^2 x_0^2} & & \\ & \ddots & \\ & & \mathrm{e}^{-\frac{1}{2}\gamma^2 x_{K-1}^2} \end{pmatrix},$$

see also (5.11).

5.2. Approach in several space dimensions

Notation. We set $\Omega = \mathbb{R}^d$ and further $\mathscr{M} = \mathbb{N}^d$.

Approach. The considerations for one space dimensions are extended to the general case.

5.2.1. Basic relations

Hermite basis functions. In d space dimensions, the Hermite basis functions $\big(\mathscr{H}_m^\gamma\big)_{m \in \mathscr{M}}$ are given by

$$\mathscr{H}_m^\gamma(x) = \mathscr{H}_{m_1}^{\gamma_1}(x_1) \cdots \mathscr{H}_{m_d}^{\gamma_d}(x_d)\,, \qquad x \in \Omega\,, \quad m \in \mathscr{M}\,,$$

see also (5.6). In particular, the orthonormality relation (5.7) holds.

Hermite series expansion. The family $\big(\mathscr{H}_m^\gamma\big)_{m\in\mathscr{M}}$ is complete in $L^2(\Omega)$, i.e., for any function $\varphi\in L^2(\Omega)$ the representation (5.8) holds with spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$.

Parseval's identity. Relations (5.7) and (5.8) imply (4.3).

Eigenvalue relation. The differential operator $\mathscr{A}=-\Delta+U_\gamma$, see also (5.1), fulfills the following eigenvalue relation with eigenfunctions $\big(\mathscr{H}_m^\gamma\big)_{m\in\mathscr{M}}$ and associated eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$

$$\big(-\Delta+U_\gamma\big)\,\mathscr{H}_m^\gamma=\lambda_m\,\mathscr{H}_m^\gamma,\quad \lambda_m=\sum_{i=1}^d\lambda_{m_i}=\sum_{i=1}^d\gamma_i^2(1+2m_i),\qquad m\in\mathscr{M}. \tag{5.14}$$

5.2.2. Discretisation

Notations. For $M,K\in\mathbb{N}^d$ with $M_i,K_i>0$ for $1\le i\le d$ we set

$$\mathscr{M}_M=\big\{m\in\mathbb{N}^d:0\le m_i\le M_i-1,1\le i\le d\big\},\qquad \mathscr{J}=\big\{j\in\mathbb{N}^d:0\le j_i\le K_i-1,1\le i\le d\big\}.$$

Further, we employ the short notation

$$\mathrm{e}^{c\,\gamma^2\cdot x^2}=\mathrm{e}^{c\sum_{i=1}^d\gamma_i^2x_i^2},\qquad c\in\mathbb{R},\quad \gamma\in\mathbb{R}^d,\quad x\in\Omega.$$

Approach. We consider a complex-valued regular function $f:\Omega\to\mathbb{C}^d$. For the quadrature approximation of a multiple integral of the form

$$\int_\Omega f(x)\,\mathrm{e}^{-\gamma^2\cdot x^2}\mathrm{d}x$$

we apply the Gauß–Hermite quadrature formula with nodes and weights $(x_j,\omega_j)_{j\in\mathscr{J}}$ given by the quadrature nodes and weights of the one-dimensional Gauß–Hermite quadrature formula

$$\sum_{j\in\mathscr{J}}\omega_j f(x_j)\approx\int_\Omega f(x)\,\mathrm{e}^{-\gamma^2\cdot x^2}\mathrm{d}x,\qquad x_j=(x_{j_1},\dots,x_{j_d}),\quad \omega_j=\omega_{j_1}\cdots\omega_{j_d},\qquad j\in\mathscr{J}. \tag{5.15}$$

Approximation of spectral coefficients. An application of the Gauß–Hermite quadrature formula (5.15) yields the following approximations to the Hermite spectral coefficients

$$\varphi_m\approx\sum_{j\in\mathscr{J}}\omega_j\,\mathrm{e}^{\frac12\gamma^2\cdot x_j^2}\varphi(x_j)\,H_m^\gamma(x_j),\qquad m\in\mathscr{M}_M, \tag{5.16}$$

see also (5.8).

Approximation of function values. On the other hand, from the Hermite spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ approximations to the values of φ at the grid points $(x_j)_{j\in\mathscr{J}}$ are retained through (5.11), see also (5.8).

5.2.3. Approximation result

Approximation result. A result on the accuracy of the Hermite spectral method is found in the recent work [26]. For $M\in\mathbb{N}^d$ with $M_i>0$ for $1\le i\le d$, we set

$$M_{\max}=\max\{M_i:1\le i\le d\},$$
$$\mathscr{M}_M=\{m\in\mathbb{N}^d:0\le m_i\le M_i-1,1\le i\le d\},\qquad \mathscr{J}=\{j\in\mathbb{N}^d:0\le j_i\le M_i-1,1\le i\le d\}.$$

Moreover, we employ the notations

$$\widetilde{\varphi}=\sum_{m\in\mathscr{M}_M}\widetilde{\varphi}_m\,\mathscr{H}_m^\gamma,\qquad \widetilde{\varphi}_m=\sum_{j\in\mathscr{J}}\omega_j\,\mathrm{e}^{\frac{1}{2}\gamma^2\cdot x^2}\varphi(x_j)\,H_m^\gamma(x_j),\quad m\in\mathscr{M}_M.$$

Then, the following spatial error estimate is valid

$$\left\|\mathscr{A}^\alpha\left(\widetilde{\varphi}-\varphi\right)\right\|_{L^2}\le C\,M_{\max}^{-\left(\beta-\alpha-\frac{d}{3}\right)}\left\|\mathscr{A}^\beta\varphi\right\|_{L^2}.$$

5.2.4. Implementation

Approach. Especially, for two space dimensions an efficient implementation of the Hermite spectral transformations (5.16) and (5.11) relies on matrix–matrix multiplications.

6. Laguerre–Fourier–Hermite spectral method

Objective. In the following, we are concerned with the numerical solution of the linear partial differential equation (3.12) involving the second order differential operator

$$\begin{gathered}\mathscr{A}(x,y,z) = -\Delta + U_\gamma(x,y,z) + \mathrm{i}\omega L(x,y)\,,\\ U_\gamma(x,y,z) = \gamma_x^4\left(x^2+y^2\right) + \gamma_z^4 z^2\,, \quad L(x,y) = x\,\partial_y - y\,\partial_x\,, \qquad (x,y,z)\in\mathbb{R}^3\,;\end{gathered} \tag{6.1}$$

furthermore, we impose asymptotic boundary conditions on the unbounded domain.

6.1. Preliminaries

6.1.1. Cylindric coordinates

In the following, we consider cylindric coordinates

$$\varphi : \mathbb{R}_{>0}\times(-\pi,\pi)\times\mathbb{R} \longrightarrow \left(\mathbb{R}^2\setminus\{0\}\right)\times\mathbb{R} : (r,\vartheta,z)^T \longmapsto (x,y,z)^T = \varphi(r,\vartheta,z) = \left(r\cos\vartheta, r\sin\vartheta, z\right)^T.$$

By means of the rule for the first derivative of the inverse function, we have

$$\begin{gathered}\frac{\partial(r,\vartheta)}{\partial(x,y)} = \left(\frac{\partial(x,y)}{\partial(r,\vartheta)}\right)^{-1},\\ \begin{pmatrix}\partial_x r & \partial_y r\\ \partial_x\vartheta & \partial_y\vartheta\end{pmatrix} = \begin{pmatrix}\partial_r x & \partial_\vartheta x\\ \partial_r y & \partial_\vartheta y\end{pmatrix}^{-1} = \begin{pmatrix}\cos\vartheta & -r\sin\vartheta\\ \sin\vartheta & r\cos\vartheta\end{pmatrix}^{-1} = \begin{pmatrix}\cos\vartheta & \sin\vartheta\\ -\frac{1}{r}\sin\vartheta & \frac{1}{r}\cos\vartheta\end{pmatrix}.\end{gathered}$$

Applying the chain rule to $f(r,\vartheta) = f\big(r(x,y),\vartheta(x,y)\big)$, it thus follows

$$\begin{aligned}\partial_x f(r,\vartheta) &= \left(\partial_x r\,\partial_r + \partial_x\vartheta\,\partial_\vartheta\right) f(r,\vartheta) = \left(\cos\vartheta\,\partial_r - \tfrac{1}{r}\sin\vartheta\,\partial_\vartheta\right) f(r,\vartheta)\,,\\ \partial_y f(r,\vartheta) &= \left(\partial_y r\,\partial_r + \partial_y\vartheta\,\partial_\vartheta\right) f(r,\vartheta) = \left(\sin\vartheta\,\partial_r + \tfrac{1}{r}\cos\vartheta\,\partial_\vartheta\right) f(r,\vartheta)\,.\end{aligned}$$

Furthermore, we obtain the relations

$$\begin{aligned}
\partial_x^2 f(r,\vartheta) &= \big(\cos\vartheta\,\partial_r - \tfrac{1}{r}\sin\vartheta\,\partial_\vartheta\big)^2 f(r,\vartheta) \\
&= \big(\cos^2\vartheta\,\partial_r^2 - \tfrac{1}{r}\sin(2\vartheta)\,\partial_{r\vartheta} + \tfrac{1}{r^2}\sin^2\vartheta\,\partial_\vartheta^2 + \tfrac{1}{r}\sin^2\vartheta\,\partial_r + \tfrac{1}{r^2}\sin(2\vartheta)\,\partial_\vartheta\big) f(r,\vartheta) \\
\partial_y^2 f(r,\vartheta) &= \big(\sin\vartheta\,\partial_r + \tfrac{1}{r}\cos\vartheta\,\partial_\vartheta\big)^2 f(r,\vartheta) \\
&= \big(\sin^2\vartheta\,\partial_r^2 + \tfrac{1}{r}\sin(2\vartheta)\,\partial_{r\vartheta} + \tfrac{1}{r^2}\cos^2\vartheta\,\partial_\vartheta^2 + \tfrac{1}{r}\cos^2\vartheta\,\partial_r - \tfrac{1}{r^2}\sin(2\vartheta)\,\partial_\vartheta\big) f(r,\vartheta)\,.
\end{aligned}$$

As a consequence, in cylindric coordinates the Laplace operator $\Delta = \partial_x^2 + \partial_y^2 + \partial_z^2$ and the operator $L(x,y) = x\partial_y - y\partial_x$, which is related to the angular momentum, take the form

$$\Delta = \partial_r^2 + \tfrac{1}{r}\partial_r + \tfrac{1}{r^2}\partial_\vartheta^2 + \partial_z^2 = \tfrac{1}{r}\partial_r(r\partial_r) + \tfrac{1}{r^2}\partial_\vartheta^2 + \partial_z^2\,, \qquad L = \partial_\vartheta\,.$$

Moreover, due to the fact that $\big|\det\varphi'(r,\vartheta,z)\big| = r$, the transformation rule for multiple integrals implies the relation

$$\int_{\mathbb{R}^3} f(x,y,z)\,\mathrm{d}(x,y,z) = \int_{\mathbb{R}_{>0}\times(-\pi,\pi)\times\mathbb{R}} r\,f\big(\varphi(r,\vartheta,z)\big)\,\mathrm{d}(r,\vartheta,z)\,.$$

6.1.2. Generalised Laguerre polynomials

Notations. We set $\Omega = (0,\infty)$ and $\mathscr{M} = \mathbb{N}$; further, we denote by $\kappa > -1$ a certain weight.

