Recent results on Magnus-type integrators and applications to quantum systems

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Guide line

Aim. Study exponential time integration methods of Magnus-type for different classes of evolution equations with explicit time-dependency.

- ♢ Identify benefits or possible limitations.
- ♢ Provide rigorous stability and error analysis.
- ♢ Improve existing methods and design novel methods.

Approach. From less involved case of linear evolution equations to more complex case of nonlinear evolution equations.

- ♢ Commutator-free quasi-Magnus (CFQM) exponential integrators for non-autonomous linear evolution equations of Schrödinger and parabolic type

  Appropriate name thanks to Arieh Iserles

- ♢ CFQM exponential integrators combined with operator splitting methods for non-autonomous nonlinear evolution equations of Schrödinger type

Focus

Focus in this talk. Joint work with SERGIO BLANES and FERNANDO CASAS.

SERGIO BLANES, FERNANDO CASAS, M. TH.
Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear evolution equations of parabolic type.
IMA J. Numer. Anal. (2017).

SERGIO BLANES, FERNANDO CASAS, M. TH.
High-order commutator-free quasi-Magnus exponential integrators and related methods for non-autonomous linear evolution equations.
Comp. Physics Commun. (2017).

SERGIO BLANES, FERNANDO CASAS, CESÁREO GONZÁLEZ, M. TH.
Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear Schrödinger equations.
Submitted (2018).

PHILIPP BADER, SERGIO BLANES, FERNANDO CASAS, M. TH.
Efficient time integration methods for Gross–Pitaevskii equations with rotation term.
Submitted (2019).

Related work. Design and analysis of local error estimators for adaptive time stepsize control. With W. AUZINGER, H. HOFSTÄTTER, O. KOCH.

CFQM exponential integrators for non-autonomous linear evolution equations

Magnus-type exponential integrators
Convergence analysis
Design of novel schemes
Schrödinger versus parabolic equations

Areas of application

Areas of application.

◇ Quantum systems

Models for oxide solar cells (with W. Auzinger, K. Held, H. Hofstätter, O. Koch)

Linear evolution equations of Schrödinger type

Linear Schrödinger equations involving space-time-dependent potentials

◇ Dissipative quantum systems

Rosen–Zener models with dissipation

Linear evolution equations of parabolic type

Variational equations related to diffusion-advection-reaction equations

Common structure. Abstract formulation as non-autonomous linear evolution equation helps to recognise common structure of complex processes.

Non-autonomous linear evolution equations

Non-autonomous evolution equations. Consider initial value problem for non-autonomous linear evolution equation

$$\begin{cases} u'(t) = A(t)\, u(t)\,, & t \in (t_0, T)\,, \\ u(t_0) \ \text{given}\,. \end{cases}$$

Exact solution not available (used only theoretically as ideal case).

Favourable numerical approximation on the basis of less involved autonomous case?

Autonomous linear evolution equations

Autonomous evolution equations. Consider initial value problem for autonomous linear evolution equation

$$\begin{cases} w'(t) = A\, w(t)\,, \quad t \in (t_0, T)\,, \\ w(t_0) \text{ given}\,. \end{cases}$$

Exact solution (formally) given by exponential

$$w(t) = \mathrm{e}^{(t-t_0)A}\, w(t_0)\,, \quad t \in [t_0, T]\,.$$

Numerical realisation. Efficient numerical approximation of exponential possibly difficult task!

Numerical realisation of exponential

Matrix exponential. Recall straightforward definition of matrix exponential by infinite series

$$A \in \mathbb{R}^{d \times d}, \quad \mathrm{e}^{tA} = \sum_{k=0}^{\infty} \frac{1}{k!} t^k A^k, \quad t \in \mathbb{R}.$$

But! Considered systems of ordinary differential equations, e.g. obtained by spatial semi-discretisations of partial differential equations, involve matrix of high dimension $d \gg 1$. Numerical realisation of exponential possibly demanding task. Standard approaches rely on series expansions and Krylov-type methods.

C. Moler, C. Van Loan. *Nineteen dubious ways to compute the exponential of a matrix, twenty-five years later. SIAM review 1/45 (2003) 3–49.*

Alternative approach. For Schrödinger equations with principal part given by Laplacian, use splitting methods and fast Fourier transform.

Magnus-type exponential integrators

Magnus expansion

Commutator. Recall short notation for commutator of linear operators

$$\big[A, B\big] = A\,B - B\,A\,.$$

Magnus expansion (Magnus, 1954). Consider non-autonomous linear evolution equation on subinterval

$$u'(t) = A(t)\,u(t)\,, \quad t \in (t_n, t_n + \tau_n)\,, \quad t_0 \leq t_n < t_n + \tau_n \leq T\,.$$

