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Splitting Methods for Nonlinear Dirac Equations

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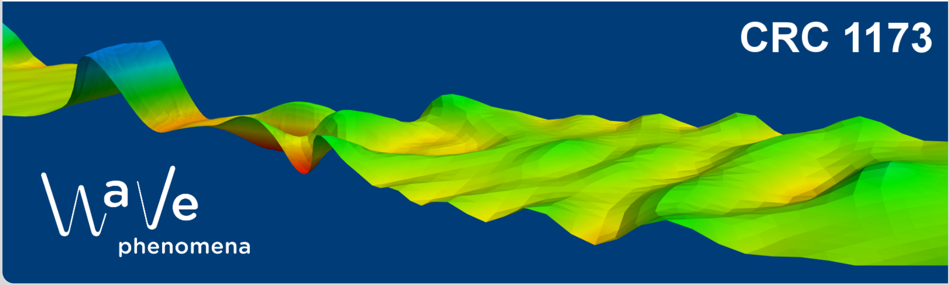

Overview

- Introduction to Dirac Systems
- Splitting Methods — a short recap
- 3-term Splitting for Nonlinear Dirac
- Error Analysis of the 3 term Splitting Scheme
- Numerical Experiments
- Summary and Outlook

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Dirac Systems

- physical description of relativistic particles (e. g. electrons) in time and space
  - v_p velocity of the particle
  - c_0 speed of light

Dirac Systems

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  - v_p velocity of the particle
  - c_0 speed of light
- $c := c_0 / v_p$ gives speed of temporal oscillations

relativistic	intermediate	non-relativistic
$c \approx 1$	$10 \lesssim c \lesssim 100$	$c \to \infty$
slow osc.	intermediate osc.	rapid osc.

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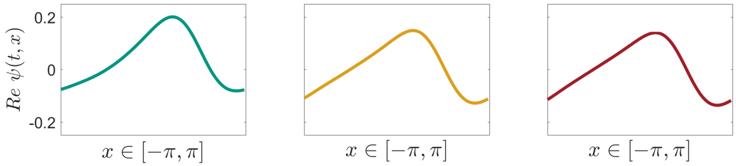

Nonlinear Dirac Equation

Consider for given initial data $\Psi(0,x) \in \mathbb{C}^4$ on $(t,x) \in [0,T] \times [-\pi,\pi]^d$

$$i\partial_t \Psi = \left(-ic \sum_{j=1}^{d} \alpha_j \partial_j + c^2 \beta \right) \Psi \; + \; \left(\phi - \sum_{j=1}^{d} \alpha_j A_j \right) \Psi \; + \; \lambda \left(\Psi \cdot \beta \overline{\Psi} \right) \beta \Psi$$

with periodic boundary conditions in space, $d = 1, 2, 3$, parameter $\lambda > 0$ fixed

- Dirac solution $\Psi(t,x) = (\psi_1(t,x), \dots, \psi_4(t,x))^\top \in \mathbb{C}^4$ *("four-spinor")*
- scalar potential $\phi(x) \in \mathbb{R}$ *("electric potential")*
- vector potential $\boldsymbol{\mathcal{A}}(x) = (A_1(x), \dots, A_d(x))^\top \in \mathbb{R}^d$ *("magnetic potential")*
- Dirac matrices $\beta,\ \alpha_j \in \mathbb{C}^{4\times 4}$, $j = 1, 2, 3$

Note: can be reduced for $d = 1, 2$ to system for **two-spinor** $\widetilde{\Psi} = (\psi_1, \psi_4)^\top$

Nonlinear Dirac Equation - the Dirac matrices

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$$i\partial_t \Psi = \left(-ic \sum_{j=1}^{d} \boldsymbol{\alpha}_j \partial_j + c^2 \boldsymbol{\beta} \right) \Psi + \left(\phi - \sum_{j=1}^{d} \boldsymbol{\alpha}_j A_j \right) \Psi + \lambda \left(\Psi \cdot \boldsymbol{\beta} \overline{\Psi} \right) \boldsymbol{\beta} \Psi$$

