

Efficient time integration methods for highly oscillatory Schrödinger equations

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Main references

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Submitted for publication.

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Highly oscillatory evolution equations

Highly oscillatory evolution equations

Highly oscillatory evolution equation. Consider nonlinear evolution equation involving **highly oscillatory linear main part**

$$\frac{d}{dt} u(t) = \frac{1}{\varepsilon} A u(t) + B(u(t)), \quad t \in (0, T), \quad 0 < \varepsilon \ll 1.$$

Basic requirements.

- (i) **Unitarity.** Unbounded linear operator $A : D(A) \subset X \rightarrow X$ generates **unitary group** $(\mathcal{E}_A(t))_{t \in \mathbb{R}}$ on underlying Banach space $(X, \|\cdot\|_X)$

$$\forall t \in \mathbb{R} \quad \forall w \in X: \quad \|\mathcal{E}_A(t)w\|_X = \|w\|_X.$$

- (ii) **Periodicity.** Associated evolution operator is **periodic** in time

$$\exists T_0 > 0 \quad \forall w \in X: \quad \mathcal{E}_A(T_0)w = w.$$

Time-dependent Schrödinger equations

Application to Schrödinger equations. Consider time-dependent nonlinear Schrödinger equation for $\psi : \Omega \times (0, T) \subseteq \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{C}$

$$i \partial_t \psi(x, t) = \frac{1}{\varepsilon} \mathcal{A}(x) \psi(x, t) + \mathcal{B}(|\psi(x, t)|) \psi(x, t), \quad (x, t) \in \Omega \times (0, T),$$

and assume that linear main part is defined by **self-adjoint operator** on Hilbert space.

- (i) **Unitarity.** Stone's theorem ensures that evolution operator $(\mathcal{E}_{-\frac{i}{\varepsilon} \mathcal{A}}(t))_{t \in \mathbb{R}}$ forms unitary group on underlying Hilbert space.
- (ii) **Periodicity.** Periodicity requirement satisfied in **mono-frequent case**, that is, eigenvalues of \mathcal{A} are integer multiples of single value.

Illustrations

Periodicity. Time-dependent Schrödinger equation with linear main part defined by self-adjoint operator satisfies additional **periodicity** requirement in **mono-frequent case**

$$i \partial_t \psi(x, t) = \frac{1}{\varepsilon} \mathcal{A}(x) \psi(x, t) + \mathcal{B}(|\psi(x, t)|) \psi(x, t), \quad (x, t) \in \Omega \times (0, T).$$

Illustrations ($d = 2$). Consider **Laplacian** on bounded domain (**Fourier basis functions**)

$$\mathcal{A} = -\Delta, \quad \Omega = (-a_1, a_1) \times (-a_2, a_2) \subset \mathbb{R}^2,$$

$$\mathcal{A} \mathcal{F}_m = \lambda_m \mathcal{F}_m, \quad m = (m_1, m_2) \in \mathbb{Z}^2,$$

$$\mathcal{F}_{m_\ell}(x_\ell) = \frac{1}{\sqrt{2a_\ell}} e^{i m_\ell \pi (x_\ell / a_\ell + 1)}, \quad x = (x_1, x_2) \in \Omega,$$

$$\mathcal{F}_m(x) = \mathcal{F}_{m_1}(x_1) \mathcal{F}_{m_2}(x_2), \quad \lambda_m = \lambda_{m_1} + \lambda_{m_2} = \pi^2 \left(\frac{m_1^2}{a_1^2} + \frac{m_2^2}{a_2^2} \right),$$

special case $a_1 = \pi = a_2$: $T_0 = 2\pi \implies (\forall m \in \mathbb{Z}^2: e^{i T_0 \lambda_m} = 1)$,

general case $\frac{a_1^2}{a_2^2} \in \mathbb{Q} \implies (\exists T_0 > 0 \forall m \in \mathbb{Z}^2: e^{i T_0 \lambda_m} = 1)$.

Similar considerations hold for additional **quadratic potential** (**Hermite basis functions**) and additional **rotation term** (**generalised Laguerre–Fourier–Hermite basis functions**).

Reformulation

Highly oscillatory evolution equation. Consider nonlinear evolution equation involving highly oscillatory linear main part

$$\frac{d}{d\tau} v(\tau) = \frac{1}{\varepsilon} A v(\tau) + B(v(\tau)), \quad \tau \in (0, T), \quad 0 < \varepsilon \ll 1.$$

Basic requirements.

- (i) *Unitarity.* Unbounded linear operator $A : D(A) \subset X \rightarrow X$ generates unitary group on underlying Banach space.
- (ii) *Periodicity.* Associated evolution operator is periodic in time.

