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Numerical Methods for an efficient integration of the Maxwell-Dirac System

Patrick Krämer, joint work with K. Schratz

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Wave phenomena

Introduction

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- Maxwell-Dirac: interaction of charged Spin-$\frac{1}{2}$ particle (e.g. electron) with its self-generated electromagnetic field

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Aim of the talk:

Uniformly accurate methods in both

- relativistic regime ($c = c_0 / v_p \approx 1$ "small") and
- non-relativistic limit regime ($c = c_0 / v_p \gg 1$ "large").

Introduction: Maxwell-Dirac (MD) system

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- MD system in Coulomb gauge (div $\mathcal{A} = 0$): $x \in \mathbb{R}^d$, $t \in [0, T]$

$$\begin{cases} i(D_0 + \sum_{j=1}^{d} \alpha_j D_j)\psi = c\beta\psi, \quad \psi(0) = \psi_0, \qquad \alpha_j, \beta \in \mathbb{C}^{4\times 4} \\ -\Delta\mathcal{V} = \rho, \\ \partial_{tt}\mathcal{A} - c^2\Delta\mathcal{A} = c\mathcal{P}\left[\boldsymbol{J}\right], \quad \mathcal{A}(0) = A, \partial_t\mathcal{A}(0) = cA' \end{cases}$$

$$D_0\psi = \left(\frac{\partial_t}{c} + i\frac{\mathcal{V}}{c}\right)\psi, \qquad D_j\psi = \left(\partial_{x_j} - i\frac{A_j}{c}\right)\psi,\ j = 1, \dots, d$$

$$\rho = |\psi|^2, \qquad J_j = c\,\mathrm{Re}\left(\psi \cdot \overline{\alpha_j\psi}\right),\ \boldsymbol{J} = (J_1, \dots, J_d)^T$$

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- ρ and $\boldsymbol{J}$ satisfy continuity equation

$$\partial_t\rho + \mathrm{div}\,\boldsymbol{J} = 0$$

MD system in the non-relativistic limit regime

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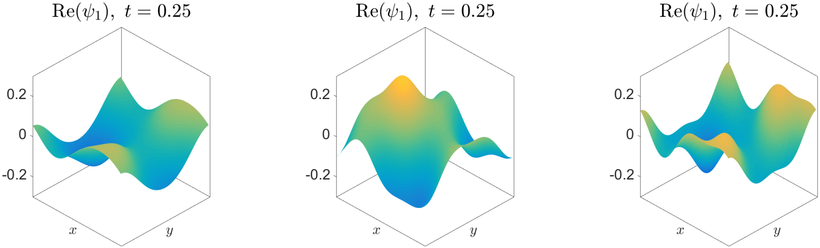

(a) $c = 4$ (b) $c = 16$ (c) $c = 32$

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Problem: severe time step restrictions for standard integrators,
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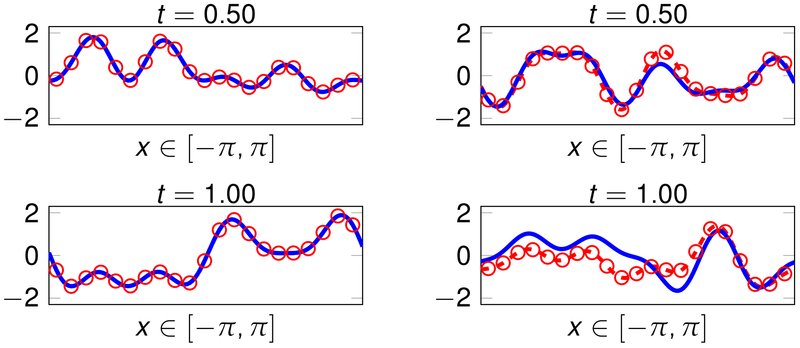

