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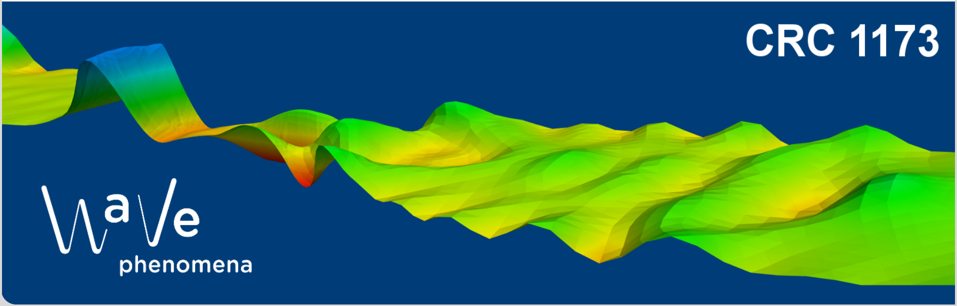
Uniformly accurate exponential-type integrators for KG equations

(Uniformly accurate exponential-type integrators for Klein-Gordon equations with asymptotic convergence to classical splitting schemes in the nonlinear Schrödinger limit)

joint work with E. Faou and K. Schratz

Simon Baumstark | October 12, 2016



Outline

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with initial conditions

$$z(0,x) = z_0(x), \quad \partial_t z(0,x) = c^2 z_0'(x),$$

for $x \in \mathbb{T} = [0, 2\pi]$ and $t \in [0, T]$.

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- **Numerical Challenge:**
  Highly oscillatory (non-relativistic) limit regime, i.e. $c \gg 1$
- Goal: Search numerical approximations $z^n \approx z(t_n)$ with $t_n = n\tau$.

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Idea:

Use Duhamel's formula and approximate integral with quadrature formula

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- Attention: $z(t_n+s) = z(t_n) + \mathcal{O}(sz')$ with $z'(t) = \mathcal{O}(c^2)$!

Gautschi-type methods

- **EWI-PS method by Bao applied to KG equation at $t_n = 1$:**

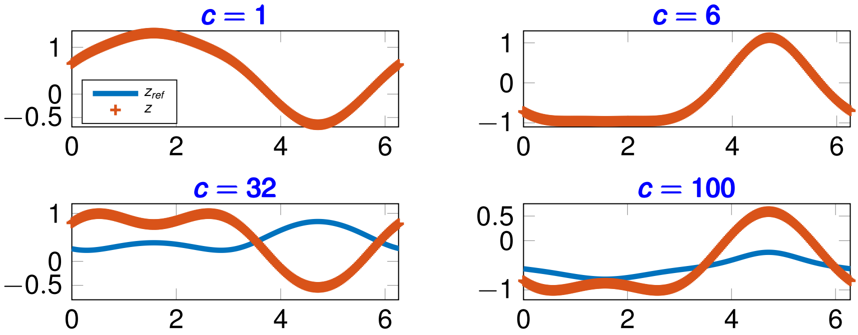

Figure: **blue line:** EWI-PS for reference solution ($\tau_{\text{ref}} \approx 10^{-6}$),
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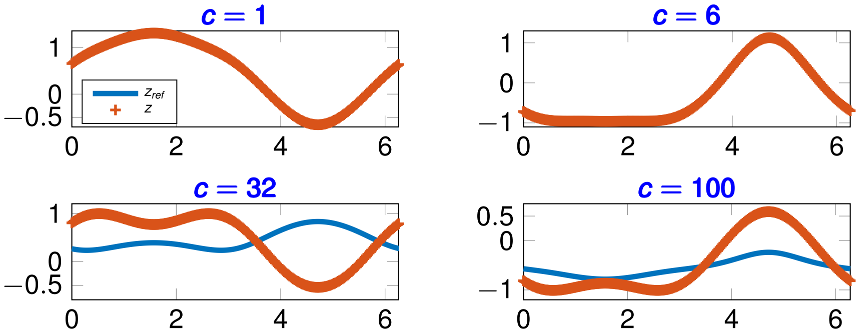

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Problem: Time step restriction for large ***c***!

