Are exponential operator splitting methods favourable for the time integration of evolutionary problems involving critical parameters?

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Theme

Splitting methods. Time integration of linear evolutionary problems by exponential operator splitting methods

$$u'(t) = A\,u(t) + B\,u(t)\,, \quad t \geq 0\,, \qquad u(0) \text{ given}\,,$$

$$u_{n+1} = \mathscr{S}(h_n)\,u_n \approx u(t_{n+1}) = u(t_n + h_n) = \mathscr{E}(h_n)\,u(t_n)\,, \qquad n \geq 0\,,$$

$$\mathscr{S}(t) = \prod_{j=1}^{s} \mathrm{e}^{b_j tB}\,\mathrm{e}^{a_j tA}\,, \quad \mathscr{E}(t) = \mathrm{e}^{t(A+B)}\,, \qquad t \geq 0\,.$$

Extension to nonlinear problems by calculus of Lie-derivatives.

Applications.

- Evolutionary Schrödinger equations
- Parabolic evolution equations

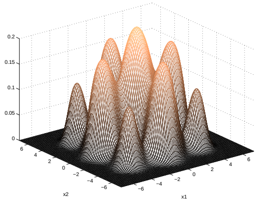
Nonlinear Schrödinger equations

Model problem. Time-dependent nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times \mathbb{R}_{\geq 0} \to \mathbb{C} : (x,t) \to \psi(x,t)$

$$\mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) = \Big(-\varepsilon^2 \Delta + U(x) + \vartheta \big|\psi(x,t)\big|^2 \Big)\, \psi(x,t)$$

subject to asymptotic boundary conditions.

Physical applications. Description of multi-component Bose–Einstein condensates by systems of coupled Gross–Pitaevskii equations.



Semi-classical regime. Study influence of critical parameter $0 < \varepsilon \ll 1$ on exact and time discrete solution.

Semi-classical regime

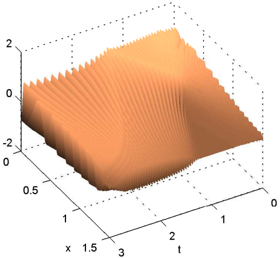
Model problem. Time-dependent Gross–Pitaevskii equation

$$\mathrm{i}\,\varepsilon\,\partial_t\psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon^2\partial_x^2 + \tfrac{1}{2}\,\omega^2 x^2 + \big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,,$$

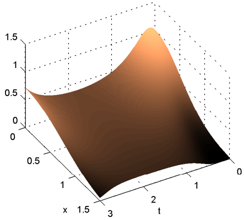
$$\psi(x,0) = \rho_0(x)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\sigma_0(x)}\,, \quad \rho_0(x) = \mathrm{e}^{-x^2}\,, \quad \sigma_0(x) = -\ln\big(\mathrm{e}^{x} + \mathrm{e}^{-x}\big)\,,$$

see BAO, JIN, AND MARKOWICH (2003).

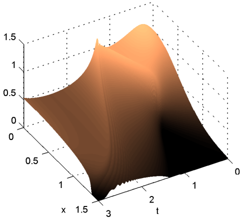
Discretisation. Space and time discretisation by the Fourier spectral method ($x \in [-8,8]$, $M = 8192$) and an embedded 4(3) time-splitting pair ($t \in [0,3]$) based on a fourth-order splitting method by BLANES AND MOAN (2002).



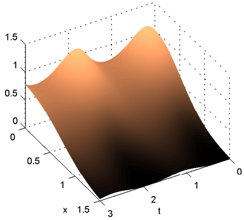
Semi-classical regime



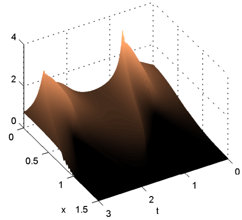
$\omega = 1, \varepsilon = 1$



$\omega = 1, \varepsilon = 10^{-2}$



$\omega = 2, \varepsilon = 1$



$\omega = 2, \varepsilon = 10^{-2}$

Objective

Error analysis of splitting methods. Specification and inspection of a local error expansion with respect to the time step

$$\mathscr{L}(h_n) = \mathscr{S}(h_n) - \mathscr{E}(h_n) = \prod_{j=1}^{s} \mathrm{e}^{b_j h_n B}\, \mathrm{e}^{a_j h_n A} - \mathrm{e}^{h_n (A+B)} = \mathscr{O}\big(h_n^{p+1}\big).$$

Local error expansion provides the basis for a convergence result

$$\big\| u_N - u(t_N) \big\|_X \leq C \left(\big\| u_0 - u(0) \big\|_X + \sum_{n=0}^{N-1} h_n^{p+1} \right).$$

Derivation of alternative local error representations particularly suitable for the investigation of certain problem classes.

