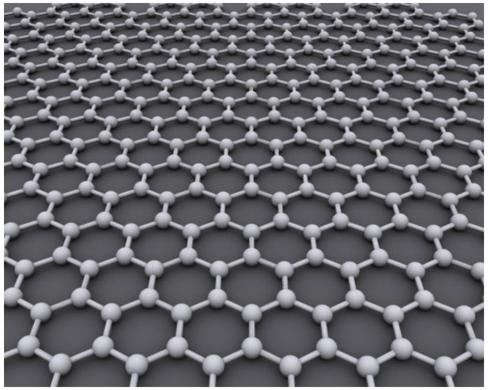
Multiscale Methods and Analysis for the Dirac Equation in the Nonrelativistic Regime



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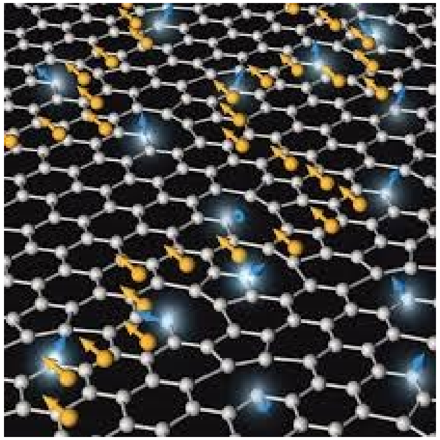
Outline

- The Dirac equation
- Numerical methods and error estimates
  - Finite difference time domain (FDTD) methods
  - Exponential wave integrator Fourier spectral (EWI-FP) method
  - Time-splitting Fourier pseudospectral (TSFP) method
- A uniformly accurate (UA) method
- Extension to nonlinear & other regimes
- Conclusion & future challenges



The Dirac equation

$$i\hbar\partial_t\Psi = \left(-ic\hbar\sum_{j=1}^{3}\alpha_j\partial_j + mc^2\beta \right)\Psi + e\left(V(\vec{x})I_4 - \sum_{j=1}^{3}A_j(\vec{x})\alpha_j \right)\Psi$$

– $\vec{x} = (x_1, x_2, x_2)^T (\text{or } (x, y, z)^T) \in \mathbb{R}^3$: spatial coordinates

– $\Psi = \Psi(t, \vec{x}) = (\psi_1, \psi_2, \psi_3, \psi_4)^T \in \mathbb{C}^4$:

complex-valued vector wave function ``spinorfield''

– $V = -A_0$: real-valued electrical potential

– $A = (A_1, A_2, A_3)^T$: real-valued magnetic potential

– $E = -\nabla V - \partial_t A = \nabla A_0 - \partial_t A$: electric field

– $B = \nabla \times A$: magnetic field

Refs: [1] P.A.M. Dirac, Proc. R. Soc. London A, 127 (1928) & 126 (1930).

[2]. Principles of Quantum Mechanics, Oxford Univ Press, 1958.

[3] http://en.wikipedia.org/wiki/Dirac_equation

The Dirac equation

- $\alpha_1, \alpha_2, \alpha_3, \beta$: 4-by-4 matrices $\quad \alpha_j^2 = \beta^2 = I_4,$ $\quad \alpha_j \alpha_l + \alpha_l \alpha_j = 0, \quad \alpha_j \beta + \beta \alpha_j = 0$

$$\alpha_1 = \begin{pmatrix} 0 & \sigma_1 \\ \sigma_1 & 0 \end{pmatrix}, \quad \alpha_2 = \begin{pmatrix} 0 & \sigma_2 \\ \sigma_2 & 0 \end{pmatrix}, \quad \alpha_3 = \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$$

- $\sigma_1, \sigma_2, \sigma_3$: 2-by-2 Pauli matrices

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

- $\gamma^0, \gamma^1, \gamma^2, \gamma^3$: 4-by-4 matrices $\quad \gamma^0 = \beta, \quad \gamma^k = \gamma^0 \alpha_k, k = 1,2,3$

- The Dirac equation

$$\left(i\hbar \gamma^\mu \partial_\mu - mc + e\gamma^\mu A_\mu \right) \Psi = 0$$

The Dirac equation

- Derived by British physicist Paul Dirac in 1928 to describe all spin-1/2 massive particles such as electrons and quarks
- It is consistent with both the principles of quantum mechanics and the theory of the special relativity
- The first theory to account fully for special relativity in quantum mechanics
- Accounted for fine details of the hydrogen spectrum in a completely rigorous way, implied the existence of a new form of matter, *antimatter* & predated experimental discovery of positron
- In special limits, it implies the Pauli, Schrodinger and Weyl equations!
- Par Dirac with Newton, Maxwell & Einstein!! Be awarded the Nobel Prize in 1933 (with Schrodinger). Host Lucasian Professor of Mathematics at the University of Cambridge at the age of 30!!