Generalised Laguerre polynomials. The generalised Laguerre polynomials $\big(\widetilde{\mathscr{L}}_j^{(\kappa)}\big)_{j\in\mathscr{M}}$ are defined through the following relations. They fulfill the relation

$$\widetilde{\mathscr{A}}(\xi)\,\widetilde{\mathscr{L}}_j^{(\kappa)}(\xi) = 0\,, \qquad j\in\mathscr{M}\,, \quad \xi\in\Omega\,,$$

with second order differential operator

$$\widetilde{\mathscr{A}}(\xi) = \xi\,\partial_\xi^2 + (\kappa+1-\xi)\,\partial_\xi + jI\,, \qquad j\in\mathscr{M}\,, \quad \xi\in\Omega\,.$$

Further, the generalised Laguerre polynomials are orthonormal with respect to the weight function $\widetilde{w}(\xi) = \xi^\kappa\,\mathrm{e}^{-\xi}$, i.e., it holds

$$\big(\widetilde{w}\widetilde{\mathscr{L}}_j^{(\kappa)}\,\big|\,\widetilde{\mathscr{L}}_{\tilde{j}}^{(\kappa)}\big)_{L^2} = \delta_{j\tilde{j}}\,, \qquad j,\tilde{j}\in\mathscr{M}\,.$$

Explicit representation. Inserting the representations

$$\widetilde{L}_j^{(\kappa)}(\xi) = \sum_{i=0}^{j}\alpha_i\,\xi^i\,,$$

$$\partial_\xi\widetilde{L}_j^{(\kappa)}(\xi) = \sum_{i=1}^{j} i\,\alpha_i\,\xi^{i-1} = \sum_{i=0}^{j-1}(i+1)\,\alpha_{i+1}\,\xi^i\,, \qquad \partial_\xi^2\widetilde{L}_j^{(\kappa)}(\xi) = \sum_{i=1}^{j-1} i\,(i+1)\,\alpha_{i+1}\,\xi^{i-1}\,,$$

into the eigenvalue relation yields

$$0 = \widetilde{\mathscr{A}}(\xi)\,\widetilde{L}_j^{(\kappa)}(\xi) = \Big(\xi\,\partial_\xi^2 + (\kappa+1)\,\partial_\xi - \xi\,\partial_\xi + j\,I\Big)\,\widetilde{L}_j^{(\kappa)}(\xi)$$
$$= \sum_{i=1}^{j-1}\Big((i+1)(\kappa+i+1)\,\alpha_{i+1} + (j-i)\,\alpha_i\Big)\,\xi^i + (\kappa+1)\alpha_1 + j\alpha_0\,,$$

which implies

$$\widetilde{L}_j^{(\kappa)}(\xi) = \sum_{i=0}^{j}\alpha_i\,\xi^i\,, \qquad \alpha_{i+1} = \tfrac{i-j}{(i+1)(\kappa+i+1)}\,\alpha_i\,, \quad 0 \le i \le j-1\,, \qquad \alpha_0 \text{ given}\,.$$

By the normalisation condition, we therefore obtain the following representation for the generalised Laguerre polynomials

$$\widetilde{\mathscr{L}}_j^{(\kappa)}(\xi) = \Big(\tfrac{1}{j!\,\Gamma(\kappa+1)}\prod_{\ell=1}^{j}(\kappa+\ell)\Big)^{\frac{1}{2}}\,\widetilde{L}_j^{(\kappa)}(\xi)\,, \qquad j \in \mathscr{M}\,.$$

Recurrence relation. The generalised Laguerre polynomials can also be constructed by means of the recurrence relation

$$\widetilde{\widetilde{L}}_0^{(\kappa)}(\xi) = 1\,, \qquad \widetilde{\widetilde{L}}_1^{(\kappa)}(\xi) = \kappa + 1 - \xi\,,$$
$$\widetilde{\widetilde{L}}_{j+1}^{(\kappa)}(\xi) = \tfrac{1}{(j+1)}\Big((\kappa+2j+1-\xi)\,\widetilde{\widetilde{L}}_j^{(\kappa)}(\xi) - (\kappa+j)\,\widetilde{\widetilde{L}}_{j-1}^{(\kappa)}(\xi)\Big), \qquad j \ge 1\,, \quad \xi \in \Omega\,.$$

Namely, by the normalisation condition it follows

$$\widetilde{\mathscr{L}}_j^{(\kappa)}(\xi) = \Big(\tfrac{j!}{\Gamma(\kappa+j+1)}\Big)^{\frac{1}{2}}\,\widetilde{\widetilde{L}}_j^{(\kappa)}(\xi)\,, \qquad j \in \mathscr{M}\,.$$

6.1.3. Scaled generalised Laguerre polynomials

Notations. As before, we set $\Omega = (0,\infty)$ and $\mathscr{M} = \mathbb{N}$; further, we denote by $\gamma > 0$ and $\kappa > -1$ a certain weight.

Scaled generalised Laguerre polynomials. We further introduce the scaled generalised Laguerre polynomials $\big(\mathscr{L}_j^{(\kappa)}\big)_{j\in\mathscr{M}}$ through

$$\mathscr{L}_j^{(\kappa)}(x) = \sqrt{2}\,\gamma^{\kappa+1}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2x^2}\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2x^2\big)\,, \qquad j \in \mathscr{M}\,, \quad x \in \Omega\,,$$

Then, the orthonormality relation

$$\big(w\,\mathscr{L}_j^{(\kappa)}\,\big|\,\mathscr{L}_{\widetilde{j}}^{(\kappa)}\big)_{L^2} = \delta_{j\widetilde{j}}\,, \qquad j, \widetilde{j} \in \mathscr{M}\,,$$

with weight function $w(x) = x$ follows. Namely, it holds

$$\begin{aligned}\big(w\mathscr{L}_j^{(\kappa)} \,\big|\, \mathscr{L}_{\tilde{j}}^{(\kappa)}\big)_{L^2} &= 2\,\gamma^{2(\kappa+1)} \int_\Omega x^{2\kappa+1}\,\mathrm{e}^{-\gamma^2 x^2}\,\widetilde{\mathscr{L}}_j^{(\kappa)}(\gamma^2 x^2)\,\widetilde{\mathscr{L}}_{\tilde{j}}^{(\kappa)}(\gamma^2 x^2)\,\mathrm{d}x \\ &= \int_\Omega \xi^\kappa\,\mathrm{e}^{-\xi}\,\widetilde{\mathscr{L}}_j^{(\kappa)}(\xi)\,\widetilde{\mathscr{L}}_{\tilde{j}}^{(\kappa)}(\xi)\,\mathrm{d}\xi \\ &= \big(\widetilde{w}\widetilde{\mathscr{L}}_j^{(\kappa)} \,\big|\, \widetilde{\mathscr{L}}_{\tilde{j}}^{(\kappa)}\big)_{L^2} = \delta_{j\tilde{j}}, \qquad j,\tilde{j} \in \mathscr{M}\,.\end{aligned}$$

Eigenvalue relation. We consider the second order differential operator

$$\mathscr{A}(x) = -\,\partial_x^2 - \tfrac{1}{x}\,\partial_x + \big(\tfrac{\kappa^2}{x^2} + \gamma^4 x^2\big)\,I\,, \qquad x \in \Omega\,.$$

A straightforward calculation shows that the first and second derivative of $\mathscr{L}_j^{(\kappa)}$ is given by

$$\begin{aligned}\partial_x \mathscr{L}_j^{(\kappa)}(x) &= \sqrt{2}\,\gamma^{\kappa+1}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\Big(2\gamma^2 x\,\partial_\xi + \big(\tfrac{\kappa}{x} - \gamma^2 x\big)\,I\Big)\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big)\,, \\ \partial_x^2 \mathscr{L}_j^{(\kappa)}(x) &= \sqrt{2}\,\gamma^{\kappa+1}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\Big(4\,\gamma^4 x^2\,\partial_\xi^2 + 4\,\gamma^2\big(\kappa - \gamma^2 x^2 + \tfrac{1}{2}\big)\,\partial_\xi \\ &\qquad + \big(\gamma^4 x^2 - (2\kappa+1)\,\gamma^2 + \tfrac{\kappa(\kappa-1)}{x^2}\big)\,I\Big)\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big)\,.\end{aligned}$$

As a consequence, this yields

$$\begin{aligned}\big(\partial_x^2 + \tfrac{1}{x}\,\partial_x\big)\,\mathscr{L}_j^{(\kappa)}(x) &= \sqrt{2}\,\gamma^{\kappa+1}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\Big(4\,\gamma^4 x^2\,\partial_\xi^2 + 4\,\gamma^2\big(\kappa + 1 - \gamma^2 x^2\big)\,\partial_\xi \\ &\qquad + \big(\gamma^4 x^2 - 2\,(\kappa+1)\,\gamma^2 + \tfrac{\kappa^2}{x^2}\big)\,I\Big)\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big)\,,\end{aligned}$$

and, furthermore, due to the fact that $\widetilde{\mathscr{A}}\,\widetilde{\mathscr{L}}_j^{(\kappa)} = 0$, it follows

$$\begin{aligned}\mathscr{A}(x)\,\mathscr{L}_j^{(\kappa)}(x) &= \Big(-\,\partial_x^2 - \tfrac{1}{x}\,\partial_x + \big(\tfrac{\kappa^2}{x^2} + \gamma^4 x^2\big)\,I\Big)\,\mathscr{L}_j^{(\kappa)}(x) \\ &= -\sqrt{2}\cdot 4\,\gamma^{\kappa+3}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\Big(\gamma^2 x^2\,\partial_\xi^2 + \big(\kappa + 1 - \gamma^2 x^2\big)\,\partial_\xi - \tfrac{1}{2}\,(\kappa+1)\,I\Big)\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big) \\ &= -\sqrt{2}\cdot 4\,\gamma^{\kappa+3}\,x^\kappa\,\mathrm{e}^{-\frac{1}{2}\gamma^2 x^2}\Big(\widetilde{\mathscr{A}}\big(\gamma^2 x^2\big) - \tfrac{1}{2}\,(2j+\kappa+1)\,I\Big)\,\widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big) \\ &= 2\,\gamma^2\big(2j+\kappa+1\big)\,\mathscr{L}_j^{(\kappa)}(x)\,,\end{aligned}$$

We thus obtain the following eigenvalue relation for the scaled Laguerre polynomials

$$\mathscr{A}(x)\,\mathscr{L}_j^{(\kappa)}(x) = 2\,\gamma^2\big(2j+\kappa+1\big)\,\mathscr{L}_j^{(\kappa)}(x)\,, \qquad j \in \mathscr{M}\,, \quad x \in \Omega\,.$$

Generalised Laguerre functions. The scaled generalised Laguerre functions $\big(\mathbf{L}_j^\kappa(x)\big)_{j\in\mathscr{M}}$ are given by $\mathbf{L}_j^\kappa(x) = \sqrt{x}\;\mathscr{L}_j^{(\kappa)}(x)$ for $j \in \mathscr{M}$ and $x \in \Omega$; they fulfill the orthonormality relation $\big(\mathbf{L}_j^\kappa \,\big|\, \mathbf{L}_{\tilde{j}}^\kappa\big)_{L^2} = \delta_{j\tilde{j}}$ for all $j,\tilde{j} \in \mathscr{M}$.

