Operator splitting methods for nonlinear Schrödinger equations

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Theme

Splitting methods. Efficient time integration of nonlinear evolution equations by exponential operator splitting methods

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), & t \in (0,T), \\ u(0) \text{ given}, \end{cases}$$

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau_{n-1}D_A}\, \mathrm{e}^{b_{s+1-j}\tau_{n-1}D_B}\, u_{n-1}$$

$$\approx\ u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1}D_F}\, u(t_{n-1}), \qquad n \in \{1,\dots,N\}.$$

Applications.

- Nonlinear Schrödinger equations (GPS, MCTDHF)
- Parabolic equations
- Wave equations

Outline

Theme. Theoretical analysis of exponential operator splitting methods for nonlinear Schrödinger equations.

Main inspiration. Work by W. BAO and CH. LUBICH.

Collaborators. Joint work with

- W. AUZINGER, H. HOFSTÄTTER, O. KOCH (Vienna)
- PH. CHARTIER, F. MÉHATS (Rennes)
- S. DESCOMBES (Nice)

Outline.

- **Applications.** Splitting methods for the time integration of the MCTDHF equations and time-dependent Gross–Pitaevskii equations.
- **Theoretical analysis.** Stability and error analysis of high-order splitting methods for linear and nonlinear Schrödinger equations.
- **Practical aspects.** Error behaviour of splitting methods for nonlinear Schrödinger equations in different regimes. Reliable and efficient time integration by local error estimation. Construction and analysis of a posteriori local error estimators for high-order splitting methods.

Nonlinear Schrödinger equations

Multi-configuration time-dependent Hartree–Fock equations
Time-dependent Gross–Pitaevskii equations

Electronic Schrödinger equations

Electronic Schrödinger equation. Model for system of unbound fermions interacting by Coulomb force. Time-dependent linear Schrödinger equation for wave function associated with D particles
$\Psi : \mathbb{R}^{3D} \times [0,T] \to \mathbb{C} : (x,t) \to \Psi(x,t)$

$$\mathrm{i}\,\partial_t \Psi(x,t) = \mathscr{H}(x)\,\Psi(x,t) = \mathscr{A}\Psi(x,t) + \mathscr{V}(x)\Psi(x,t)$$

subject to asymptotic boundary conditions and initial condition.

- Differential operator $\mathscr{A}$ comprises second derivatives with respect to each spatial coordinate

$$\mathscr{A} = -\tfrac{1}{2}\Delta\,, \qquad \Delta = \Delta_{x_1} + \cdots + \Delta_{x_D}\,, \qquad x = (x_1,\ldots,x_D) \in \mathbb{R}^{3D}\,,$$
$$\Delta_{x_j} = \partial^2_{x_{j1}} + \partial^2_{x_{j2}} + \partial^2_{x_{j3}}\,, \qquad x_j = (x_{j1},x_{j2},x_{j3})\,, \qquad j \in \{1,\ldots,D\}\,.$$

- Multiplication operator $\mathscr{V}$ takes pairwise Coulomb interaction of particles into account

$$\mathscr{V}(x) = \sum_{1\le j<k\le D} \frac{1}{|x_j - x_k|}\,, \qquad x = (x_1,\ldots,x_D) \in \mathbb{R}^{3D}\,.$$

MCTDHF approach

MCTDHF approach. Multi-configuration time-dependent Hartree–Fock approach allows to replace high-dimensional linear Schrödinger equation by system of coupled linear ordinary differential equations and nonlinear partial differential equations in three space dimensions (computationally treatable problem).

- **Approximation.** Replace multi-particle wave function by linear combination of Hartree products with orbitals depending on coordinates of single particle and satisfying additional orthogonality and gauge conditions

$$\Psi(x,t) \approx U(x,t) = \sum_{\mu\in\mathcal{M}} a_\mu(t)\,\Phi_\mu(x,t) = \sum_{\mu\in\mathcal{M}} a_\mu(t)\,\varphi_{\mu_1}(x_1,t)\cdots\varphi_{\mu_D}(x_D,t)\,.$$

- **Pauli exclusion principle.** Reduction to antisymmetrised products.
- **MCTDHF equations.** Derivation of equations of motion for orbitals and coefficients in linear combination of Hartree products via Dirac–Frenkel variational principle

$$\mathrm{i}\partial_t U - \mathscr{H}U \perp \delta U\,.$$

Approximation

Approximation. Approximation of multi-particle wave function by linear combination of Hartree products involving orbitals $\varphi_k : \mathbb{R}^3 \times [0,T] \to \mathbb{C}$ for $k \in \{1,\dots,K\}$

$$\Psi(x,t) \;\approx\; U(x,t) = \sum_{\mu \in \mathcal{M}} a_\mu(t)\, \Phi_\mu(x,t)\,,$$

$$\mathcal{M} = \Big\{ \mu = (\mu_1,\dots,\mu_D) \in \mathbb{N}^D : \mu_j \in \{1,\dots,K\} \text{ for } j \in \{1,\dots,D\} \Big\},$$

$$\Phi_\mu(x,t) = \Big(\bigotimes_{j=1}^{D} \varphi_{\mu_j} \Big)(x,t) = \varphi_{\mu_1}(x_1,t) \cdots \varphi_{\mu_D}(x_D,t)\,, \qquad x = (x_1,\dots,x_D) \in \mathbb{R}^{3D}\,, \qquad t \in (0,T)\,.$$

Pauli exclusion principle. Significant reduction from K^D to $\binom{K}{D}$ different coefficients due to additional requirement of antisymmetry (permutation $\sigma : \{1,\dots,D\} \to \{1,\dots,D\}$)

$$a_{\sigma(\mu)} = \operatorname{sign}(\sigma)\, a_\mu\,, \qquad \sigma(\mu) = \big(\mu_{\sigma(1)},\dots,\mu_{\sigma(D)}\big)\,, \qquad \mu = (\mu_1,\dots,\mu_D) \in \mathcal{M}\,.$$

In particular $a_\mu = 0$ if $\mu_j = \mu_k$ for some $1 \le j < k \le D$.

Two-particles case involves $\binom{K}{2} = \frac{1}{2} K(K-1)$ different coefficients: Consideration of $\sigma = (12)$ with $\operatorname{sign}(\sigma) = -1$ implies $a_{\mu_2\mu_1} = -a_{\mu_1\mu_2}$ and in particular $a_{\mu_1\mu_1} = -a_{\mu_1\mu_1} = 0$ for $\mu_1,\mu_2 \in \{1,\dots,K\}$.

Orthogonality and gauge conditions. Additional orthogonality and gauge conditions on orbitals (with self-adjoint operator $\mathcal{A}_0 = -\frac{1}{2}\Delta$, $t \in [0,T]$, $k,\ell \in \{1,\dots,K\}$)

$$\big(\varphi_k(\cdot,t) \,|\, \varphi_\ell(\cdot,t)\big)_{L^2} = \delta_{k\ell}\,, \qquad \big(\varphi_k(\cdot,t) \,|\, \mathrm{i}\,\partial_t \varphi_\ell(\cdot,t) - \mathcal{A}_0\, \varphi_\ell(\cdot,t)\big)_{L^2} = 0\,.$$

MCTDHF equations

MCTDHF equations. Application of Dirac–Frenkel variational principle yields associated equations of motion. MCTDHF equations constitute system of ordinary differential equations for coefficients $a_\mu : [0,T] \to \mathbb{C}$ ($\mu \in \mathscr{M}$) and partial differential equations for orbitals $\varphi_k : \mathbb{R}^3 \times [0,T] \to \mathbb{C}$ ($k \in \{1,\dots,K\}$)

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,a_\mu(t) = \sum_{\nu\in\mathscr{M}} \big(\Phi_\mu(\cdot,t)\,|\,\mathscr{V}\,\Phi_\nu(\cdot,t)\big)_{L^2}\,a_\nu(t)\,,$$

$$\mathrm{i}\,\partial_t\varphi_k(\xi,t) = \mathscr{A}_0\,\varphi_k(\xi,t) + (I-P)\sum_{\ell,m=1}^{K}\rho^{-1}_{k\ell}(t)\,\big(\Psi_\ell(\cdot,t)\,|\,\mathscr{V}\,\Psi_m(\cdot,t)\big)_{L^2}\,\varphi_m(\xi,t)\,,$$

$$\xi\in\mathbb{R}^3\,,\quad t\in[0,T]\,,\quad k\in\{1,\dots,K\}\,,\quad \mu\in\mathscr{M}\,,$$

subject to asymptotic boundary conditions and initial conditions.