Quantum Mechanics with Relativistics

$$\psi(\vec{x},t) = Ae^{i\vec{k}\bullet\vec{x}-i\omega t} \;\&\; V \equiv 0$$
$$\overset{\hbar=m=1}{\Rightarrow} \omega := \omega(\vec{k}) = \frac{1}{2}\vec{k}^2$$
$$\Rightarrow \vec{v} = \nabla\omega(\vec{k}) = \vec{k}$$

- Making the Schroedinger equation relativistic

$$E = \frac{\vec{p}^2}{2m} + V(x) \overset{E\to i\hbar\partial_t;\, \vec{p}\to -i\hbar\nabla}{\Longrightarrow} i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi := H\psi$$

$$\rho := |\psi|^2,\; J := \mathrm{Im}(\overline{\psi}\nabla\psi)$$
$$\partial_t\rho + \nabla\bullet J = 0$$

- Klein-Gordon equation for spinless –pion (Oskar Klein&Walter Gordon, 1926)

$$E^2 = m^2c^4 + (c\vec{p})^2 \Leftrightarrow \frac{E^2}{c^2} - \vec{p}^2 = m^2c^2$$

$$\overset{E\to i\hbar\partial_t;\, \vec{p}\to -i\hbar\nabla}{\Longrightarrow} \left(\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\phi = \frac{m^2c^2}{\hbar^2}\phi$$

$$\rho := \overline{\phi}\,\partial_t\phi - \phi\,\partial_t\overline{\phi}$$
$$J := \phi\nabla\overline{\phi} - \overline{\phi}\nabla\phi$$
$$\partial_t\rho + \nabla\bullet J = 0$$

Quantum Mechanics with Relativistics

$$E=\sqrt{(\vec{p}c)^2+(mc^2)^2} \Leftrightarrow \sqrt{\frac{E^2}{c^2}-\vec{p}^2}=mc \Leftrightarrow \sqrt{\frac{E^2}{c^2}-\vec{p}^2}-mc=0$$

- Dirac's coup
  - Square-root of an operator

$$\frac{E^2}{c^2}-\vec{p}^2=m^2c^2 \Rightarrow \nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}=\left(A\partial_x+B\partial_y+C\partial_z+\frac{i}{c}D\partial_t\right)^2=\frac{m^2c^2}{\hbar^2}$$

$$AB+BA=0, \quad \ldots \quad \& \quad A^2=B^2=\ldots=1$$

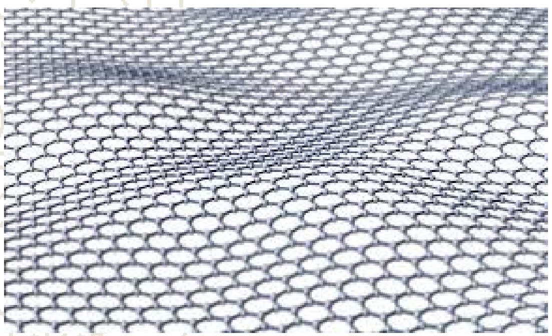
$$\Rightarrow A=i\beta\alpha_1, \quad B=i\beta\alpha_2, \quad C=i\beta\alpha_3, \quad D=\beta \Leftrightarrow \text{Clifford Algebra over 4d!!}$$

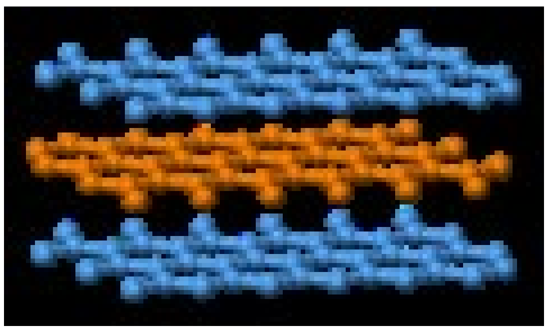
  - Dirac equation $\sqrt{\frac{E^2}{c^2}-\vec{p}^2}-mc=0 \Rightarrow \left(A\partial_x+B\partial_y+C\partial_z+\frac{i}{c}D\partial_t-\frac{mc}{\hbar}\right)\psi=0$