Reformulation. Convenient to employ time scaling

$$\begin{aligned} v : [0, T] &\longrightarrow X : \tau \longmapsto v(\tau), \\ \tau = \varepsilon t &\iff t = \frac{\tau}{\varepsilon}, \\ u : [0, \frac{T}{\varepsilon}] &\longrightarrow X : t \longmapsto u(t) = v(\varepsilon t), \end{aligned}$$

which leads to **long-term problem**

$$\frac{d}{dt} u(t) = A u(t) + \varepsilon B(u(t)), \quad t \in (0, \frac{T}{\varepsilon}), \quad 0 < \varepsilon \ll 1.$$

Space and time discretisation of highly oscillatory evolution equations

Approach

Evolution operator. Consider highly oscillatory nonlinear evolution equation

$$\frac{d}{dt} u(t) = A u(t) + \varepsilon B(u(t)), \quad t \in (0, \frac{T}{\varepsilon}), \quad 0 < \varepsilon \ll 1.$$

Employ formally linear notation for **associated evolution operator**

$$u(t) = \mathcal{E}_{A+\varepsilon B}(t) u(0), \quad t \in [0, \frac{T}{\varepsilon}].$$

Objective. Introduce efficient space and time discretisation methods for computation of **approximation** to exact solution value at final time

$$u(\frac{T}{\varepsilon}) = \mathcal{E}_{A+\varepsilon B}(\frac{T}{\varepsilon}) u(0).$$

Approach. Use approach studied in CHARTIER, MAKAZAGA, MURUA, VILMART (2012).
 Employ simplifying assumption that final time is **multiple of period** (otherwise perform additional short time integration)

$$\text{final time } \frac{T}{\varepsilon} = \text{integer number} \times \text{period } T_0.$$

Use decomposition into equidistant subintervals

$$\text{final time } \frac{T}{\varepsilon} = \text{number of macro steps } N \times \text{subinterval of length } N_0 T_0$$

with **macro stepsize** $H = \varepsilon N_0 > 0$ chosen such that $0 < H = \varepsilon N_0 < 1$,

Approach

Objective. Compute **approximation** at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \hat{u}_N = u\left(\frac{T}{\varepsilon}\right) = \mathcal{E}_{A+\varepsilon B}(N N_0 T_0) u(0).$$

Basic idea. Replace **exact value** at multiple of period by **composition**

$$\begin{aligned} u_n &= \prod_{j=1}^r \left(\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0) \right) u_{n-1} \\ &\approx \hat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_{n-1}, \quad n \in \{1, 2, \dots, N\}. \end{aligned}$$

Suitable choice of coefficients $(\alpha_j, \beta_j)_{j=1}^r$ in dependence of $N_0 > 0$ leads to **higher-order multi-revolution composition methods**.

Remark. Solution of evolution equations with modified parameters required

$$\begin{aligned} u(t) &= \mathcal{E}_{A+\varepsilon B}(t) u(0), & \frac{d}{dt} u(t) &= A u(t) + \varepsilon B(u(t)), \\ v(t) &= \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(t) v(0), & \frac{d}{dt} v(t) &= A v(t) + \alpha_j \varepsilon N_0 B(v(t)), \\ w(t) &= \mathcal{E}_{A-\beta_j \varepsilon N_0 B}(t) w(0), & \frac{d}{dt} w(t) &= A w(t) - \beta_j \varepsilon N_0 B(w(t)). \end{aligned}$$

Approach

Objective. Compute **approximation** at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \hat{u}_N = u\left(\frac{T}{\varepsilon}\right) = \mathcal{E}_{A+\varepsilon B}(N N_0 T_0) u(0).$$

Basic idea. Replace **exact value** at multiple of period by **composition**

$$\begin{aligned} u_n &= \prod_{j=1}^r (\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)) u_{n-1} \\ &\approx \hat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_{n-1}, \quad n \in \{1, 2, \dots, N\}. \end{aligned}$$

Realisation. Realisation of **multi-revolution composition method** for low-dimensional time-dependent nonlinear Schrödinger equations relies on **exponential operator splitting method** for time discretisation combined with **pseudo-spectral method** for space discretisation.

Remark. Favourable behaviour of **time-splitting pseudo-spectral methods** for numerical solution of low-dimensional nonlinear Schrödinger equations confirmed by

- **numerical comparisons** (see various contributions by W. BAO and collaborators) and
- **theoretical investigations** (see work by CH. LUBICH and collaborators).