Error analysis

Standard approaches.

- Expansion of exponential functions
- Baker–Campbell–Hausdorff formula

Alternative approaches.

- **Quadrature formulas.** Optimal bounds regarding the regularity of the exact solution by techniques studied in Jahnke and Lubich (2000), Koch, Neuhauser, and Th. (2010), Lubich (2008), and Th. (2008).
- **Differential equations.** Investigation of evolutionary problems involving critical parameters in Descombes, Dumont, Louvet, and Massot (2007). Suitable local error expansion exploited in Descombes and Schatzman (2002) and Descombes and Th. (2010).

Contents

Contents.

- Exponential operator splitting methods
- Local error expansions
    - Baker–Campbell–Hausdorff formula
    - Quadrature formulas
    - Differential equations

Exponential operator splitting methods

Exponential operator splitting methods

Aim. For a linear evolutionary problem on a Banach space X

$$u'(t) = A\,u(t) + B\,u(t)\,, \quad t \geq 0\,, \qquad u(0) \text{ given}\,,$$

determine numerical approximations at certain time grid points $0 = t_0 < t_1 < \cdots < t_N$ through the recurrence relation

$$u_{n+1} = \mathscr{S}(h_n)\,u_n \approx u(t_{n+1}) = u(t_n + h_n) = \mathscr{E}(h_n)\,u(t_n)\,, \qquad n \geq 0\,.$$

Approach. Exponential operator splitting methods rely on a suitable decomposition of the right-hand side and the presumption that the initial value problems

$$v'(t) = A\,v(t)\,, \quad v(t) = \mathrm{e}^{tA}\,v(0)\,, \qquad t \geq 0\,,$$
$$w'(t) = B\,w(t)\,, \quad w(t) = \mathrm{e}^{tB}\,w(0)\,, \qquad t \geq 0\,,$$

are solvable in an accurate and efficient way.

Exponential operator splitting methods (Examples)

- Lie–Trotter splitting method yields first-order approximation

$$\mathscr{S}(t) = \mathrm{e}^{tB}\,\mathrm{e}^{tA}, \qquad \mathscr{S}(t) = \mathrm{e}^{tA}\,\mathrm{e}^{tB}.$$

- Second-order Strang splitting method given through

$$\mathscr{S}(t) = \mathrm{e}^{\frac{1}{2}tA}\,\mathrm{e}^{tB}\,\mathrm{e}^{\frac{1}{2}tA}, \qquad \mathscr{S}(t) = \mathrm{e}^{\frac{1}{2}tB}\,\mathrm{e}^{tA}\,\mathrm{e}^{\frac{1}{2}tB}.$$

- Higher-order splitting methods by Blanes and Moan, Kahan and Li, McLachlan, Suzuki, and Yoshida are cast into form

$$\mathscr{S}(t) = \prod_{j=1}^{s} \mathrm{e}^{b_j tB}\,\mathrm{e}^{a_j tA} \approx \mathscr{E}(t) = \mathrm{e}^{t(A+B)}$$

with certain (real or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$.

Practical realisation (Schrödinger equations)

First part. The numerical solution of the initial value problem

$$v'(t) = A\, v(t)\,, \quad t \geq 0\,, \qquad v(0) \text{ given}\,,$$

involving the differential operator A (related to the Laplacian) relies on a spectral decomposition

$$v(t) = \mathrm{e}^{tA}\, v(0) = \sum_m v_m\, \mathrm{e}^{t\,\mu_m} \mathscr{B}_m\,,$$

$$v(0) = \sum_m v_m \mathscr{B}_m\,, \qquad A\,\mathscr{B}_m = \mu_m \mathscr{B}_m\,.$$

Second part. The numerical solution of the initial value problem

$$w'(t) = B\, w(t)\,, \quad t \geq 0\,, \qquad w(0) \text{ given}\,,$$

involving the (unbounded) multiplication operator B (related to the potential) relies on a pointwise multiplication

$$\big(w(t)\big)(x) = \big(\mathrm{e}^{tB}\, w(0)\big)(x) = \mathrm{e}^{tB(x)}\, \big(w(0)\big)(x)\,.$$