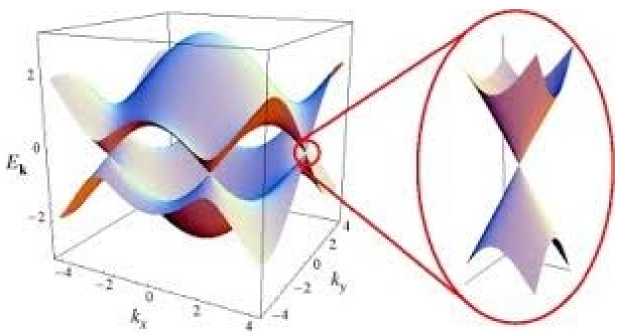
$$E=\sqrt{(\vec{p}c)^2+(mc^2)^2} \overset{E\to i\hbar\partial_t;\,\vec{p}\to -i\hbar\nabla}{\Longrightarrow} i\hbar\partial_t\Psi=\left(-ic\hbar\sum_{j=1}^{3}\alpha_j\partial_j+mc^2\beta\right)\Psi$$

Typical Applications

- Graphene/graphites and/or 2D materials – K. Novoselov, A. Geim, etc., Science, 2004; K. Novoselov, A. Geim , etc., Nature, 2005; K. Novoselov, …, A. Geim, Science, 2007; D.A. Abanin, etc., Science, 2011; A.H.C. Neto, etc., Rev. Mod. Phys., 2009, … (Nobel Prize in 2010)







  – Same dispersion relation at Dirac cone

- Chiral confinement of quasirelativistic BEC – M. Merkl et al., PRL,2010
- Atto-second laser on molecule -F. Fillion-Gourdeau, E. Lorin and A.D. Bandrauk, PRL, 13'&JCP14
- Neutron interaction in nuclear physics--H. Liang, J. Meng &Z.G. Zhou, Phys. Rep., 15'

The Dirac equation

$$i\hbar\partial_t\Psi = \left(-ic\hbar\sum_{j=1}^{3}\alpha_j\partial_j + mc^2\beta\right)\Psi + e\left(V(\vec{x})I_4 - \sum_{j=1}^{3}A_j(\vec{x})\alpha_j\right)\Psi$$

- Dimensionless Dirac equation in *d*-dimension (d=3,2,1)

$$i\eta\partial_t\Psi = \left(-\frac{i\eta}{\varepsilon}\sum_{j=1}^{d}\alpha_j\partial_j + \frac{\lambda}{\varepsilon^2}\beta\right)\Psi + \left(V(\vec{x})I_4 - \sum_{j=1}^{d}A_j(\vec{x})\alpha_j\right)\Psi, \quad \vec{x}\in\mathbb{R}^d$$

$$0<\varepsilon := \frac{x_s}{t_s c} = \frac{v_s}{c} \le 1; \quad 0<\eta := \frac{\hbar t_s}{m_s x_s^2} \le 1; \quad 0<\lambda := \frac{m}{m_s} \le 1$$

- Different parameter regimes
  - Standard scaling: $\varepsilon = \eta = \lambda = 1$
  - Semiclassical regime: $\varepsilon = \lambda = 1 \,\&\, 0<\eta \ll 1$
  - Nonrelativistic regime: $\eta = \lambda = 1 \,\&\, 0<\varepsilon \ll 1$
  - Massless regime: $\varepsilon = \eta = 1 \,\&\, 0<\lambda \ll 1$

Different limits of the Dirac equation

Dirac Equation

$\mu = 1, \varepsilon = 1$

$\lambda \to 0 (m \to 0)$

massless ⇐ **Weyl Equation**

$\eta = 1, \lambda = 1$

$\varepsilon \to 0 (c \to \infty)$

nonrelativistic ⇒ **Schrodinger or Pauli Equation**

$\lambda = 1, \varepsilon = 1$

$\eta \to 0 (\hbar \to 0)$

semiclasical ⇓ **relativistic Euler Equation**

$\lambda = 1$

$\varepsilon \to 0 (c \to \infty)$

⇓ (from relativistic Euler Equation) **Euler equation**

$\lambda = 1$

$\eta \to 0$

$(\hbar \to 0)$

⇓ (from Schrodinger or Pauli Equation) **Euler equation**

$$i\eta\partial_t\Psi = \left(-\frac{i\eta}{\varepsilon}\sum_{j=1}^{d}\alpha_j\partial_j + \frac{\lambda}{\varepsilon^2}\beta\right)\Psi + \left(V(\vec{x})I_4 - \sum_{j=1}^{d}A_j(\vec{x})\alpha_j\right)\Psi,$$