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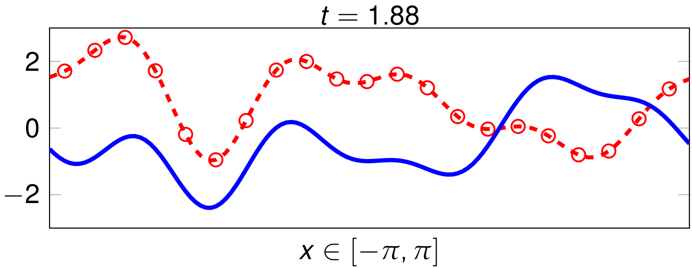

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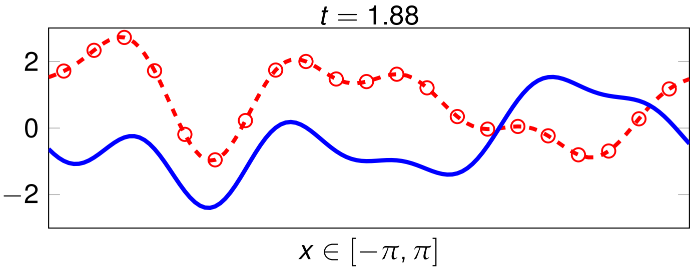

(c) $c = 64$

numerical challenge: what if $c = 10^3, 10^6, \ldots$?

Idea: asymptotic expansion

(e.g. Analysis: Masmoudi & Nakanishi 2003)

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

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$$\begin{cases} i\partial_t \begin{pmatrix} u_\infty \\ v_\infty \end{pmatrix} = \frac{1}{2}\Delta \begin{pmatrix} u_\infty \\ u_\infty \end{pmatrix} + \mathcal{V}_\infty \begin{pmatrix} u_\infty \\ -v_\infty \end{pmatrix}, \\ -\Delta \mathcal{V}_\infty = \frac{1}{4}\left(|u_\infty|^2 + |v_\infty|^2\right) \end{cases} \qquad \begin{pmatrix} u_\infty \\ v_\infty \end{pmatrix}(0) \text{ suitably chosen}$$

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- cf. Modulated Fourier expansion (MFE) (cf. Gauckler, Hairer, Lubich, . . .)

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- solve this limit system efficiently by splitting methods (cf. Lubich 2008)
- cf. Modulated Fourier expansion (MFE) (cf. Gauckler, Hairer, Lubich, ...)
- see also K. & Schratz (16') for numerical results in case of the Maxwell-Klein-Gordon system

Q: Does this ansatz work?

$$\psi(t) = \frac{1}{2}\left(u_\infty(t)e^{ic^2 t} + \overline{v_\infty}(t)e^{-ic^2 t}\right) + \mathcal{O}\left(c^{-1}\right) = \psi_\infty(t) + \mathcal{O}\left(c^{-1}\right)$$

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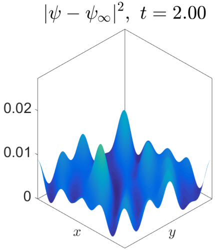
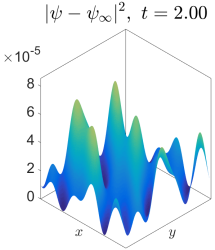


(a) $c = 2$,

max 10^{-2}



(b) $c = 32$,

max 10^{-5}

The numerical approximation

$$\psi(t) = \frac{1}{2}\left(u_\infty(t)e^{ic^2 t} + \overline{v_\infty}(t)e^{-ic^2 t}\right) + \mathcal{O}\left(c^{-1}\right) = \psi_\infty(t) + \mathcal{O}\left(c^{-1}\right)$$

- time integration of the SP system with Strang splitting, step size τ:

$$\psi_\infty(t_n) = \psi_\infty^n + \mathcal{O}\left(\tau^2\right), \quad t_n = n\tau,\ n = 0, 1, 2, \dots,$$

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$$\Rightarrow \|\psi(t_n) - \psi_\infty^n\|_r$$

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asymptotic approx. error (cf. Masmoudi & Nakanishi, 2003)

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Drawback:

Only works in the nonrelativistic limit ($c \gg 1$).