Nonlinearity. Nonlinearity comprises terms of the form

$$\int_{\mathbb{R}^3}\frac{1}{|\xi-\eta|}\,\overline{f_1(\xi)}\,g_1(\xi)\,\mathrm{d}\xi\;f_2(\eta)\,,\qquad \eta\in\mathbb{R}^3\,,\qquad \iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{1}{|\xi-\eta|}\,\overline{f_1(\xi)\,f_2(\eta)}\,g_1(\xi)\,g_2(\eta)\,\mathrm{d}\xi\,\mathrm{d}\eta\,.$$

Remark. Second iterated commutator of Laplacian and nonlinearity comprises certain combinations of orbitals

$$\overline{f_1}\,f_2\,\Delta f_3\,,\qquad f_3\,\overline{\nabla f_1}\cdot\nabla f_3\,.$$

Essential for error analysis of splitting methods (considerations for MCTDHF equations in principle similar to considerations for cubic Schrödinger equation).

Existence and regularity result

Existence result. Theoretial result ensuring existence and uniqueness of regular solution to MCTDHF equations essential for stability and convergence analysis of splitting methods.

Theorem (Koch and Lubich, 2008)

Let $m \in \mathbb{N}_{\geq 2}$. Provided that the initial density matrix $\rho(0)$ is non-singular and that the initial values for the orbitals satisfy $\varphi_k(\cdot,0) \in H^m(\mathbb{R}^3)$ for $k \in \{1,\dots,K\}$, there exists a unique strong solution to the MCTDHF equations such that

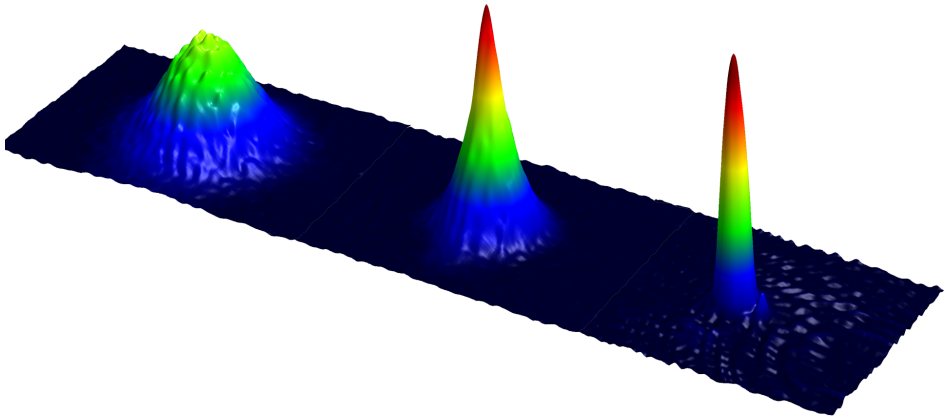
$$\varphi_k(\cdot,t) \in H^m(\mathbb{R}^3), \qquad k \in \{1,\dots,K\}, \qquad t \in [0,T),$$

where either $T = \infty$ or $\rho(t)$ becomes singular for $t \uparrow T$.

Bose–Einstein condensation

In our laboratories temperatures are measured in micro- or nanokelvin ... In this ultracold world ... atoms move at a snail's pace ... and behave like matter waves. Interesting and fascinating new states of quantum matter are formed and investigated in our experiments.

(GRIMM ET AL., Innsbruck)

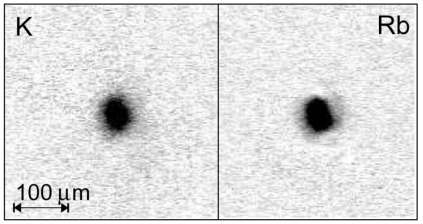


Bose–Einstein condensation in dilute gases. In 1925 Albert Einstein predicted that at (very) low temperatures particles in a (dilute) gas could all reside in the same quantum state. This peculiar gaseous state, a Bose–Einstein condensate, was produced in the laboratory for the first time in 1995 using the powerful laser-cooling methods developed in recent years. These condensates exhibit quantum phenomena on a large scale, and investigating them has become one of the most active areas of research in contemporary physics. See PETHICK, SMITH (2002).

Physical experiments (University of Innsbruck). Realisation of ground state and investigation of time evolution (H.-C. NÄGERL, M. MARK).

Gross–Pitaevskii equations

Physical experiments. Observation of multi-component Bose–Einstein condensates. Realisation of double species ^{87}Rb ^{41}K BEC at LENS, see G. THALHAMMER ET AL. (2008).



Theoretical model. Mathematical description (of certain aspects) of multi-component Bose–Einstein condensate by system of coupled time-dependent Gross–Pitaevskii equations for macroscopic wave function $\Psi : \mathbb{R}^d \times [0,T] \to \mathbb{C}^J : (x,t) \mapsto \Psi(x,t)$

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

$$V_j(x) \approx \sum_{\ell=1}^{d} \Big(\frac{m_j}{2}\,\omega_{j\ell}^2\,(x_\ell - \zeta_{j\ell})^2 + \kappa_{j\ell} \big(\sin(q_{j\ell}\,x_\ell)\big)^2 \Big), \qquad \big\|\Psi_j(\cdot,0)\big\|_{L^2}^2 = N_j\,,$$

$$x \in \mathbb{R}^d\,, \qquad t \in [0,T]\,, \qquad j \in \{1,\ldots,J\}\,.$$

Model equation

Model problem. Consider nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = \left(-\frac{1}{2}\Delta + U(x) + \vartheta \left|\psi(x,t)\right|^2 \right) \psi(x,t)\,, \\ \psi(x,0) \text{ given}, \qquad (x,t) \in \mathbb{R}^d \times [0,T]\,, \end{cases}$$

subject to asymptotic boundary conditions.

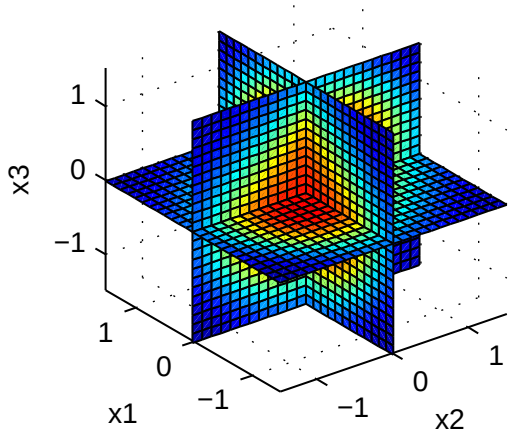


Illustration. Solution profile $|\psi|^2$ of GPE in 3D ($\omega = \vartheta = 1$, $T = 3$, $M = 128^3$, tol $= 10^{-6}$).

Geometric properties. Preservation of particle number $\|\psi(\cdot,t)\|_{L^2}^2$ and energy functional

$$E\big(\psi(\cdot,t)\big) = \Big(\big(-\tfrac{1}{2}\Delta + U + \tfrac{1}{2}\vartheta\,|\psi(\cdot,t)|^2 \big)\,\psi(\cdot,t) \,\Big|\, \psi(\cdot,t) \Big)_{L^2}\,, \qquad t \in [0,T]\,.$$

Ground state. Solution of special form $\psi(x,t) = \mathrm{e}^{-\mathrm{i}\mu t}\,\varphi(x)$ that minimises energy functional. Useful as reliable reference solution in time integration.