6.2. Laguerre–Fourier–Hermite spectral method

Notation. We let $\Omega = \{(r,\vartheta,z) \in \mathbb{R}^3 : r > 0, -\pi < \vartheta < \pi\}$.

Objective. We are concerned with the efficient numerical solution of the linear partial differential equation $\mathrm{i}\,\partial_t \psi = \mathscr{A}\,\psi$, $t \geq 0$, involving the second order differential operator

$$\begin{aligned} \mathscr{A}(x,y,z) &= -\Delta + U_\gamma(x,y,z) + \mathrm{i}\omega L(x,y)\,, \\ U_\gamma(x,y,z) = \gamma_x^4\left(x^2+y^2\right) + \gamma_z^4 z^2\,, &\quad L(x,y) = x\,\partial_y - y\,\partial_x\,, \qquad (x,y,z) \in \mathbb{R}^3\,; \end{aligned}$$

furthermore, we impose asymptotic boundary conditions on the unbounded domain.

Cylindric coordinates. Employing cylindric coordinates, by means of the previous considerations, we obtain

$$\mathscr{A}(r,\vartheta,z) = -\partial_r^2 - \tfrac{1}{r^2}\,\partial_\vartheta^2 - \partial_z^2 - \tfrac{1}{r}\,\partial_r + \mathrm{i}\,\omega\,\partial_\vartheta + \gamma_x^4 r^2\, I + \gamma_z^4 z^2\, I\,, \qquad (r,\vartheta,z) \in \Omega\,.$$

6.2.1. Laguerre–Fourier–Hermite spectral decomposition

Notation. We set $\mathscr{M} = \{m = (j,k,\ell) \in \mathbb{N} \times \mathbb{Z} \times \mathbb{N}\}$.

Objective. In the following, we are concerned with constructing orthonormal basis functions $\left(\mathscr{B}_m\right)_{m\in\mathscr{M}}$ which fulfill the eigenvalue relation

$$\mathscr{A}\,\mathscr{B}_m = \lambda_m\,\mathscr{B}_m\,, \quad m \in \mathscr{M}\,, \tag{6.2}$$

with associated eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$. Then, the solution of $\mathrm{i}\,\partial_t\psi = \mathscr{A}\,\psi$ is given by

$$\psi(\cdot,t) = \mathrm{e}^{-\mathrm{i}\,t\,\mathscr{A}}\psi(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_m(0)\,\mathrm{e}^{-\mathrm{i}\,t\,\lambda_m}\,\mathscr{B}_m\,, \quad t \geq 0\,, \qquad \psi(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_m(0)\,\mathscr{B}_m\,.$$

Approach. We employ the following representation

$$\mathscr{B}_m(r,\vartheta,z) = \mathscr{L}_j^{(|k|)}(r)\,\mathscr{F}_k(\vartheta)\,\mathscr{H}_\ell^{\gamma_z}(z)\,, \qquad m \in \mathscr{M}\,, \quad (r,\vartheta,z) \in \Omega\,, \tag{6.3}$$

involving the scaled generalised Laguerre *polynomials,* the Fourier basis functions which are given by $\mathscr{F}_k(\vartheta) = \frac{1}{\sqrt{2\pi}}\,(-1)^k\,\mathrm{e}^{\mathrm{i}\,k\,\vartheta}$ for $-\pi < \vartheta < \pi$ and $k \in \mathbb{Z}$, and further the Hermite basis functions. We note that the basis functions $\left(\mathscr{B}_m\right)_{m\in\mathscr{M}}$ fulfill the orthonormality relation

$$\left(w\,\mathscr{B}_m \,\middle|\, \mathscr{B}_{\tilde{m}}\right)_{L^2} = \delta_{m\tilde{m}}\,, \qquad m, \tilde{m} \in \mathscr{M}\,,$$

involving the weight function $w(r,\vartheta,z) = r$. Inserting (6.3) into (6.2) and using that the eigenvalue relations

$$\begin{gathered}\Big(-\partial_r^2 - \tfrac{1}{r}\partial_r + \tfrac{k^2}{r^2} I + \gamma_x^4 r^2 I\Big)\mathscr{L}_j^{(|k|)}(r) = 2\,\gamma_x^2\big(2j+|k|+1\big)\mathscr{L}_j^{(|k|)}(r), \qquad j\in\mathbb{N},\ k\in\mathbb{Z}, \quad r>0,\\ \partial_\vartheta \mathscr{F}_k(\vartheta) = \mathrm{i}\,k\,\mathscr{F}_k(\vartheta), \quad \partial_\vartheta^2 \mathscr{F}_k(\vartheta) = -k^2\,\mathscr{F}_k(\vartheta), \qquad k\in\mathbb{Z}, \quad -\pi<\vartheta<\pi,\\ \big(-\partial_z^2 + \gamma_z^4 z^2 I\big)\mathscr{H}_\ell^{\gamma_z}(z) = \gamma_z^2\big(1+2\,\ell\big)\mathscr{H}_\ell^{\gamma_z}(z), \qquad \ell\in\mathbb{N}, \quad z\in\mathbb{R},\end{gathered}$$

are satisfied, we find that

$$\begin{aligned}\mathscr{A}(r,\vartheta,z)\,\mathscr{B}_m(r,\vartheta,z) &= \Big(-\partial_r^2 - \tfrac{1}{r^2}\partial_\vartheta^2 - \partial_z^2 - \tfrac{1}{r}\partial_r + \mathrm{i}\,\omega\,\partial_\vartheta + \gamma_x^4 r^2 I + \gamma_z^4 z^2 I\Big)\mathscr{B}_m(r,\vartheta,z)\\ &= \mathscr{F}_k(\vartheta)\Big(-\partial_r^2 + \tfrac{k^2}{r^2} - \partial_z^2 - \tfrac{1}{r}\partial_r - k\,\omega + \gamma_x^4 r^2 I + \gamma_z^4 z^2 I\Big)\mathscr{L}_j^{(|k|)}(r)\,\mathscr{H}_\ell^{\gamma_z}(z)\\ &= \mathscr{F}_k(\vartheta)\,\mathscr{H}_\ell^{\gamma_z}(z)\Big(-\partial_r^2 - \tfrac{1}{r}\partial_r + \tfrac{k^2}{r^2} + \gamma_x^4 r^2 I\Big)\mathscr{L}_j^{(|k|)}(r)\\ &\quad + \mathscr{F}_k(\vartheta)\,\mathscr{L}_j^{(|k|)}(r)\Big(-\partial_z^2 + \gamma_z^4 z^2 I\Big)\mathscr{H}_\ell^{\gamma_z}(z) - k\,\omega\,\mathscr{B}_m(r,\vartheta,z)\\ &= \Big(2\,\gamma_x^2\big(2j+|k|+1\big) + \gamma_z^2\big(1+2\,\ell\big) - k\,\omega\Big)\mathscr{B}_m(r,\vartheta,z).\end{aligned}$$

We therefore have that

$$\mathscr{A}\mathscr{B}_m = \lambda_m\mathscr{B}_m, \quad \lambda_m = 2\,\gamma_x^2\big(2j+|k|+1\big) + \gamma_z^2\big(1+2\,\ell\big) - k\,\omega, \qquad m=(j,k,\ell)\in\mathscr{M}.$$

Spectral decomposition. For any function $\varphi\in L^2(\Omega)$, the spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$ with respect to $\big(\mathscr{B}_m\big)_{m\in\mathscr{M}}$ are given by

$$\begin{gathered}\varphi = \sum_{m\in\mathscr{M}} \varphi_m\,\mathscr{B}_m,\\ \varphi_m = \big(w\,\varphi\,\big|\,\mathscr{B}_m\big)_{L^2} = \int_{\mathbb{R}_{>0}\times(-\pi,\pi)\times\mathbb{R}} r\,\varphi(r,\vartheta,z)\,\overline{\mathscr{B}_m(r,\vartheta,z)}\,\mathrm{d}(r,\vartheta,z).\end{gathered}$$

6.3. Discretisation

Notation. For integers $M_i>0$ and $J_i>0$, $1\le i\le 3$, we set

$$\begin{gathered}\mathscr{M}_M = \big\{m=(j,k,\ell)\in\mathbb{N}\times\mathbb{Z}\times\mathbb{N} : j\le M_1, k\le M_2, \ell\le M_3\big\},\\ \mathscr{J} = \big\{j=(j_1,j_2,j_3)\in\mathbb{N}^3 : 0\le j_i\le J_i-1\big\}.\end{gathered}$$

Approach. The generalised Gauß–Laguerre quadrature formula (with $\kappa=0$) is used for the quadrature approximation of an integral of the form

$$\sum_{j=0}^{J-1}\omega_j f(r_j) \approx \int_{\mathbb{R}>0} \mathrm{e}^{-r} f(r)\,\mathrm{d}r,$$

where $f : \mathbb{R}_{>0} \to \mathbb{C}$ is a regular function; the quadrature nodes and weights $(r_j, \omega_j)_{j=0}^{J-1}$ are computed in a similar manner as the Gauß–Hermite quadrature nodes and weights.

Approximation of spectral coefficients. In the following, we let $\big(r_{j_1}, \omega_{j_1}^{(1)}\big)_{j_1=0}^{J_1-1}$ denote the Gauß–Laguerre quadrature nodes and weights, $\big(\vartheta_{j_2}, \omega_{j_2}^{(2)}\big)_{j_2=0}^{J_2-1}$ the trapezoid quadrature nodes and weights, and $\big(z_{j_3}, \omega_{j_3}^{(3)}\big)_{j_3=0}^{J_3-1}$ the Gauß–Hermite quadrature nodes and weights. Then, for $\varphi \in L^2(\Omega)$ approximations to the spectral coefficients $(\varphi_m)_{m\in\mathscr{M}}$ with respect to $\big(\mathscr{B}_m\big)_{m\in\mathscr{M}}$ are given by

$$\varphi_m \approx \sum_{j\in\mathscr{J}} \omega_{j_1}^{(1)}\, \omega_{j_2}^{(2)}\, \omega_{j_3}^{(3)}\, r_{j_1}\, \mathrm{e}^{r_{j_1}}\, \mathrm{e}^{\frac{1}{2}\gamma_z^2 z_{j_3}^2}\, \varphi(r_{j_1}, \vartheta_{j_2}, z_{j_3})\, \overline{\mathscr{B}_m(r_{j_1}, \vartheta_{j_2}, z_{j_3})}\,, \qquad m \in \mathscr{M}_M\,.$$

Approximation of function values. From the spectral coefficients $(\varphi_m)_{m\in\mathscr{M}_M}$ approximations to the values of φ at the grid points $(r_{j_1}, \vartheta_{j_2}, z_{j_3})_{j_i \le J_i - 1, 1\le i\le 3}$ are retained through

$$\varphi(r_{j_1}, \vartheta_{j_2}, z_{j_3}) \approx \sum_{m\in\mathscr{M}_M} \varphi_m\, \mathscr{B}_m(r_{j_1}, \vartheta_{j_2}, z_{j_3})\,, \qquad j \in \mathscr{J}\,.$$

6.3.1. Gauß–Laguerre quadrature formula

Approach. The Gauß–Laguerre quadrature formula is used for the quadrature approximation of an integral of the form

$$\sum_{j=0}^{J-1} \widetilde{\omega}_j f(\widetilde{r}_j) \approx \int_{\mathbb{R}>0} \mathrm{e}^{-r} f(r)\, \mathrm{d}r\,,$$

where $f : \mathbb{R}_{>0} \to \mathbb{C}$ is a regular function; the quadrature nodes and weights $(\widetilde{r}_j, \widetilde{\omega}_j)_{j=0}^{J-1}$ are computed in a similar manner as the Gauß–Hermite quadrature nodes and weights, i.e. the roots of $\widetilde{\mathscr{L}}_J^{(0)}$ are obtained through the numerical solution of an associated eigenvalue problem. The Gauß–Laguerre quadrature formula $(\widetilde{r}_j, \widetilde{\omega}_j)_{j=0}^{J-1}$ is of order $2J$, i.e, the quadrature formula approximation is exact for any polynomial f of degree $\deg f \le 2J-1$.