Fourier pseudo-spectral method

Spectral decomposition. Let $\Omega = [-a_1, a_1] \times \cdots \times [-a_d, a_d]$ with $a_\ell > 0$ for $1 \leq \ell \leq d$. The Fourier basis functions $(\mathcal{F}_m)_{m \in \mathbb{Z}^d}$ form an orthonormal basis of $L^2(\Omega)$ and satisfy an eigenvalue relation

$$\psi(\cdot, t) = \sum_m \psi_m(t)\, \mathcal{F}_m\,, \qquad \psi_m(t) = \big(\psi(\cdot, t) \,|\, \mathcal{F}_m\big)_{L^2}\,,$$

$$-\Delta \mathcal{F}_m = \lambda_m \mathcal{F}_m\,,$$

$$\mathcal{F}_m(x) = \prod_{\ell=1}^{d} \left(\frac{1}{\sqrt{2a_\ell}}\, \mathrm{e}^{\,\mathrm{i}\,\pi m_\ell \left(\frac{x_\ell}{a_\ell}+1\right)} \right), \qquad \lambda_m = \sum_{\ell=1}^{d} \frac{\pi^2 m_\ell^2}{a_\ell^2}\,.$$

Numerical approximation. Truncation of the infinite sum and application of the trapezoid quadrature formula

$$\psi_M(\cdot, t) = \sum_m{}_M\, \psi_m(t)\, \mathcal{F}_m\,,$$

$$\psi_m(t) = \int_\Omega \psi(\xi, t)\, \mathcal{F}_m(\xi)\, \mathrm{d}\xi \approx \sum_k{}_M\, \omega_k\, \psi(\xi_k, t)\, \mathcal{F}_m(\xi_k)\,.$$

Local error expansions

Baker–Campbell–Hausdorff formula

Baker–Campbell–Hausdorff formula. The BCH formula implies

$$\mathrm{e}^{tL}\,\mathrm{e}^{tK} = \mathrm{e}^{tS(t)}\,, \qquad S(t) = K + L - \tfrac{1}{2}\,t\,\big[K,L\big] + \mathscr{O}\big(t^2\big)\,.$$

Local error expansion (Strang splitting). For exponential operator splitting methods involving two compositions

$$\mathscr{S}(t) = \mathrm{e}^{b_2 tB}\,\mathrm{e}^{a_2 tA}\,\mathrm{e}^{b_1 tB}\,\mathrm{e}^{a_1 tA} = \mathrm{e}^{tS(t)} \approx \mathscr{E}(t) = \mathrm{e}^{t(A+B)}$$

the above relation yields the expansion

$$\begin{aligned} S(t) &= (a_1+a_2)A + (b_1+b_2)B \\ &\qquad - \tfrac{1}{2}\,t\,\big(a_1(b_1+b_2) + a_2(b_2-b_1)\big)\,\big[A,B\big] + \mathscr{O}\big(t^2\big) \approx A+B\,. \end{aligned}$$

Difficulties. Justify approach for unbounded operators A, B. Capture precise form of remainder and obtain optimal regularity requirements on the exact solution.

Quadrature formulas

Approach. Alternative local error expansion provides optimal error bounds regarding the regularity of the exact solution for (non)linear evolutionary Schrödinger equations with (un)bounded potentials.

- **Linear problems.** Jahnke and Lubich (2000), Neuhauser and Th. (2009), Th. (2008)
- **Nonlinear problems.** Gauckler (2010), Koch, Neuhauser, and Th. (2010), Lubich (2008)

Main tools.

- Variation-of-constants formula
- Stepwise expansion of e^{tB}
- Quadrature formulas for multiple integrals
- Bounds for iterated commutators
- Characterise domains of unbounded operators

Local error expansion (Strang splitting)

Assumptions. Suppose $a_1 + a_2 = 1$ and

$$\big\|\,[A,B]\,u\big\|_X + \big\|\,[A,[A,B]]\,u\big\|_X \leq C_{\mathrm{ad}}\,\|u\|_D\,,$$

$$\|B\|_{X\leftarrow X} \leq C_B\,, \quad \big\|\mathrm{e}^{tA}\big\|_{X\leftarrow X} \leq \mathrm{e}^{M_A|t|}\,, \quad \big\|\mathrm{e}^{tB}\big\|_{X\leftarrow X} \leq \mathrm{e}^{M_B|t|}\,.$$

