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The Dirac Equation and its Nonrelativistic Limit

Patrick Krämer, joint work with K. Schratz

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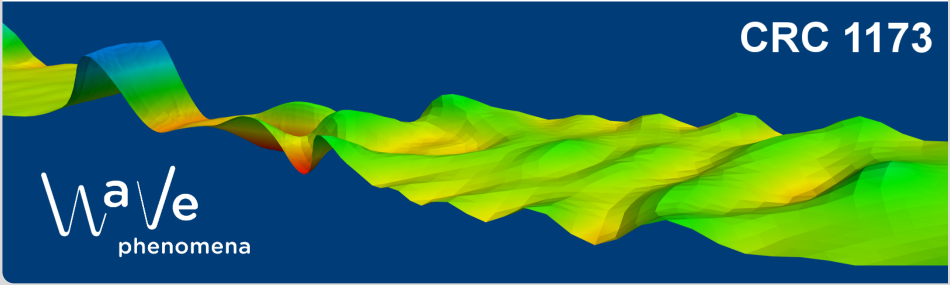

Outline

- Motivation and Background
- Introduction to Covariant Derivatives and Four-Vectors
- Free Dirac Equation
- Coupling to Electromagnetic Field
- Asymptotic approximation
- Numerical Experiments (Free Dirac)
- Outlook

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Motivation and Background

- Klein-Gordon (KG) equation (1927) only good for **spinless** particles (e.g. Higgs Boson)
  $\Rightarrow$ allows negative probability density for particles with spin

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Motivation and Background

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  $\Rightarrow$ allows negative probability density for particles with spin
- Dirac (1928): relativistic wave equation for particles with **spin 1/2** (Fermions)
- **Dirac equation** for a so-called four-vector spinor $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T$,

$$i(\partial_t \psi + c \sum_{j=1}^{d} \gamma_j \partial_j)\psi = c^2 \beta \psi, \quad \psi(0) = \psi_0, \quad \gamma_j, \beta \in \mathbb{C}^{4\times 4}, \ j = 1, \dots, d.$$

- $c \gg 1$ (nonrelativistic regime) $\Rightarrow$ highly oscillatory wave equation

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Covariant Derivatives and Four-Vectors

- let $x^\mu = (x_0, x_1, x_2, x_3)$ **contravariant** space-time coordinates
- let $x_\mu = (x_0, -x_1, -x_2, -x_3)$ **covariant** space-time coordinates

with

$$x_0 = ct, \quad x_1 = x, \quad x_2 = y, \quad x_3 = z.$$

- **contravariant** derivative $\partial_\mu = \frac{\partial}{\partial x^\mu} = (\partial_t / c, \nabla)$
- **covariant** derivative $\partial^\mu = \frac{\partial}{\partial x_\mu} = (\partial_t / c, -\nabla)$

Covariant Derivatives and Four-Vectors

- **four-vector definition:**

$$A^\mu = (A_0, A_1, A_2, A_3) \quad \Longleftrightarrow \quad A_\mu = (A_0, -A_1, -A_2, -A_3),$$
$$B^\mu = (B_0, B_1, B_2, B_3) \quad \Longleftrightarrow \quad B_\mu = (B_0, -B_1, -B_2, -B_3)$$

- summation convention for repeated indices:

$$A_\mu B^\mu = A_0 B_0 - \sum_{j=1}^{3} A_j B_j$$

- in particular for $\partial^\mu = (\partial_t / c, -\nabla)$:

$$\partial_\mu \partial^\mu = \partial_t^2 / c^2 - \nabla^2 \quad \text{(d'Alembert operator).}$$

- for example Klein-Gordon equation

$$\partial_\mu \partial^\mu \psi + c^2 \psi = 0 \quad \Longleftrightarrow \quad c^{-2} \partial_t^2 \psi + (-\Delta + c^2) \psi = 0.$$