Formal representation of solution based on Magnus expansion

$$u(t_n + \tau_n) = \mathrm{e}^{\Omega(\tau_n, t_n)}\,u(t_n)\,,$$

$$\begin{aligned}\Omega(\tau_n, t_n) = &\int_{t_n}^{t_n+\tau_n} A(\sigma)\,\mathrm{d}\sigma \\ &+ \tfrac{1}{2}\int_{t_n}^{t_n+\tau_n}\int_{t_n}^{\sigma_1}\big[A(\sigma_1), A(\sigma_2)\big]\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1 \\ &+ \tfrac{1}{6}\int_{t_n}^{t_n+\tau_n}\int_{t_n}^{\sigma_1}\int_{t_n}^{\sigma_2}\Big(\big[A(\sigma_1),\big[A(\sigma_2), A(\sigma_3)\big]\big] \\ &\qquad + \big[A(\sigma_3),\big[A(\sigma_2), A(\sigma_1)\big]\big]\Big)\,\mathrm{d}\sigma_3\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1 + \dots\end{aligned}$$

Magnus integrators

Magnus integrators. Truncation of Magnus expansion

$$\Omega(\tau_n, t_n) = \int_{t_n}^{t_n+\tau_n} A(\sigma)\,\mathrm{d}\sigma + \tfrac{1}{2}\int_{t_n}^{t_n+\tau_n}\int_{t_n}^{\sigma_1} \big[A(\sigma_1), A(\sigma_2)\big]\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1 + \dots$$

and application of quadrature formulae for approximation of multiple integrals leads to class of Magnus integrators.

- Second-order Magnus integrator (exponential midpoint rule)

$$\tau_n\, A\big(t_n + \tfrac{\tau_n}{2}\big) \;\approx\; \Omega(\tau_n, t_n)\,.$$

- Fourth-order Magnus integrator, see Blanes, Casas, Ros (2000)

$$\tfrac{1}{6}\,\tau_n\,\Big(A(t_n) + 4\,A\big(t_n + \tfrac{\tau_n}{2}\big) + A(t_n+\tau_n)\Big) - \tfrac{1}{12}\,\tau_n^2\,\big[A(t_n), A(t_n+\tau_n)\big] \;\approx\; \Omega(\tau_n, t_n)\,.$$

Issue. In context of large-scale problems, presence of (iterated) commutators disadvantageous.

Magnus-type integrators

Disadvantages. Presence of iterated commutators causes

- loss of structure (issues of well-definedness and stability for PDEs involving differential operators).
- large computational cost (for realisation of action of arising matrix-exponentials on vectors by Krylov-type methods, e.g.).

Alternative. Commutator-free quasi-Magnus exponential integrators provide useful alternative to interpolatory Magnus integrators.

A. Alvermann, H. Fehske, P. B. Littlewood.
Numerical time propagation of quantum systems in radiation fields.
New Journal of Physics 14 (2012) 105008.

... We explain the use of commutator-free exponential time propagators for the numerical solution of the associated Schrödinger or master equations with a time-dependent Hamilton operator. These time propagators are based on the Magnus series but avoid the computation of commutators, which makes them suitable for the efficient propagation of systems with a large number of degrees of freedom. ...

CFQM exponential integrators

Situation. Consider non-autonomous linear evolution equation

$$\begin{cases} u'(t) = A(t)\, u(t)\,, & t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,. \end{cases}$$

General format. Determine numerical approximations at certain time grid points $t_0 < t_1 < \cdots < t_N \leq T$ by recurrence

$$u_{n+1} = \mathcal{S}(\tau_n, t_n)\, u_n \approx u(t_{n+1}) = \mathcal{E}(\tau_n, t_n)\, u(t_n)\,,$$
$$\tau_n = t_{n+1} - t_n\,, \quad n \in \{0, 1, \dots, N-1\}\,.$$

Cast high-order commutator-free quasi-Magnus (CFQM) exponential integrators into general form

$$\mathcal{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n B_{nJ}} \cdots \mathrm{e}^{\tau_n B_{n1}}\,,$$

$$B_{nj} = \sum_{k=1}^{K} a_{jk}\, A_{nk}\,, \quad A_{nk} = A(t_n + c_k \tau_n)\,.$$

Advantages and numerical realisation

Comparison. CFQM exponential integrators generalise exponential operator splitting methods defined by coefficients $(\alpha_\ell, \beta_\ell)_{\ell=1}^{s}$ (freeze time by adding differential equation $\frac{\mathrm{d}}{\mathrm{d}t}\, t = 1$)

$$u_{n+1} = \mathrm{e}^{\tau_n \alpha_s A_{ns}} \cdots \mathrm{e}^{\tau_n \alpha_1 A_{n1}}\, u_n\,, \quad A_{nk} = A(t_n + c_k \tau_n)\,, \quad c_k = \sum_{\ell=1}^{k} \beta_\ell\,,$$

with the merit of a significantly reduced number of exponentials for higher-order schemes, which enhances efficiency.

Numerical realisation.

- Action of arising matrix-exponentials on vectors commonly computed by Krylov-type methods. Computational effort determined by cost for matrix-vector products.
- In context of certain classes of linear Schrödinger equations involving Laplace operator, favourable approach relies on use of fast Fourier transform and its inverse.