Local error expansion. For exponential operator splitting methods involving two compositions it follows

$$\begin{aligned}\mathscr{L}(h_n)\,u(t_n) &= \Big(\mathrm{e}^{b_2h_nB}\,\mathrm{e}^{a_2h_nA}\,\mathrm{e}^{b_1h_nB}\,\mathrm{e}^{a_1h_nA} - \mathrm{e}^{h_n(A+B)}\Big)\,u(t_n)\\ &= h_n\,\big(b_1+b_2-1\big)\,\mathrm{e}^{h_nA}B\,u(t_n)\\ &\qquad - h_n^2\,\mathrm{e}^{h_nA}\Big(\big(a_1b_1+b_2-\tfrac12\big)\,\big[A,B\big] + \tfrac12\,\big((b_1+b_2)^2-1\big)\,B^2\Big)\,u(t_n)\\ &\qquad + \mathscr{O}\,\big(h_n^3, C_B^3, M_A, M_B, C_{\mathrm{ad}}, \|u(t_n)\|_D\big)\,.\end{aligned}$$

Linear Schrödinger equations. Choose $X = L^2(\Omega)$, $D = H^2(\Omega)$, and $M_A = M_B = 0$, see Th. (2008).

Order conditions (Strang splitting)

Order conditions. Requirement $\mathscr{L}(h_n) = \mathscr{O}\big(h_n^{p+1}\big)$ for $p = 1, 2$ implies (classical) order conditions

$$a_1 + a_2 = 1\,, \qquad b_1 + b_2 = 1\,, \qquad (p = 1)$$
$$(1 - a_1)\, b_1 = \tfrac{1}{2}\,. \qquad (p = 2)$$

Examples. Retain first order Lie–Trotter splitting

$$s = 1\,, \qquad a_1 = 1\,, \quad b_1 = 1\,,$$
$$s = 2\,, \qquad a_1 = 0\,, \quad a_2 = 1\,, \quad b_1 = 1\,, \quad b_2 = 0\,,$$

and second order Strang splitting

$$s = 2\,, \qquad a_1 = \tfrac{1}{2} = a_2\,, \quad b_1 = 1\,, \quad b_2 = 0\,,$$
$$s = 2\,, \qquad a_1 = 0\,, \quad a_2 = 1\,, \quad b_1 = \tfrac{1}{2} = b_2\,.$$

Local error expansion

Extension. Local error expansion for high-order splitting methods applied to nonlinear problems, see KOCH, NEUHAUSER, AND TH., *High-order splitting methods for nonlinear evolution equations and application to the MCTDHF equations in electron dynamics* (2010).

Theorem (Local error expansion)

The defect operator of an exponential operator splitting method admits the (formal) expansion

$$D(t,v) = \sum_{k=1}^{p} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|\le p-k}} \frac{1}{\mu!}\, t^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} ad_{D_A}^{\mu_{ell}}(D_B)\, e^{tD_A}\, v + R_{p+1}(t,v)\,,$$

$$C_{k\mu} = \sum_{\lambda\in L_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\, c_{\lambda_\ell}^{\mu_\ell} - \prod_{\ell=1}^{k} \frac{1}{\mu_\ell+\dots+\mu_k+k-\ell+1}\,.$$

Differential equations

Approach. Alternative local error representation exploited in Descombes et al. (2007), Descombes and Schatzman (2002), and Descombes and Th. (2010). Investigation of evolutionary problems involving critical parameters.

Basic idea. Deduce differential equation for splitting operator

$$\mathscr{S}(t) = \prod_{j=1}^{s} \mathrm{e}^{b_j t B}\, \mathrm{e}^{a_j t A}, \qquad t \geq 0,$$

that is closely related to differential equation for evolution operator

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

Main tools. Variation-of-constants formula, iterated commutators.

Local error representation (Lie–Trotter splitting)

Consider first order Lie–Trotter splitting. Determine first time derivative of $\mathscr{S}(t) = \mathrm{e}^{tB}\,\mathrm{e}^{tA}$

$$\mathscr{S}'(t) = B\,\mathscr{S}(t) + \mathrm{e}^{tB} A\,\mathrm{e}^{tA} = (A+B)\,\mathscr{S}(t) + \left(\mathrm{e}^{tB} A - A\,\mathrm{e}^{tB}\right)\mathrm{e}^{tA}$$

and obtain following initial value problem for splitting operator

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

Compare with initial value problem for evolution operator

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

By variation-of-constants formula it follows for $\mathscr{L} = \mathscr{S} - \mathscr{E}$

$$\mathscr{L}(t) = \int_0^t \mathscr{E}(t-\tau)\,\mathscr{R}(\tau)\,\mathrm{d}\tau\,, \quad \mathscr{R}(t) = \left[\mathrm{e}^{tB}, A\right]\mathrm{e}^{tA}\,, \qquad t \geq 0\,.$$