Illustration (Ground state computation, Time evolution)

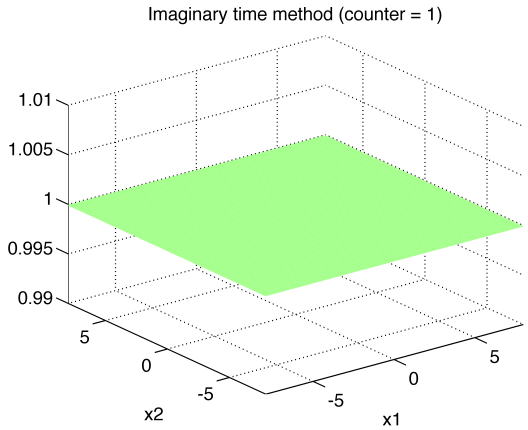
Simulation. Model equation with harmonic potential ($d = 2$, $\vartheta = 10$). Computation of groundstate solution ($\omega_1 = 1 = \omega_2$) and time evolution ($\omega_1 = 2 = \omega_2$) for

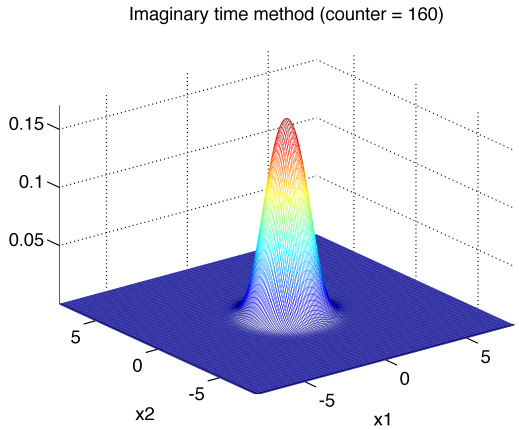
$$\mathrm{i}\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\Delta + U(x) + \vartheta\,|\psi(x,t)|^2 \Big)\,\psi(x,t)\,.$$

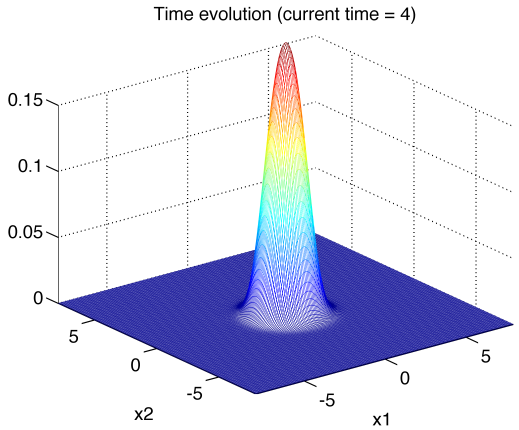
Space discretisation by Fourier pseudo-spectral method ($x \in [-8,8] \times [-8,8]$, $M = 200 \times 200$). Artificial time integration by 2(1) pair based on Strang and Lie–Trotter splitting methods. Time integration by embedded 4(3) pair based on 4th-order splitting method by BLANES, MOAN (2002) ($t \in [0,4]$, $\mathrm{tol} = 10^{-6}$).

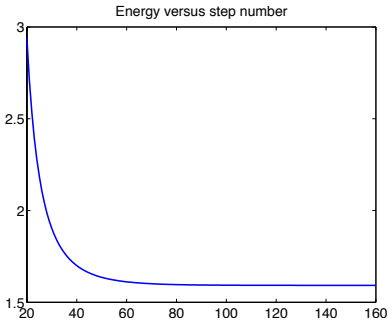
Movie
Ground state, Time Evolution, Energy, Time stepsizes (MATLAB)

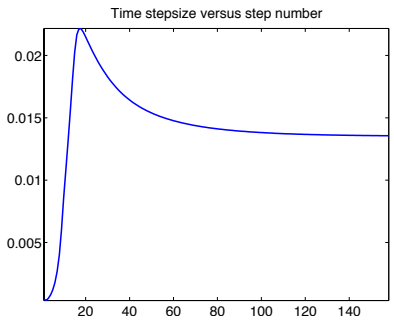
Illustrations (Ground state computation, Time evolution)

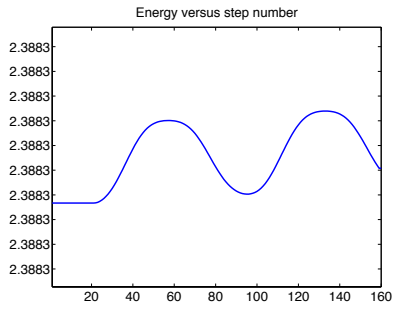


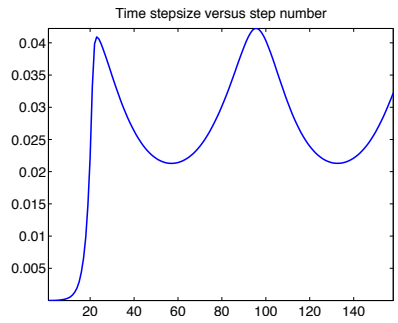












Abstract formulation

Abstract formulation. Compact formulation of model equation as nonlinear evolution equation on Hilbert space $(X, (\cdot\,|\,\cdot)_X, \|\cdot\|_X)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\, u(t) + B\big(u(t)\big)\, u(t)\,, \qquad t \in (0,T)\,.$$

- **Linear subproblem.** Solution representation for subproblem involving linear differential operator A (related to Laplacian) often relies on spectral decomposition (employ eigenrelation $A\mathscr{B}_m = \mu_m \mathscr{B}_m$ for $m \in \mathscr{M}$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = A\, v(t)\,, \qquad t \in (0,T)\,,$$

$$v(0) = \sum_{m\in\mathscr{M}} v_m \mathscr{B}_m\,, \qquad v(t) = \mathrm{e}^{tA}\, v(0) = \sum_{m\in\mathscr{M}} v_m\, \mathrm{e}^{t\mu_m}\, \mathscr{B}_m\,, \quad t \in [0,T]\,.$$

- **Nonlinear subproblem.** Special invariance property of solution to subproblem involving (unbounded) nonlinear multiplication operator B (related to potential and nonlinearity) allows to compute solution by pointwise multiplication

$$\frac{\mathrm{d}}{\mathrm{d}t}\, w(t) = B\big(w(t)\big)\, w(t) = B(w(0))\, w(t)\,, \qquad t \in (0,T)\,,$$

$$\big(w(t)\big)(x) = \big(\mathrm{e}^{tB(w(0))}\, w(0)\big)(x) = \mathrm{e}^{t\,(B(w_0))(x)}\, w_0(x)\,, \qquad (x,t) \in \mathbb{R}^d \times [0,T]\,.$$

Explanation. Analytical solution of $\partial_t \psi(x,t) = -\mathrm{i}\,\big(U(x) + \vartheta\,|\psi(x,t)|^2\big)\,\psi(x,t)$ satisfies relation

$$\partial_t\, |\psi(x,t)|^2 = \partial_t\big(\overline{\psi(x,t)}\,\psi(x,t)\big) = 2\,\Re\big(\overline{\psi(x,t)}\,\partial_t\psi(x,t)\big) = 2\,\Re\big(-\mathrm{i}\,\big(U(x) + \vartheta\,|\psi(x,t)|^2\big)\,|\psi(x,t)|^2\big) = 0\,.$$

Highly oscillatory problems, Semi-classical regime

Additional small parameter $0 < \varepsilon \ll 1$.