Limit approximation

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- Rewrite KG equation as a first-order system $z = \frac{1}{2}(u + \overline{u})$ with

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- **Multiscale expansion:** Introduce $u(t,x) = U(t, c^2 t, x)$ and expand

$$U = \sum_{n\in\mathbb{N}_0} c^{-2n}U_n(t, c^2 t, x) = U_0(t, c^2 t, x) + \mathcal{O}(c^{-2}),$$

$$\boxed{c\langle\nabla\rangle_c = c^2 - \tfrac{1}{2}\Delta} + \mathcal{O}(c^{-2}), \qquad \boxed{c\langle\nabla\rangle_c^{-1} = 1} + \mathcal{O}(c^{-2}).$$

Limit approximation

- This yields the cubic nonlinear Schrödinger (NLS) limit system:

$$(\star) \qquad i\partial_t u_\infty = \frac{1}{2}\Delta u_\infty + \frac{3}{8}|u_\infty|^2 u_\infty, \qquad u_\infty = z_0 - iz_0'$$

such that (for suff. smooth solutions)

$$z = \frac{1}{2}\left(u_\infty e^{ic^2 t} + c.c.\right) + \mathcal{O}(c^{-2}).$$

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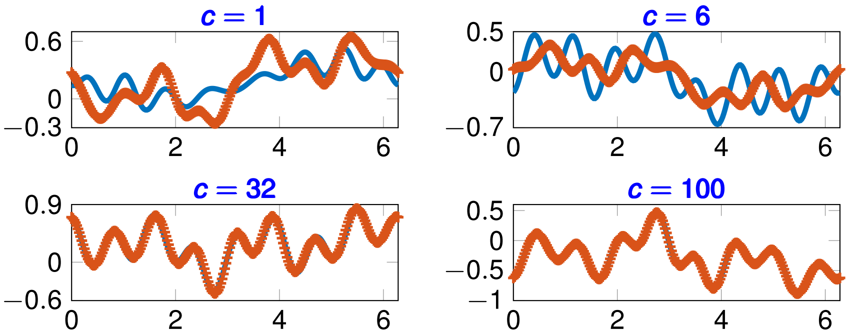
- **Advantage:**
  Only solve non-oscillatory cubic NLS $(\star)$ numerically, e.g. with Strang splitting (see Faou/Schratz 2014)

Limit approximation

- **Limit approximation vs. reference solution at $t_n = 1$:**



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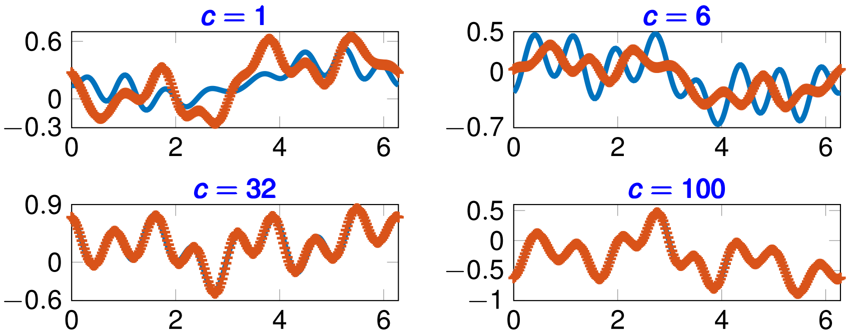

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Problem: Good approximation only for $c \gg 1$!

Uniformly accurate scheme

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Uniformly accurate scheme

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Aim: Scheme that works well for small AND large c.

Idea:

- Derive Duhamel's formula in "twisted variables"
- Integrate the highly-oscillatory phases exactly

Uniformly accurate scheme

What are these "twisted variables"?