- Dirac matrices (defined via Pauli matrices $\boldsymbol{\sigma}_j \in \mathbb{C}^{2\times 2},\ j = 1, 2, 3$)

$$\boldsymbol{\beta} = \begin{pmatrix} \mathcal{I}_2 & 0 \\ 0 & -\mathcal{I}_2 \end{pmatrix}, \qquad \boldsymbol{\alpha}_j = \begin{pmatrix} 0 & \boldsymbol{\sigma}_j \\ \boldsymbol{\sigma}_j & 0 \end{pmatrix} \in \mathbb{C}^{4\times 4},\ j = 1, 2, 3$$

- Hermite property: $\boldsymbol{\alpha}_j = \boldsymbol{\alpha}_j^H = (\overline{\boldsymbol{\alpha}_j})^\top \quad \Rightarrow \quad \boldsymbol{\alpha}_j^\top = \overline{\boldsymbol{\alpha}_j}$
- Important **anti-commuting** properties for $j, k = 1, 2, 3$:

$$\boldsymbol{\alpha}_j \boldsymbol{\beta} + \boldsymbol{\beta} \boldsymbol{\alpha}_j = 0, \qquad \boldsymbol{\alpha}_j \boldsymbol{\alpha}_k + \boldsymbol{\alpha}_k \boldsymbol{\alpha}_j = 2\delta_{j,k} \mathcal{I}_4, \qquad \boldsymbol{\beta}^2 = \mathcal{I}_4 = \boldsymbol{\alpha}_j^2.$$

$\Rightarrow$ commutator $[\boldsymbol{\alpha}_j, \boldsymbol{\beta}] = \boldsymbol{\alpha}_j \boldsymbol{\beta} - \boldsymbol{\beta} \boldsymbol{\alpha}_j = 2\boldsymbol{\alpha}_j \boldsymbol{\beta}$

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Splitting Methods — a short recap

Consider ODE

$$y' = F(y) = f_1(y) + f_2(y), \quad y(0) = y_0 \in \mathbb{C}^N$$

with "nice" functions f_1, f_2 and corresponding subproblems

$$w' = f_1(w), \quad w(0) = w_0 \quad (S1), \qquad z' = f_2(z), \quad z(0) = z_0 \quad (S2)$$

- exact flows φ_1^t and φ_2^t, i.e. $w(t) = \varphi_1^t(w_0)$, $z(t) = \varphi_2^t(z_0)$
- **Lie splitting** (with step size τ at time $t_n = n\tau,\ n = 0, 1, 2, 3, \dots$)

$$\left(\Phi_{\text{Lie}}^{\tau}\right)^n (y_0) = \left(\varphi_1^{\tau} \circ \varphi_2^{\tau}\right)^n (y_0) = y(t_n) + \mathcal{O}(\tau)$$

- **Strang splitting**

$$\left(\Phi_{\text{Strang}}^{\tau}\right)^n (y_0) = \left(\varphi_1^{\tau/2} \circ \varphi_2^{\tau} \circ \varphi_1^{\tau/2}\right)^n (y_0) = y(t_n) + \mathcal{O}\left(\tau^2\right)$$

Splitting Methods — Commutators

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Now consider the linear case $f_1(y) = Ay$, $f_2(y) = By$, $A, B \in \mathbb{R}^{N\times N}$.
Dependency of the error constant in case of

- **Lie splitting** on norm of commutator

$$[A, B]y_0 = (AB - BA)y_0$$

- **Strang splitting** on norm of double commutators

$$[A, [A, B]]y_0 \qquad \text{and} \qquad [B, [B, A]]y_0$$

Generalization to evolution equations: $A(v)$, $B(v)$ nonlinear operators
(cf. [Lubich 2008], [Descombes 2013], ...)

$$[A, B](v)w = A'(v)B(v)w - B'(v)A(v)w$$

Splitting Methods — Example of NLS

Classical splitting for NLS with p.b.c.