Highly oscillatory equations. Consider highly oscillatory equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = \frac{1}{\varepsilon}\, A\, u(t) + B\big(u(t)\big)\, u(t)\,, \qquad t \in (0, T)\,.$$

Rescaling leads to problem over long times

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + \varepsilon\, B\big(u(t)\big)\, u(t)\,, \qquad t \in \Big(0, \frac{T}{\varepsilon}\Big)\,.$$

Semi-classical regime. Consider nonlinear Schrödinger equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = \varepsilon\, A\, u(t) + \frac{1}{\varepsilon}\, B\big(u(t)\big)\, u(t)\,, \qquad t \in (0, T)\,.$$

Problems of similar form arise in applications from solid state physics, see Bao, Jin, Markowich (2002/03).

Illustration (Small parameter, Solution behaviour)

Simulation. Consider model equation with harmonic potential and additional small parameter ($d = 1$, $\varepsilon = 10^{-2}$, $\omega = 1$, $\vartheta = 1$)

$$\mathrm{i}\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon\,\Delta + \tfrac{1}{\varepsilon}\,U(x) + \tfrac{1}{\varepsilon}\,\vartheta\,|\psi(x,t)|^2 \Big)\,\psi(x,t)\,.$$

Space and time discretisation by Fourier pseudo-spectral method and embedded 4(3) pair based on 4th-order splitting method by BLANES, MOAN (2002) ($x \in [-8,8]$, $M = 8192$, $t \in [0,3]$, $\mathrm{tol} = 10^{-6}$, $N = 2178$).

Movie
Solution behaviour in presence of small parameter (MATLAB)

Exponential operator splitting methods for nonlinear Schrödinger equations

Exponential operator splitting methods

Time-stepping approach. For nonlinear evolution equation on Banach space $(X, \|\cdot\|_X)$

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad t \in (0,T), \qquad u(0) \text{ given},$$

determine approximations at time grid points $0 = t_0 < \cdots < t_N \le T$ with associated stepsizes $\tau_{n-1} = t_n - t_{n-1}$ for $n \in \{1,\ldots,N\}$ by recurrence

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1}).$$

Splitting methods. Time-splitting methods rely on suitable decomposition of right-hand side and presumption that subproblems

$$\frac{\mathrm{d}}{\mathrm{d}t} v(t) = A\big(v(t)\big), \quad v(t) = \mathrm{e}^{tD_A}\, v(0), \qquad t \in (0,T),$$
$$\frac{\mathrm{d}}{\mathrm{d}t} w(t) = B\big(w(t)\big), \quad w(t) = \mathrm{e}^{tD_B}\, w(0), \qquad t \in (0,T),$$

are solvable in accurate and efficient manner.

General form. High-order splitting methods are cast into following form with real (or complex) method coefficients $(a_j, b_j)_{j=1}^s$

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, tD_A}\, \mathrm{e}^{b_{s+1-j}\, tD_B} \;\approx\; \mathscr{E}_F(t,\cdot) = \mathrm{e}^{tD_F} = \mathrm{e}^{t(D_A+D_B)}.$$

Calculus of Lie-derivatives

Formal calculus. Calculus of Lie-derivatives is suggestive of less involved linear case, see for instance HAIRER, LUBICH, WANNER (2002) and SANZ-SERNA, CALVO (1994).

Problem. Consider nonlinear evolution equation on Banach space involving (unbounded) nonlinear operator $F : D(F) \subseteq X \to X$

$$\frac{\mathrm{d}}{\mathrm{d}t} u(t) = F\big(u(t)\big), \qquad t \in (0, T).$$

Employ formal notation for exact solution

$$u(t) = \mathscr{E}_F\big(t, u(0)\big) = \mathrm{e}^{tD_F} u(0), \qquad t \in [0, T].$$

Evolution operator, Lie-derivative. For (unbounded) nonlinear operator $G : D(G) \subseteq X \to X$ define evolution operator and Lie-derivative by

$$\mathrm{e}^{tD_F} G\, v = G\big(\mathscr{E}_F(t, v)\big), \quad t \in (0, T), \qquad D_F G\, v = G'(v)\, F(v).$$

Remark. Definition of Lie-derivative is natural extension of identity $L = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \mathrm{e}^{tL}$

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \mathrm{e}^{tD_F} G\, v &= \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} G\big(\mathscr{E}_F(t, v)\big) = G'\big(\mathscr{E}_F(t, v)\big)\, F\big(\mathscr{E}_F(t, v)\big)\Big|_{t=0} = G'(v)\, F(v) \\ &= D_F G\, v.\end{aligned}$$

Example methods

General form. High-order splitting methods are cast into following form with real (or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, tD_A}\, \mathrm{e}^{b_{s+1-j}\, tD_B} \approx \mathscr{E}_F(t,\cdot) = \mathrm{e}^{tD_F} = \mathrm{e}^{t(D_A+D_B)}.$$

Low-order methods. First-order Lie–Trotter splitting method and second-order Strang splitting method

$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{tD_B}\, \mathrm{e}^{tD_A}, \qquad \mathscr{S}_F(t,\cdot) = \mathrm{e}^{\frac{1}{2}tD_A}\, \mathrm{e}^{tD_B}\, \mathrm{e}^{\frac{1}{2}tD_A}.$$

Higher-order method. Symmetric fourth-order splitting method by Blanes, Moan (2002).

j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.3963098014983680
3,6	0.6048726657110 80	3,5	−0.0390563049223486
4,5	$1/2-(a_2+a_3)$	4	$1-2(b_1+b_2+b_3)$

Practical realisation by pseudo-spectral methods

Spectral decomposition. Numerical solution of subproblem involving linear differential operator A (related to Laplacian) relies on spectral decomposition (employ eigenrelation $A\mathscr{B}_m = \mu_m \mathscr{B}_m$ for $m \in \mathscr{M}$)

$$\frac{\mathrm{d}}{\mathrm{d}t} v(t) = A\, v(t)\,, \quad t \in (0,T)\,, \qquad v(0) \text{ given}\,,$$

$$v(0) = \sum_{m\in\mathscr{M}} v_m \mathscr{B}_m\,, \qquad v(t) = \mathrm{e}^{tA} v(0) = \sum_{m\in\mathscr{M}} v_m \mathrm{e}^{t\mu_m} \mathscr{B}_m\,, \quad t \in [0,T]\,.$$

Fourier spectral decomposition. Let $\Omega = (-a_1, a_1) \times \cdots \times (-a_d, a_d)$ (sufficiently large). Fourier basis functions form complete orthonormal system in $L^2(\Omega)$ and satisfy

$$\psi(\cdot,t) = \sum_{m\in\mathscr{M}} \psi_m(t)\, \mathscr{F}_m\,, \qquad \psi_m(t) = \big(\psi(\cdot,t) \,|\, \mathscr{F}_m\big)_{L^2}\,,$$

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

Numerical approximation. Truncation of infinite sum and application of trapezoid quadrature formula yields approximation (realisation by Fast Fourier Techniques)

$$\mathscr{Q}_M \psi(\cdot,t) = \sum_{|m|\le M} \psi_m(t)\, \mathscr{F}_m\,, \qquad \psi_m(t) = \int_\Omega \psi(x,t)\, \overline{\mathscr{F}_m(x)}\, \mathrm{d}x \approx \sum_{k\in\mathscr{K}} \omega_k\, \psi(\xi_k,t)\, \overline{\mathscr{F}_m(\xi_k)}\,.$$

Remark. Analogous relations for Sine, Hermite, and generalised Laguerre–Fourier Hermite pseudo-spectral methods.

Illustration (GPE with rotation, Time evolution)

Simulation. Time-dependent Gross–Pitaevskii equation with additional rotation term (EXAMPLE IN BAO, LI, SHEN, 2009).