Example (Nonstiff orders $p = 2, 4$)

Order 2 (Exponential midpoint rule). Magnus / CFQM exponential integrator based on single Gaussian quadrature node involves single exponential at each time step

$$p = 2, \quad J = 1 = K, \quad c_1 = \tfrac{1}{2}, \quad a_{11} = 1, \quad A_{n1} = A\big(t_n + \tfrac{\tau_n}{2}\big),$$
$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n A(t_n + \frac{1}{2}\tau_n)}.$$

Order 4. Fourth-order CFQM exponential integrator based on two Gaussian quadrature nodes requires evaluation of two exponentials

$$p = 4, \quad J = 2 = K, \quad c_k = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}, \quad a_{1k} = \tfrac{1}{4} \pm \tfrac{\sqrt{3}}{6},$$
$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n (a_{12} A_{n1} + a_{11} A_{n2})} \, \mathrm{e}^{\tau_n (a_{11} A_{n1} + a_{12} A_{n2})}.$$

Scheme suitable for evolution equations of Schrödinger type and of parabolic type, since

$$b_1 = a_{11} + a_{12} = \tfrac{1}{2} = a_{21} + a_{22} = b_2 .$$

Examples (Nonstiff order $p = 6$)

Order 6. Sixth-order CFQM exponential integrator obtained from coefficients given in ALVERMANN, FEHSKE. Scheme suitable for evolution equations of Schrödinger type, but poor stability behaviour observed for evolution equations of parabolic type, since

$$\exists\, j \in \{1, \dots, J\}: \quad b_j = \sum_{k=1}^{K} a_{jk} < 0\,.$$

Higher-order schemes.

- With regard to efficiency desirable to use higher-order schemes (in context of partial differential equations, typically $p \in \{4, 5, 6\}$).
- *Secret of success* lies in *suitable and smart* choice of arising coefficients.

First illustration (Parabolic equation)

Practice in numerical methods is the only way of learning it. H. Jeffreys, B. Jeffreys

Test equation. Consider nonlinear diffusion-advection-reaction equation

$$\partial_t U(x,t) = f_2\big(U(x,t)\big)\,\partial_{xx} U(x,t) + f_1\big(U(x,t)\big)\,\partial_x U(x,t) + f_0\big(U(x,t)\big) + g(x,t)\,.$$

Associated variational equation has form of non-autonomous linear evolution equation

$$\partial_t u(x,t) = \alpha_2(x,t)\,\partial_{xx} u(x,t) + \alpha_1(x,t)\,\partial_x u(x,t) + \alpha_0(x,t)\,u(x,t)\,.$$

Impose periodic boundary conditions and regular initial condition.

First illustration (Parabolic equation)

Test equation. Consider non-autonomous linear evolution equation

$$\partial_t u(x,t) = \alpha_2(x,t)\,\partial_{xx} u(x,t) + \alpha_1(x,t)\,\partial_x u(x,t) + \alpha_0(x,t)\,u(x,t)\,.$$

Impose periodic boundary conditions and regular initial condition.

Special choice. In particular, set

$$(x,t) \in \Omega \times [0,T]\,, \quad \Omega = [0,1]\,, \quad T = 1\,,$$

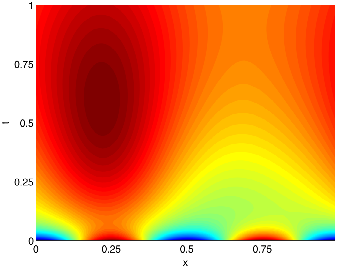
$$U(x,t) = \mathrm{e}^{-t} \sin(2\pi x)\,, \quad u(x,0) = \big(\sin(2\pi x)\big)^2\,,$$

$$f_2(w) = \tfrac{1}{10}\,\big(\cos(w) + \tfrac{11}{10}\big)\,, \quad f_1(w) = \tfrac{1}{10}\,w\,,$$

$$f_0(w) = w\,\big(w - \tfrac{1}{2}\big)\,,$$

$$\alpha_2(x,t) = f_2\big(U(x,t)\big)\,, \quad \alpha_1(x,t) = f_1\big(U(x,t)\big)\,,$$

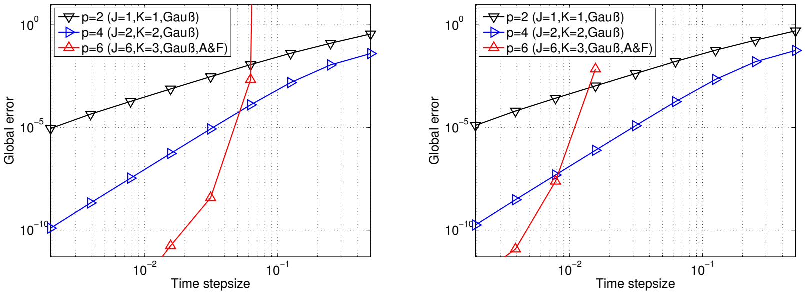
$$\alpha_0(x,t) = f_2'\big(U(x,t)\big)\,\partial_{xx} U(x,t) + f_1'\big(U(x,t)\big)\,\partial_x U(x,t) + f_0'\big(U(x,t)\big)\,.$$



First illustration (Parabolic equation, Global errors)

One must watch the convergence of a numerical code as carefully as a father watching his four year old play near a busy road. J. P. Boyd

Numerical experiment. Apply CFQM exponential integrators of nonstiff orders $p = 2,4,6$ to parabolic test equation (see before). Display global errors versus time stepsizes for $M = 50$ (left) and $M = 100$ (right) space grid points. Sixth-order scheme shows poor stability behaviour.