The Dirac equation $\eta = \lambda = 1$

$$\Psi = (\psi_1, \psi_2, \psi_3, \psi_4)^T \in \mathbb{C}^4$$

- Dimensionless Dirac equation in *d*-dimension (d=3,2,1)

$$i\partial_t \Psi = \left(-\frac{i}{\varepsilon} \sum_{j=1}^{d} \alpha_j \partial_j + \frac{1}{\varepsilon^2} \beta \right) \Psi + \left(V(\vec{x}) I_4 - \sum_{j=1}^{d} A_j(\vec{x}) \alpha_j \right) \Psi, \quad \vec{x} \in \mathbb{R}^d$$

  – Initial data

$$0 < \varepsilon := \frac{x_s}{t_s c} = \frac{v}{c} \le 1$$

$$\Psi(0, \vec{x}) = \Psi_0(\vec{x}), \quad \vec{x} \in \mathbb{R}^d$$

  – Dispersive PDE & time symmetric

  – Mass & energy conservation

Conservations laws

$$i\partial_t\Psi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\alpha_j\partial_j + \frac{1}{\varepsilon^2}\beta\right)\Psi + \left(V(\vec{x})I_4 - \sum_{j=1}^{d}A_j(\vec{x})\alpha_j\right)\Psi$$

- Position and current densities

$$\rho := \Psi^*\Psi = \sum_{j=1}^{4}\left|\psi_j\right|^2, \qquad \vec{J} = (J_1, J_2, J_3)^T \quad \text{with} \quad J_l := \frac{1}{\varepsilon}\Psi^*\alpha_l\Psi$$

- Conservation law $\qquad \partial_t\rho + \nabla\bullet\vec{J} = 0, \quad \vec{x}\in\mathbb{R}^d$
- Mass conservation

$$\|\Psi\|^2 := \int_{\mathbb{R}^d}\left|\Psi(t,\vec{x})\right|^2 d\vec{x} \equiv \int_{\mathbb{R}^d}\left|\Psi_0(\vec{x})\right|^2 d\vec{x} = 1$$

- Energy (or Hamiltonian) conservation

$$E(t) := \int_{\mathbb{R}^d}\left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\Psi^*\alpha_j\partial_j\Psi + \frac{1}{\varepsilon^2}\Psi^*\beta\Psi + V(\vec{x})\left|\Psi\right|^2 - \sum_{j=1}^{d}A_j(\vec{x})\Psi^*\alpha_j\Psi\right)d\vec{x} \equiv E(0)$$

The Dirac equation

$$i\partial_t \psi_1 = -\frac{i}{\varepsilon}\left(\partial_x - i\partial_y\right)\psi_4 + \frac{1}{\varepsilon^2}\psi_1 + V(t,\mathbf{x})\psi_1 - \left[A_1(t,\mathbf{x}) - iA_2(t,\mathbf{x})\right]\psi_4,$$
$$i\partial_t \psi_4 = -\frac{i}{\varepsilon}\left(\partial_x + i\partial_y\right)\psi_1 - \frac{1}{\varepsilon^2}\psi_4 + V(t,\mathbf{x})\psi_4 - \left[A_1(t,\mathbf{x}) + iA_2(t,\mathbf{x})\right]\psi_1,$$

$$i\partial_t \psi_2 = -\frac{i}{\varepsilon}\left(\partial_x + i\partial_y\right)\psi_3 + \frac{1}{\varepsilon^2}\psi_2 + V(t,\mathbf{x})\psi_2 - \left[A_1(t,\mathbf{x}) + iA_2(t,\mathbf{x})\right]\psi_3,$$
$$i\partial_t \psi_3 = -\frac{i}{\varepsilon}\left(\partial_x - i\partial_y\right)\psi_2 - \frac{1}{\varepsilon^2}\psi_3 + V(t,\mathbf{x})\psi_3 - \left[A_1(t,\mathbf{x}) - iA_2(t,\mathbf{x})\right]\psi_2.$$