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Free Dirac Equation

- in covariant notation for $\psi : [0, T] \times \mathbb{R}^d \to \mathbb{C}^4$

$$i\gamma^\mu \partial_\mu \psi = c\beta\psi, \quad \psi(0,x) = \psi_0(x)$$

$$\Longleftrightarrow \quad i\left(\frac{\partial_t}{c} + \sum_{j=1}^{d} \gamma_j \partial_j\right)\psi = c\beta\psi, \quad \psi(0,x) = \psi_0(x)$$

with

$$\beta = \begin{pmatrix} Id_2 & 0 \\ 0 & -Id_2 \end{pmatrix}, \quad \gamma_0 = Id_4, \quad \gamma_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, \quad j = 1, 2, 3$$

- Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Free Dirac Equation

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- In standard notation

$$i\partial_t\psi = -ic\sum_{j=1}^{d}\gamma_j\partial_j\psi + c^2\beta\psi, \quad \psi(0) = \psi_0.$$

- Properties of the matrices $\beta, \gamma_j, j = 1, 2, 3$:

$$\gamma_j\gamma_k + \gamma_k\gamma_j = 2\delta_{jk}Id_4, \quad \gamma_j\beta + \beta\gamma_j = 0, \quad \beta^2 = Id_4, \qquad j, k = 1, 2, 3$$

- differentiating w.r.t. time t yields for smooth ψ

$$\partial_t^2\psi = -c^2(-\Delta + c^2)\psi,$$

$$\psi(0) = \psi_0, \quad \partial_t\psi(0) = -c\sum_{j=1}^{d}\gamma_j\partial_j\psi_0 - ic^2\beta\psi_0.$$

$\Rightarrow$ components of ψ satisfy linear KG equation!

Free Dirac Equation

- for $d = 1, 2$ Dirac system for $\psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T$ can be reduced
- let $\Phi = (\psi_1, \psi_4)^T$ or $\Phi = (\psi_2, \psi_3)^T$, $\Phi : [0, T] \times \mathbb{R}^d \to \mathbb{C}^2$, then

$$i\partial_t \Phi = -ic \sum_{j=1}^{d} \sigma_j \partial_j \Phi + c^2 \sigma_3 \Phi, \quad \Phi(0) = \Phi^0.$$

- denote $\Phi = (\Phi_1, \Phi_2)^T$, and let $d = 2$ then

$$\begin{cases} i\partial_t \Phi_1 = -ic(\partial_x - i\partial_y)\Phi_2 + c^2 \Phi_1 \\ i\partial_t \Phi_2 = -ic(\partial_x + i\partial_y)\Phi_1 - c^2 \Phi_2 \end{cases}, \quad \Phi(0) = \Phi^0$$

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- Free Dirac **exactly** solvable!

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- Free Dirac **exactly** solvable!
- components Φ_j, $j = 1, 2$ satisfy linear Klein-Gordon equation

$$\Longrightarrow \quad \begin{cases} \partial_t^2 \Phi = -c^2(-\Delta + c^2)\Phi \\ \Phi(0) = \Phi^0, \quad \partial_t \Phi(0) = -c \sum_{j=1}^{d} \sigma_j \partial_j \Phi^0 - ic^2 \sigma_3 \Phi^0 \end{cases}$$

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Coupling to Electromagnetic (EM) Field

- electric scalar potential $V : [0, T] \times \mathbb{R}^3 \to \mathbb{R}$
- magnetic vector potential $A : [0, T] \times \mathbb{R}^3 \to \mathbb{R}^3$, $A = (A_1, A_2, A_3)$

$$\Rightarrow \quad \textbf{real four-vector potential} \quad \mathcal{A}^\mu = (V, A_1, A_2, A_3)$$

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$$\partial_\mu \quad \mapsto \quad D_\mu := \partial_\mu + i\frac{\mathcal{A}_\mu}{c}$$

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$$\frac{\partial_t}{c} \mapsto \frac{\partial_t}{c} + i\frac{V}{c}, \qquad \nabla \mapsto \nabla - i\frac{A}{c}.$$