First conclusions

Observations and first conclusions.

- Order barrier at order four, i.e. CFQM exponential integrators of order five or higher necessarily involve negative coefficients which cause integration backward in time (ill-posed problem).
- Close connexion to class of time-splitting methods gives reasons for the study of *unconventional* CFQM exponential integrators involving complex coefficients under additional positivity condition.

Our starting point for a series of works ...

Complete the big picture ...

- **Stability and error analysis** of CFQM exponential integrators for parabolic evolution equations and for Schrödinger equations with time-dependent Hamiltonian of form $A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$

  Sergio Blanes, Fernando Casas, M. Th.
  Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear evolution equations of parabolic type.
  IMA J. Numer. Anal. (2017).

  Sergio Blanes, Fernando Casas, Cesáreo González, M. Th.
  Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear Schrödinger equations.
  Submitted (2018).

- **Design of efficient schemes**

  Sergio Blanes, Fernando Casas, M. Th.
  High-order commutator-free quasi-Magnus exponential integrators and related methods for non-autonomous linear evolution equations.
  Comp. Physics Commun. (2017).

Convergence analysis

Schrödinger equations
Parabolic equations

Analytical framework

Analytical framework. Suitable functional analytical framework for evolution equations of Schrödinger or parabolic type based on

- selfadjoint operators and unitary evolution operators on Hilbert spaces or
- sectorial operators and analytic semigroups on Banach spaces.

Hypotheses (Parabolic case). Domain of $A(t) : D \subset X \to X$ time-independent, dense and continuously embedded. Linear operator $A(t) : D \subset X \to X$ sectorial, uniformly in $t \in [t_0, T]$, i.e., there exist $a \in \mathbb{R}$, $0 < \phi < \frac{\pi}{2}$, $C_1 > 0$ such that

$$\|(\lambda I - A(t))^{-1}\|_{X \leftarrow X} \le \frac{C_1}{|\lambda - a|}\,, \qquad t \in [t_0, T]\,, \qquad \lambda \notin S_\phi(a) = \{a\} \cup \big\{\mu \in \mathbb{C} : |\arg(a-\mu)| \le \phi\big\}\,.$$

Graph norm of $A(t)$ and norm in D equivalent for $t \in [t_0, T]$, i.e., there exists $C_2 > 0$ such that

$$C_2^{-1}\|x\|_D \le \|x\|_X + \|A(t)\,x\|_X \le C_2\|x\|_D\,, \qquad t \in [t_0, T]\,, \qquad x \in D\,.$$

Defining operator family is Hölder-continuous for some exponent $\vartheta \in (0, 1]$, i.e., there exists $C_3 > 0$ such that

$$\|A(t) - A(s)\|_{X \leftarrow D} \le C_3\,|t-s|^\vartheta\,, \qquad s, t \in [t_0, T]\,.$$

Consequence. Sectorial operator $A(t)$ generates analytic semigroup $\big(\mathrm{e}^{\sigma A(t)}\big)_{\sigma \in [0,\infty)}$ on X. By integral formula of Cauchy, representation follows

$$\mathrm{e}^{\sigma A(t)} = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \mathrm{e}^\lambda \big(\lambda I - \sigma A(t)\big)^{-1}\,\mathrm{d}\lambda\,, \quad \sigma > 0\,, \qquad \mathrm{e}^{\sigma A(t)} = I\,, \quad \sigma = 0\,.$$

Basic assumptions on methods

CFQM exponential integrators. High-order CFQM exponential integrators cast into form

$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n B_{nJ}} \cdots \mathrm{e}^{\tau_n B_{n1}}\,, \qquad B_{nj} = \sum_{k=1}^{K} a_{jk}\, A_{nk}\,, \qquad A_{nk} = A(t_n + c_k \tau_n)\,.$$

Employ standard assumption that ratios of subsequent time stepsizes remain bounded

$$\varrho_{\min} \le \frac{\tau_{n+1}}{\tau_n} \le \varrho_{\max}\,, \qquad n \in \{0, 1, \dots, N-2\}\,.$$

Nodes and coefficients. Relate nodes to quadrature nodes and suppose

$$0 \le c_1 < \cdots < c_K \le 1\,.$$

Assume basic consistency condition to be satisfied (direct consequence of elementary requirement $\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n A}$ for time-independent operator A)

$$\sum_{j=1}^{J} b_j = 1\,, \qquad b_j = \sum_{k=1}^{K} a_{jk}\,, \qquad j \in \{1, \dots, J\}\,.$$

In connection with evolution equations of parabolic type employ positivity condition, which ensures well-definededness of CFQM exponential integrators within analytical framework of sectorial operators and analytic semigroups

$$\Re\, b_j > 0\,, \qquad j \in \{1, \dots, J\}\,.$$

Convergence result

Situation.