Movie
Time evolution of GPE with rotation term (MATLAB)

Stability and error analysis of exponential operator splitting methods for nonlinear Schrödinger equations

Objectives

Mein Verzicht auf das Restglied war leichtsinnig. (W. ROMBERG, 1979)

Situation. Time integration of nonlinear evolution equations by splitting methods

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \qquad t \in (0,T), \qquad u(0) \text{ given},$$

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau_{n-1} D_A}\, \mathrm{e}^{b_{s+1-j}\tau_{n-1} D_B}\, u_{n-1}$$

$$\approx\ u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1}), \qquad n \in \{1,\dots,N\}.$$

Reasonable requirements in connection with nonlinear Schrödinger equations (regular solution, WKB initial condition, with $k \in \mathbb{N}$)

$$\sup_{t\in[0,T]} \|u(t)\|_D \le C, \qquad \varepsilon^j \, \|\partial_x^k u(0)\|_X \le C.$$

Local error representations. Deduce local error representations for high-order splitting methods suitable for problems involving unbounded operators and critical parameters

$$\mathscr{L}_F(\tau, v) = \mathscr{S}_F(\tau, v) - \mathscr{E}_F(\tau, v) = \mathscr{O}\big(\tau^{p+1}, \|v\|_D\big).$$

Convergence analysis. Derivation of convergence result relies on stability bounds and local error estimates. Extension to full discretisations by time-splitting pseudo-spectral methods

$$\|u_{NM} - u(t_N)\|_X \le C\Big(\|u_0 - u(0)\|_X + \tau^p + M^{-q}\Big).$$

Derivation of local error expansions

Standard approaches.

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

Approaches for nonlinear evolution equations.

- **Quadrature formulas.** Obtain optimal error bounds with respect to regularity of solution, see JAHNKE, LUBICH (2000), LUBICH (2008).

  Extension to high-order splitting methods TH. (2008, 2012), KOCH, NEUHAUSER, TH. (2013), HOFSTÄTTER, KOCH, TH. (2014).

- **Differential equations.** Obtain exact local error representations for evolution equations involving critical parameters, see DESCOMBES, SCHATZMAN (2002), DESCOMBES, DUMONT, LOUVET, MASSOT (2007).

  Application to Schrödinger equations in semi-classical regime, see DESCOMBES, TH. (2010, 2012). Related techniques studied in AUZINGER, KOCH, TH. (2012, 2014).

Highly oscillatory problems. Recent study of multi-revolution composition time-splitting pseudo-spectral methods for highly oscillatory problems (with CHARTIER, MÉHATS).

Approach based on quadrature formulas

Quadrature formulas

Approach. Suitable local error expansions for high-order splitting methods allow to deduce error estimates for linear and nonlinear Schrödinger equations. Numerical experiments confirm optimality with respect to regularity of exact solution.

$$\mathscr{L}_F(t,v) = \mathscr{S}_F(t,v) - \mathscr{E}_F(t,v) = \mathscr{O}\left(t^{p+1}, \|v\|_D\right)$$

Guiding principle. Linear problems versus nonlinear problems

$$D = H^p(\Omega), \qquad D = H^{2p}(\Omega).$$

Numerical experiments confirm order reduction for less regular solutions.

Main tools.

- Variation-of-constants formula (Gröbner–Alekseev)
- Stepwise expansion of e^{tD_B}
- Quadrature formulas for multiple integrals
- Bounds for iterated Lie-commutators
- Characterise domains of unbounded operators

Local error expansion (Linear evolution equations)

Situation. Splitting method involving two compositions applied to linear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A\,u(t) + B\,u(t)\,, \qquad \mathscr{S}_F(t,\cdot) = \mathrm{e}^{b_2\,tB}\,\mathrm{e}^{a_2\,tA}\,\mathrm{e}^{b_1\,tB}\,\mathrm{e}^{a_1\,tA} \approx \mathscr{E}_F(t,\cdot) = \mathrm{e}^{t(A+B)}\,.$$

Derivation of local error expansion. Assume that $\|B\|_{X\leftarrow X} \le C_B$ and $\|\mathrm{e}^{tC}\|_{X\leftarrow X} \le \mathrm{e}^{M_C\,t}$.
Variation-of-constants formula yields suitable representation for exact solution

$$\mathscr{E}_F(t,\cdot) = \mathrm{e}^{tA} + I_1 + I_2 + \mathscr{O}\big(t^3, C_B^3, M_A, M_{A+B}\big)\,,$$

$$I_1 = \int_0^t \mathrm{e}^{(h-\tau_1)A}\,B\,\mathrm{e}^{\tau_1 A}\,\mathrm{d}\tau_1\,, \qquad I_2 = \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)A}\,B\,\mathrm{e}^{(\tau_1-\tau_2)A}\,B\,\mathrm{e}^{\tau_2 A}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,.$$

Stepwise expansion of e^{tB} yields suitable representation for numerical solution

$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{t(a_1+a_2)A} + Q_1 + Q_2 + \mathscr{O}\big(t^3, C_B^3, M_A, M_B\big)\,,$$

$$Q_1 = t\,\big(b_1\,\mathrm{e}^{a_2\,tA}B\,\mathrm{e}^{a_1\,tA} + b_2\,B\,\mathrm{e}^{t(a_1+a_2)A}\big)\,,$$

$$Q_2 = \tfrac{1}{2}\,t^2\,\big(b_1^2\,\mathrm{e}^{a_2\,tA}B^2\mathrm{e}^{a_1\,tA} + 2\,b_1\,b_2\,B\,\mathrm{e}^{a_2\,tA}\,B\,\mathrm{e}^{a_1\,tA} + b_2^2\,B^2\,\mathrm{e}^{t(a_1+a_2)A}\big)\,.$$

Under basic consistency condition $a_1 + a_2 = 1$ obtain local error expansion involving multiple integrals I_1, I_2, and iterated quadrature approximations Q_1, Q_2

$$\mathscr{L}_F(t,\cdot) = Q_1 - I_1 + Q_2 - I_2 + \mathscr{O}\big(t^3, C_B^3, M_A, M_B, M_{A+B}\big)\,.$$

Taylor series expansions of integrands involve iterated Lie-commutators $[A,B]$, $[A,[A,B]]$.

Local error expansion (Linear evolution equations)

Assumptions. Assume $a_1 + a_2 = 1$ and furthermore

$$\|B\|_{X \leftarrow X} \leq C_B\,, \qquad \|\mathrm{e}^{tC}\|_{X \leftarrow X} \leq \mathrm{e}^{M_C t}\,, \quad C \in \{A, B, A+B\}\,,$$
$$\|[A,B]\,v\|_X + \|[A,[A,B]]\,v\|_X \leq C_{\mathrm{ad}}\,\|v\|_D\,.$$

Local error expansion. Splitting method involving two compositions fulfills local error expansion (Strang $a_1 = \frac{1}{2} = a_2$, $b_1 = 1$, $b_2 = 0$)

$$\begin{aligned}\mathscr{L}_F(t,v) &= \left(\mathrm{e}^{b_2 tB}\,\mathrm{e}^{a_2 tA}\,\mathrm{e}^{b_1 tB}\,\mathrm{e}^{a_1 tA} - \mathrm{e}^{t(A+B)}\right) v \\ &= t\left(b_1 + b_2 - 1\right)\mathrm{e}^{tA}\,B\,v \\ &\quad - t^2\,\mathrm{e}^{tA}\left(\left(a_1 b_1 + b_2 - \tfrac{1}{2}\right)[A,B] + \tfrac{1}{2}\left((b_1+b_2)^2 - 1\right)B^2\right) v \\ &\quad + \mathscr{O}\left(t^3, C_B^3, M_A, M_B, M_{A+B}, C_{\mathrm{ad}}, \|v\|_D\right).\end{aligned}$$

Applications (Schrödinger equations). Extension to high-order splitting methods for nonlinear Schrödinger equations (GPE), see Th. (2008, 2012).

- Natural choice $X = L^2(\Omega)$ ensures $M_A = M_B = M_{A+B} = 0$ (unitarity of evolution operators). Iterated Lie-commutators related to differential operators. Explains regularity requirements $D = H^{2p}(\Omega)$ (nonlinear case) and $D = H^p(\Omega)$ (linear case).
- **Drawback.** Numerical illustrations show that approach not optimal with respect to critical parameter ($B = U/\varepsilon$).

Local error expansion (Nonlinear evolution equations)

Result. Local error expansion for high-order splitting methods applied to linear and nonlinear evolution equations.