Modification. Let

$$r_j = \tfrac{1}{\gamma}\sqrt{\widetilde{r}_j}\,, \quad \omega_j = \tfrac{1}{2\gamma^2}\,\widetilde{\omega}_j\, \mathrm{e}^{\widetilde{r}_j}\,, \qquad 0 \le j \le J-1\,.$$

Then, it holds with $w(\xi) = \xi$

$$\sum_{j=0}^{J-1} \omega_j\, f(r_j)\, \mathscr{L}_m^{(\kappa)}(r_j) \approx \big(wf \,\big|\, \mathscr{L}_m^{(\kappa)}\big)_{L^2} = \int_{\mathbb{R}>0} \xi\, f(\xi)\, \mathscr{L}_m^{(\kappa)}(\xi)\, \mathrm{d}\xi$$

and in particular for $f = \mathscr{L}_{\widetilde{j}}^{(\kappa)}$ (equalitity in quadrature approximation)

$$\sum_{j=0}^{J-1} \omega_j \, \mathscr{L}_j^{(\kappa)}(r_j) \, \mathscr{L}_{\widetilde{j}}^{(\kappa)}(r_j) = \big(w \, \mathscr{L}_j^{(\kappa)} \,\big|\, \mathscr{L}_{\widetilde{j}}^{(\kappa)} \big)_{L^2} = \delta_{j\widetilde{j}}, \qquad j, \widetilde{j} \in \mathscr{M}.$$

Namely, using that

$$\begin{aligned} \mathscr{L}_j^{(\kappa)}(x) &= \sqrt{2}\, \gamma^{\kappa+1} \, x^{\kappa} \, \mathrm{e}^{-\frac{1}{2}\gamma^2 x^2} \, \widetilde{\mathscr{L}}_j^{(\kappa)}\big(\gamma^2 x^2\big), \qquad j \in \mathscr{M}, \quad x \in \Omega, \\ \widetilde{\mathscr{L}}_j^{(\kappa)}(y) &= \tfrac{1}{\sqrt{2}\gamma} \, y^{-\frac{1}{2}\kappa} \, \mathrm{e}^{\frac{1}{2}y} \, \mathscr{L}_j^{(\kappa)}\big(\tfrac{1}{\gamma}\sqrt{y}\big), \qquad j \in \mathscr{M}, \quad y \in \Omega, \end{aligned}$$

and employing the transformation $\xi = \frac{1}{\gamma}\sqrt{r}$, $r = \gamma^2 \xi^2$, $\mathrm{d}r = 2\gamma^2 \, \xi$, we obtain

$$\begin{aligned} \sum_{j=0}^{J-1} \omega_j f(r_j) \mathscr{L}_j^{(\kappa)}(r_j) &= \tfrac{1}{2\gamma^2} \sum_{j=0}^{J-1} \widetilde{\omega}_j \, \mathrm{e}^{\widetilde{r}_j} f\Big(\tfrac{1}{\gamma}\sqrt{\widetilde{r}_j}\Big) \mathscr{L}_j^{(\kappa)}\Big(\tfrac{1}{\gamma}\sqrt{\widetilde{r}_j}\Big) \\ &= \tfrac{1}{\sqrt{2}\gamma} \sum_{j=0}^{J-1} \widetilde{\omega}_j \, \widetilde{r}_j^{\frac{\kappa}{2}} \, \mathrm{e}^{\frac{1}{2}\widetilde{r}_j} \, f\Big(\tfrac{1}{\gamma}\sqrt{\widetilde{r}_j}\Big) \, \widetilde{\mathscr{L}}_j^{(\kappa)}(\widetilde{r}_j) \\ &\approx \tfrac{1}{\sqrt{2}\gamma} \int_{\mathbb{R}>0} \mathrm{e}^{-r} \, r^{\frac{\kappa}{2}} \, \mathrm{e}^{\frac{1}{2}r} \, f\Big(\tfrac{1}{\gamma}\sqrt{r}\Big) \, \widetilde{\mathscr{L}}_j^{(\kappa)}(r) \, \mathrm{d}r \\ &= \tfrac{1}{2\gamma^2} \int_{\mathbb{R}>0} f\Big(\tfrac{1}{\gamma}\sqrt{r}\Big) \, \mathscr{L}_j^{(\kappa)}\big(\tfrac{1}{\gamma}\sqrt{r}\big) \, \mathrm{d}r \\ &= \int_{\mathbb{R}>0} \xi \, f(\xi) \, \mathscr{L}_j^{(\kappa)}(\xi) \, \mathrm{d}\xi \\ &= \big(w \, f \,\big|\, \mathscr{L}_j^{(\kappa)} \big)_{L^2} \end{aligned}$$

with weight function $w(\xi) = \xi$.

Numerical approximation of spectral coefficients. Furthermore, an application of the Gauss–Laguerre formula and the trapezoidal rule yields

$$\begin{aligned} \varphi = \sum_{m \in \mathscr{M}} \varphi_m \, \mathscr{B}_m, \quad \mathscr{B}_m(r,\vartheta) = \mathscr{L}_{m_1}^{(|m_2|)}(r) \, \mathscr{F}_{m_2}(\vartheta), \qquad 0 < r < \infty, \quad -\pi < \vartheta < \pi, \\ \varphi_m = \big(w\varphi \,\big|\, \mathscr{B}_m \big)_{L^2} = \int_{\mathbb{R}_{>0}\times(-\pi,\pi)} r \, \varphi(r,\vartheta) \, \overline{\mathscr{B}_m(r,\vartheta)} \, \mathrm{d}(r,\vartheta) \\ \approx \sum_{j_1=0}^{J_1-1} \sum_{j_2=0}^{J_2-1} \omega_{j1}\omega_{j2} \varphi(r_{j_1}, \vartheta_{j_2}) \mathscr{L}_{m_1}^{(|m_2|)}(r_{j_1}) \, \overline{\mathscr{F}_{m_2}(\vartheta_{j_2})}, \end{aligned}$$

$$r_{j_1} = \tfrac{1}{\gamma}\sqrt{\widetilde{r}_{j_1}}, \quad \omega_{j_1} = \tfrac{1}{2\gamma^2} \, \widetilde{\omega}_{j_1} \, \mathrm{e}^{\widetilde{r}_{j_1}}, \qquad \vartheta_{j_2} = -\pi + \tfrac{2\pi}{J_2} j_2, \quad \omega_{j_2} = \tfrac{2\pi}{J_2}, \qquad 0 \le j_1 \le J_1 - 1, \quad 0 \le j_2 \le J_2 - 1.$$

Part III.

Time integration of Gross–Pitaevskii systems

7. Gross–Pitaevskii systems

7.1. Original formulation

Gross–Pitaevskii systems. In certain respects, a multi-component Bose–Einstein condensate is well described by a system of J coupled Gross–Pitaevskii equations

$$\begin{aligned} \mathrm{i}\hbar\,\partial_t \Psi_j(x,t) &= \Big(-\tfrac{\hbar^2}{2m_j}\,\Delta + V_j(x) + \hbar^2 \sum_{k=1}^{J} g_{jk} \big|\Psi_k(x,t)\big|^2 \Big)\, \Psi_j(x,t)\,, \\ \big\|\Psi_j(\cdot,0)\big\|_{L^2}^2 &= N_j\,, \qquad x \in \mathbb{R}^d\,, \quad t \geq 0\,, \quad 1 \leq j \leq J\,. \end{aligned} \tag{7.1}$$

Here, we denote by $\Psi_j : \mathbb{R}^d \times \mathbb{R}_{\geq 0} \to \mathbb{C} : (x,t) \mapsto \Psi_j(x,t)$ the order parameters (wave functions), by $\hbar \approx 1.054571628 \cdot 10^{-34}$ Planck's constant, by m_j the masses of the atomic species, and by N_j their total particle numbers, $1 \leq j \leq J$. In the most relevant case of three space dimensions, the intra-species coupling constants g_{jj} and the inter-species coupling constants g_{jk} are given by $g_{jk} = 2\pi\,\sigma_{jk}\frac{m_j+m_k}{m_j m_k}$ with scattering lengths σ_{jk}, where $\sigma_{jk} = \sigma_{kj}$, $1 \leq j,k \leq J$. The external trapping potentials are described by real-valued functions $V_j : \mathbb{R}^d \to \mathbb{R}$, $1 \leq j \leq J$. Further, the partial differential equations in (7.1) are subject to asymptotic boundary conditions and certain initial conditions.

External potentials. In many cases, the external trapping potentials are modelled by scaled harmonic potentials

$$V_j(x) = \tfrac{m_j}{2} \sum_{i=1}^{d} \omega_{ji}^2\,(x_i - \zeta_{ji})^2\,, \qquad x \in \mathbb{R}^d\,, \quad 1 \leq j \leq J\,,$$

with positive weights $\omega_{ji} > 0$ and center displacements $\zeta_{ji} \in \mathbb{R}$, $1 \leq i \leq d$, $1 \leq j \leq J$.

7.2. Normalised formulation

Normalisation. Employing a linear transformation of the spatial variable

$$\xi = \sqrt{c}\,x\,, \qquad c = \tfrac{1}{\hbar}\sqrt[J]{m_1 \cdots m_J}\,,$$

$$\psi_j(\xi,t) = \tfrac{1}{C}\,\Psi_j(x,t)\,, \qquad C = \sqrt[4]{c^d}\,, \qquad U_j(\xi) = \tfrac{1}{\hbar}\,V_j(x)\,, \qquad \vartheta_{jk} = \hbar\,C^2 g_{jk}\,, \qquad 1 \leq j,k \leq J\,,$$

we obtain the following normalised formulation of the Gross–Pitaevskii system (7.1)

$$\begin{gathered} \mathrm{i}\,\partial_t \psi_j(\xi,t) = \Big(-c_j\,\Delta + U_j(\xi) + \sum_{k=1}^{J} \vartheta_{jk} \left|\psi_k(\xi,t)\right|^2 \Big)\,\psi_j(\xi,t)\,, \quad c_j = \tfrac{\sqrt[J]{m_1\cdots m_J}}{2m_j}\,, \\ \left\|\psi_j(\cdot,0)\right\|_{L^2}^2 = N_j\,, \qquad \xi\in\mathbb{R}^d\,, \quad t\geq 0\,, \quad 1\leq j\leq J\,. \end{gathered} \tag{7.2}$$

In accordance with (7.1), the partial differential equations in (7.2) are subject to asymptotic boundary conditions and certain initial conditions. The constant C is chosen such that the total particle numbers are conserved.