A uniformly accurate scheme: Overview (1)

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Goal: uniform convergence for all $c \geq 1$

Approximate exact solution $\psi(t_n)$ by numerical approximation ψ_*^n such that

$$\|\psi(t_n) - \psi_*^n\|_r \leq K\tau,$$

with constant K independent of c.

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- compute ψ_*^n by

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Approximate exact solution $\psi(t_n)$ by numerical approximation ψ_*^n such that

$$\|\psi(t_n) - \psi_*^n\|_r \leq K\tau,$$

with constant K independent of c.

- rewrite MD system such that

$$\psi(t) = \frac{1}{2}\left(u_*(t)e^{ic^2 t} + \overline{v_*}(t)e^{-ic^2 t}\right)$$

- $w_* = (u_*, v_*)^T$ satisfies $i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2 t} F_*(e^{ic^2 t} w_*)$
- $\mathcal{L}_c w_*$ and $F_*(e^{ic^2 t} w_*)$ bounded with respect to $c \geq 1$
- compute ψ_*^n by
  - integrating highly oscillatory phases $e^{m \cdot ic^2 t}$ exactly, $m = -4, -2, 0, 2$

  in nonlinearity $F(e^{ic^2 t} w_*)$

A uniformly accurate scheme: Overview (1)

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- compute ψ_*^n by
  - integrating highly oscillatory phases $e^{m\cdot ic^2t}$ exactly, $m = -4, -2, 0, 2$
  - freezing slowly varying parts

  in nonlinearity $F(e^{ic^2t}w_*)$

A uniformly accurate scheme: Overview (2)

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Maxwell-Dirac $iD_0\psi = -i\sum_{j=1}^{d}\alpha_j D_j\psi + c\beta\psi$

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First order system $w = (u, v)^T$ $\quad i\partial_t w = -c\langle\nabla\rangle_c w + F[w, \mathcal{V}, \boldsymbol{\mathcal{A}}]$

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"Twisted" system $w_* = (u_*, v_*)^T$ $i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2t}F_*[w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*]$

Twisted system

Dirac Equation for ψ:

$$iD_0\psi = -i\sum_{j=1}^{d}\alpha_j(\partial_j - i\frac{A_j}{c})\psi + c\beta\psi, \quad \psi(0) = \psi_0$$

The "twisted" system for twisted variables $w_* = e^{-ic^2t}w = (u_*, v_*)^T$:

$$\boxed{i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2t}F_*[w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*]}, \quad w_*(0) = \begin{pmatrix} \psi_0 - i\langle\nabla\rangle_c^{-1} D_0\psi_0 \\ \overline{\psi_0} - i\langle\nabla\rangle_c^{-1} \overline{D_0\psi_0} \end{pmatrix}$$

- define $\langle\nabla\rangle_c := \sqrt{-\Delta + c^2}$,
- $\mathcal{L}_c = c\langle\nabla\rangle_c - c^2$
- $\|\mathcal{L}_c w\|_r \leq K\left\|\frac{1}{2}\Delta w\right\|_r$,

Twisted system

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- $\|\mathcal{L}_c w\|_r \leq K\left\|\frac{1}{2}\Delta w\right\|_r$, as $\sqrt{1+x^2} \leq 1 + \frac{x^2}{2}$

MD system: simplification

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$$\begin{cases} i\left(D_0 + \sum_{j=1}^{d} \alpha_j D_j\right)\psi = c\beta\psi, \quad \psi(0) = \psi_0, \qquad \alpha_j, \beta \in \mathbb{C}^{4\times 4} \\ -\Delta\mathcal{V} = |\psi|^2, \\ \partial_{tt}\boldsymbol{\mathcal{A}} - c^2\Delta\boldsymbol{\mathcal{A}} = c\mathcal{P}\left[\boldsymbol{J}\right], \quad \boldsymbol{\mathcal{A}}(0) = A, \partial_t\boldsymbol{\mathcal{A}}(0) = cA' \end{cases}$$

$$D_0\psi = \left(\frac{\partial_t}{c} + i\frac{\mathcal{V}}{c}\right)\psi, \qquad D_j\psi = \left(\partial_{x_j} - i\frac{A_j}{c}\right)\psi, \; j = 1, \ldots, d$$