Theorem (Th. 2008, Th. 2012, Koch & Neuhauser & Th. 2013)

Any exponential operator splitting method of (nonstiff) order p admits the (formal) expansion

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

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

Remarks.

- Application to Gross–Pitaevskii equations and MCTDHF equations.
- Local error expansion suitable for parabolic problems.

Convergence result (MCTDHF equations)

Situation and assumptions.

- Consider an exponential operator splitting method of (nonstiff) order $p \geq 1$.
- Set $m = p = 2$ or $m = 2p - 3$ for $p \in \mathbb{N}_{\geq 3}$.
- Suppose that the MCTDHF equations possess a uniquely determined sufficiently regular solution on the time interval $[0, T]$ such that

$$\|u(t)\|_{X_m} \leq M_m\,, \qquad u(t) = \big(a(t), \varphi(\cdot, t)\big)^T\,, \qquad X_m = \mathbb{C}^{|\mathcal{M}|} \times \big(H^m(\mathbb{R}^3)\big)^K\,, \qquad t \in [0, T]\,.$$

- Assume that the associated density matrix $\rho(t)$ is nonsingular for $t \in [0, T]$.

Theorem (Koch & Neuhauser & Th., 2013)

The global error estimate

$$\|u_n - u(t_n)\|_{X_0} \leq C\tau^p\,, \qquad n \in \{0, \ldots, N\}, \quad t_N \leq T\,,$$

holds with constant $C > 0$ depending on M_m.

Global error estimate (Full discretisations)

Discretisation. Space and time discretisation of nonlinear Schrödinger equations (GPE) by different pseudo-spectral methods (Fourier, Sine, Hermite) and high-order variable stepsize time-splitting methods.

Theorem (Th. 2012)

Provided that exact solution remains bounded in fractional power space X_β defined by principal linear part for $\beta \geq p$, the global error estimate holds

$$\left\| u_{NM} - u(t_N) \right\|_{X_0} \leq C \left(\left\| u_0 - u(0) \right\|_{X_0} + \tau_{\max}^p + M^{-q} \right).$$

Extensions.

- Time-dependent Gross–Pitaevskii equations with additional rotation term, see Hofstätter, Koch, Th. (2014).
- Multi-revolution composition time-splitting pseudo-spectral methods for highly oscillatory problems (with Chartier, Méhats).

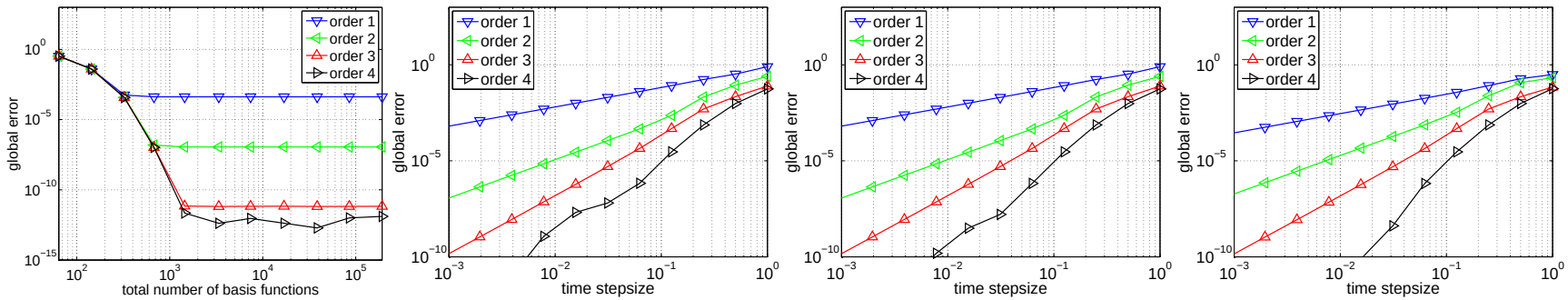
Global error estimate (Full discretisations)

Theorem (Th. 2012)

Global error estimate for regular solutions

$$\left\| u_{NM} - u(t_N) \right\|_{X_0} \leq C \left(\left\| u_0 - u(0) \right\|_{X_0} + \tau_{\max}^p + M^{-q} \right).$$

Illustration. Discretisation of Gross–Pitaevskii equation ($d = 2$, $\varepsilon = \omega = T = 1$) by different pseudo-spectral methods ($M = 256 \times 256$) and time-splitting methods of (nonstiff) orders $p = 1, 2, 3, 4$. Dependence of global error on total number of basis functions ($\vartheta = 0$, dominant error term related to linear part, Fourier, Hermite basis function as exact reference solution, temporal error dominates global error). Numerically observed orders of convergence in time ($\vartheta = 1$, Fourier, Sine, Hermite, smooth initial value, numerical reference solution).



Approach based on differential equations

Differential equations

Approach. Derivation of compact local error representation for splitting methods applied to (non)linear evolution equations involving critical parameters. Related approach studied for construction and analysis of a posteriori local error estimators (with W. AUZINGER, O. KOCH).

Basic idea. Deduce differential equation for splitting operator that is closely related to differential equation for evolution operator

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\,tD_A}\,\mathrm{e}^{b_{s+1-j}\,tD_B}\,, \quad t\in(0,T)\,, \qquad \mathscr{S}_F(0,\cdot) = I\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t,\cdot) = D_F\,\mathscr{E}_F(t,\cdot) = (D_A+D_B)\,\mathscr{E}_F(t,\cdot)\,, \quad t\in(0,T)\,, \qquad \mathscr{E}_F(0,\cdot) = I\,.$$

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

Theorem (Descombes & Th. 2012)

The defect of the Lie–Trotter splitting method admits the integral representation

$$\mathscr{L}_F(t,\cdot) = \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\,\mathrm{e}^{\tau_2 D_B}\,[D_A,D_B]\,\mathrm{e}^{(\tau_1-\tau_2)D_B}\,\mathrm{e}^{(t-\tau_1)D_F}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1$$

$$= \int_0^t \int_0^{\tau_1} \partial_2\mathscr{E}_F\big(t-\tau_1,\mathscr{S}_F(\tau_1,\cdot)\big)\,\partial_2\mathscr{E}_B\big(\tau_1-\tau_2,\mathscr{E}_A(\tau_1,\cdot)\big)\,[B,A]\big(\mathscr{E}_B\big(\tau_2,\mathscr{E}_A(\tau_1,\cdot)\big)\big)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,.$$

Remark. Extension to higher-order splitting methods involved! Corresponding result for high-order splitting methods applied to linear problems deduced in DESCOMBES, TH. (2010).

Application (Equations with critical parameters)

Application. Error analysis of splitting methods for Schrödinger equations involving critical parameters $0 < \varepsilon \ll 1$

$$\mathrm{i}\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon\,\Delta + \tfrac{1}{\varepsilon}\,U(x) + \tfrac{1}{\varepsilon}\,\vartheta\,\big|\psi(x,t)\big|^2 \Big)\,\psi(x,t)\,, \qquad t \in (0,T)\,,$$

see DESCOMBES, TH. (2010, 2012).

- High-order splitting methods for linear Schrödinger equations

$$\text{local error} = \mathcal{O}\big(\tfrac{\tau^{p+1}}{\varepsilon}\big)\,.$$

- Lie–Trotter splitting method for nonlinear evolution equations

$$\begin{aligned} &\text{smooth initial value:} && \text{local error} = C\big(\tfrac{\tau}{\varepsilon}\big)\,\tau^2\,, \\ &\text{WKB initial value:} && \text{local error} = C\big(\tfrac{\tau}{\varepsilon}\big)\,\tau\,. \end{aligned}$$

Remark. Difficult task to adjust time stepsize in suitable manner. Reliable time integration of Schrödinger equations with critical parameters based on adaptive time stepsize control.