Explanation. Multiplying the partial differential equation in (7.1) with $\frac{1}{\hbar}$ yields

$$\mathrm{i}\,\partial_t \Psi_j(x,t) = \Big(-\tfrac{\hbar}{2m_j}\,\Delta + \tfrac{1}{\hbar}\,V_j(x) + \hbar \sum_{k=1}^{J} g_{jk} \left|\Psi_k(x,t)\right|^2 \Big)\,\Psi_j(x,t)\,.$$

Note that $\partial_{x_i} = \sqrt{c}\,\partial_{\xi_i}$, $1\leq i\leq d$, and thus $\Delta_x = c\,\Delta_\xi$; therefore, substituting $\Psi_j(x,t) = C\,\psi_j(\xi,t)$ as well as $V_j(x) = \hbar\,U_j(\xi)$ gives

$$\mathrm{i}C\,\partial_t \psi_j(\xi,t) = C\Big(-\tfrac{\hbar c}{2m_j}\,\Delta + U_j(\xi) + \hbar\,C^2 \sum_{k=1}^{J} g_{jk} \left|\psi_k(\xi,t)\right|^2 \Big)\,\psi_j(\xi,t)\,.$$

Multiplying with $\frac{1}{C}$ and using that $\hbar\,c = \sqrt[J]{m_1\cdots m_J}$ and $\vartheta_{jk} = \hbar\,C^2 g_{jk}$, yields the partial differential equation in (7.2). Further, due to $\mathrm{d}\xi = \sqrt{c^d}\,\mathrm{d}x = C^2\,\mathrm{d}x$, it follows

$$\left\|\psi_j(\cdot,0)\right\|_{L^2}^2 = \int_{\mathbb{R}^d} \left|\psi_j(\xi,0)\right|^2 \mathrm{d}\xi = \int_{\mathbb{R}^d} \left|\Psi_j(x,0)\right|^2 \mathrm{d}x = \left\|\Psi_j(\cdot,0)\right\|_{L^2}^2\,.$$

7.3. Special case

Special case. As an illustration, we specify a Gross–Pitaevskii system in three space dimensions involving two coupled equations, that is, we set $J=2$ and $d=3$ in (7.1) and obtain

$$\begin{gathered} \mathrm{i}\hbar\,\partial_t \Psi_1(x,t) = \Big(-\tfrac{\hbar^2}{2m_1}\,\Delta + V_1(x) + \hbar^2 g_{11} \left|\Psi_1(x,t)\right|^2 + \hbar^2 g_{12} \left|\Psi_2(x,t)\right|^2 \Big)\,\Psi_1(x,t)\,, \\ \mathrm{i}\hbar\,\partial_t \Psi_2(x,t) = \Big(-\tfrac{\hbar^2}{2m_2}\,\Delta + V_2(x) + \hbar^2 g_{12} \left|\Psi_1(x,t)\right|^2 + \hbar^2 g_{22} \left|\Psi_2(x,t)\right|^2 \Big)\,\Psi_2(x,t)\,, \\ \left\|\Psi_1(\cdot,0)\right\|_{L^2}^2 = N_1\,, \qquad \left\|\Psi_2(\cdot,0)\right\|_{L^2}^2 = N_2\,, \qquad x\in\mathbb{R}^3\,, \quad t\geq 0\,; \end{gathered}$$

the scaled harmonic potentials are of the form

$$\begin{aligned} V_1(x) &= \tfrac{m_1}{2}\left(\omega_{11}^2(x_1-\zeta_{11})^2 + \omega_{12}^2(x_2-\zeta_{12})^2 + \omega_{13}^2(x_3-\zeta_{13})^2\right), \qquad x\in\mathbb{R}^3\,, \\ V_2(x) &= \tfrac{m_2}{2}\left(\omega_{21}^2(x_1-\zeta_{21})^2 + \omega_{22}^2(x_2-\zeta_{22})^2 + \omega_{23}^2(x_3-\zeta_{23})^2\right), \qquad x\in\mathbb{R}^3\,. \end{aligned}$$

In compact vector and matrix notation, we have

$$m = (m_1, m_2) \in \mathbb{R}^2\,, \qquad N = (N_1, N_2) \in \mathbb{R}^2\,,$$
$$g = \begin{pmatrix} g_{11} & g_{12} \\ g_{12} & g_{22} \end{pmatrix} \in \mathbb{R}^{2\times 2}\,, \qquad \omega = \begin{pmatrix} \omega_{11} & \omega_{12} & \omega_{13} \\ \omega_{21} & \omega_{22} & \omega_{23} \end{pmatrix} \in \mathbb{R}^{2\times 3}\,, \qquad \zeta = \begin{pmatrix} \zeta_{11} & \zeta_{12} & \zeta_{13} \\ \zeta_{21} & \zeta_{22} & \zeta_{23} \end{pmatrix} \in \mathbb{R}^{2\times 3}\,.$$

In the present situation, the linear transformation

$$\xi = \sqrt{c}\,x\,, \qquad c = \tfrac{\sqrt{m_1 m_2}}{\hbar}\,,$$
$$\psi_j(\xi,t) = \tfrac{1}{C}\,\Psi_j(x,t)\,, \qquad C = \sqrt[4]{c^3}\,, \qquad U_j(\xi) = \tfrac{1}{\hbar}\,V_j(x)\,, \quad j = 1,2\,, \qquad \vartheta = \hbar\,C^2 g\,,$$

yields the following normalised system

$$\mathrm{i}\,\partial_t \psi_1(\xi,t) = \Big(-\tfrac{\sqrt{m_1 m_2}}{2m_1}\,\Delta + U_1(\xi) + \vartheta_{11}\,\big|\psi_1(\xi,t)\big|^2 + \vartheta_{12}\,\big|\psi_2(\xi,t)\big|^2 \Big)\,\psi_1(\xi,t)\,,$$
$$\mathrm{i}\,\partial_t \psi_2(\xi,t) = \Big(-\tfrac{\sqrt{m_1 m_2}}{2m_2}\,\Delta + U_2(\xi) + \vartheta_{12}\,\big|\psi_1(\xi,t)\big|^2 + \vartheta_{22}\,\big|\psi_2(\xi,t)\big|^2 \Big)\,\psi_2(\xi,t)\,,$$
$$\big\|\psi_1(\cdot,0)\big\|_{L^2}^2 = N_1\,, \qquad \big\|\psi_2(\cdot,0)\big\|_{L^2}^2 = N_2\,, \qquad \xi \in \mathbb{R}^3\,, \quad t \geq 0\,.$$

8. Ground state solution

8.1. Energy functional

Energy functional. For a nonlinear Schrödinger equation such as (7.2), the energy functional E is given by

$$\begin{aligned} E(\varphi) &= \sum_{j=1}^{J} E_j(\varphi)\,, \\ E_j(\varphi) &= \Big(\big(-c_j\,\Delta + U_j \big)\,\varphi_j \,\Big|\, \varphi_j \Big)_{L^2} + \tfrac{1}{2} \sum_{k=1}^{J} \vartheta_{jk} \Big(|\varphi_k|^2 \varphi_j \,\Big|\, \varphi_j \Big)_{L^2}\,, \qquad 1 \le j \le J\,, \end{aligned} \tag{8.1}$$

where $\varphi = \big(\varphi_1, \dots, \varphi_J\big)$ with $\varphi_j : \mathbb{R}^d \to \mathbb{C}$ for $1 \le j \le J$.

Notations. In accordance with the eigenvalue relation (5.14) for the Hermite basis functions, we henceforth denote

$$\begin{aligned} \mathscr{G}_j(\varphi) &= \big(\mathscr{A}_j + \mathscr{B}_j(\varphi) \big)\,\varphi_j\,, \quad \widetilde{\mathscr{G}}_j(\varphi) = \big(\mathscr{A}_j + \widetilde{\mathscr{B}}_j(\varphi) \big)\,\varphi_j\,, \\ \mathscr{B}_j(\varphi) &= \mathscr{B}_j^{(0)} + \sum_{k=1}^{J} \vartheta_{jk}\,\mathscr{B}_j^{(k)}(\varphi)\,, \quad \widetilde{\mathscr{B}}_j(\varphi) = \mathscr{B}_j^{(0)} + \tfrac{1}{2} \sum_{k=1}^{J} \vartheta_{jk}\,\mathscr{B}_j^{(k)}(\varphi)\,, \\ \mathscr{A}_j &= c_j \big(-\Delta + U_\gamma \big), \quad \mathscr{B}_j^{(0)} = U_j - c_j\,U_\gamma\,, \quad \mathscr{B}_j^{(k)}(\varphi) = |\varphi_k|^2\,, \qquad 1 \le j \le J\,. \end{aligned} \tag{8.2}$$

With these abbrevitaions, the partial differential equations in (7.2) and the associated energies are written in compact form

$$\mathrm{i}\,\partial_t \psi_j(\xi, t) = \mathscr{G}_j\big(\psi(\xi, t)\big), \quad E_j(\varphi) = \Big(\widetilde{\mathscr{G}}_j(\varphi) \,\Big|\, \varphi_j \Big)_{L^2}\,, \qquad 1 \le j \le J\,,$$

see also (8.1).