Approach

Approach. Compute **approximation** at final time $\frac{T}{\varepsilon} = N N_0 T_0$ (recall $0 < H = \varepsilon N_0 < 1$)

$$w_N \approx \hat{u}_N = u\left(\frac{T}{\varepsilon}\right) = \mathcal{E}_{A+\varepsilon B}(N N_0 T_0) u(0).$$

Step 1. Replace exact value at multiple of period by **composition** (macro stepsize $H = \varepsilon N_0$)

$$\prod_{j=1}^r (\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)) v \approx \mathcal{E}_{A+\varepsilon B}(N_0 T_0) v.$$

Step 2. Apply **time-splitting method** (micro time stepsize $h = \frac{T_0}{K}$)

$$\prod_{k=1}^K \prod_{\ell=1}^s \left(\mathcal{E}_{\gamma B}(b_\ell \frac{T_0}{K}) \mathcal{E}_A(a_\ell \frac{T_0}{K}) \right) v \approx \mathcal{E}_{A+\gamma B}(T_0) v.$$

Step 3. Apply **pseudo-spectral method** (projection, quadrature approximation)

$$\mathcal{E}_A(t) \mathcal{Q}_M v \approx \mathcal{E}_A(t) v.$$

For Fourier spectral method discrete solution given by (1D)

$$\sum_{m=-\frac{M}{2}}^{\frac{M}{2}-1} \sum_{k=1}^M \omega_k v(\xi_k) \overline{\mathcal{F}_m(\xi_k)} e^{-i\lambda_m t} \mathcal{F}_m \approx \sum_{m \in \mathbb{Z}} \int_{\Omega} v(x) \overline{\mathcal{F}_m(x)} dx e^{-i\lambda_m t} \mathcal{F}_m.$$

Full discretisation

Multi-revolution composition time-splitting pseudo-spectral method. Resulting fully discrete solution with macro stepsize $H = \varepsilon N_0$ and micro time stepsize $h = \frac{T_0}{K}$ given by

$$w_n = \prod_{j=1}^r \left(\prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{-\beta_j HB}(-b_\ell h) \mathcal{E}_A(-a_\ell h) \mathcal{Q}_M) \prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{\alpha_j HB}(b_\ell h) \mathcal{E}_A(a_\ell h) \mathcal{Q}_M) \right) w_{n-1}$$

$$\approx \hat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_{n-1}, \quad n \in \{1, 2, \dots, N\}.$$

Examples. First-order composition method and first-order Lie–Trotter splitting method

$$w_n = \prod_{k=1}^K (\mathcal{E}_{HB}(h) \mathcal{E}_A(h) \mathcal{Q}_M) w_{n-1}.$$

Second-order composition method and second-order Strang splitting method

$$\alpha_1 = \frac{1}{2} \left(1 + \frac{1}{N_0} \right), \quad \beta_1 = \frac{1}{2} \left(1 - \frac{1}{N_0} \right),$$

$$w_n = \prod_{k=1}^K \left(\mathcal{E}_{-\beta_1 HB} \left(-\frac{h}{2} \right) \mathcal{E}_A(-h) \mathcal{Q}_M \mathcal{E}_{-\beta_1 HB} \left(-\frac{h}{2} \right) \right) \prod_{k=1}^K \left(\mathcal{E}_{\alpha_1 HB} \left(\frac{h}{2} \right) \mathcal{E}_A(h) \mathcal{Q}_M \mathcal{E}_{\alpha_1 HB} \left(\frac{h}{2} \right) \right) w_{n-1}.$$

Computational cost

Computational cost. Realisation of r -stage multi-revolution composition method based on s -stage time-splitting pseudo-spectral method requires $N \times 2r \times Ks$ spectral transforms (macro stepsize $H = \varepsilon N_0$, micro stepsize $h = \frac{T_0}{K}$)

$$w_n = \prod_{j=1}^r \left(\prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{-\beta_j HB}(-b_\ell h) \mathcal{E}_A(-a_\ell h) \mathcal{Q}_M) \prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{\alpha_j HB}(b_\ell h) \mathcal{E}_A(a_\ell h) \mathcal{Q}_M) \right) w_{n-1}$$

$$\approx \hat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_{n-1}, \quad n \in \{1, 2, \dots, N\}.$$

Sole application of s -stage time-splitting pseudo-spectral method with time stepsize $h = \frac{T_0}{K}$ requires in total $N \times N_0 \times Ks$ spectral transforms.