- Employ standard hypotheses on operator family defining non-autonomous linear evolution equation of parabolic or Schrödinger type. See paper (parabolic case) and preprint (Schrödinger case, special structure).
- Use that coefficients of considered high-order CFQM exponential integrators fulfill basic assumptions (positivity condition for parabolic case) and order conditions.

Theorem

Provided that operator family and exact solution are sufficiently regular, following estimate holds in underlying Banach space with constant $C > 0$ independent of n and time increments

$$\big\| u_n - u(t_n) \big\|_X \leq C \Big(\big\| u_0 - u(t_0) \big\|_X + \tau_{\max}^p \Big), \quad 0 < \tau_n \leq \tau_{\max}, \quad n \in \{0, 1, \dots, N\}.$$

Crucial point. Specify regularity and compatibility requirements on exact solution.

- Parabolic test equation with $X = \mathscr{C}(\Omega, \mathbb{R})$: Obtain regularity requirement on solution $u(t) \in \mathscr{C}^{2p}(\Omega, \mathbb{R})$ for $t \in [t_0, T]$.
- Schrödinger equation with $A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$: For $X = L^2(\Omega, \mathbb{C})$ weaker assumption $\partial_x^p u(t) \in L^2(\Omega, \mathbb{C})$ for $t \in [t_0, T]$ sufficient.

Main tools of proof

Stability. Relate stability function of CFQM exponential integrator to analytic semigroup (suitable choice of frozen time t)

$$\Delta_{n_0}^{n} = \prod_{i=n_0}^{n} \mathscr{S}_i(\tau_i, t_i) - \mathrm{e}^{(t_{n+1}-t_{n_0})\,A(t)}\,, \quad \|\mathrm{e}^{sA(t)}\|_{X\leftarrow X} + s\,\|\mathrm{e}^{sA(t)}\|_{D\leftarrow X} \leq C\,.$$

Employ telescopic identity, bounds for analytic semigroup, Hölder-continuity of defining operator family, and Gronwall-type inequality to deduce desired stability bound

$$\Big\| \prod_{i=n_0}^{n} \mathscr{S}_i(\tau_i, t_i) \Big\|_{X\leftarrow X} \leq C\,.$$

Local error. Repeated application of variation-of-constants formula yields suitable representation which is starting point for further expansions

$$u(t_{n+1}) - \mathscr{S}(\tau_n, t_n)\,u(t_n) = \sum_{j=1}^{J}\sum_{k=1}^{K} a_{jk} \Big(\prod_{i=j+1}^{J} \mathrm{e}^{\tau_n B_{ni}(\tau_n)} \Big) \int_0^{\tau_n} \mathrm{e}^{(\tau_n-\sigma) B_{nj}(\tau_n)}\, g_{njk}(\sigma)\,\mathrm{d}\sigma\,,$$

$$g_{njk}(\sigma) = \big(A(t_n + d_{j-1}\tau_n + b_j\sigma) - A(t_n + c_k\tau_n) \big)\, u(t_n + d_{j-1}\tau_n + b_j\sigma)\,.$$

Resulting local error representation involved for high-order schemes.

Design of novel schemes

Numerical comparisons for dissipative quantum system

Derivation of order conditions

Approach.

- Focus on design of efficient schemes of non-stiff orders $p = 4, 5$ involving $K = 3$ Gaussian quadrature nodes. By time-symmetry of schemes achieve $p = 6$.
- Employ advantageous reformulation (suffices to study first time step, indicate dependence on time stepsize $\tau > 0$)

$$\prod_{j=1}^{J} \mathrm{e}^{\tau(a_{j1} A_1(\tau) + a_{j2} A_2(\tau) + a_{j3} A_3(\tau))} = \prod_{j=1}^{J} \mathrm{e}^{x_{j1} \alpha_1(\tau) + x_{j2} \alpha_2(\tau) + x_{j3} \alpha_3(\tau)} + \mathcal{O}\big(\tau^{p+1}\big), \quad \alpha_k(\tau) = \mathcal{O}\big(\tau^k\big).$$

- Determine set of independent order conditions (obtain $q = 10$ conditions for $p = 5$, use Lyndon multi-index $(1,2)$ and corresponding word $\alpha_1 \alpha_2$ etc.)