Energy conservation. For the solution of the normalised Gross–Pitaevskii system (7.2) the total energy (8.1) is a conserved quantity, that is, it holds

$$E\big(\psi(\cdot, t)\big) = E\big(\psi(\cdot, 0)\big)\,, \qquad t \ge 0\,. \tag{8.3}$$

8.2. Ground state solution

Ground state solution. The ground state solution of the normalised Gross–Pitaevskii system (7.2) is a solution of the special form

$$\psi_j(\xi,t) = \mathrm{e}^{-\mathrm{i}\,\mu_j t}\,\varphi_j(\xi)\,, \qquad \xi\in\mathbb{R}^d\,, \quad t\geq 0\,, \quad 1\leq j\leq J\,,$$

that minimises the energy functional E, see (8.1). Hereby, the chemical potentials $\mu_j\in\mathbb{R}$, $1\leq j\leq J$, are given by

$$N_j\,\mu_j = \Big(\mathscr{G}_j(\varphi)\,\Big|\,\varphi_j\Big)_{L^2} = \Big(\big(-c_j\,\Delta + U_j\big)\,\varphi_j\,\Big|\,\varphi_j\Big)_{L^2} + \sum_{k=1}^{J}\vartheta_{jk}\,\Big(|\varphi_k|^2\varphi_j\,\Big|\,\varphi_j\Big)_{L^2}\,, \qquad 1\leq j\leq J\,.$$

8.3. A single Gross–Pitaevskii equation

Gross–Pitaevskii equation. For simplicity, we meanwhile consider a single Gross–Pitaevskii equation of the form

$$\begin{aligned} \mathrm{i}\,\partial_t\psi(\xi,t) &= \Big(-\tfrac{1}{2}\,\Delta + U(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2\Big)\,\psi(\xi,t)\,,\\ \big\|\psi(\cdot,0)\big\|_{L^2}^2 &= N\,, \qquad \xi\in\mathbb{R}^d\,, \quad t\geq 0\,, \end{aligned} \tag{8.4}$$

see also (7.2); in accordance with (8.2), we denote

$$\begin{aligned} \mathscr{G}(\varphi) &= \big(\mathscr{A}+\mathscr{B}(\varphi)\big)\,\varphi\,, \quad \widetilde{\mathscr{G}}(\varphi) = \big(\mathscr{A}+\widetilde{\mathscr{B}}(\varphi)\big)\,\varphi\,,\\ \mathscr{B}(\varphi) &= \mathscr{B}^{(0)} + \vartheta\,\mathscr{B}^{(1)}(\varphi)\,, \quad \widetilde{\mathscr{B}}(\varphi) = \mathscr{B}^{(0)} + \tfrac{1}{2}\,\vartheta\,\mathscr{B}^{(1)}(\varphi)\,,\\ \mathscr{A} &= \tfrac{1}{2}\big(-\Delta + U_\gamma\big)\,, \quad \mathscr{B}^{(0)} = U - \tfrac{1}{2}\,U_\gamma\,, \quad \mathscr{B}^{(1)}(\varphi) = |\varphi|^2\,. \end{aligned}$$

Particle number conservation. With the help of the eigenvalue relation (5.14) and Parseval's identity (4.3), it it seen that

$$\Big(\psi(\cdot,t)\,\Big|\,\mathscr{G}\big(\psi(\cdot,t)\big)\Big)_{L^2}\in\mathbb{R}\,.$$

As a consequence, for the solution of (8.4) we further obtain

$$\begin{aligned} \partial_t\big\|\psi(\xi,t)\big\|_{L^2}^2 &= \big(\partial_t\psi(\xi,t)\,\big|\,\psi(\xi,t)\big)_{L^2} + \big(\psi(\xi,t)\,\big|\,\partial_t\psi(\xi,t)\big)_{L^2} = 2\,\Re\big(\psi(\xi,t)\,\big|\,\partial_t\psi(\xi,t)\big)_{L^2}\\ &= 2\,\Re\Big(-\mathrm{i}\Big(\psi(\cdot,t)\,\Big|\,\mathscr{G}\big(\psi(\cdot,t)\big)\Big)_{L^2}\Big) = 0\,, \qquad t\geq 0\,, \end{aligned}$$

which shows that the total particle number is conserved.

Energy conservation. In the present situation, the energy functional is given by

$$E(\varphi) = \big(\widetilde{\mathscr{G}}(\varphi)\,\big|\,\varphi\big)_{L^2} = \Big(\big(-\tfrac{1}{2}\,\Delta + U + \tfrac{1}{2}\,\vartheta\,|\varphi|^2\big)\,\varphi\,\Big|\,\varphi\Big)_{L^2}\,.$$

We note that $\partial_\varphi |\varphi|^2 = \overline{\varphi}\,(\cdot) + \varphi\,\overline{(\cdot)}$ and further

$$\tfrac{1}{2}\,\vartheta\,\big(\varphi\,\overline{\varphi}\,(\cdot) + \varphi^2\,\overline{(\cdot)}\,\big|\,\varphi\big)_{L^2} = \tfrac{1}{2}\,\vartheta\,\big(|\varphi|^2\varphi\,\big|\,(\cdot)\big)_{L^2} + \tfrac{1}{2}\,\vartheta\,\big((\cdot)\,\big|\,|\varphi|^2\varphi\big)_{L^2}\,.$$

Thus, making use of the fact that the Laplacian is a selfadjoint operator and that the potential U is real-valued, the Fréchet derivative of E equals

$$\partial_\varphi E(\varphi) = \Big(\big(-\tfrac{1}{2}\,\Delta + U + \vartheta\,|\varphi|^2\big)\,\varphi\,\Big|\,(\cdot)\Big)_{L^2} + \Big(\big(-\tfrac{1}{2}\,\Delta + U + \vartheta\,|\varphi|^2\big)\,(\cdot)\,\Big|\,\varphi\Big)_{L^2} = 2\,\Re\,\big(\mathscr{G}(\varphi)\,\big|\,(\cdot)\big)_{L^2}\,.$$

As a consequence, the energy conservation (8.3) follows; namely, for the solution of (8.4), we obtain

$$\begin{aligned}\partial_t E\big(\psi(\cdot,t)\big) &= \partial_\varphi E\big(\psi(\cdot,t)\big)\,\partial_t\psi(\cdot,t) = 2\,\Re\,\Big(\mathscr{G}\big(\psi(\cdot,t)\big)\,\Big|\,\partial_t\psi(\cdot,t)\Big)_{L^2} = 2\,\Re\,\Big(-\mathrm{i}\big\|\mathscr{G}\big(\psi(\cdot,t)\big)\big\|_{L^2}^2\Big)\\ &= 0\,, \qquad t \geq 0\,.\end{aligned}$$

Generalisation. Similar considerations apply to Gross–Pitaevskii systems (7.2) showing that the total particle numbers and the total energy is conserved; more precisely, it follows

$$\begin{gathered}\partial_{\varphi_j} E(\varphi) = 2\,\Re\,\big(\mathscr{G}_j(\varphi)\,\big|\,(\cdot)\big)_{L^2}\,, \quad \partial_t\big\|\psi_j(\cdot,t)\big\|_{L^2} = 0\,,\\ \partial_t E\big(\psi(\cdot,t)\big) = \partial_\varphi E\big(\psi(\cdot,t)\big)\,\partial_t\psi(\cdot,t) = 0\,, \qquad t \geq 0\,, \quad 1 \leq j \leq J\,.\end{gathered}$$

8.3.1. Groundstate solution

We next determine the ground state solution of the Gross–Pitaevskii equation (8.4) for the limiting cases $\vartheta = 0$ and $\vartheta \gg 1$; in particular, we consider a scaled harmonic potential

$$U(\xi) = \tfrac{1}{2}\sum_{i=1}^{d} \omega_i^2\,\xi_i^2\,, \qquad \omega_i > 0\,, \quad \xi \in \mathbb{R}^d\,.$$

These special solutions will serve as suitable initial values in the ground state computation by the imaginary time method and a minimisation approach, respectively.

Linear Schrödinger equations

For $\vartheta = 0$, problem (8.4) simplifies to a linear Schrödinger equation. In the above situation, the ground state solution is given by the first Hermite basis function. More precisely, it holds

$$\begin{gathered}\psi(\xi,t) = \sqrt{N}\,\mathrm{e}^{-\mathrm{i}\mu t}\varphi(\xi)\,, \qquad \xi \in \mathbb{R}^d\,, \quad t \geq 0\,,\\ \varphi = \mathscr{H}_0^\gamma\,, \qquad \gamma_i = \sqrt{\omega_i}\,, \quad 1 \leq i \leq d\,, \qquad \mu = \tfrac{1}{2}\sum_{i=1}^{d}\omega_i\,.\end{gathered}$$

Namely, inserting into (8.4) yields (due to $\lambda_0 = \gamma_1^2 + \cdots + \gamma_d^2 = \omega_1 + \cdots + \omega_d$)

$$\begin{aligned}\mu\,\psi(\xi,t) = \mathrm{i}\,\partial_t\psi(\xi,t) &= \big(-\tfrac{1}{2}\,\Delta + U(\xi)\big)\,\psi(\xi,t) = \tfrac{1}{2}\sqrt{N}\,\mathrm{e}^{-\mathrm{i}\mu t}\,\big(-\Delta + U_\gamma(\xi)\big)\,\mathscr{H}_0^\gamma(\xi)\\ &= \tfrac{1}{2}\sqrt{N}\,\mathrm{e}^{-\mathrm{i}\mu t}\lambda_0\,\mathscr{H}_0^\gamma(\xi) = \tfrac{1}{2}\sum_{i=1}^{d}\omega_i\,\psi(\xi,t)\,,\end{aligned}$$

see also (5.14). Note that this is consistent with

$$\mu = \tfrac{1}{N}\Big(\tfrac{1}{2}\big(-\Delta + U_\gamma\big)\,\psi(\cdot,t)\,\Big|\,\psi(\cdot,t)\Big)_{L^2} = \tfrac{1}{2}\,\big(\lambda_0\,\mathscr{H}_0^\gamma\,\big|\,\mathscr{H}_0^\gamma\big)_{L^2} = \tfrac{1}{2}\,\lambda_0 = \tfrac{1}{2}\sum_{i=1}^{d}\omega_i\,.$$

Thomas–Fermi approximation

For large values of ϑ, neglecting the Laplace operator in (8.4), the *Thomas–Fermi approximation* yields an approximate ground state through

$$\psi(\xi,t) = \sqrt{N}\,\mathrm{e}^{-\mathrm{i}\mu t}\varphi(\xi)\,,$$

$$\varphi(\xi) = \begin{cases}\sqrt{\frac{1}{N\vartheta}\,\big(\mu - U(\xi)\big)}\,, & \text{if } U(\xi) < \mu\,,\\ 0\,, & \text{otherwise}\,,\end{cases}\,,\quad \|\varphi\|_{L^2} = 1\,,\qquad \xi\in\mathbb{R}^d\,,\quad t\geq 0\,.$$

This is seen by inserting the above relation into the differential equation

$$\mu\,\psi(\xi,t) = \mathrm{i}\,\partial_t\psi(\xi,t) = \Big(U(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2\Big)\,\psi(\xi,t)$$

which yields $\mu = U(\xi) + \vartheta\,\big|\psi(\xi,t)\big|^2$. In particular, for a scaled harmonic potential U_γ, due to the normalisation condition

$$1 = \|\varphi\|_{L^2}^2 = \tfrac{1}{N\vartheta}\int_{U(\xi)<\mu}\big(\mu - U(\xi)\big)\,\mathrm{d}\xi$$

the chemical potential μ is given by

$$\mu = \begin{cases}\frac{1}{4}\,\sqrt[3]{18\,\big(N\vartheta\,\omega_1\big)^2}\,, & d=1\,,\\ \sqrt[2]{\frac{1}{\pi}N\vartheta\,\omega_1\omega_2}\,, & d=2\,,\\ \frac{1}{4}\,\sqrt[5]{450\,\big(\frac{1}{\pi}N\vartheta\,\omega_1\omega_2\,\omega_3\big)^2}\,, & d=3\,.\end{cases}$$

9. Time-splitting pseudo-spectral methods

9.1. Abstract formulation

Abstract evolutionary problem. For the specification of the time integration method as well as for theoretical considerations, it is convenient to formulate a nonlinear Schrödinger equation as an abstract ordinary differential equation on a function space by formally omitting the spatial variable. In particular, for the normalised Gross–Pitaevskii system (7.2) this yields the following abstract initial value problem for $u(t) = \psi(\cdot, t) = \big(\psi_1(\cdot, t), \dots, \psi_J(\cdot, t)\big)$

$$\mathrm{i}\, u'(t) = A\, u(t) + B\big(u(t)\big)\, u(t)\,, \quad t \geq 0\,, \qquad u(0) \text{ given}\,. \tag{9.1}$$

Approach. In the following, we apply time-splitting spectral methods for discretising Gross–Pitaevskii systems in space and time. More precisely, the time integration of (7.2) and (9.1), respectively, relies on high-order exponential operator splitting methods, see Part I. For the numerical solution of the associated initial value problems

$$\mathrm{i}\, u'(t) = A\, u(t)\,, \quad t \geq 0\,, \qquad u(0) \text{ given}\,, \tag{9.2a}$$

$$\mathrm{i}\, u'(t) = B\big(u(t)\big)\, u(t)\,, \quad t \geq 0\,, \qquad u(0) \text{ given}\,, \tag{9.2b}$$

we make use of Hermite and Fourier spectral methods, see Part II. In the subsequent Sections 9.2 and 9.3, we specify the definition of the unbounded operators $A : D(A) \subset X \to X$ and $B(v) : D(B) \subset X \to X$, $v \in V$, which is closely related to the choice of the spectral method. Moreover, we briefly discuss the numerical solution of the initial value problems (9.2).