Conclusion. For smaller value of decisive parameter $0 < \varepsilon \ll 1$, which corresponds to larger final time $\frac{T}{\varepsilon} = N N_0 T_0 \gg 1$, reasonable assumption $0 < H = \varepsilon N_0 < 1$ with $N_0 \gg 1$ implies

$$N \times 2r \times Ks \ll N \times N_0 \times Ks.$$

Numerical illustrations. Numerical illustrations for cubic Schrödinger equation given in CHARTIER, MAKAZAGA, MURUA, VILMART (2012) confirm that second- and fourth-order multi-revolution composition methods combined with second-order Strang time-splitting Fourier pseudo-spectral method are **superior in efficiency** compared to sole application of time-splitting method for long-term integration (in regime $0 < \varepsilon \ll 1$, $\frac{T}{\varepsilon} = N N_0 T_0 \gg 1$).

Convergence analysis

Convergence analysis

Situation. Consider multi-revolution composition time-splitting pseudo-spectral method in regime $0 < \varepsilon \ll 1$ ($\frac{T}{\varepsilon} = NN_0 T_0 \gg 1$, macro stepsize $H = \varepsilon N_0$, micro stepsize $h = \frac{T_0}{K}$)

$$w_n = \prod_{j=1}^r \left(\prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{-\beta_j HB}(-b_\ell h) \mathcal{E}_A(-a_\ell h) \mathcal{Q}_M) \prod_{k=1}^K \prod_{\ell=1}^s (\mathcal{E}_{\alpha_j HB}(b_\ell h) \mathcal{E}_A(a_\ell h) \mathcal{Q}_M) \right) w_{n-1} \\ \approx \hat{u}_n = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_{n-1}, \quad n \in \{1, 2, \dots, N\}.$$

Aim. For evolution equation with **regular solution** analyse stability and error behaviour of full discretisation based on

- multi-revolution composition method of order P
- time-splitting method of order p
- pseudo-spectral method

and deduce convergence estimate of form

$$\text{global error} = \mathcal{O}(H^P) + \mathcal{O}(h^p) + \mathcal{O}(M^{-\rho}).$$

Stability and error analysis of multi-revolution composition methods

Stability analysis

Objective. Stability analysis of multi-revolution composition method

$$\begin{cases} \frac{d}{dt} u(t) = A u(t) + \varepsilon B(u(t)), & t \in (0, \frac{T}{\varepsilon}), \\ u(0) = u_0, \end{cases} \quad 0 < \varepsilon \ll 1,$$
$$u_{n+1} = \prod_{j=1}^r (\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)) u_n$$
$$\approx \hat{u}_{n+1} = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_n, \quad n \in \{0, 1, \dots, N-1\}.$$

Stability. Due to unitarity of evolution operator associated with nonlinear time-dependent Schrödinger equation involving real-valued potential and real parameter $\gamma \in \mathbb{R}$

$$i \partial_t \psi(x, t) = -\Delta \psi(x, t) + V(x) \psi(x, t) + \gamma \mathcal{B}(|\psi(x, t)|) \psi(x, t), \quad (x, t) \in \Omega \times \mathbb{R},$$
$$\|\psi(\cdot, t)\|_{L^2} = \|\psi(\cdot, 0)\|_{L^2}, \quad t \in \mathbb{R},$$

stability of multi-revolution composition method in Lebesgue-space $X = L^2(\Omega, \mathbb{C})$ is evident

$$\|u_{n+1}\|_X = \|u_n\|_X, \quad n \in \{0, 1, \dots, N-1\}.$$

Remark. Stability in Sobolev-space of higher degree is more involved task.

Objective

Objective. Error analysis of multi-revolution composition method applied to highly oscillatory evolution equation

$$\begin{cases} \frac{d}{dt} u(t) = A u(t) + \varepsilon B(u(t)), & t \in (0, \frac{T}{\varepsilon}), \\ u(0) = u_0, \end{cases} \quad 0 < \varepsilon \ll 1,$$

$$\begin{aligned} u_{n+1} &= \prod_{j=1}^r (\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)) u_n \\ &\approx \hat{u}_{n+1} = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) \hat{u}_n, \quad n \in \{0, 1, \dots, N-1\}. \end{aligned}$$

Approach. Employ stepwise expansion of solution value $\mathcal{E}_{A+\gamma B}(t) v$ based on variation-of-constants formula and specify remainder terms.

First step. As first step provide rigorous analysis for linear case with bounded operator B .

Remark. Error analysis given in CHARTIER, MAKAZAGA, MURUA, VILMART (2012) relies on infinite Taylor series expansions of $\mathcal{E}_{A+\gamma B}(t)$. Presence of unbounded operators A, B requires to adapt strategies for deducing error estimates for multi-revolution composition methods.