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$$

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- for sake of simplicity set $\boldsymbol{J} \equiv 0$
- $\boldsymbol{\mathcal{A}}(t) = \cos(ct\sqrt{-\Delta})A + \frac{\sin(ct\sqrt{-\Delta})}{\sqrt{-\Delta}}A'$ linear

Uniform system

$$e^{-ic^2 t} F_*(t) = F_{*,0}(t) + e^{2ic^2 t} F_{*,2}(t) + e^{-2ic^2 t} F_{*,-2}(t) + e^{-4ic^2 t} F_{*,-4}(t)$$

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- $-\Delta\mathcal{V}_* = \frac{1}{4}\left|e^{ic^2t}u_* + e^{-ic^2t}\overline{v_*}\right|^2 \quad \Rightarrow \quad \mathcal{V}_* = \mathcal{V}_*^0 + e^{2ic^2t}\mathcal{V}_*^1 + e^{-2ic^2t}\overline{\mathcal{V}_*^1}$
- $$\mathfrak{D}_{\text{div}}[\mathcal{V}] = \sum_{j=1}^{d}\alpha_j(\partial_j\mathcal{V}), \quad \mathfrak{D}_0[\boldsymbol{\mathcal{A}}] = \sum_{j=1}^{d}\alpha_j(\frac{\partial_t}{c}A_j), \quad \mathfrak{D}_{\text{curl}}[\boldsymbol{\mathcal{A}}] = -\frac{1}{2}\sum_{j,k=1}^{d}\alpha_j\alpha_k(\partial_jA_k - \partial_kA_j)$$
- $\boldsymbol{\mathcal{A}}_* = \boldsymbol{\mathcal{A}}$, as $\boldsymbol{\mathcal{A}}$ is linear

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for example

$$\begin{aligned} F_{*,0} =& \frac{1}{2}\left(\mathcal{V}_*^0 + \langle\nabla\rangle_c^{-1}\mathcal{V}_*^0\langle\nabla\rangle_c\right)\begin{pmatrix} u_* \\ -v_* \end{pmatrix} + \frac{1}{2}\left(\mathcal{V}_*^1 - \langle\nabla\rangle_c^{-1}\mathcal{V}_*^1\langle\nabla\rangle_c\right)\begin{pmatrix} \overline{v_*} \\ -\overline{u_*} \end{pmatrix} \\ & - \langle\nabla\rangle_c^{-1}\Bigg[\frac{|\boldsymbol{\mathcal{A}}_*|^2}{2c}\begin{pmatrix} u_* \\ v_* \end{pmatrix} + i\begin{pmatrix} \boldsymbol{\mathcal{A}}_*\cdot\nabla u_* \\ -\boldsymbol{\mathcal{A}}_*\cdot\nabla v_* \end{pmatrix} + \frac{i}{2}\begin{pmatrix} -\mathfrak{D}_{\mathrm{div}}[\mathcal{V}_*^1]\cdot\overline{v_*} \\ \overline{\mathfrak{D}_{\mathrm{div}}[\mathcal{V}_*^1]}\cdot\overline{u_*} \end{pmatrix} \\ & + \frac{i}{2}\begin{pmatrix} -[\mathfrak{D}_{\mathrm{div}}[\mathcal{V}_*^0] + \mathfrak{D}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}_*] + \mathfrak{D}_0[\boldsymbol{\mathcal{A}}_*]]\cdot u_* \\ [\overline{\mathfrak{D}_{\mathrm{div}}[\mathcal{V}_*^0]} + \overline{\mathfrak{D}_{\mathrm{curl}}[\boldsymbol{\mathcal{A}}_*]} + \overline{\mathfrak{D}_0[\boldsymbol{\mathcal{A}}_*]}]\cdot v_* \end{pmatrix}\Bigg] \end{aligned}$$