- coupled Dirac equation for $\psi : [0, T] \times \mathbb{R}^d \to \mathbb{C}^4$, $\psi(0, x) = \psi_0(x)$

$$i\gamma^\mu D_\mu \psi = c\beta\psi$$

$$\iff i\left(\frac{\partial_t}{c} + \sum_{j=1}^{d} \gamma_j \partial_j\right)\psi = c\beta\psi + \frac{1}{c}(V - \sum_{j=1}^{d} \gamma_j A_j)\psi.$$

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Asymptotic approximation

- Bao et al, 2015: severe **time step restrictions** required in standard numerical time integration schemes for **coupled** Dirac
  - CNFD method: $\tau \sim c^{-3}$
  - EWI-FP method: $\tau \sim c^{-2}$
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Idea: (cf. Masmoudi & Nakanishi, 2003; Bao et al, 2015)

$$\Phi(t) = \frac{1}{2} u_0(t) e^{ic^2 t} + \frac{1}{2} \overline{v_0(t)} e^{-ic^2 t} + \mathcal{O}\left(c^{-2}\right).$$

- filter out high frequencies $e^{\pm ic^2 t} \Rightarrow u_0, v_0$ **nice functions**
- u_0, v_0 satisfy **Schrödinger system independent of c**

$$\begin{cases} i\partial_t u_0 = \frac{1}{2}\Delta u_0 + V(t) u_0, \\ i\partial_t v_0 = \frac{1}{2}\Delta v_0 - V(t) v_0, \end{cases} + \text{suitable initial data.}$$

- Schrödinger system can be solved **efficiently by Strang splitting**

Asymptotic approximation for free Dirac

- **free Dirac** for $d = 2$: $\quad i\partial_t\Phi = -ic\sum_{j=1}^{d}\sigma_j\partial_j\Phi + c^2\sigma_3\Phi, \quad \Phi(0) = \Phi_0.$
- components $\Phi_j, j = 1, 2$ satisfy **Klein-Gordon equation**

$$\begin{cases} \partial_t^2\Phi = -c^2(-\Delta + c^2)\Phi \\ \Phi(0) = \Phi^0, \quad \partial_t\Phi(0) = -c\sum_{j=1}^{d}\sigma_j\partial_j\Phi^0 - ic^2\sigma_3\Phi^0 =: \Phi^{0\prime}. \end{cases}$$

$\langle\nabla\rangle_c = \sqrt{-\Delta + c^2}$

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- Rewrite the KG equation as a **first order system**

$$\begin{cases} i\partial_t u = -c \langle \nabla \rangle_c u, \quad u(0) = \Phi^0 - ic^{-1} \langle \nabla \rangle_c^{-1} \Phi^{0\prime}, \\ i\partial_t v = -c \langle \nabla \rangle_c v, \quad v(0) = \overline{\Phi^0} - ic^{-1} \langle \nabla \rangle_c^{-1} \overline{\Phi^{0\prime}}, \end{cases}$$

where $u = (u^1, u^2)^T,\ v = (v^1, v^2)^T : [0, T] \times \mathbb{R}^d \to \mathbb{C}^2$

- in particular $\Phi = \frac{1}{2}(u + \overline{v})$.

$\langle \nabla \rangle_c = \sqrt{-\Delta + c^2}$

Asymptotic approximation for free Dirac

$$i\partial_t u = \underbrace{-c\left\langle \nabla \right\rangle_c u}_{=-(c^2-\frac{1}{2}\Delta)u+\mathcal{O}\left(c^{-2}\right)}, \qquad u(0) = \Phi^0 - ic^{-1}\left\langle \nabla \right\rangle_c^{-1} \Phi^{0\prime},$$

Taylor:

$$c\left\langle \nabla \right\rangle_c u = (c^2 - \frac{1}{2}\Delta)u + \mathcal{O}\left(c^{-2}\Delta^2 u\right).$$

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Formal asymptotic expansion of u:

$$u(t) = e^{ic^2 t}u_0(t) + \mathcal{O}\left(c^{-2}\right)$$

u_0 nice, not depending on c

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Asymptotic approximation for free Dirac

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u_0 nice, not depending on c $\quad\Rightarrow\quad$ Free Schrödinger equation

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Asymptotic approximation for free Dirac