$$(1):\ y_J = \sum_{\ell=1}^{J} x_{\ell 1} = 1, \quad (2):\ z_J = \sum_{\ell=1}^{J} x_{\ell 2} = 0, \quad (3):\ \sum_{j=1}^{J} x_{j3} = \tfrac{1}{12},$$

$$(1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1} + 2\,y_{j-1}) = -\tfrac{1}{6}, \quad (1,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j1} + 2\,y_{j-1}) = \tfrac{1}{12}, \quad (2,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j2} + 2\,z_{j-1}) = \tfrac{1}{120},$$

$$(1,1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1}^2 + 3\,y_{j-1}^2 + 3\,x_{j1}\,y_{j-1}) = -\tfrac{1}{4}, \quad (1,1,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j1}^2 + 3\,y_{j-1}^2 + 3\,x_{j1}\,y_{j-1}) = \tfrac{1}{10},$$

$$(1,2,2):\ \sum_{j=1}^{J} x_{j1}\,(x_{j2}^2 - 3\,x_{j2}\,z_j + 3\,z_j^2) = \tfrac{1}{40}, \quad (1,1,1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1}^3 + 4\,y_{j-1}^3 + 6\,x_{j1}\,y_{j-1}^2 + 4\,x_{j1}^2\,y_{j-1}) = \tfrac{3}{10}.$$

Design of novel schemes

Additional practical constraints.

- In certain cases, require time-symmetry to further reduce number of order conditions (for $p = 6$ obtain $q = 7$ conditions (1), (3), (1,2), (2,3), (1,1,3), (1,2,2), (1,1,1,2))

$$\Psi_J^{[r]}(-\tau) = \left(\Psi_J^{[r]}(\tau)\right)^{-1}, \qquad x_{J+1-j,k} = (-1)^{k+1} x_{jk}.$$

- In certain cases, express solutions to order conditions in terms of few coefficients and minimise amount by which high-order conditions (e.g. at order seven) are not satisfied.

Favourable novel schemes. Illustrate favourable behaviour of resulting novel schemes for dissipative quantum system (Rosen–Zener model).

Dissipative quantum system

Rosen–Zener model with dissipation. For Rosen–Zener model with dissipation, associated Schrödinger equation in normalised form reads

$$u'(t) = A(t)\,u(t) = -\mathrm{i}\,H(t)\,u(t)\,, \quad t \in (t_0, T)\,,$$

$$H(t) = f_1(t)\,\sigma_1 \otimes I + f_2(t)\,\sigma_2 \otimes R + \delta D \in \mathbb{C}^{d\times d}\,, \quad d = 2\,k\,,$$

$$I = \mathrm{diag}\big(1\big) \in \mathbb{R}^{k\times k}\,, \quad R = \mathrm{tridiag}\big(1,0,1\big) \in \mathbb{R}^{k\times k}\,, \quad D = -\mathrm{i}\,\mathrm{diag}\big(1^2, 2^2, \dots, d^2\big) \in \mathbb{C}^{d\times d}\,.$$

Notation and special choice. Recall definitions of Pauli matrices and Kronecker product

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_1 \otimes I = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \sigma_2 \otimes R = \begin{pmatrix} 0 & -\mathrm{i}R \\ \mathrm{i}R & 0 \end{pmatrix}.$$

Special choice of arising functions and parameters

$$d = 10\,, \quad T_0 = 1\,, \quad t_0 = -4\,T_0\,, \quad T = 4\,T_0\,, \quad V_0 = \tfrac{1}{2}\,, \quad \omega = 5\,, \quad \delta = 10^{-1}\,,$$

$$f_1(t) = V_0\,\cos(\omega\,t)\,\big(\cosh\big(\tfrac{t}{T}\big)\big)^{-1}\,, \quad f_2(t) = -\,V_0\,\sin(\omega\,t)\big(\cosh\big(\tfrac{t}{T}\big)\big)^{-1}\,.$$

Remark.

- Ordinary differential equation of simple form that shows characteristics of parabolic equations if $\delta > 0$ and $d \gg 1$.
- Straightforward realisation of matrix-exponentials by low-order Taylor series expansions.

Favourable novel schemes ($p = 4$)

Favourable fourth-order schemes. Design fourth-order time-symmetric CFQM exponential integrator with real coefficients satisfying positivity condition

$$\forall\, j \in \{1, \dots, J\}: \quad x_{j1} > 0\,.$$

Use additional degrees of freedom due to inclusion of sixth-order quadrature nodes and further exponentials to verify certain conditions at order five and to minimise deviation of the remaining fifth-order conditions without increasing the overall computational cost

$$p = 4: \quad \mathrm{CF}_4^{[4]}\,, \quad \mathrm{CF}_5^{[4]}\,.$$

Compare novel schemes with optimised CFQM exponential integrator proposed in ALVERMANN, FEHSKE (see eq. (43))

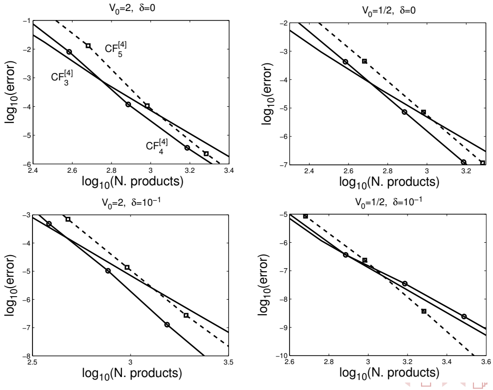
$$p = 4: \quad \mathrm{CF}_3^{[4]}\,.$$

Illustration ($p = 4$)

Numerical results. Time integration of Rosen–Zener model by fourth-order schemes

$$p = 4: \quad \mathrm{CF}_3^{[4]}\ (\mathrm{A}\ \&\ \mathrm{F}), \quad \mathrm{CF}_4^{[4]}, \mathrm{CF}_5^{[4]}\ (\text{novel}).$$

Implementation by Taylor series approximation of order $M = 6$. Display global errors in fundamental matrix solution at final time versus number of matrix-vector products. Novel schemes favourable for higher accuracy.