$$i\partial_t\psi = -\Delta\psi + |\psi|^2\psi, \quad \psi(0) = \psi_0, \quad (t,x) \in [0,T] \times [-\pi,\pi]^d$$

into

$$i\partial_t w = -\Delta w, \quad w(0) = w_0 \quad (S1), \qquad i\partial_t z = |z|^2 z, \quad z(0) = z_0 \quad (S2)$$

- solve $(S1)$ exactly in Fourier space

$$\varphi_1^t(w_0) = \exp(it\Delta)w_0 \qquad \sim \qquad \exp(it(-|k|^2))\widehat{(w_0)}_k \quad \forall k \in \mathbb{Z}^d$$

- in $(S2)$ exploit that

$$\boxed{\partial_t |z|^2 = \partial_t (z \cdot \overline{z}) = 0, \quad \text{i.e.} \quad |z(t,x)|^2 = |z_0(x)|^2}$$

$$\Rightarrow \quad \varphi_2^t(z_0(x)) = \exp(-it|z_0(x)|^2)z_0(x) \qquad \forall x \in [-\pi,\pi]^d,$$

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Time Splitting Fourier Pseudospectral Scheme

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$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j + c^2\boldsymbol{\beta}\right)\Psi}_{=:\, H\Psi =:\, \mathcal{H}(\Psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)\Psi}_{=:\, \mathcal{V}(\Psi)} + \underbrace{\lambda\left(\Psi\cdot\boldsymbol{\beta}\overline{\Psi}\right)\boldsymbol{\beta}\Psi}_{=:\, \mathcal{N}(\Psi)}$$

Time Splitting Fourier Pseudospectral Scheme

$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j + c^2\boldsymbol{\beta}\right)\Psi}_{=:\, H\Psi =:\, \mathcal{H}(\Psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)\Psi}_{=:\, \mathcal{V}(\psi)}$$

for $\lambda = 0$:

- exponential 2-term **Strang splitting** successfull (TSFP scheme in [Bao2017])
- exact flows ($D_k,\ \widetilde{D}_x \in \mathbb{R}^{4\times 4}$ diagonal)

$$\varphi_{\mathcal{H}}^t(\Psi_0) = e^{-itH}\Psi_0 \quad \sim \quad Q_k\, e^{-itD_k}\, Q_k^{\mathrm{H}}\, \widehat{(\Psi_0)}_k \quad \forall k \in \mathbb{Z}^d$$

$$\varphi_{\mathcal{V}}^t(\Psi_0) = e^{-it\left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)}\Psi_0 \quad \sim \quad P_x\, e^{-it\widetilde{D}_x}\, P_x^{\mathrm{H}}\, \widehat{(\Psi_0)}_k \quad \forall x \in [-\pi, \pi]^d$$

- $\varphi_{\mathcal{H}}^t$ **isometry** in H^r $\rightsquigarrow$ **stability** of scheme
- second order global error involves commutators

$$[\mathcal{H}, [\mathcal{H}, \mathcal{V}]](\Psi) = c^4 \sum_{j=1}^{d} A_j\, [\boldsymbol{\beta}, [\boldsymbol{\beta}, \boldsymbol{\alpha}_j]] + \mathcal{O}\left(c^3\right)$$

Splitting Methods for Nonlinear Dirac

$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j + c^2\boldsymbol{\beta}\right)\Psi}_{\mathcal{H}(\psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)\Psi}_{\mathcal{V}(\psi)} + \underbrace{\lambda\left(\Psi\cdot\boldsymbol{\beta}\overline{\Psi}\right)\boldsymbol{\beta}\Psi}_{\mathcal{N}(\psi)}$$

for $\lambda \neq 0$:

- $\varphi^t_{\mathcal{H}}(\Psi_0)$ as before, but
- **Complication:** within subproblem $i\partial_t\Psi = \mathcal{V}(\Psi) + \mathcal{N}(\Psi)$ $\quad (S2)$

$$\partial_t\left(\Psi\cdot\boldsymbol{\beta}\overline{\Psi}\right) = \partial_t\Psi\cdot\boldsymbol{\beta}\overline{\Psi} + \Psi\cdot\boldsymbol{\beta}\overline{\partial_t\Psi} = \cdots = i\Psi\cdot\left(\sum_{j=1}^{d} A_j\left(\overline{\boldsymbol{\alpha}_j}\boldsymbol{\beta} - \boldsymbol{\beta}\overline{\boldsymbol{\alpha}_j}\right)\right)\overline{\Psi} \neq 0$$

$\Rightarrow$ no explicit expression for **exact flow** of $(S2)$ if $\boldsymbol{\mathcal{A}} = (A_1, \ldots, A_d)^\top \neq 0$

How to explicitly formulate a Strang splitting ???

$$\left(\varphi^{\tau/2}_{\mathcal{H}} \circ \underbrace{\varphi^{\tau}_{\mathcal{V}+\mathcal{N}}}_{=\,???} \circ \varphi^{\tau/2}_{\mathcal{H}}\right)^n(\Psi_0) \approx \Psi(t_n)$$

Splitting Methods for Nonlinear Dirac

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$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\alpha_j\partial_j + c^2\beta\right)\Psi}_{\mathcal{H}(\psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\alpha_j A_j\right)\Psi}_{\mathcal{V}(\psi)} + \underbrace{\lambda\left(\Psi\cdot\beta\overline{\Psi}\right)\beta\Psi}_{\mathcal{N}(\psi)}$$

Problem: $\varphi^{\tau}_{\mathcal{V}+\mathcal{N}}(\Psi) = ???$

Idea: approximate $\varphi^{\tau}_{\mathcal{V}+\mathcal{N}}$ by another Strang Splitting Scheme

$$\varphi^{\tau}_{\mathcal{V}+\mathcal{N}}(\Psi_0) \approx \Phi^{\tau}_{\mathcal{V}+\mathcal{N}}(\Psi_0) := \left(\varphi^{\tau/2}_{\mathcal{N}} \circ \varphi^{\tau}_{\mathcal{V}} \circ \varphi^{\tau/2}_{\mathcal{N}}\right)(\Psi_0)$$

Advantage: $\partial_t\left(\Psi\cdot\beta\overline{\Psi}\right) \equiv 0$ within subproblem

$$i\partial_t\Psi = \lambda\left(\Psi\cdot\beta\overline{\Psi}\right)\beta\Psi, \quad \Psi(0) = \Psi_0$$

$\Rightarrow$ explicit and cheap evaluation of $\varphi^{t}_{\mathcal{N}}(\Psi_0) = \exp\left(-it\lambda\left(\Psi_0\cdot\beta\overline{\Psi_0}\right)\beta\right)\Psi_0$

$$i\partial_t\Psi = \mathcal{H}(\psi) + \mathcal{V}(\psi) + \mathcal{N}(\psi)$$

3 Term Strang Splitting for Nonlinear Dirac

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$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\alpha_j\partial_j + c^2\beta\right)\Psi}_{\mathcal{H}(\psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\alpha_j A_j\right)\Psi}_{\mathcal{V}(\psi)} + \underbrace{\lambda\left(\Psi\cdot\beta\overline{\Psi}\right)\beta\Psi}_{\mathcal{N}(\psi)}$$

3-term Strang splitting scheme

$$\left(\Phi^{\tau}_{\text{Strang}}\right)^n(\Psi_0) = \left(\varphi^{\tau/2}_{\mathcal{H}} \circ \underbrace{\varphi^{\tau/2}_{\mathcal{N}} \circ \varphi^{\tau}_{\mathcal{V}} \circ \varphi^{\tau/2}_{\mathcal{N}}}_{=\Phi^{\tau}_{\mathcal{V}+\mathcal{N}} \approx \varphi^{\tau}_{\mathcal{V}+\mathcal{N}}} \circ \varphi^{\tau/2}_{\mathcal{H}}\right)^n(\Psi_0) \approx \Psi(t_n)$$

perturbation of the 2-term scheme

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Error Analysis of the 3 term Splitting