- In 2D/1D

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\sigma_j\partial_j + \frac{1}{\varepsilon^2}\sigma_3\right)\Phi + \left(V(\vec{x})I_2 - \sum_{j=1}^{d}A_j(\vec{x})\sigma_j\right)\Phi, \quad \vec{x}\in\mathbb{R}^d$$

  - Initial data $\Phi = (\phi_1,\phi_2)^T$ with $\Phi=(\psi_1,\psi_4)^T$ or $(\psi_2,\psi_3)^T$

$$\Phi(0,\vec{x}) = \Phi_0(\vec{x}), \quad \vec{x}\in\mathbb{R}^d$$

  - Dispersive PDE & time symmetric
  - Mass & energy conservation

Conservations laws

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d} \sigma_j \partial_j + \frac{1}{\varepsilon^2}\sigma_3 \right)\Phi + \left(V(\vec{x}) I_2 - \sum_{j=1}^{d} A_j(\vec{x})\sigma_j \right)\Phi$$

- Position and current densities

$$\rho := \Phi^*\Phi = \sum_{j=1}^{2} |\phi_j|^2, \qquad \vec{J} = (J_1, J_2)^T \quad \text{with} \quad J_l := \frac{1}{\varepsilon}\Phi^*\sigma_l\Phi$$

- Conservation law $\quad \partial_t \rho + \nabla \bullet \vec{J} = 0, \quad \vec{x} \in \mathbb{R}^d$
- Mass conservation

$$\|\Phi\|^2 := \int_{\mathbb{R}^d} |\Phi(t,\vec{x})|^2 \, d\vec{x} \equiv \int_{\mathbb{R}^d} |\Phi_0(\vec{x})|^2 \, d\vec{x} = 1$$

- Energy (or Hamiltonian) conservation

$$E(t) := \int_{\mathbb{R}^d} \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d} \Phi^*\sigma_j\partial_j\Phi + \frac{1}{\varepsilon^2}\Phi^*\sigma_3\Phi + V(\vec{x})|\Phi|^2 - \sum_{j=1}^{d} A_j(\vec{x})\Phi^*\sigma_j\Phi \right) d\vec{x}$$

Two typical regimes & results

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\sigma_j\partial_j + \frac{1}{\varepsilon^2}\sigma_3 \right)\Phi + \left(V(\vec{x})I_2 - \sum_{j=1}^{d} A_j(\vec{x})\sigma_j \right)\Phi$$

- Standard regime $\quad v = O(c) \Leftrightarrow \varepsilon = 1$
  - Analytical study on existence & multiplicity of solutions: Gross, 66'; Gesztesy, Grosse & Thaller, 84'; Das & Kay, 89'; Das, 93'; Esteban & Sere, 97'; Dolbeault, Esteban & Sere, 00'; Esteban & Sere, 02'; Booth, Legg & Jarvis, 01'; Fefferman & Weistein, J. Amer. Math. Soc., 12'; CMP, 14; Ablowitz & Zhu, 12'; ……
  - Numerical methods
    - Leap-frog finite difference (LFFD) method: Shebalin, 97'; Nraun, Su & Grobe, 99'; Xu, Shao & Tang, 13'; Brinkman, Heitzinger & Markowich, 14'; Hammer, Potz & Arnold, 15'; Antoine, Lorin, Sater, Fillion-Gourdeau & Bandrauk, 15', …..
    - Time-splitting Fourier pseudospectral (TSFP) method: Bao & Li, 04'; Huang, Jin, Markowich, Sparber & Zheng, 05'; Xu, Shao & Tang, 13'; …..
    - Gaussian beam method: Wu, Huang, Jin & Yin, 12', ….
- Nonrelativistic regime

$$v \ll c \Leftrightarrow 0 < \varepsilon \ll 1 \Rightarrow \omega = \varepsilon^{-2} + O(1)$$

Existing results in nonrelativistic regime

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\sigma_j\partial_j + \frac{1}{\varepsilon^2}\sigma_3\right)\Phi + \left(V(\vec{x})I_2 - \sum_{j=1}^{d}A_j(\vec{x})\sigma_j\right)\Phi$$

- Nonrelativistic limits: Gross, 66'; Hunziker, 75'; Foldy & Wouthuysen, 78'; Schoene, 79'; Cirincione & Chernoff, 81'; Grigore, Nenciu & Purice, 89'; Najman, 92'; Gerad, Markowich, Mauser & Poupaud, 97'; Bechouche, Mauser & Poupaud, 98'; Bolte & Keppeler, 99'; Spohn, 00'; Kammerer, 04'; Bechouche, Mauser & Selberg, 05; ……