Favourable novel scheme ($p = 6$, commutator)

Favourable novel scheme (commutator). Design unconventional scheme of order six involving single commutator

$$p = 6\,, \quad J = 5\,, \quad K = 3\,,$$

$$\mathrm{CF}_{5C}^{[6]}(\tau) = \prod_{j=4}^{5} \mathrm{e}^{\tau a_{j1} A_1(\tau) + \tau a_{j2} A_2(\tau) + \tau a_{j3} A_3(\tau)}\, \mathrm{e}^{D} \prod_{j=1}^{2} \mathrm{e}^{\tau a_{j1} A_1(\tau) + \tau a_{j2} A_2(\tau) + \tau a_{j3} A_3(\tau)}\,,$$

$$D = \tau^2 \big[C_1(\tau), C_2(\tau)\big]\,, \quad C_1(\tau) = e_1 \big(A_1(\tau) + A_3(\tau)\big) + e_2\, A_2(\tau)\,, \quad C_2(\tau) = A_3(\tau) - A_1(\tau)\,.$$

Contrary to classical interpolatory Magnus integrators, where arising commutators only of first order, additional computational cost low due to

$$D \simeq \big[d_1\, \alpha_1(\tau) + d_2\, \alpha_3(\tau), \alpha_2(\tau)\big] = \mathcal{O}\big(\tau^3\big)\,, \quad \alpha_k(\tau) = \mathcal{O}\big(\tau^k\big)\,.$$

Compare novel scheme with optimised CFQM exponential integrator proposed in ALVERMANN, FEHSKE (see Table 3, stability issues for $\delta > 0$)

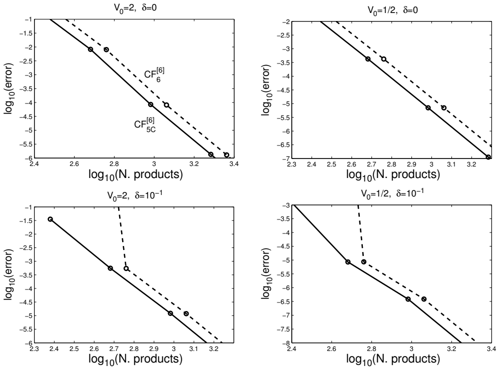
$$p = 6: \quad \mathrm{CF}_6^{[6]}\,.$$

Illustration ($p = 6$)

Numerical results. Time integration of Rosen–Zener model by sixth-order schemes

$$p = 6 : \quad \mathrm{CF}_6^{[6]} \text{ (A \& F)}, \quad \mathrm{CF}_{5C}^{[6]} \text{ (novel)}.$$

Implementation by Taylor series approximation of order $M = 6$. Display global errors in fundamental matrix solution at final time versus number of matrix-vector products. Novel schemes favourable in all cases.



Favourable novel schemes ($p = 5, 6$, complex)

Favourable novel schemes (complex coefficients). Design CFQM exponential integrator with complex coefficients satisfying positivity condition

$$p = 5: \quad \mathrm{CF}_3^{[5]}, \qquad p = 6: \quad \mathrm{CF}_4^{[6]}, \quad \mathrm{CF}_5^{[6]}.$$

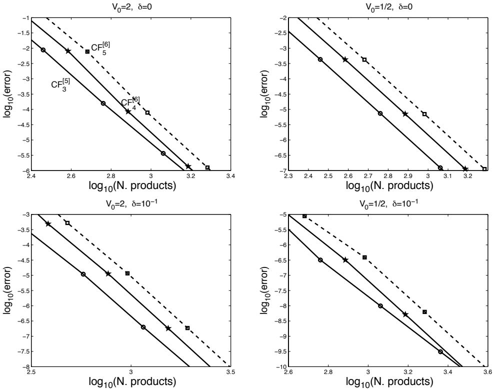
- Expect schemes to remain stable for $\delta > 0$.
- Expect scheme with $J = 3$ to be most efficient.

Favourable novel schemes ($p = 5, 6$, complex), Illustration

Numerical results. Time integration of Rosen–Zener model by fifth-order scheme and sixth-order schemes

$$p = 5: \quad CF_3^{[5]}, \qquad p = 6: \quad CF_4^{[6]}, \quad CF_5^{[6]}.$$

Implementation by Taylor series approximation of order $M = 6$. Display global errors in fundamental matrix solution at final time versus number of matrix-vector products. Novel schemes remain stable for $\delta > 0$.