Local error representation (Lie–Trotter splitting)

Consider remainder $\mathscr{R}(t) = \big[\mathrm{e}^{tB}, A\big]\,\mathrm{e}^{tA}$. Determine first time derivative of $r(t) = \big[\mathrm{e}^{tB}, A\big] = \mathrm{e}^{tB} A - A\,\mathrm{e}^{tB}$

$$r'(t) = B\,\mathrm{e}^{tB} A - A\,B\,\mathrm{e}^{tB} = B\,r(t) + \big(B\,A - A\,B\big)\,\mathrm{e}^{tB}$$

and obtain following initial value problem

$$r'(t) = B\,r(t) + \big[B, A\big]\,\mathrm{e}^{tB}\,, \quad t \geq 0\,, \qquad r(0) = 0\,.$$

By variation-of-constants formula it follows

$$r(t) = \int_0^t \mathrm{e}^{\tau B}\big[B, A\big]\,\mathrm{e}^{(t-\tau)B}\,\mathrm{d}\tau\,, \qquad t \geq 0\,.$$

Local error representation (Lie–Trotter splitting)

Local error. Above considerations imply local error representation

$$\begin{aligned}\mathscr{L}(h_n) &= \left(\mathrm{e}^{h_n B}\,\mathrm{e}^{h_n A} - \mathrm{e}^{h_n (A+B)}\right) u(t_n)\\ &= \int_0^{h_n}\int_0^{\tau_1} \mathscr{E}(h_n-\tau_1)\,\mathrm{e}^{\tau_2 B}\,[B,A]\,\mathrm{e}^{-\tau_2 B}\,\mathscr{S}(\tau_1)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,.\end{aligned}$$

If $\left\|\mathscr{E}(h_n-\tau_1)\,\mathrm{e}^{\tau_2 B}\,[B,A]\,\mathrm{e}^{-\tau_2 B}\,\mathscr{S}(\tau_1)\,u(t_n)\right\|_X \le C\,\|u(t_n)\|_D$ local error estimate follows at once

$$\left\|\mathscr{L}(h_n)\,u(t_n)\right\|_X \le C\,h_n^2\,.$$

Extension. Exact local error representation for high-order splitting methods deduced in DESCOMBES AND TH. (2010).

Objective. Study local error representation for evolutionary problems involving critical parameters.

Local error representation

Theorem (Local error representation)

$$\mathscr{L}(t) = \int_0^t \mathscr{E}(t-\tau)\,\mathscr{R}(\tau)\,d\tau\,, \quad t \geq 0\,, \qquad \mathscr{R} = \mathscr{S}_{\sigma+1}^{s}\,\mathscr{T}\,\mathscr{S}_1^{\sigma}\,,$$

$$\sigma = \begin{cases} \frac{1}{2}\,s\,, & s \text{ even}, \\ \frac{1}{2}\,(s+1)\,, & s \text{ odd}, \end{cases} \qquad \mathscr{T} = \sum_{j=0}^{\sigma-1} C_{\sigma-j,j} + \sum_{j=0}^{s-\sigma-1} D_{\sigma+1+j,j}\,,$$

$$\mathscr{I}_{\pm}(L_1,L_2,t) = \int_0^t e^{\pm tL_1}\,[L_1,L_2]\,e^{\mp tL_1}\,d\tau\,,$$

$$C_{k,0} = c_k\,\mathscr{I}_+(B_k,A) + d_{k-1}\,\mathscr{I}_+(A_k,B) + d_{k-1}\mathscr{I}_+\big(B_k,\mathscr{I}_+(A_k,B)\big)\,,$$

$$C_{k,j} = C_{k,j-1} + \mathscr{I}_+(A_{k+j},C_{k,j-1}) + \mathscr{I}_+(B_{k+j},C_{k,j-1})$$
$$+ \mathscr{I}_+\big(B_{k+j},\mathscr{I}_+(A_{k+j},C_{k,j-1})\big)\,, \quad 1 \leq k \leq \sigma\,,\ 0 \leq j \leq \sigma-1\,,$$

$$D_{k,0} = c_k\,\mathscr{I}_-(B_k,A) - c_k\,\mathscr{I}_-\big(A_k,\mathscr{I}_-(B_k,A)\big) + d_{k-1}\,\mathscr{I}_-(A_k,B)\,,$$

$$D_{k,j} = D_{k,j-1} - \mathscr{I}_-(A_{k-j},D_{k,j-1}) - \mathscr{I}_-(B_{k-j},D_{k,j-1})$$
$$+ \mathscr{I}_-\big(A_{k-j},\mathscr{I}_-(B_{k-j},D_{k,j-1})\big)\,, \quad \sigma+1 \leq k \leq s\,,\ 0 \leq j \leq s-\sigma-1\,.$$