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- KG eq. rewritten as first-order system in time with $z = \frac{1}{2}(u + \overline{u})$

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- Look at "twisted variable" $u_*(t) = e^{-ic^2 t}u(t)$ which satisfies

$$i\partial_t u_* = -(\underbrace{c\langle\nabla\rangle_c - c^2}_{=:\mathcal{A}_c})u_* + \frac{1}{8}c\langle\nabla\rangle_c^{-1}e^{-ic^2 t}\left(e^{ic^2 t}u_* + e^{-ic^2 t}\overline{u_*}\right)^3.$$

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- $\mathcal{A}_c$ and $c\langle\nabla\rangle_c^{-1}$ are uniformly bounded in c:

$$\|\mathcal{A}_c u\|_r^2 \leq \frac{1}{2}\|u\|_{r+2}^2, \qquad \|c\langle\nabla\rangle_c^{-1}u\|_r \leq \|u\|_r.$$

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Advantage:

All operators uniformly bounded in c $\boxed{\rightsquigarrow \partial_t u_* \text{ bounded in } c!}$

Uniformly accurate scheme

A first-order uniformly accurate scheme

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- Duhamel's formula yields

$$u_*(t_n+\tau) = e^{i\tau\mathcal{A}_c} u_*(t_n) - \frac{i}{8} c \langle\nabla\rangle_c^{-1} e^{i\tau\mathcal{A}_c} \int_0^\tau e^{-is\mathcal{A}_c} \quad e^{-ic^2(t_n+s)} \Big(e^{ic^2(t_n+s)} \quad u_*(t_n+s) \quad + c.c. \Big)^3 ds.$$

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$$e^{-is\mathcal{A}_c} = 1 + \mathcal{O}(s\mathcal{A}_c) = 1 + \mathcal{O}(s\Delta),$$
$$u_*(t_n+s) = u_*(t_n) + \mathcal{O}\Big(s \cdot \partial_t u_*(t_n+\xi)\Big).$$

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A first-order uniformly accurate scheme

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- Now we integrate the highly-oscillatory phases $e^{\pm ikc^2 s}$ exactly

Uniformly accurate scheme

- Yields **first-order uniformly accurate scheme:**

$$
\begin{aligned}
u_*^{n+1} = {} & e^{i\tau\mathcal{A}_c} e^{-i\tau\frac{3}{8}|u_*^n|^2} u_*^n \\
& - i\tau\frac{3}{8}\left(c\langle\nabla\rangle_c^{-1} - 1\right) e^{i\tau\mathcal{A}_c}|u_*^n|^2 u_*^n \\
& - \tau\frac{i}{8} c\langle\nabla\rangle^{-1} e^{i\tau\mathcal{A}_c}\Big\{ e^{-2ic^2 t_n}\,\varphi_1(-2ic^2\tau)3|u_*^n|^2\overline{u_*^n} \\
& \qquad + e^{2ic^2 t_n}\,\varphi_1(2ic^2\tau)(u_*^n)^3 \\
& \qquad + e^{-4ic^2 t_n}\varphi_1(-4ic^2\tau)(\overline{u_*^n})^3 \Big\}
\end{aligned}
$$

with $u_*^0 = z(0) - ic^{-1}\langle\nabla\rangle_c^{-1}\, z'(0)$ and $\varphi_1(x) := \frac{e^x - 1}{x}$.