Nonrelativistic limit for u:

$$i\partial_t u_0 = \frac{1}{2}\Delta u_0,$$

- suitable initial data such that $u(0) = u_0(0) + \mathcal{O}\left(c^{-2}\right)$!!

$$u(0) = \Phi^0 - ic^{-1}\langle\nabla\rangle_c^{-1}\Phi^{0\prime},$$

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Taylor:

$$c^{-1}\left\langle \nabla \right\rangle_c^{-1} u = c^{-2}u + \mathcal{O}\left(c^{-4}\Delta u\right).$$

- Reminder: $\Phi^{0\prime} = -c\sum_{j=1}^{d}\sigma_j\partial_j\Phi^0 - ic^2\sigma_3\Phi^0$

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$$\Rightarrow u(0) = (Id_2 - \sigma_3)\Phi^0 + ic^{-1}\sum_{j=1}^{d}\sigma_j\partial_j\Phi^0 + \mathcal{O}\left(c^{-2}\right) =: u_0(0) + \mathcal{O}\left(c^{-2}\right)$$

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$\left\langle\nabla\right\rangle_c = \sqrt{-\Delta + c^2}$

Asymptotic approximation for free Dirac

- Finally $\Phi(t) = \widetilde{\Phi}_0(t) + \mathcal{O}\left(c^{-2}\right)$ with **limit approximation**

$$\widetilde{\Phi}_0(t) := \frac{1}{2}\left(e^{ic^2 t} u_0(t) + e^{-ic^2 t}\overline{v_0(t)}\right).$$

- nice functions u_0, v_0 satisfy the **limit system**

$$\begin{cases} i\partial_t u_0 = \frac{1}{2}\Delta u_0 \\ i\partial_t v_0 = \frac{1}{2}\Delta v_0 \end{cases}$$

with initial data

$$u_0(0) = \begin{pmatrix} ic^{-1}(\partial_x - i\partial_y)\Phi_2^0 \\ 2\Phi_2^0 + ic^{-1}(\partial_x + i\partial_y)\Phi_1^0 \end{pmatrix}, \quad v_0(0) = \begin{pmatrix} 2\overline{\Phi_1^0} + ic^{-1}(\partial_x + i\partial_y)\overline{\Phi_2^0} \\ ic^{-1}(\partial_x - i\partial_y)\overline{\Phi_1^0} \end{pmatrix}$$

- blue terms in initial data crucial for error $\mathcal{O}\left(c^{-2}\right)$

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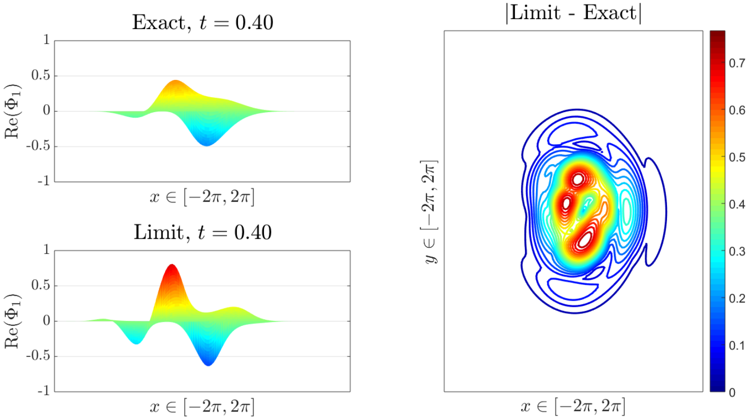
Free Dirac equation with

(a) $c = 1$:



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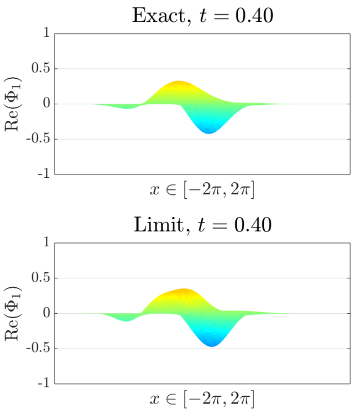
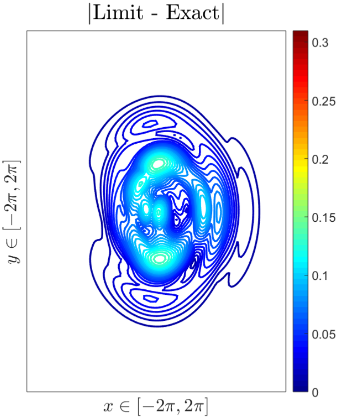
Free Dirac equation with