Application to linear Schrödinger equations

Model problem. Consider linear Schrödinger equation

$$\partial_t \psi(x,t) = \mathrm{i}\,\varepsilon\,\partial_x^2\,\psi(x,t) - \tfrac{\mathrm{i}}{\varepsilon}\,U(x)\,\psi(x,t)$$

under periodic boundary condition on a bounded interval $\Omega \subset \mathbb{R}$.

Abstract formulation. Employ abstract formulation

$$u'(t) = A\,u(t) + B\,u(t)\,, \qquad A = \mathrm{i}\,\varepsilon\,\partial_x^2\,, \quad B = -\tfrac{\mathrm{i}}{\varepsilon}\,U\,.$$

Stone's Theorem implies that the unbounded differential operator A and the multiplication operaror B generate unitary evolution operators for any $\varepsilon \in \mathbb{R}$ and $t \in \mathbb{R}$

$$\big\| \mathrm{e}^{t(A+B)} \big\|_{L^2 \leftarrow L^2} = 1\,, \quad \big\| \mathrm{e}^{tA} \big\|_{L^2 \leftarrow L^2} = 1\,, \quad \big\| \mathrm{e}^{tB} \big\|_{L^2 \leftarrow L^2} = 1\,.$$

Application to linear Schrödinger equations

Employ above local error representation

$$\mathscr{L}(h_n) = \int_0^{h_n} \int_0^{\tau_1} \mathrm{e}^{(h_n-\tau_1)(A+B)}\, \mathrm{e}^{\tau_2 B} \big[B, A\big]\, \mathrm{e}^{(\tau_1-\tau_2)B}\, \mathrm{e}^{\tau_1 A}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \,.$$

Determine bound for first Lie-commutator

$$\big[A, B\big]\, u = \big[\partial_x^2, U\big]\, u = \partial_x^2 (U u) - U\, \partial_x^2 u = \big(2\, \partial_x U\, \partial_x + \partial_x^2 U\, I\big)\, u\,,$$

$$\big\| [A, B]\, u \big\|_{L^2} \leq C\big(\partial_x^2 U\big)\, \|u\|_{H^1}\,, \qquad C(\partial_x^2 U) = \max\{2\, \|\partial_x U\|_{L^\infty}, \|\partial_x^2 U\|_{L^\infty}\}\,.$$

Together with the above bounds this further implies the estimate

$$\begin{aligned} \big\|\mathscr{L}(h_n)\, u(t_n)\big\|_{L^2} &\leq C\big(\partial_x^2 U\big) \int_0^{h_n} \int_0^{\tau_1} \Big\| \mathrm{e}^{-\mathrm{i}\,(\tau_1-\tau_2)\, U/\varepsilon}\, \mathrm{e}^{\mathrm{i}\,\varepsilon\,\tau_1 \partial_x^2}\, u(t_n) \Big\|_{H^1} \mathrm{d}\tau_2\, \mathrm{d}\tau_1 \\ &\leq C\big(\partial_x^2 U\big)\, \frac{h_n^2}{\varepsilon} \Big(h_n\, \|\partial_x U\|_{L^\infty} \|u(t_n)\|_{L^2} + \varepsilon\, \|u(t_n)\|_{H^1} \Big)\,. \end{aligned}$$

Application to linear Schrödinger equations

Local error estimate. Due to $\|u(t_n)\|_{L^2} = \|u(0)\|_{L^2}$ it holds

$$\big\|\mathscr{L}(h_n)\,u(t_n)\big\|_{L^2} \leq C\big(\partial_x^2 U\big)\,\frac{h_n^2}{\varepsilon}\,\Big(h_n\,\|\partial_x U\|_{L^\infty}\,\|u(0)\|_{L^2} + \varepsilon\,\|u(t_n)\|_{H^1}\Big).$$