Reliable and efficient time integration of nonlinear Schrödinger equations

Adaptive stepsize control

Adaptive stepsize control. Standard strategy for adaptive time stepsize control

$$\tau_{\text{optimal}} = \tau \cdot \min\left(\alpha_{\max}, \max\left(\alpha_{\min}, \sqrt[p+1]{\alpha \cdot \frac{\text{tol}}{\text{err}_{\text{local}}}}\right)\right).$$

Local error estimators. Construction of local error estimators for splitting methods.

- A posteriori local error estimators, see AUZINGER, KOCH, TH. (2012, 2014).
- Embedded splitting methods, see KOCH, NEUHAUSER, TH. (2013).

Example. Fourth-order splitting method (BLANES, MOAN) and embedded third-order splitting method (KOCH, TH.).

j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.3963098014983680
3,6	0.604872665711080	3,5	−0.0390563049223486
4,5	$1/2-(a_2+a_3)$	4	$1-2(b_1+b_2+b_3)$

j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	−0.0060995324486253
7	−1.3630829287974774	7	0

A posteriori error estimators (Linear evolution equations)

Basic idea. Consider linear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t) = \big(A+B\big)\,\mathscr{E}_F(t)\,, \quad t\in[0,T]\,, \qquad \mathscr{E}_F(0) = I\,.$$

For p-th order splitting method determine related differential equation involving defect

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}_F(t) = \big(A+B\big)\,\mathscr{S}_F(t) + \mathscr{D}_F(t)\,, \quad t\in[0,T]\,, \qquad \mathscr{S}_F(0) = I\,.$$

Use integral representation for local error $\mathscr{L}_F = \mathscr{S}_F - \mathscr{E}_F$ (variation-of-constants formula)

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{L}_F(t) = \big(A+B\big)\,\mathscr{L}_F(t) + \mathscr{D}_F(t)\,, \quad t\in[0,T]\,, \qquad \mathscr{L}_F(0) = 0\,,$$

$$\mathscr{L}_F(t) = \int_0^t \mathrm{e}^{(t-\tau)(A+B)}\,\mathscr{D}_F(\tau)\,\mathrm{d}\tau\,.$$

Apply Hermite quadrature approximation and show that $f(0) = \cdots = f^{(p-1)}(0) = 0$ due to validity of order conditions

$$\sum_{\ell=0}^{p-1} \omega_\ell\, t^{\ell+1}\, f^{(\ell)}(0) + \tfrac{1}{p+1}\, t\, f(t) - \int_0^t f(\tau)\,\mathrm{d}\tau = \mathscr{O}\big(t^{p+2}\big)\,.$$

Obtain asymptotically correct a posteriori local error estimator

$$\mathscr{P}_F(t) = \tfrac{1}{p+1}\, t\, \mathscr{D}_F(t)\,, \qquad \mathscr{P}_F(t) - \mathscr{L}_F(t) = \mathscr{O}\big(t^{p+2}\big)\,.$$

A posteriori local error estimators

Result. Asymptotically correct a posteriori local error estimator associated with high-order splitting method

$$\mathscr{S}_F = \mathscr{S}_1^s \approx \mathscr{E}_F, \qquad \mathscr{S}_k^m(t) = \prod_{j=k}^{m} \mathrm{e}^{b_j\, tB}\, \mathrm{e}^{a_j\, tA},$$

$$\mathscr{P}_F = \frac{1}{p+1}\, t\, \mathscr{D}_F, \qquad \mathscr{P}_F(t) - \mathscr{L}_F(t) = \mathscr{O}\big(t^{p+2}\big),$$

$$\mathscr{D}_F = \sum_{k=1}^{s} \mathscr{S}_k^s\, a_k A\, \mathscr{S}_1^{k-1} + \sum_{k=1}^{s-1} \mathscr{S}_{k+1}^s\, b_k B\, \mathscr{S}_1^k - \big(A + (1-b_s)\, B\big)\, \mathscr{S}_F(t).$$

Extension to nonlinear evolution equations by calculus of Lie-derivatives.

Rigorous analysis. Detailed treatment of high-order splitting methods for nonlinear evolution equations involved! Theoretical analysis completed for Strang splitting method and linear equations, see AUZINGER, KOCH, TH. (2012, 2014).

- Suitable representations for higher-order derivatives of defect.
- Rigorous proof of asymptotical correctness in context of Schrödinger equation (optimal regularity requirements on exact solution).

A posteriori error estimator (Lie–Trotter splitting method)

Special case. A posteriori local error estimator for Lie–Trotter splitting method applied to linear evolution equation given by

$$\mathscr{P}_F(t,v) = \tfrac{1}{2}\, t\, \mathscr{D}_F(t,v), \qquad \mathscr{D}_F(t,v) = \big(\mathrm{e}^{tB}\,\mathrm{e}^{tA}A - A\,\mathrm{e}^{tB}\,\mathrm{e}^{tA}\big)\,v.$$

Extension to nonlinear case yields

$$\mathscr{D}_F(t,v) = \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,\partial_2\mathscr{E}_A(t,v)\,A\,v - A\,\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big).$$

Explanation. Extension by formal calculus of Lie-derivatives implies $\mathscr{D}_F(t,v) = D_A\,\mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,v - \mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,D_A\,v$ and

$$G(v) = \mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,v = \mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big), \quad G'(v) = \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,\partial_2\mathscr{E}_A(t,v),$$

$$\mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,D_A\,v = A\,\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big), \quad D_A\,\mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,v = G'(v)\,A\,v = \partial_2\mathscr{E}_B\big(t,\mathscr{E}_A(t,v)\big)\,\partial_2\mathscr{E}_A(t,v)\,A\,v.$$

Remark. Improved approximation $\mathscr{S}_F(t,\cdot) - \mathscr{P}_F(t,\cdot) = \mathscr{E}_F(t,\cdot) + \mathscr{O}\big(t^{p+2}\big)$.

Realisation and computational effort. Realisation for nonlinear Schrödinger equations (Gross–Pitaevskii equation) straightforward. Computational effort comparable with splitting pair Lie/Strang (two additional applications of A required, FFT).

$$\mathscr{P}(t,v) = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\Big(A\,w - \mathrm{i}\vartheta t\big(A\,w\,|w|^2 + \overline{A\,w}\,w^2\big)\Big) - A\,\mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\,w, \quad w = \mathrm{e}^{tA}\,v.$$

Explanation. With $G(v) = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\,w$, $G'(v) = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\Big(\mathrm{e}^{tA}(\cdot) - \mathrm{i}\vartheta t\big(\overline{w}\,\mathrm{e}^{tA}(\cdot) + w\,\overline{\mathrm{e}^{tA}(\cdot)}\big)\,w\Big)$ obtain

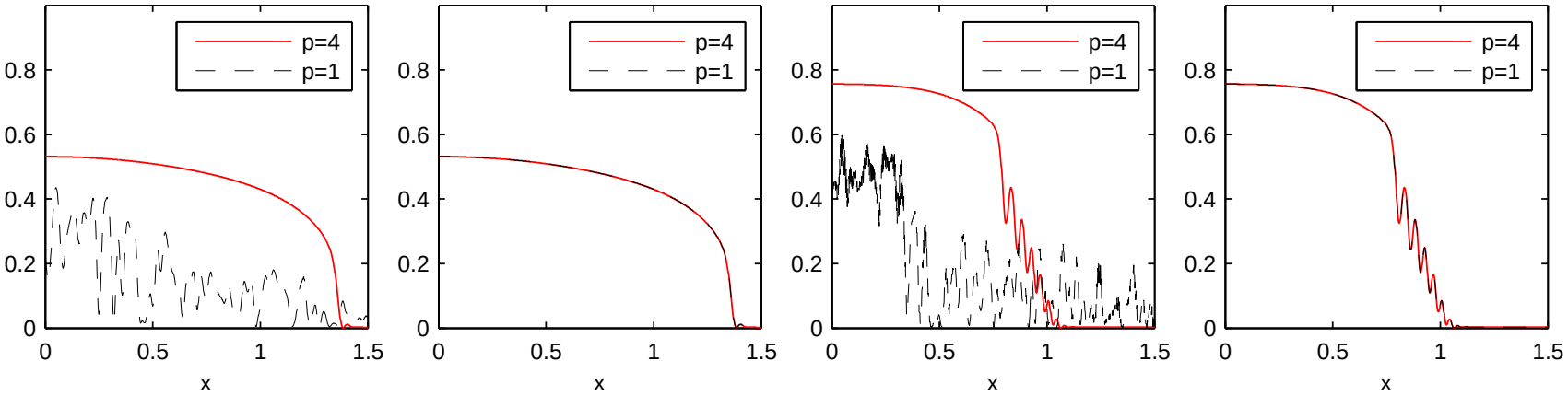
$$\mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,D_A\,v = A\,\mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\,w, \qquad D_A\,\mathrm{e}^{tD_A}\,\mathrm{e}^{tD_B}\,v = \mathrm{e}^{-\mathrm{i}t\,(U+\vartheta|w|^2)}\Big(A\,w - \mathrm{i}\vartheta\,t\,\big(Aw\,|w|^2 + \overline{A\,w}\,w^2\big)\Big).$$