9.2. Time-splitting Fourier pseudo-spectral method

For the Fourier spectral method, the numerical solution of the associated initial value problem (9.2a) relies on techniques that were the content of Section 4.2. Due to the fact that Gross–Pitaevskii systems fulfill a certain invariance properties, the exact solution of (9.2b) is available.

9.2.1. First part

Initial value problem. Regarding (9.2a), we consider the following initial value problem

$$\mathrm{i}\, \partial_t \psi(\cdot, t) = \mathscr{A} \psi(\cdot, t)\,, \quad t \geq 0\,, \qquad \psi(\cdot, 0) \text{ given}\,, \tag{9.3a}$$

where the application of the Fourier spectral method suggests the choice

$$\mathscr{A} = \begin{pmatrix} \mathscr{A}_1 & & \\ & \ddots & \\ & & \mathscr{A}_J \end{pmatrix}, \qquad \mathscr{A}_j = -\,c_j\,\Delta\,, \quad c_j = \frac{\sqrt[J]{m_1\cdots m_J}}{2m_j}\,, \quad 1 \le j \le J\,. \tag{9.3b}$$

We are thus concerned with the componentwise numerical solution of the above problem, i.e., we consider

$$\mathrm{i}\,\partial_t \psi_j(\cdot,t) = \mathscr{A}_j\,\psi_j(\cdot,t)\,, \quad t \ge 0\,, \qquad \psi_j(\cdot,0) \text{ given}\,, \qquad 1 \le j \le J\,. \tag{9.3c}$$

Exact solution. It is straightforward to extend the approach of Section 4.2. The eigenvalue relation (4.9) for the differential operator $-\Delta$ with corresponding eigenfunctions $(\mathscr{F}_m)_{m\in\mathscr{M}}$ and eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$ implies

$$\mathscr{A}_j\,\mathscr{F}_m = c_j\,\lambda_m\,\mathscr{F}_m\,, \qquad m \in \mathscr{M}\,, \qquad 1 \le j \le J\,.$$

Employing a spectral decomposition of the initial value into Fourier basis functions, we thus obtain the following representation

$$\psi_j(\cdot,t) = \sum_{m\in\mathscr{M}} \mathrm{e}^{-\mathrm{i}\,c_j\lambda_m t}\,\psi_{jm}(0)\,\mathscr{F}_m\,, \qquad \psi_j(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_{jm}(0)\,\mathscr{F}_m\,, \qquad 1 \le j \le J\,, \tag{9.4}$$

see also (4.2) and (9.3).

Numerical solution. The numerical realisation of (9.4) relies on techniques that were discussed in Section 4.2.2.

9.2.2. Second part

Initial value problem. Regarding (9.2b), we consider the initial value problem

$$\mathrm{i}\,\partial_t \psi(\cdot,t) = \mathscr{B}\big(\psi(\cdot,t)\big)\,\psi(\cdot,t)\,, \quad t \ge 0\,, \qquad \psi(\cdot,0) \text{ given}\,, \tag{9.5a}$$

where the application of the Fourier spectral method for the first part (9.3) suggests the following choice

$$\mathscr{B}\big(\psi(\cdot,t)\big) = \begin{pmatrix} \mathscr{B}_1\big(\psi(\cdot,t)\big) & & \\ & \ddots & \\ & & \mathscr{B}_J\big(\psi(\cdot,t)\big) \end{pmatrix}, \tag{9.5b}$$

$$\mathscr{B}_j\big(\psi(\cdot,t)\big) = U_j + \sum_{k=1}^{J} \vartheta_{jk}\,\big|\psi_k(\cdot,t)\big|^2\,, \qquad 1 \le j \le J\,.$$

We are thus concerned with the numerical solution of the initial value problem

$$\mathrm{i}\,\partial_t \psi_j(\cdot,t) = \mathscr{B}_j\big(\psi(\cdot,t)\big)\,\psi_j(\cdot,t)\,, \qquad \psi_j(\cdot,0) \text{ given}\,, \qquad 1 \le j \le J\,. \tag{9.5c}$$

Invariance and exact solution. Noting that the exact solution of (9.5) fulfills

$$\partial_t \big|\psi_j(\cdot,t)\big|^2 = 2\,\Re\Big(\overline{\psi_j(\cdot,t)}\,\partial_t \psi_j(\cdot,t)\Big) = 2\,\Re\Big(-\mathrm{i}\,\mathscr{B}_j\big(\psi(\cdot,t)\big)\,\big|\psi_j(\cdot,t)\big|^2\Big) = 0\,,$$

we conclude that the following invariance property holds

$$\mathscr{B}_j\big(\psi(\cdot,t)\big) = \mathscr{B}_j\big(\psi(\cdot,0)\big)\,, \qquad t \ge 0\,, \qquad 1 \le j \le J\,. \tag{9.6}$$

Consequently, the exact solution of the initial value problem (9.5) is obtained by a pointwise multiplication

$$\psi_j(\xi,t) = \mathrm{e}^{-\mathrm{i}\,t\,\mathscr{B}_j(\psi(\xi,0))}\,\psi_j(\xi,0)\,, \qquad \xi \in \Omega\,, \quad t \ge 0\,. \tag{9.7}$$

Numerical solution. The numerical realisation of (9.7) relies on collocation at the trapezoid quadrature nodes, see also Section 4.2.2.

9.3. Time-splitting Hermite pseudo-spectral method

For the Hermite spectral method, the numerical solution of the associated initial value problem (9.2a) relies on techniques that were the content of Section 5.2, see also Section 8.1. Due to the fact that Gross–Pitaevskii systems fulfill a certain invariance properties, the exact solution of (9.2b) is available. We recall the definition of the scaled harmonic potential

$$U_\gamma(\xi) = \sum_{i=1}^{d} \gamma_i^4\,\xi_i^2\,, \qquad \gamma_i > 0\,, \quad \xi \in \mathbb{R}^d\,, \quad 1 \le i \le d\,,$$

see also (5.1).

9.3.1. First part

Initial value problem. Regarding (9.2a), we consider the initial value problem (9.3a), where the application of the Hermite spectral method suggests the choice

$$\mathscr{A} = \begin{pmatrix} \mathscr{A}_1 & & \\ & \ddots & \\ & & \mathscr{A}_J \end{pmatrix}, \qquad \mathscr{A}_j = -\,c_j\,\big(\Delta - U_\gamma\big)\,, \quad c_j = \frac{\sqrt[J]{m_1 \cdots m_J}}{2m_j}\,, \quad 1 \le j \le J\,.$$

In the same way as for the Fourier spectral method, we are thus concerned with the numerical solution of (9.3c).

Exact solution. It is straightforward to extend the approach of Section 5.2. The eigenvalue relation (5.14) for the differential operator $-\Delta + U_\gamma$ with eigenfunctions $(\mathscr{H}_m^\gamma)_{m\in\mathscr{M}}$ and eigenvalues $(\lambda_m)_{m\in\mathscr{M}}$ implies

$$\mathscr{A}_j \mathscr{H}_m^\gamma = c_j \lambda_m \mathscr{H}_m^\gamma, \qquad m \in \mathscr{M}, \qquad 1 \le j \le J.$$

Employing a spectral decomposition of the initial value into Hermite basis functions, we thus obtain the following representation

$$\psi_j(\cdot,t) = \sum_{m\in\mathscr{M}} \mathrm{e}^{-\mathrm{i}c_j\lambda_m t}\, \psi_{jm}(0)\, \mathscr{H}_m^\gamma, \qquad \psi_j(\cdot,0) = \sum_{m\in\mathscr{M}} \psi_{jm}(0)\, \mathscr{H}_m^\gamma, \qquad 1 \le j \le J, \tag{9.8}$$

see also (5.8) and (9.3c).

Numerical solution. The numerical realisation of (9.8) relies on techniques that were discussed in Section 5.2.2.

9.3.2. Second part

Initial value problem. Regarding (9.2b), we consider the initial value problem (9.5a), where the application of the Hermite spectral method for the first part suggests the choice

$$\mathscr{B}\big(\psi(\cdot,t)\big) = \begin{pmatrix} \mathscr{B}_1\big(\psi(\cdot,t)\big) & & \\ & \ddots & \\ & & \mathscr{B}_J\big(\psi(\cdot,t)\big) \end{pmatrix},$$

$$\mathscr{B}_j\big(\psi(\cdot,t)\big) = U_j - c_j\, U_\gamma + \sum_{k=1}^{J} \vartheta_{jk} \big|\psi_k(\cdot,t)\big|^2, \qquad 1 \le j \le J.$$

Similarly to before, due to the validity of the invariance property (9.6), the numerical solution of (9.5c) is realised by a pointwise multiplication and collocation at the Gauß–Hermite quadrature nodes, see also Section 5.2.2.

9.4. Numerical illustrations

In the following, we illustrate the favourable behaviour of time-splitting Fourier and Hermite pseudo-spectral methods for systems of coupled Gross–Pitaevskii equations (7.1). A detailed description of the numerical examples is found in [13], see also [36, 44].

9.4.1. Computation time

A comparison of the computation time of the Fourier and Hermite spectral method in one and two space dimensions is given in Figure 1.

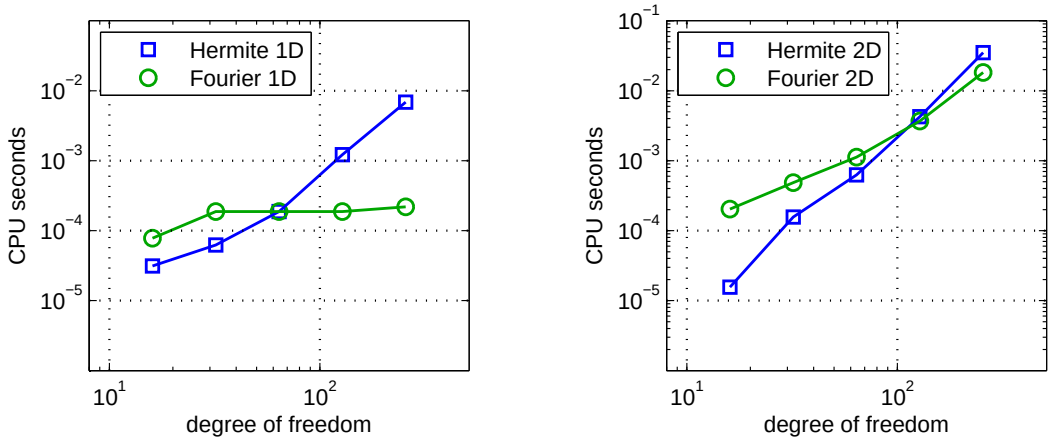

Figure 1.: Computation time of the Fourier and Hermite spectral methods in one (left picture) and two (right picture) space dimensions.