Auxiliary estimate. First spatial derivative $\chi = \partial_x \psi$ satisfies

$$\begin{aligned}\partial_t \psi(x,t) &= \mathrm{i}\,\varepsilon\,\partial_x^2\,\psi(x,t) - \tfrac{\mathrm{i}}{\varepsilon}\,U(x)\,\psi(x,t)\,,\\ \partial_t \chi(x,t) &= \mathrm{i}\,\varepsilon\,\partial_x^2\,\chi(x,t) - \tfrac{\mathrm{i}}{\varepsilon}\,U(x)\,\chi(x,t) - \tfrac{\mathrm{i}}{\varepsilon}\,\partial_x U(x)\,\psi(x,t)\,.\end{aligned}$$

In abstract form with $v(t) = \chi(\cdot,t)$

$$v'(t) = (A+B)\,v(t) + \partial_x B\,u(t)\,,\quad t \geq 0\,,\qquad v(0)\ \text{given}\,.$$

By means of the variation-of-constants formula it follows

$$\varepsilon\,\|u(t_n)\|_{H^1} \leq \sqrt{2}\,\varepsilon\,\|u(0)\|_{H^1} + t_n\,\|\partial_x U\|_{L^\infty}\,\|u(0)\|_{L^2}\,.$$

Application to linear Schrödinger equations

Global error estimate. Employ Lady Windermere's Fan argument

$$u_N - u(t_N) = \prod_{j=0}^{N-1} \mathscr{S}(h_j)\big(u_0 - u(0)\big) + \sum_{n=0}^{N-1} \prod_{j=n+1}^{N-1} \mathscr{S}(h_j)\,\mathscr{L}(h_n)\,u(t_n)$$

to obtain global error estimate

$$\|u_N - u(t_N)\|_{L^2} \le \|u_0 - u(0)\|_{L^2} + \sum_{n=0}^{N-1} \|\mathscr{L}(h_n)\,u(t_n)\|_{L^2}$$

$$\le \|u_0 - u(0)\|_{L^2}$$

$$+ C\big(\partial_x^2 U\big) \sum_{n=0}^{N-1} \frac{h_n^2}{\varepsilon} \Big(h_n \|\partial_x U\|_{L^\infty} \|u(t_n)\|_{L^2} + \varepsilon \|u(t_n)\|_{H^1}\Big)$$

$$\le \|u_0 - u(0)\|_{L^2}$$

$$+ C\big(\partial_x^2 U\big) \sum_{n=0}^{N-1} \frac{h_n^2}{\varepsilon} \Big((h_n + t_n)\,\|\partial_x U\|_{L^\infty}\,\|u(0)\|_{L^2} + \sqrt{2}\,\varepsilon\,\|u(0)\|_{H^1}\Big).$$

Global error estimate (Lie-Trotter splitting)

Theorem (Global error estimate, Lie-Trotter splitting)

Suppose that the potential $U : \Omega \to \mathbb{R}$ is twice differentiable with bounded derivatives and that the initial value $u(0)$ remains bounded in $H^1(\Omega)$. Then, the following global error estimate holds for the Lie–Trotter splitting method

$$\|u_N - u(t_N)\|_{L^2} \leq \|u_0 - u(0)\|_{L^2} + C\big(\partial_x^2 U\big) \sum_{n=0}^{N-1} \frac{h_n^2}{\varepsilon} \Big(t_n \|\partial_x U\|_{L^\infty} \|u(0)\|_{L^2} + \varepsilon \|u(0)\|_{H^1}\Big)$$

with constant $C(\partial_x^2 U) = 2 \max\{2\|\partial_x U\|_{L^\infty}, \|\partial_x^2 U\|_{L^\infty}\}$.

Global error estimate

Theorem (Global error estimate)

Assume that an exponential operator splitting method satisfies the (classical) pth-order conditions for $p \geq 1$. Suppose further that the potential $U : \Omega \to \mathbb{R}$ is $2p$ times differentiable with bounded derivatives and that the initial value $u(0)$ remains bounded in $H^p(\Omega)$. Then, the following global error estimate is valid

$$\left\| u_N - u(t_N) \right\|_{L^2} \leq \left\| u_0 - u(0) \right\|_{L^2} + C \sum_{n=0}^{N-1} \frac{h_n^{p+1}}{\varepsilon} \sum_{j=0}^{p} \varepsilon^j \left\| u(0) \right\|_{H^j}$$

with constant $C > 0$ depending on $\left\| \partial_x^j U \right\|_{L^\infty}$, $0 \leq j \leq 2p$, and t_N.