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- **stability** bounds for $\varphi^t_{\mathcal{H}}$, $\varphi^t_{\mathcal{V}}$, $\varphi^t_{\mathcal{N}}$ in H^r, $r > d/2$ $\qquad (\|uv\|_r \leq K\,\|u\|_r\,\|v\|_r)$
- **local error** analysis: $\Psi(\tau) - \Phi^{\tau}_{\text{Strang}}(\Psi_0)$

$$\Big\| \Psi(\tau) - \left(\varphi_{\mathcal{H}}^{\tau/2} \circ \varphi^{\tau}_{\mathcal{V}+\mathcal{N}} \circ \varphi_{\mathcal{H}}^{\tau/2}\right)(\Psi_0) + \left(\varphi_{\mathcal{H}}^{\tau/2} \circ \varphi^{\tau}_{\mathcal{V}+\mathcal{N}} \circ \varphi_{\mathcal{H}}^{\tau/2}\right)(\Psi_0) - \left(\varphi_{\mathcal{H}}^{\tau/2} \circ \varphi_{\mathcal{N}}^{\tau/2} \circ \varphi_{\mathcal{V}}^{\tau} \circ \varphi_{\mathcal{N}}^{\tau/2} \circ \varphi_{\mathcal{H}}^{\tau/2}\right)(\Psi_0) \Big\|_r$$

Error Analysis of the 3 term Splitting

3-term Strang splitting scheme

$$\left(\Phi^{\tau}_{\text{Strang}}\right)^n(\Psi_0) = \Big(\varphi^{\tau/2}_{\mathcal{H}} \circ \underbrace{\varphi^{\tau/2}_{\mathcal{N}} \circ \varphi^{\tau}_{\mathcal{V}} \circ \varphi^{\tau/2}_{\mathcal{N}}}_{=\Phi^{\tau}_{\mathcal{V}+\mathcal{N}} \approx \varphi^{\tau}_{\mathcal{V}+\mathcal{N}}} \circ \varphi^{\tau/2}_{\mathcal{H}}\Big)^n(\Psi_0) \approx \Psi(t_n)$$

- **stability** bounds for $\varphi^t_{\mathcal{H}}$, $\varphi^t_{\mathcal{V}}$, $\varphi^t_{\mathcal{N}}$ in H^r, $r > d/2$ $\qquad (\|uv\|_r \le K\,\|u\|_r\,\|v\|_r)$
- **local error** analysis: $\Psi(\tau) - \Phi^{\tau}_{\text{Strang}}(\Psi_0)$

$$\begin{aligned} &\Big\| \Psi(\tau) - \left(\varphi^{\tau/2}_{\mathcal{H}} \circ \varphi^{\tau}_{\mathcal{V}+\mathcal{N}} \circ \varphi^{\tau/2}_{\mathcal{H}}\right)(\Psi_0) \\ &\qquad + \varphi^{\tau/2}_{\mathcal{H}}\left(\varphi^{\tau}_{\mathcal{V}+\mathcal{N}}\left(\varphi^{\tau/2}_{\mathcal{H}}(\Psi_0)\right) - \left(\varphi^{\tau/2}_{\mathcal{N}} \circ \varphi^{\tau}_{\mathcal{V}} \circ \varphi^{\tau/2}_{\mathcal{N}}\right)\left(\varphi^{\tau/2}_{\mathcal{H}}(\Psi_0)\right) \right) \Big\|_r \\ \le\ & \tau^3 \left(\|[\mathcal{H},[\mathcal{H},\mathcal{V}+\mathcal{N}]](\Psi_0)\|_r + \dots\right) \qquad \text{"local error 2-term Strang"} \\ &+ \tau^3 \left(\left\|[\mathcal{V},[\mathcal{V},\mathcal{N}]]\left(\varphi^{\tau/2}_{\mathcal{H}}(\Psi_0)\right)\right\|_r + \dots\right) \qquad \text{"perturbation"} \end{aligned}$$