9.4.2. Spatial error

The accuracy of the Fourier and Hermite spectral methods is illustrated in Figure 2.

9.4.3. Temporal convergence order

The numerical convergence orders of various exponential operator splitting methods applied to a two-dimensional Gross–Pitaevskii equation with external harmonic potential and coupling constant $\vartheta = 1$ and $\vartheta = 100$, respectively, are given in Figures 3 and 4.

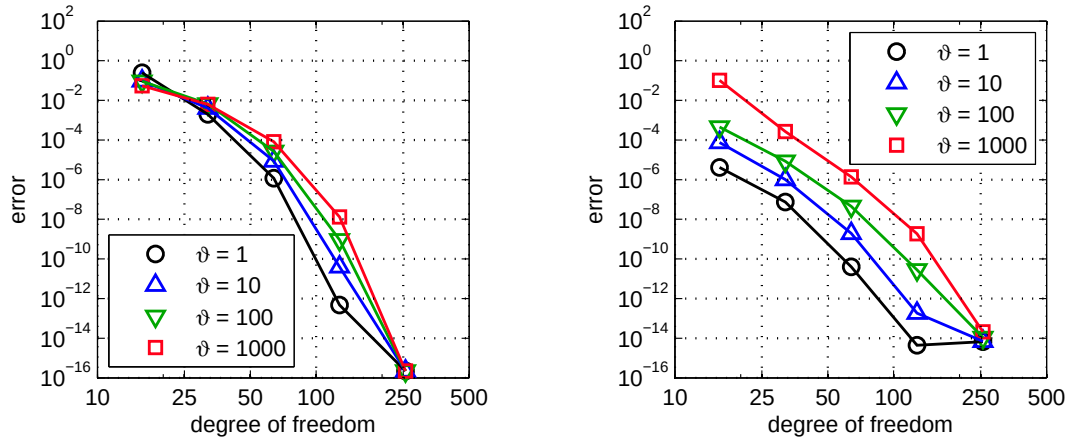

Figure 2.: Spatial error of the Fourier (left picture) and Hermite (right picture) spectral method.

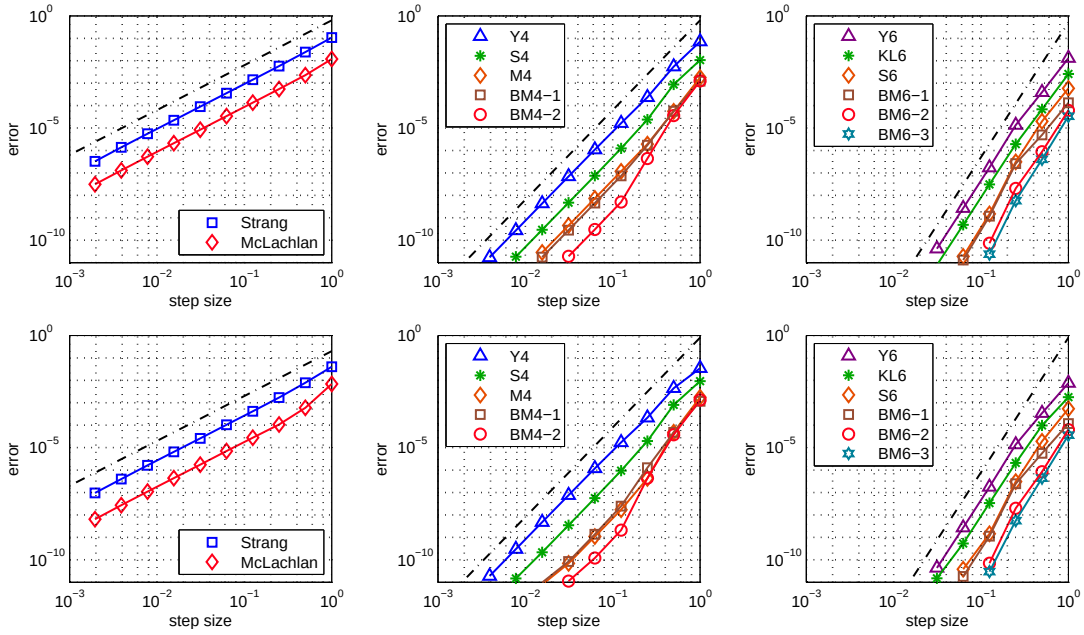

Figure 3.: Temporal orders of various time-splitting Fourier (first row) and Hermite (second row) spectral methods when applied to a Gross–Pitaevskii equation with $\vartheta = 1$.

9.4.4. Long-term integration

The long-term behaviour of time-splitting Fourier and Hermite spectral methods for a two-dimensional Gross–Pitaevskii equation with external harmonic potential and coupling constant $\vartheta = 1$ is illustrated in Table 1. For the time integration, the second-order Strang splitting method, fourth- and sixth-order splitting methods proposed by BLANES & MOAN, and fourth-order explicit Runge–Kutta methods are applied, see also Table 1. For a certain prescribed tolerance, the required number of basis functions, the number of spectral transformations, the particle number conservation error $\Delta_{\mathrm{pn}} = \left| \left\| \psi(\cdot,0) \right\|_{L^2}^2 - \left\| \psi(\cdot,T) \right\|_{L^2}^2 \right|$, and the energy conservation error $\Delta_E = \left| E\big(\psi(\cdot,0)\big) - E\big(\psi(\cdot,T)\big) \right|$ are displayed.

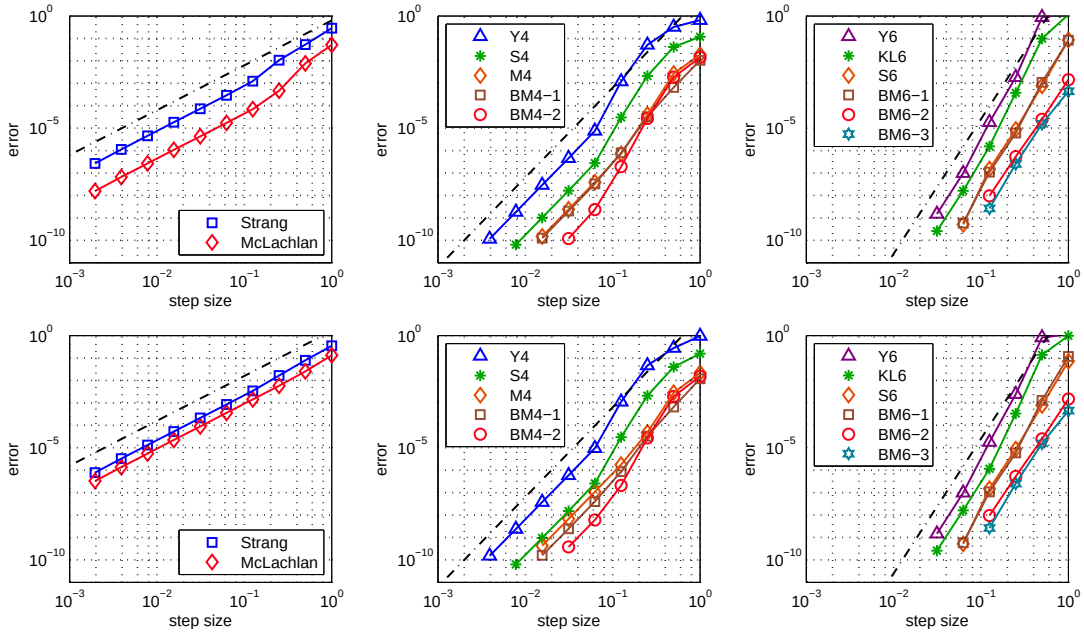

Figure 4.: Temporal orders of various time-splitting Fourier (first row) and Hermite (second row) spectral methods when applied to a Gross–Pitaevskii equation with $\vartheta = 100$.

tol.	method	d.o.f.	#transf.	Δ_{pn}	Δ_E
$< 10^{-2}$	Hermite 2	32×32	16384	$2.6 \cdot 10^{-11}$	$4.2 \cdot 10^{-6}$
$< 10^{-2}$	Fourier 2	64×64	32768	$3.6 \cdot 10^{-13}$	$1.6 \cdot 10^{-6}$
$< 10^{-2}$	Hermite 4	32×32	6144	$9.7 \cdot 10^{-12}$	$1.1 \cdot 10^{-5}$
$< 10^{-2}$	Fourier 4	64×64	12288	$1.7 \cdot 10^{-13}$	$9.1 \cdot 10^{-7}$
$< 10^{-2}$	Hermite 6	32×32	14337	$2.3 \cdot 10^{-11}$	$3.2 \cdot 10^{-8}$
$< 10^{-2}$	Fourier 6	64×64	7169	$1.1 \cdot 10^{-13}$	$6.8 \cdot 10^{-6}$
$< 10^{-2}$	Hermite rk4	32×32	65532	$2.1 \cdot 10^{-5}$	$1.2 \cdot 10^{-4}$
$< 10^{-2}$	Fourier rk4	64×64	524284	$6.4 \cdot 10^{-10}$	$3.7 \cdot 10^{-9}$
$< 10^{-2}$	Hermite ode45	32×32	208376	$2.6 \cdot 10^{-8}$	$1.5 \cdot 10^{-7}$
$< 10^{-2}$	Fourier ode45	64×64	1132436	$5.6 \cdot 10^{-12}$	$3.1 \cdot 10^{-11}$
$< 10^{-6}$	Hermite 4	64×64	24576	$1.0 \cdot 10^{-10}$	$1.1 \cdot 10^{-10}$
$< 10^{-6}$	Fourier 4	128×128	49152	$6.7 \cdot 10^{-12}$	$1.2 \cdot 10^{-11}$
$< 10^{-6}$	Hermite 6	64×64	28673	$1.2 \cdot 10^{-8}$	$2.1 \cdot 10^{-10}$
$< 10^{-6}$	Fourier 6	128×128	28673	$4.2 \cdot 10^{-12}$	$8.7 \cdot 10^{-12}$
$< 10^{-6}$	Hermite rk4	64×64	524284	$6.4 \cdot 10^{-10}$	$3.7 \cdot 10^{-9}$
$< 10^{-6}$	Fourier rk4	128×128	524284	$6.4 \cdot 10^{-10}$	$3.7 \cdot 10^{-9}$
$< 10^{-6}$	Hermite ode45	64×64	509816	$3.6 \cdot 10^{-10}$	$2.1 \cdot 10^{-9}$
$< 10^{-6}$	Fourier ode45	128×128	1411448	$2.2 \cdot 10^{-12}$	$1.1 \cdot 10^{-11}$

Table 1.: Time integration of a two-dimensional Gross–Pitaevskii equation up to $T = 400$. For a tolerance (tol.), the degree of freedom (d.o.f.), the number of spectral transformations (#transf.), the particle number conservation error Δ_{pn}, and the energy conservation error Δ_E are displayed.

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