Classical Wentzel–Kramers–Brillouin initial values. If $\varepsilon^j \left\| u(0) \right\|_{H^j} \leq M_j$ it follows with $h = \max\{h_n, 0 \leq n \leq N-1\}$

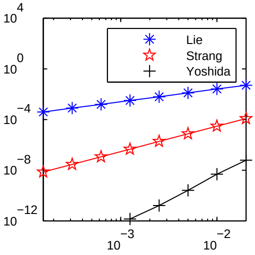
$$\left\| u_N - u(t_N) \right\|_{L^2} \leq \left\| u_0 - u(0) \right\|_{L^2} + C \, \frac{h^p}{\varepsilon} \, .$$

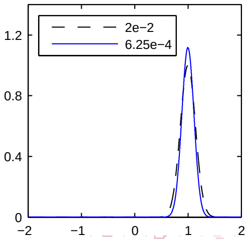
Numerical example

Model problem. Consider linear Schrödinger equation

$$\mathrm{i}\,\varepsilon\,\partial_t\psi(x,t) = -\tfrac{1}{2}\,\varepsilon^2\Delta\,\psi(x,t) + \tfrac{1}{2}\,x^2\,\psi(x,t)\,,$$
$$\psi(x,0) = \mathrm{e}^{-25\,(x-1/2)^2}\,\mathrm{e}^{\mathrm{i}\,(1+x)/\varepsilon}\,,\qquad -2\le x\le 2\,,\quad 0\le t\le 0.64\,,$$

subject to periodic boundary conditions, see also BAO, JIN, AND MARKOWICH (2002). Time integration by time-splitting Fourier spectral methods.





Numerical example

Dependence on critical parameter. For a fixed time stepsize h and different parameter values ε determine the temporal error $\mathrm{err}(\varepsilon)$ and the corresponding ratios

$$\mathrm{ratio}(\varepsilon) = \log\left(\frac{\mathrm{err}(\varepsilon)}{\mathrm{err}(\varepsilon/2)}\right) / \log(2).$$

critical parameter	global error ($p = 1$)	ratio ($p = 1$)
0.020000	1.9083138555435586e-001	-9.546799767444528e-001
0.010000	3.698597849512038e-001	-8.876216181670132e-001
0.005000	6.842862992889865e-001	-5.347591837576926e-001
0.002500	9.913257778242306e-001	

critical parameter	global error ($p = 1$, $h/4$)	ratio ($p = 1$, $h/4$)
0.020000	4.759083334913000e-002	-9.795186767037100e-001
0.010000	9.383995971552103e-002	-9.887465227244113e-001
0.005000	1.862216516131053e-001	-9.728227523631063e-001
0.002500	3.654929489758708e-001	-8.940389596804734e-001
0.001250	6.792216918020555e-001	-5.448625017980767e-001
0.000625	9.909038225216962e-001	

Numerical example

Conclusion. Higher-order exponential operator splitting methods are favourable for the time-integration of linear Schrödinger equations in the semi-classical regime, provided that the time stepsize fulfills the requirement h sufficiently smaller than $\sqrt[p]{\varepsilon}$.

critical parameter	global error ($p = 2$)	ratio ($p = 2$)
0.020000	7.729399568231682e-004	-9.118303667208469e-001
0.010000	1.454233181843335e-003	-9.763859382146316e-001
0.005000	2.861248016688788e-003	-9.939800245764093e-001
0.002500	5.698667358149775e-003	-9.984569484384943e-001
0.001250	1.138515107875544e-002	-9.994894832381450e-001
0.000625	2.276224600976379e-002	

critical parameter	global error ($p = 4$)	ratio ($p = 4$)
0.020000	1.760514889939917e-006	-9.667658211629046e-001
0.010000	3.440845825158100e-006	-9.914955815231308e-001
0.005000	6.841244690937256e-006	-9.978612083014881e-001
0.002500	1.366222015470383e-005	-9.994645019027982e-001
0.001250	2.731429993314372e-005	-9.998660746803390e-001
0.000625	5.462352893104207e-005	

Conclusions and future work

Contents. Derivation of different local error expansions for high-order exponential operator splitting methods applied to evolutionary problems.

- Local error expansion based on quadrature formulas.
- Local error representation based on differential equations.

Applications to linear evolutionary Schrödinger equations in the semi-classical regime.

Future work. Error analysis for high-order splitting methods applied to nonlinear evolutionary problems involving critical parameters. First results for Lie-Trotter splitting method.