Global Error of the 3 term Splitting

$$\left(\Phi^{\tau}_{\text{Strang}}\right)^n(\Psi_0) = \Big(\varphi^{\tau/2}_{\mathcal{H}} \circ \underbrace{\varphi^{\tau/2}_{\mathcal{N}} \circ \varphi^{\tau}_{\mathcal{V}} \circ \varphi^{\tau/2}_{\mathcal{N}}}_{=\Phi^{\tau}_{\mathcal{V}+\mathcal{N}} \approx \varphi^{\tau}_{\mathcal{V}+\mathcal{N}}} \circ \varphi^{\tau/2}_{\mathcal{H}}\Big)^n(\Psi_0) \approx \Psi(t_n)$$

- **global error** = **stability** + **local error** in H^r, $r > d/2$

$$\left\| \Psi(t_n) - \left(\Phi^{\tau}_{\text{Strang}}\right)^n(\Psi_0)\right\|_r$$
$$\leq \tau^2 K \left(\|[\mathcal{H},[\mathcal{H},\mathcal{V}+\mathcal{N}]](\Psi_0)\|_r, \left\|[\mathcal{V},[\mathcal{V},\mathcal{N}]]\left(\varphi^{\tau/2}_{\mathcal{H}}(\Psi_0)\right)\right\|_r, \dots \right)$$

- $[\mathcal{H},[\mathcal{H},\mathcal{V}+\mathcal{N}]](\Psi_0) = c^4 \sum_{j=1}^{d} A_j [\boldsymbol{\beta},[\boldsymbol{\beta},\boldsymbol{\alpha}_j]]\Psi_0 + \mathcal{O}(c^3)$

- $[\mathcal{V},[\mathcal{V},\mathcal{N}]]\left(\varphi^{\tau/2}_{\mathcal{H}}(\Psi_0)\right) = \mathcal{O}(c^0)$

$$i\partial_t \Psi = \underbrace{\left(-ic\sum_{j=1}^{d}\boldsymbol{\alpha}_j\partial_j + c^2\boldsymbol{\beta}\right)\Psi}_{\mathcal{H}(\psi)} + \underbrace{\left(\phi - \sum_{j=1}^{d}\boldsymbol{\alpha}_j A_j\right)\Psi}_{\mathcal{V}(\psi)} + \underbrace{\lambda\left(\Psi\cdot\boldsymbol{\beta}\overline{\Psi}\right)\boldsymbol{\beta}\Psi}_{\mathcal{N}(\psi)}$$

Theorem

- let $r > d/2$, $c \geq 1$ and $\lambda \geq 0$
- let initial data $\Psi(0) \in H^{r+2}$, potentials $\phi, \boldsymbol{\mathcal{A}} \in H^{r+2}$
- $0 < \tau \leq 1$ small step size, $t_n = n\tau \in [0, T]$

Then the 3-term Strang splitting scheme

$$\Psi^{n+1} = \Phi^{\tau}_{\text{Strang}}(\Psi^n) = \left(\varphi_{\mathcal{H}}^{\tau/2} \circ \underbrace{\varphi_{\mathcal{N}}^{\tau/2} \circ \varphi_{\mathcal{V}}^{\tau} \circ \varphi_{\mathcal{N}}^{\tau/2}}_{=\Phi^{\tau}_{\mathcal{V}+\mathcal{N}} \approx \varphi^{\tau}_{\mathcal{V}+\mathcal{N}}} \circ \varphi_{\mathcal{H}}^{\tau/2} \right)(\Psi^n), \quad \Psi^0 = \Psi(0)$$

satisfies

$$\|\Psi(t_n) - \Psi^n\|_r \leq \tau^2 \left(c^4 K_{\boldsymbol{\mathcal{A}}} + c^3 K \right),$$

- $K_{\boldsymbol{\mathcal{A}}}$, K depend on T, r, Ψ, Φ, $\boldsymbol{\mathcal{A}}$ but **not** on c, τ
- $K_{\boldsymbol{\mathcal{A}}} = 0$ for $\boldsymbol{\mathcal{A}} \equiv 0$