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- $\boldsymbol{\mathcal{A}}_* = \boldsymbol{\mathcal{A}}$, as $\boldsymbol{\mathcal{A}}$ is linear
- $F_{*,2}, F_{*,-2}, F_{*,-4}$ similar

Uniform system

$$i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2 t} F_*[w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*]$$

- nonlinearity

$$e^{-ic^2 t} F_*(t) = F_{*,0}(t) + e^{2ic^2 t} F_{*,2}(t) + e^{-2ic^2 t} F_{*,-2}(t) + e^{-4ic^2 t} F_{*,-4}(t)$$

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- $F_{*,m}$, $m = -4, -2, 0, 2$ nice (slowly varying), i.e.

$$\|F_{*,m}(t+s) - F_{*,m}(t)\|_r \leq sK\left(\|F_{*,m}(t)\|_{r+2} + \sup_{0 \leq \xi \leq s} \|F_{*,m}(t+\xi)\|_r \right),$$

with K independent of $c \geq 1$.

Uniform system

$$i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2 t} F_*[w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*]$$

- Duhamel's formula

$$w_*(t+\tau) = e^{i\mathcal{L}_c \tau} w_*(t) - i \int_0^\tau e^{i\mathcal{L}_c(\tau - s)} \sum_{m \in \{-4,-2,0,2\}} e^{m \cdot ic^2 (t+s)} F_{*,m}(t+s) ds$$

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- $\left\| e^{-i\mathcal{L}_c s} w - w \right\|_r \le Ks \left\| \frac{1}{2}\Delta w \right\|_r$
- $\left\| F_{*,m}(t+s) - F_{*,m}(t) \right\|_r \le Ks \quad \Rightarrow \quad$ freeze $F_{*,m}(t)$

Uniform system

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- $\left\| e^{-i\mathcal{L}_c s} w - w \right\|_r \leq Ks \left\| \frac{1}{2}\Delta w \right\|_r$
- $\| F_{*,m}(t+s) - F_{*,m}(t) \|_r \leq Ks \quad \Rightarrow \quad$ freeze $F_{*,m}(t)$
- $\| \mathcal{R}(\tau, t, w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*) \|_r \leq \tau^2 K(\|w_*(t)\|_{r+2} + \|\mathcal{V}_*(t)\|_{r+2} + \|\boldsymbol{\mathcal{A}}_*(t)\|_{r+2})$

Uniform system

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$$= e^{i\mathcal{L}_c\tau}\left(w_*(t) - i\sum_{m\in\{-4,-2,0,2\}} e^{m\cdot ic^2 t} F_{*,m}(t)\int_0^\tau e^{m\cdot ic^2 s}ds\right)$$

$$+ \mathcal{R}(\tau, t, w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*).$$

- $\left\| e^{-i\mathcal{L}_c s} w - w\right\|_r \le Ks\left\|\frac{1}{2}\Delta w\right\|_r$
- $\|F_{*,m}(t+s) - F_{*,m}(t)\|_r \le Ks \quad \Rightarrow$ freeze $F_{*,m}(t)$
- $\|\mathcal{R}(\tau, t, w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*)\|_r \le \tau^2 K(\|w_*(t)\|_{r+2} + \|\mathcal{V}_*(t)\|_{r+2} + \|\boldsymbol{\mathcal{A}}_*(t)\|_{r+2})$
- Integrate $\int_0^\tau e^{m\cdot ic^2 s}ds = \tau\varphi_1(m\cdot ic^2\tau)$ exactly, $\quad \varphi_1(x) = \dfrac{e^x - 1}{x}$