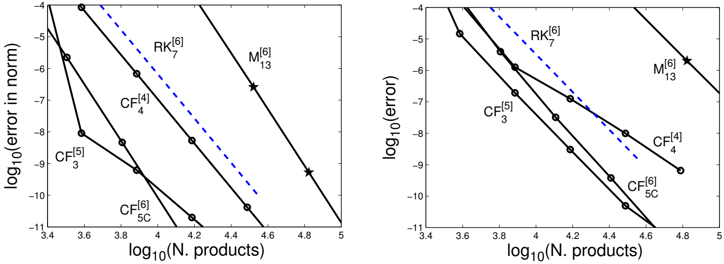
Comparison

Numerical results. Time integration of Rosen–Zener model with vanishing diffusion

$$\delta = 0, \quad V_0 = 5, \quad \omega = \tfrac{1}{2}, \quad T = 20, \quad d = 20.$$

Comparison of CFQM exponential integrators with standard explicit Runge–Kutta method and Magnus integrator.

- Global errors in fundamental matrix solution U versus total number of matrix–vector products (left).
- Corresponding errors in preservation of norm $\|U(T) - 1\|$ (right).



Extension to non-autonomous nonlinear evolution equations

Areas of application

Situation. Consider nonlinear evolution equations of form

$$u'(t) = A(t)\, u(t) + B\big(u(t)\big), \quad t \in (t_0, T).$$

Areas of application. In context of Bose–Einstein condensates and their description by nonlinear Schrödinger equations, study

- Gross–Pitaevskii equations with opening trap
- Gross–Pitaevskii equations with rotation (moving frame)

PHILIPP BADER, SERGIO BLANES, FERNANDO CASAS, M. TH. *Efficient time integration methods for Gross–Pitaevskii equations with rotation term. Submitted (2019).*

Numerical realisation by operator splitting

Approach. Apply CFQM exponential integrators in combination with operator splitting methods to nonlinear evolution equations of form

$$\begin{cases} u'(t) = A(t)\,u(t) + B\big(u(t)\big)\,, & t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,. \end{cases}$$

In each time step, resolve (small number of) autonomous nonlinear evolution equations (*frozen time*), and employ suitable compositions of solutions to associated subproblems

$$v'(t) = A(t_*)\,v(t)\,, \quad w'(t) = B\big(w(t)\big)\,.$$

Example. Second-order splitting method (Strang, specification for autonomous linear equation, first step)

$$u'(t) = A\,u(t) + B\,u(t)\,,$$

$$\mathrm{e}^{\frac{\tau}{2}A}\,\mathrm{e}^{\tau B}\,\mathrm{e}^{\frac{\tau}{2}A}u_0 \approx u(t_0+\tau) = \mathrm{e}^{\tau(A+B)}u(t_0)\,.$$

Illustration (BEC)

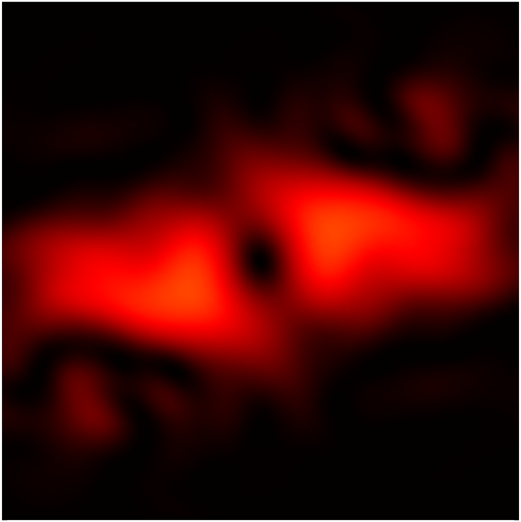
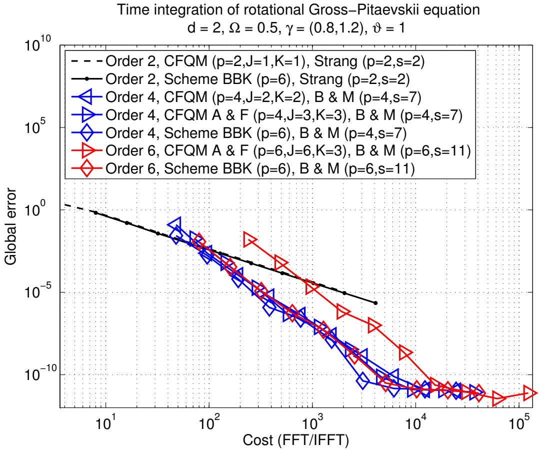


Illustration (BEC)



Conclusions

Summary.

- Commutator-free quasi-Magnus (CFQM) exponential integrators form favourable class of time discretisation methods for linear evolution equations of Schrödinger type and of parabolic type.
- Theoretical analysis contributes to deeper understanding (reveals approach to resolve stability issues, explains order reductions causing signifcant loss of accuracy).

Current and future work.

- Extension of CFQM exponential integrators combined with operator splitting methods to nonlinear Schrödinger equations.

Thank you!