Uniformly accurate scheme

Asymptotic convergence to classical splitting schemes

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Asymptotic convergence to classical splitting schemes

- Applied Lie splitting scheme to the Schrödinger limit (see F./S. 2014)

$$u_\infty^{n+1} = e^{-\tau \frac{i}{2}\Delta} e^{-i\tau \frac{3}{8}|u_\infty^n|^2} u_\infty^n$$

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Asymptotic convergence to classical splitting schemes

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With $\|\tau\varphi_1(ilc^2\tau)\|_r = \mathcal{O}(c^{-2})$

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$$u_*^{n+1} = u_\infty^{n+1} + \mathcal{O}(c^{-2})$$

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Theorem (Convergence bound for the first-order scheme)

Fix $r > d/2$ and assume that

$$\|z(0)\|_{r+2} + \|c^{-1}\langle\nabla\rangle_c^{-1} z'(0)\|_{r+2} \leq M$$

uniformly in c. For u_*^n defined in the first-order scheme we set

$$z^n \ := \frac{1}{2}\left(e^{ic^2 t_n} u_*^n + e^{-ic^2 t_n}\overline{u_*^n}\right).$$

Then, there exists a $T_r > 0$ and $\tau_0 > 0$ such that for all $\tau \leq \tau_0$ and $t_n \leq T_r$ we have for all $c > 0$ that

$$\|z(t_n) - z^n\|_r \ \leq \tau K^*_{r,M,t_n},$$

where the constant K^*_{r,M,t_n} can be chosen independently of c.

Uniformly accurate scheme

Remark

Uniformly accurate scheme

Karlsruhe Institute of Technology

Remark

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  Insert Duhamel's formula for $u_*(t_n + s)$ into $u_*(t_n + \tau)$ and go on analogously to derivation of the first-order scheme

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- Generalization to higher order schemes:
  Insert Duhamel's formula for $u_*(t_n + s)$ into $u_*(t_n + \tau)$ and go on analogously to derivation of the first-order scheme
- Second-order scheme converges in the limit $c \to \infty$ to the classical Strang splitting method for the corresponding nonlinear Schrödinger equation

$$u_*^{n+1} = \text{ Strang for limit NLS} + \mathcal{O}(c^{-2}).$$

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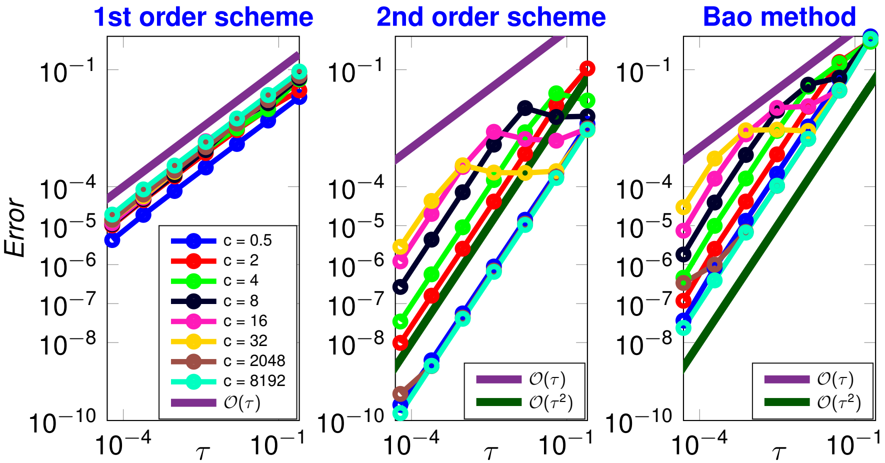
Uniformly accurate scheme

Other uniformly accurate schemes:

Bao/Cai/Zhao (2014)	Chartier et al (2015)
• Multiscale decomposition • Only linear convergence rate $\mathcal{O}(\tau)$ for all $c \in [1, \infty)$ • Derivation is complicated	• Chapman-Enskog expansion • Convergence proof needs higher regularity assumptions: First order $\rightarrow H^{r+4}$ Second order $\rightarrow H^{r+8}$

Uniformly accurate scheme



Simulation on $x \in [-16, 16]$, $t \in [0, 1]$, $\tau_{ref} \approx 10^{-6}$ and $M = 256$.

Outlook

- Derive a first-order uniformly accurate scheme for the Klein-Gordon-Zakharov (KGZ) system in the different limit regimes
- Construct higher-order methods
- Error analysis for the uniformly accurate schemes for the KGZ system

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