Error analysis (Linear case, $P = 1$)

Aim. For multi-revolution composition method applied to **linear evolution equation** deduce expansion with respect to $H = \varepsilon N_0$ (initial step)

$$\frac{d}{dt} u(t) = A u(t) + \varepsilon B u(t), \quad t \in (0, \frac{T}{\varepsilon}), \quad 0 < \varepsilon \ll 1,$$

$$u_1 = \prod_{j=1}^r (\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0)) u_0 \approx \hat{u}_1 = \mathcal{E}_{A+\varepsilon B}(N_0 T_0) u_0,$$

$$u_1 - \hat{u}_1 = \mathcal{O}(H^{P+1}).$$

Special case. Focus on simple approximation

$$P = 1: \quad u_1 - \hat{u}_1 = \mathcal{E}_{A+\varepsilon N_0 B}(T_0) u_0 - \mathcal{E}_{A+\varepsilon B}(N_0 T_0) u_0 = \mathcal{O}(H^{P+1}).$$

Fundamental tool. Employ linear variation-of-constants formula and use periodicity $\mathcal{E}_A(T_0) = I$ (evolution operator **near-identity map**, smooth dependence on parameter)

$$u(t) = \mathcal{E}_{A+\varepsilon B}(t) u_0 = \mathcal{E}_A(t) u_0 + \varepsilon \int_0^t \mathcal{E}_A(t-\tau) B \mathcal{E}_{A+\varepsilon B}(\tau) u_0 d\tau, \quad t \in [0, \frac{T}{\varepsilon}],$$

$$\mathcal{E}_{A+\varepsilon B}(nT_0) = I + \varepsilon \int_0^{nT_0} \mathcal{E}_A(-\tau) B \mathcal{E}_{A+\varepsilon B}(\tau) d\tau, \quad n \in \mathbb{Z}.$$

Explanation (Linear case, $P = 1$)

Explanation. Repeated application of linear variation-of-constants formula and periodicity requirement $\mathcal{E}_A(T_0) = I$ leads to expansion of exact value involving T_0 -periodic integrand (remainder bounded in underlying function space)

$$\begin{aligned} \mathcal{E}_{A+\varepsilon B}(N_0 T_0) &= I + \varepsilon \int_0^{N_0 T_0} \mathcal{E}_A(-\tau) B \mathcal{E}_{A+\varepsilon B}(\tau) \, d\tau \\ &= I + \varepsilon \int_0^{N_0 T_0} \mathcal{E}_A(-\tau) B \mathcal{E}_A(\tau) \, d\tau + \varepsilon^2 \int_0^{N_0 T_0} \int_0^\tau \mathcal{E}_A(-\tau) B \mathcal{E}_A(\tau - \sigma) B \mathcal{E}_{A+\varepsilon B}(\sigma) \, d\sigma \, d\tau, \\ &= I + \varepsilon \int_0^{N_0 T_0} f(\tau) \, d\tau + \mathcal{O}(H^2), \quad f(\tau + T_0) = f(\tau), \quad H = \varepsilon N_0. \end{aligned}$$

Decomposition of interval $[0, N_0 T_0]$ and suitable integral transformation permits **reduction to primary interval** $[0, T_0]$

$$\begin{aligned} \mathcal{E}_{A+\varepsilon B}(N_0 T_0) &= I + \varepsilon \sum_{\ell=1}^{N_0} \int_0^{T_0} f(\tau + (\ell - 1)T_0) \, d\tau + \mathcal{O}(H^2) \\ &= I + \varepsilon N_0 \int_0^{T_0} f(\tau) \, d\tau + \mathcal{O}(H^2) = \mathcal{E}_{A+\varepsilon N_0 B}(T_0) + \mathcal{O}(H^2). \end{aligned}$$

Suggests to consider **first-order multi-revolution composition method** (leading terms of expansions coincide) and proves error relation

$$P = 1: \quad u_1 - \hat{u}_1 = \mathcal{E}_{A+\varepsilon N_0 B}(T_0) u_0 - \mathcal{E}_{A+\varepsilon B}(N_0 T_0) u_0 = \mathcal{O}(H^{P+1}), \quad H = \varepsilon N_0.$$

Error analysis (Linear case)

Extension. Consider **multi-revolution composition method** of classical order $P \in \mathbb{N}_{\geq 1}$.

- Derivatives of evolution operator with respect to decisive parameter satisfy bound

$$\|\partial_\varepsilon^k \mathcal{E}_{A+\varepsilon B}(t)v\|_X \leq (\|B\|_{X \leftarrow X} |t|)^k \|v\|_X, \quad t \in \mathbb{R}, \quad k \in \mathbb{N}, \quad v \in X.$$

- Employ Taylor series expansions of exact and numerical evolution operator with respect to decisive parameter.
- Validity of order conditions ensures that dominant terms in expansions cancel.
- Suitable estimation of remainder yields error estimate.