Extensions

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$$i\partial_t\Psi = \left(-ic\sum_{j=1}^{d}\alpha_j\partial_j + c^2\beta\right)\Psi + \left(\phi - \sum_{j=1}^{d}\alpha_j A_j\right)\Psi + \lambda\left(\Psi\cdot\beta\overline{\Psi}\right)\beta\Psi$$

- allow **time dependent potentials** $\phi(t,x)$, $\boldsymbol{\mathcal{A}}(t,x)$
  $\rightsquigarrow$ approximate exact flow in $[t_n, t_n+\tau]$ via exponential trapezoidal rule

$$\varphi_{\mathcal{V}}^{\tau} = e^{-i\int_{t_n}^{t_n+\tau}\left(\phi(s)-\sum_{j=1}^{d}\alpha_j A_j(s)\right)ds} \approx e^{-i\frac{\tau}{2}\left(\phi(t_n)+\phi(t_n+\tau)-\sum_{j=1}^{d}\alpha_j(A_j(t_n)+A_j(t_n+\tau))\right)}$$

(cf. TSFP scheme in [Bao2017] for the linear case $\lambda = 0$)

- **Dirac-Poisson** equation: combine Dirac (for Ψ) with Poisson (for ϕ)

$$-\Delta\phi = |\Psi|^2$$

$\rightsquigarrow$ solve for ϕ within subproblem $i\partial_t\Psi = \mathcal{V}(\Psi)$
$\rightsquigarrow$ within this subproblem $\phi(t) = \phi(0)$

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Numerical Framework for 3-term Strang

Simulation on 2D torus $[-\pi, \pi]^2$, periodic boundary conditions and on finite time interval $[0, T = 1]$, parameter $\lambda = 0.5$

- consider reduced **two-spinor** system
- initial data:

$$\widetilde{\Psi}(0, x) = \begin{pmatrix} \dfrac{\cos^2(3x_1)\sin(2x_1)}{2-\cos(x_1)} + \dfrac{\cos(2x_2)}{2-\sin(x_2)} \\ \dfrac{\cos(2x_1)}{2-\cos(x_1)} + \dfrac{\sin(2x_2)}{2-\cos(x_2)} \end{pmatrix}$$

- potentials:

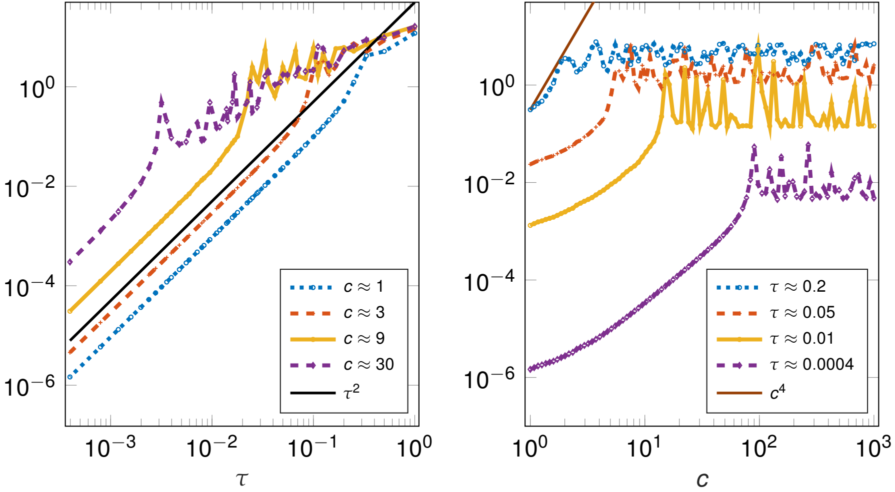
$$\phi(x) = \frac{\cos(2x_1) + \sin(3x_2)}{2 - \sin(2x_1)\cos(x_2)}$$

$$\boldsymbol{\mathcal{A}}(x) = \begin{pmatrix} \dfrac{\sin(2x_1) + \sin(3x_2)}{2 - \cos(2x_1)\cos(x_2)} \\ \dfrac{\cos(3x_1)\sin(x_2) + \cos(2x_2)}{2 - \sin(x_1)\sin(2x_2)} \end{pmatrix} = \begin{pmatrix} A_1(x) \\ A_2(x) \end{pmatrix} \quad (\text{or } \boldsymbol{\mathcal{A}} \equiv 0)$$