(b) $c = 2$:

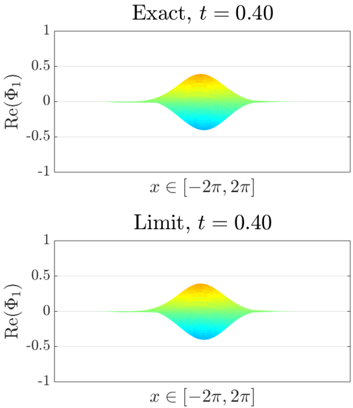


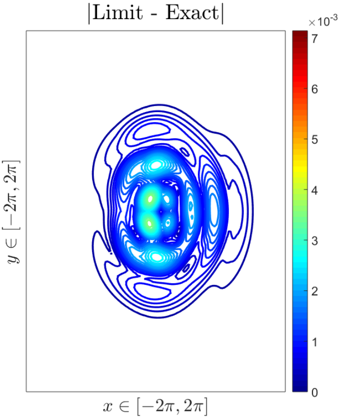


Numerical Experiments (Free Dirac)

Free Dirac equation with

(c) $c = 16$:



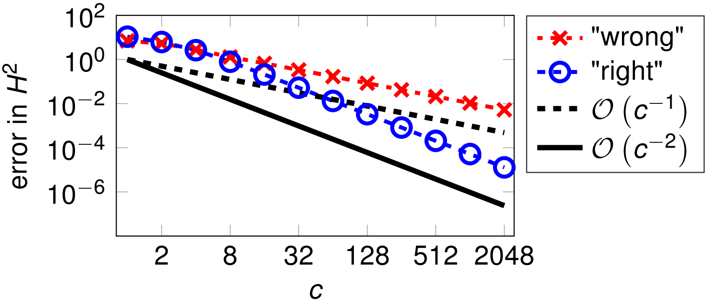


Numerical Experiments (Free Dirac)

Karlsruhe Institute of Technology

Simulation for $d = 2$, $T = 2$, $(x, y) \in [-2\pi, 2\pi]^2$, p.b.c.,

$$\Phi(0, x, y) = \left(e^{-0.5(x^2+y^2)} \sin(y), e^{-0.5((x-1)^2+y^2)} \cos(x)\right)^T$$



$\Phi - \widetilde{\Phi}_0$: wrong limit initial data (neglecting c^{-1} terms)

$\Phi - \widetilde{\Phi}_0$: correct limit initial data (respecting c^{-1} terms)

- Motivation and Background
- Introduction to Covariant Derivatives and Four-Vectors
- Free Dirac Equation
- Coupling to Electromagnetic Field
- Asymptotic approximation
- Numerical Experiments (Free Dirac)
- Outlook

Outlook

- apply the same ideas to the coupled Dirac equation (cf. Bao et al, 2015)
- generalize the results on the coupled Dirac equation to the Maxwell-Dirac system
  $\Rightarrow$ **Schrödinger-Poisson limit** system (Masmoudi & Nakanishi, 2003)

Outlook

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  $\Rightarrow$ **Schrödinger-Poisson limit** system (Masmoudi & Nakanishi, 2003)

Challenges:

- understanding the steps:
  Maxwell-**Dirac** $\rightarrow$ Maxwell-**Klein-Gordon** $\rightarrow$ Schrödinger-Poisson
- potential V satisfies a **Poisson equation** depending on the Dirac solution Φ
- potential A satisfies a **highly-oscillatory wave equation** depending on the Dirac solution Φ
  $\Rightarrow$ coupled **nonlinear system** for Φ, V, A