Lemma

$$\begin{aligned} & \left\| \prod_{j=1}^r \left(\mathcal{E}_{A-\beta_j \varepsilon N_0 B}(-T_0) \mathcal{E}_{A+\alpha_j \varepsilon N_0 B}(T_0) \right) v - \mathcal{E}_{A+\varepsilon B}(N_0 T_0) v \right\|_X \\ & \leq \frac{C}{(P+1)!} \|B\|_{X \leftarrow X}^{P+1} T_0^{P+1} H^{P+1} \|v\|_X, \quad v \in X. \end{aligned}$$

Remark. Rigorous extension to nonlinear problems more involved.

Convergence result

Convergence result (Linear case)

Convergence analysis. For evolution equation with **regular solution** analyse stability and error behaviour of full discretisation based on

- multi-revolution composition method of order P
- time-splitting method of order p
- pseudo-spectral method

and deduce convergence estimate of form

$$\text{global error} = \mathcal{O}(H^P) + \mathcal{O}(h^p) + \mathcal{O}(M^{-\rho}).$$

Dependence on macro and micro stepsizes. Above considerations explain dependence of global error on **macro stepsize**. Dependence on **micro stepsize** and superconvergent behaviour of symmetric versus non-symmetric time-splitting methods explained in CHARTIER, MÉHATS, TH., ZHANG (2015). Illustration by numerical examples.

Convergence result (Linear case)

Theorem (Global error estimate)

Assume that the unbounded linear operator A satisfies the stated requirements and that the linear operator B is bounded. For the full discretisation of the linear Schrödinger equation

$$\frac{d}{dt} u(t) = A u(t) + \varepsilon B u(t), \quad t \in (0, \frac{T}{\varepsilon}], \quad 0 < \varepsilon \ll 1,$$

combine a multi-revolution composition method of nonstiff order $P \in \mathbb{N}_{\geq 1}$, applied with macro stepsize H , a time-splitting method of nonstiff order $p \in \mathbb{N}_{\geq 1}$, applied with micro time stepsize h , and a pseudo-spectral method applied with M_0^d basis functions. Under the assumption that the exact solution remains bounded in the fractional power space X_ϑ for some $\vartheta \geq \frac{p}{2}$, the global error estimate

$$\begin{aligned} \|u_{MN} - u(\frac{T}{\varepsilon})\|_X &\leq \|u_0 - u(0)\|_X + CH^P + CM_0^{-\rho} \\ &\quad + \begin{cases} C(h^{2\vartheta} + Hh^p) & \text{if splitting non-symmetric,} \\ C(h^{2\vartheta} + \varepsilon h^p) & \text{if splitting symmetric,} \end{cases} \end{aligned}$$

is valid with $\rho = \rho(\vartheta) > 0$ depending on the considered pseudo-spectral method and $C > 0$ depending in particular on upper bounds for $\max\{\|u(t)\|_{X_\vartheta} : 0 \leq t \leq \frac{T}{\varepsilon}\}$, where $\frac{T}{\varepsilon} = NN_0 T_0$.

Numerical illustrations

Illustrations

Model problem. Consider **time-dependent nonlinear Schrödinger equation** with regular solution ($d = 1$, $T_0 = 2\pi$)

$$i \partial_t \psi(x, t) = -\partial_{xx} \psi(x, t) + \varepsilon V(x) |\psi(x, t)|^2 \psi(x, t),$$

$$V(x) = 2 \cos(2x), \quad \psi(x, 0) = \cos(x) + \sin(x), \quad (x, t) \in (-\pi, \pi) \times \left(0, \frac{T}{\varepsilon}\right].$$

Space discretisation. Apply Fourier pseudo-spectral method for **space discretisation** (spatial error for $M = 256$ basis functions insignificant).

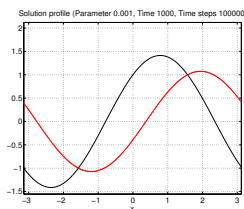
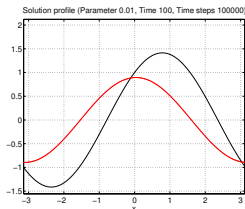
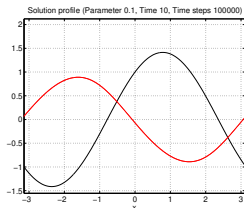
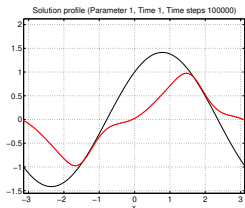
Illustrations.