Illustration (Smaller parameter)

Integration without preparation is frustration. (REVEREND LEON SULLIVAN,)

Situation. Time and space discretisation of model problem ($d = 1$, $\varepsilon = 10^{-2}$, $\vartheta = 1$, $(x,t) \in [-8,8] \times [0,3]$) by splitting methods and Fourier pseudo-spectral method ($M = 8192$).

Illustration. Harmonic potential with $\omega = 1$ (col. 1 & 2) or $\omega = 2$ (col. 3 & 4), respectively. Splitting methods ($p = 1, 4$) applied with constant time stepsizes. Comparison of solution profiles $|\psi(x,t)|^2$ for $x \in [0, 1.5]$ at time $t = 3$. Stepsizes $\tau = \frac{\varepsilon}{20}$ (col. 1 & 3) or $\tau = \frac{\varepsilon}{50}$ (col. 2 & 4) if $p = 1$, and $\tau = \frac{\varepsilon}{20}$ if $p = 4$.

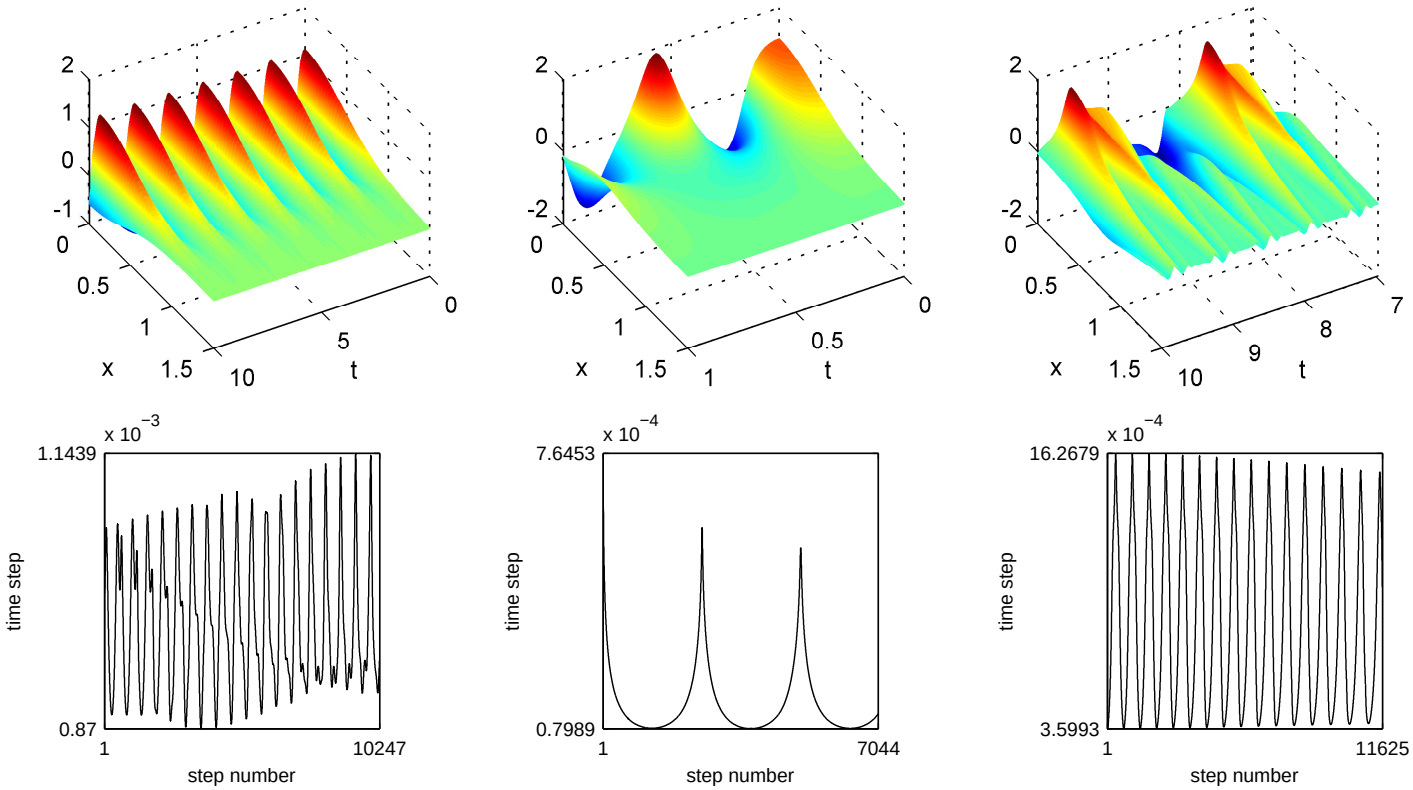


Movie

Time integration by embedded 4(3) splitting pair. Solution profile $|\psi(x,t)|^2$ for $\mathrm{tol} = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-6}$ ($N = 951, 2342, 2452, 3560$). (MATLAB)

Illustration (Reliable time integration)

Further illustrations. Time integration of model equation ($d = 1$, $\varepsilon = 1$, $\omega = 5$) by embedded 4(3) pair (tol $= 10^{-10}$). Solution profiles $\Re\psi$ for $(x,t) \in [0,1.5] \times [T_0, T]$ and associated time stepsizes. Left: Additional lattice potential with $\kappa = 10$ and defocusing nonlinearity with $\vartheta = 1$ for $t \in [0,10]$. Middle: Focusing nonlinearity with $\vartheta = -10$ for $t \in [0,1]$. Right: Defocusing nonlinearity with $\vartheta = 1$ and sharp initial Gaussian with $\gamma = 4$ for $t \in [0,10]$.



Conclusions and future work

Conclusions.

- Theoretical analysis of space and time discretisations based spectral and splitting methods.
- Adaptivity in time essential for reliable numerical simulations.

Open questions.

- Asymptotical correctness of higher-order a posteriori local error estimators for nonlinear Schrödinger equations.
- Convergence analysis of higher-order time-splitting pseudo-spectral methods for nonlinear Schrödinger equations involving small parameters $\mathrm{i}u' = Au + \frac{1}{\varepsilon}B(u)$.
- Convergence analysis of multi-revolution compositon methods combined with time-splitting pseudo-spectral methods for Schrödinger equations $\mathrm{i}u' = \frac{1}{\varepsilon}Au + B(u)$.

Thank you!

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2. P. Chartier, F. Méhats, M. Thalhammer, Y. Zhang. *Superconvergence of Strang splitting for NLS in* T^d.

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1. P. Chartier, F. Méhats, M. Thalhammer, Y. Zhang. *Convergence analysis of multi-revolution composition time-splitting pseudo-spectral methods for linear Schrödinger equations.*

Lecture note. *Time-splitting spectral methods for nonlinear Schrödinger equations.*