Uniform Time integration scheme

$$i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2 t} F_*[w_*, \mathcal{V}_*, \boldsymbol{\mathcal{A}}_*]$$

- Duhamel's formula

$$w_*(t+\tau) = e^{i\mathcal{L}_c\tau}\left(w_*(t) - i\tau \sum_{m\in\{-4,-2,0,2\}} e^{m\cdot ic^2 t}\varphi_1(m\cdot ic^2\tau) F_{*,m}(t)\right) + \mathcal{O}\left(\tau^2\right)$$

Uniform Time integration scheme

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- First order time integration scheme: $\left(\varphi_1(x) = \frac{e^x - 1}{x}\right)$

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Uniform Time integration scheme

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$$i\partial_t w_* = -\mathcal{L}_c w_* + e^{-ic^2 t} F_*[w_*, \mathcal{V}_*, \mathcal{A}_*]$$

- Duhamel's formula

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Global error

Linear convergence, i.e. $\|w_*(t_n) - w_*^n\|_r \leq K\tau$, K independent of $c \geq 1$.

Summary: Comparison MD Limit vs Uniform

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Limit approx.:

$$\psi_\infty^n = \frac{1}{2}(e^{ic^2 t_n} u_\infty^n + e^{-ic^2 t_n} \overline{v_\infty^n})$$

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Good approx for

large $c \gg 1$, $c \in [\tau^{-2}, \infty)$.

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Good Approx. for

all $c \geq 1$.

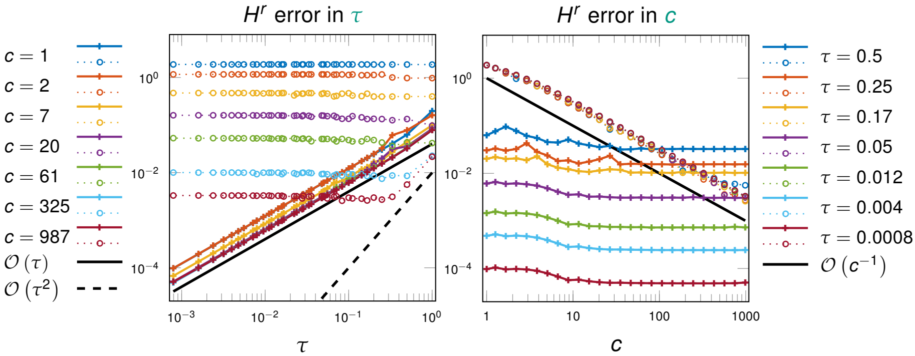
Numerical Experiments

Karlsruhe Institute of Technology

Simulation with $d = 2$, $T = 1$, $r = 2$, smooth initial data

Uniform: ——+—— Limit: ···o···

$$\max_{t_n\in[0,T]} \|\psi(t_n) - \psi_*^n\|_r = \mathcal{O}\left(\tau \cdot c^0\right), \qquad \max_{t_n\in[0,T]} \|\psi(t_n) - \psi_\infty^n\|_r = \mathcal{O}\left(\tau^2 + c^{-1}\right)$$



$t \in [0, T]$, $x \in [-\pi, \pi]^d$, $\tau_{ref} \approx 7 \cdot 10^{-6}$, $N = 256$ grid points

Outlook

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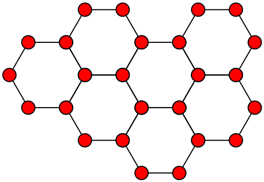
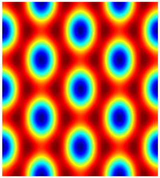
- include external potential V_{ex} into model

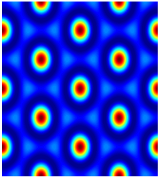
$\Rightarrow$ efficient simulation of electrons in graphene?
(together with group of Kurt Busch (HU Berlin))



$|\psi|^2$



$|V_{ex}|^2$



Literature

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