- Solution behaviour in dependence of decisive parameter
- Error behaviour of time-splitting methods
- Error behaviour of multi-revolution composition time-splitting methods

Solution behaviour

Solution behaviour. Illustrate behaviour of solution to nonlinear Schrödinger equation in dependence of decisive parameter (real part, $T = 1$). Apply Strang-splitting method with time stepsize Δt (verify result for refined time stepsize)

$$\begin{aligned} \varepsilon = 1, \quad \frac{T}{\varepsilon} = 1, \quad \Delta t = 10^{-5}, & \quad \varepsilon = 10^{-1}, \quad \frac{T}{\varepsilon} = 10, \quad \Delta t = 10^{-4}, \\ \varepsilon = 10^{-2}, \quad \frac{T}{\varepsilon} = 100, \quad \Delta t = 10^{-3}, & \quad \varepsilon = 10^{-3}, \quad \frac{T}{\varepsilon} = 1000, \quad \Delta t = 10^{-2}. \end{aligned}$$



Time-splitting methods

Error behaviour. Analyse error behaviour of **sole application** of first-order Lie–Trotter splitting method ($p = 1$), second-order Strang splitting method ($p = 2$), and fourth-order splitting method by Yoshida ($p = 4$) for time integration of nonlinear Schrödinger equation

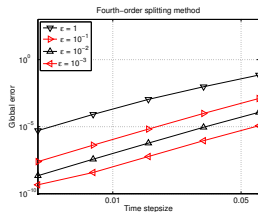
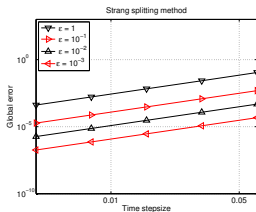
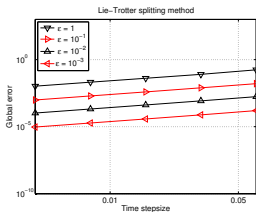
$$i \partial_t \psi(x, t) = -\partial_{xx} \psi(x, t) + \varepsilon V(x) |\psi(x, t)|^2 \psi(x, t),$$

$$V(x) = 2 \cos(2x), \quad \psi(x, 0) = \cos(x) + \sin(x), \quad (x, t) \in (-\pi, \pi) \times \left(0, \frac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solution

$$\text{global error at final time } \frac{T}{\varepsilon} = \mathcal{O}(\varepsilon h^p), \quad \frac{T}{\varepsilon} = N \Delta t,$$

see **theoretical error estimate** deduced in CHARTIER, MÉHATS, TH., ZHANG (2014).



Time-splitting methods

Error behaviour. Analyse error behaviour of **sole application** of first-order Lie–Trotter splitting method ($p = 1$), second-order Strang splitting method ($p = 2$), and fourth-order splitting method by Yoshida ($p = 4$) for time integration of nonlinear Schrödinger equation

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Numerical results. Numerical results confirm error relation for regular solutions

$$\text{global error at final time } \frac{T}{\varepsilon} : \quad \text{err}_\varepsilon = \mathcal{O}(\varepsilon h^p), \quad \frac{T}{\varepsilon} = Nh,$$

see **theoretical error estimate** deduced in CHARTIER, MÉHATS, TH., ZHANG (2014).

Drawback! Number of time steps N increases in dependence of parameter!

h	N	$\text{err}_{10^{-1}}$	p	N	$\text{err}_{10^{-2}}$	p	N	$\text{err}_{10^{-3}}$	p
$6.2 \cdot 10^{-2}$	160	$1.2 \cdot 10^{-3}$		1600	$1.1 \cdot 10^{-4}$		16000	$1.1 \cdot 10^{-5}$	
$3.1 \cdot 10^{-2}$	320	$9.6 \cdot 10^{-5}$	3.7	3200	$9.0 \cdot 10^{-6}$	3.7	32000	$8.9 \cdot 10^{-7}$	3.7
$1.5 \cdot 10^{-2}$	640	$6.5 \cdot 10^{-6}$	3.8	6400	$5.9 \cdot 10^{-7}$	3.9	64000	$5.9 \cdot 10^{-8}$	3.9
$7.8 \cdot 10^{-3}$	1280	$4.1 \cdot 10^{-7}$	3.9	12800	$3.7 \cdot 10^{-8}$	3.9	128000	$3.8 \cdot 10^{-9}$	3.9
$3.9 \cdot 10^{-3}$	2560	$2.4 \cdot 10^{-8}$	4.0	25600	$2.2 \cdot 10^{-9}$	4.0	256000	$4.5 \cdot 10^{-10}$	3.0