- Fourier Pseudospectral discretization in space, $N \times N$ grid points ($N = 64$)
- reference solution: 3-term Strang splitting with $\tau_{\text{ref}} = 3.1 \cdot 10^{-6}$

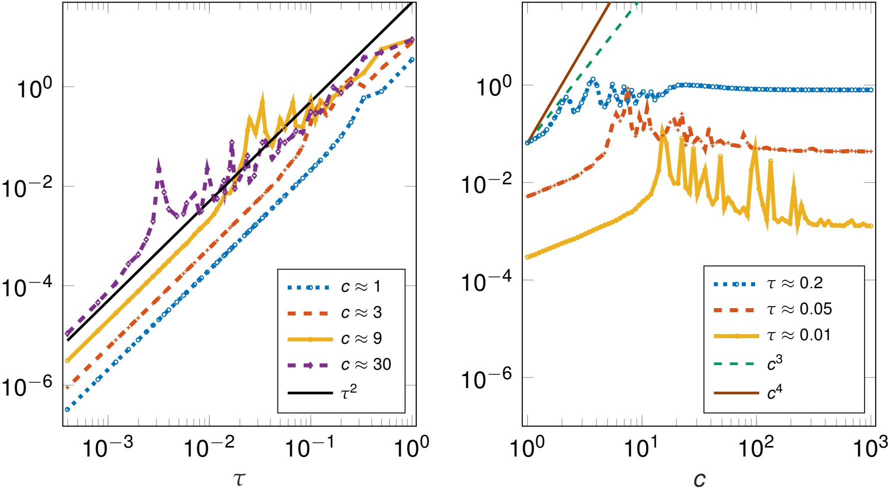
Experiment 1: $\mathcal{A} \neq 0$

Error $\max_{t_n \in [0,1]} \|\Psi(t_n) - \Psi^n\|_{H^2} = \mathcal{O}\left(\tau^2 c^4\right)$



Experiment 2: $\mathcal{A} \equiv 0$

Error $\max_{t_n \in [0,1]} \|\Psi(t_n) - \Psi^n\|_{H^2} = \mathcal{O}\left(\tau^2 c^3\right)$



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Summary

3-term exponential Strang splitting for nonlinear Dirac Equations

- 2nd order global convergence, i.e. error $\mathcal{O}\left(\tau^2(c^4 K_{\mathcal{A}} + c^3 K)\right)$
- $K_{\mathcal{A}} = 0$ for $\boldsymbol{\mathcal{A}} \equiv 0$
- extendable to
  - time dependent potentials
  - nonlinear Dirac-Poisson system

Outlook: Further interesting schemes

Ansatz

$$\Psi = \frac{1}{2}\left(U + \overline{V}\right)$$

([Faou/Schratz2014], [Baumstark/Faou/Schratz2017], [K./Schratz2017],...)

- Nonrelativistic Limit Scheme $c \to \infty$

$$\text{Dirac(-Poisson)} \xrightarrow{c \to \infty} \text{nonlinear Schrödinger(-Poisson) (SP)}$$

  - $U(t) = e^{ic^2 t} U_\infty(t) + \mathcal{O}\left(c^{-1}\right), \quad V(t) = \dots$
  - error $\mathcal{O}\left(\tau^p + c^{-1}\right)$ (solve SP with method of order p)

- Uniformly Accurate Scheme

  - twisted variables $U_*(t) = e^{-ic^2 t} U(t)$, $V_*(t) = \dots$

$$\text{Dirac(-Poisson)} \overset{\text{twisted Variables}}{\rightsquigarrow} \text{"nice" first order system for } (U_*, V_*)$$

  - error $\mathcal{O}\left(\tau^p\right)$ (uni. in c) for exp. type integrator (c-independent)