Global errors of fourth-order splitting method by Yoshida for $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}$

Multi-revolution composition time-splitting methods

Error behaviour (Composition). Study error behaviour of **second-order multi-revolution composition method** ($P = 2$) for time integration of nonlinear Schrödinger equation

$$i \partial_t \psi(x, t) = -\partial_{xx} \psi(x, t) + \varepsilon V(x) |\psi(x, t)|^2 \psi(x, t),$$

$$V(x) = 2 \cos(2x), \quad \psi(x, 0) = \cos(x) + \sin(x), \quad (x, t) \in (-\pi, \pi) \times \left(0, \frac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solutions (if micro stepsize $h = \frac{T_0}{K}$ sufficiently small)

$$\text{global error at final time } \frac{T}{\varepsilon} = \mathcal{O}(H^P), \quad \frac{T}{\varepsilon} = N N_0 T_0, \quad H = \varepsilon N_0,$$

see **theoretical error estimate** deduced in CHARTIER, MÉHATS, TH., ZHANG (2015).

N	1000	500	250	125
N_0	2	4	8	16
H	$2 \cdot 10^{-3}$	$4 \cdot 10^{-3}$	$8 \cdot 10^{-3}$	$16 \cdot 10^{-3}$
error	$6.58 \cdot 10^{-7}$	$3.31 \cdot 10^{-6}$	$1.39 \cdot 10^{-5}$	$5.64 \cdot 10^{-5}$
P		2.33	2.07	2.01

Global errors of second-order multi-revolution composition method for $\varepsilon = 10^{-3}$ and $T = 4\pi$.

Error of time-splitting method insignificant for $p = 4$, $K = 10^3$.

Reference solution computed for refined macro stepsize $H = 10^{-3}$ ($N = 2000$, $N_0 = 1$).

Multi-revolution composition time-splitting methods

Error behaviour (Splitting). Study error behaviour of multi-revolution composition method ($P = 2$) combined with **symmetric second-order Strang splitting method** ($p = 2$) for time integration of nonlinear Schrödinger equation

$$i \partial_t \psi(x, t) = -\partial_{xx} \psi(x, t) + \varepsilon V(x) |\psi(x, t)|^2 \psi(x, t),$$

$$V(x) = 2 \cos(2x), \quad \psi(x, 0) = \cos(x) + \sin(x), \quad (x, t) \in (-\pi, \pi) \times \left(0, \frac{T}{\varepsilon}\right].$$

Numerical results. Numerical results confirm error relation for regular solutions (if macro stepsize $H = \varepsilon N_0$ sufficiently small)

$$\text{global error at final time } \frac{T}{\varepsilon} = \mathcal{O}(\varepsilon h^p), \quad \frac{T}{\varepsilon} = N N_0 T_0, \quad h = \frac{T_0}{K},$$

see **theoretical error estimate** deduced in CHARTIER, MÉHATS, TH., ZHANG (2015).

h	$3.9 \cdot 10^{-1}$	$1.9 \cdot 10^{-1}$	$9.8 \cdot 10^{-2}$	$4.9 \cdot 10^{-2}$	$2.4 \cdot 10^{-2}$
error(ε)	$2.23 \cdot 10^{-2}$	$6.85 \cdot 10^{-3}$	$1.46 \cdot 10^{-3}$	$3.61 \cdot 10^{-4}$	$9.34 \cdot 10^{-5}$
error(2ε)	$4.46 \cdot 10^{-2}$	$1.37 \cdot 10^{-2}$	$2.93 \cdot 10^{-3}$	$7.22 \cdot 10^{-4}$	$1.86 \cdot 10^{-4}$
$\frac{\text{error}(2\varepsilon)}{\text{error}(\varepsilon)}$	2.00	2.00	2.00	2.00	2.00
p		1.70	2.22	2.01	1.95

Global errors at $T = 4\pi$ for symmetric second-order splitting, where $\varepsilon = 10^{-3}$, $N = 2000$, $N_0 = 1$ and $2\varepsilon = 2 \cdot 10^{-3}$, $N = 1000$, $N_0 = 1$, respectively. Error of composition method insignificant for $P = 2$.
 Reference solution computed by fourth-order splitting method.

Conclusions and future work

Conclusions. Multi-revolution composition methods combined with time-splitting pseudo-spectral methods for highly oscillatory evolution equations.

- Rigorous convergence analysis completed for linear case.
- Superconvergent behaviour of symmetric splitting methods explained for nonlinear case.

Future work. Treatment of Dirac equation in non-relativistic regime.

Thank you!