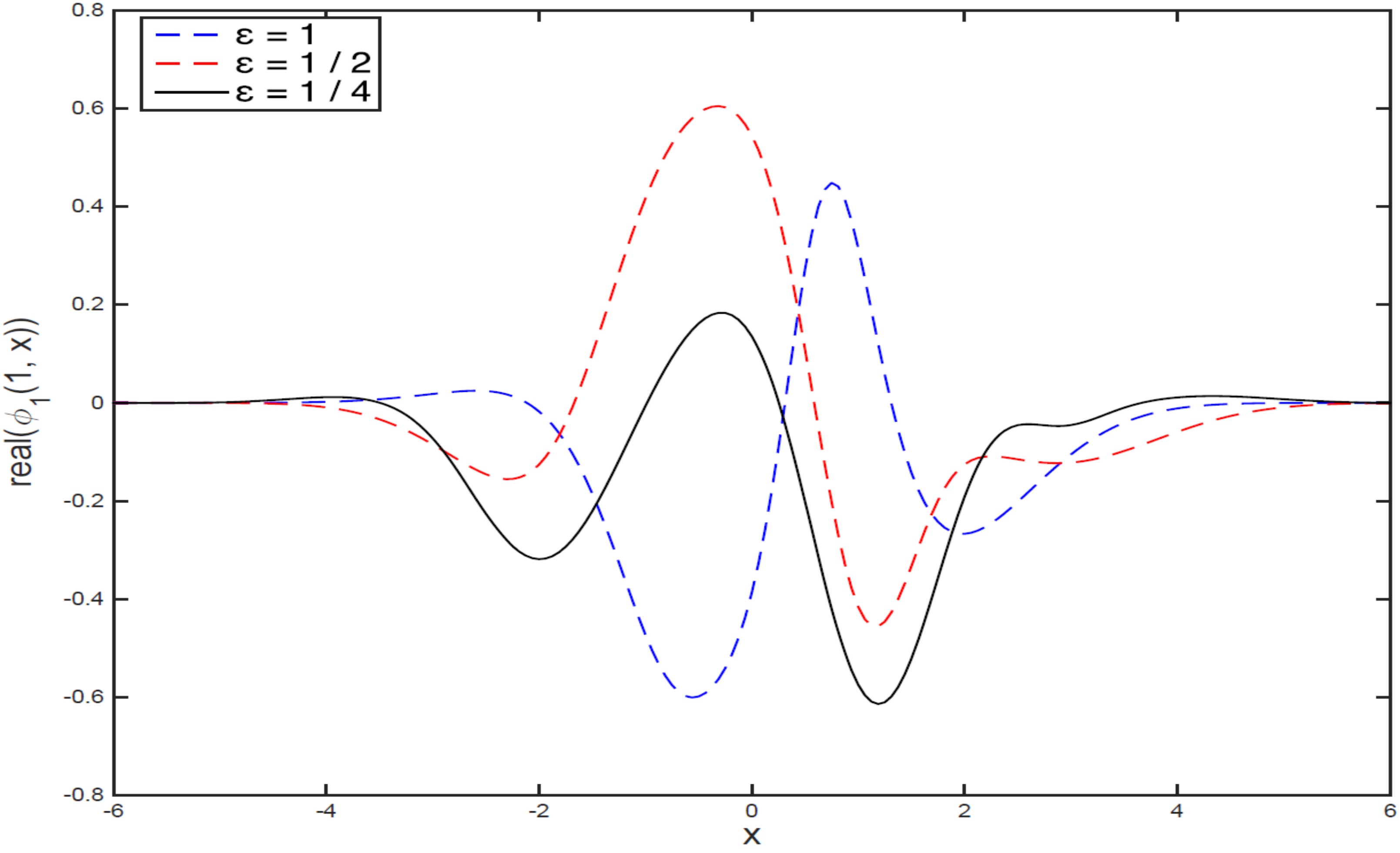
$$\Psi := \Psi^{\varepsilon} \quad (\text{or } \Phi := \Phi^{\varepsilon}) \to ??? \quad \text{when} \quad \varepsilon \to 0$$

  – Main difficulty: $E(t)$ is indefinite & unbounded when $\varepsilon \to 0$!!!

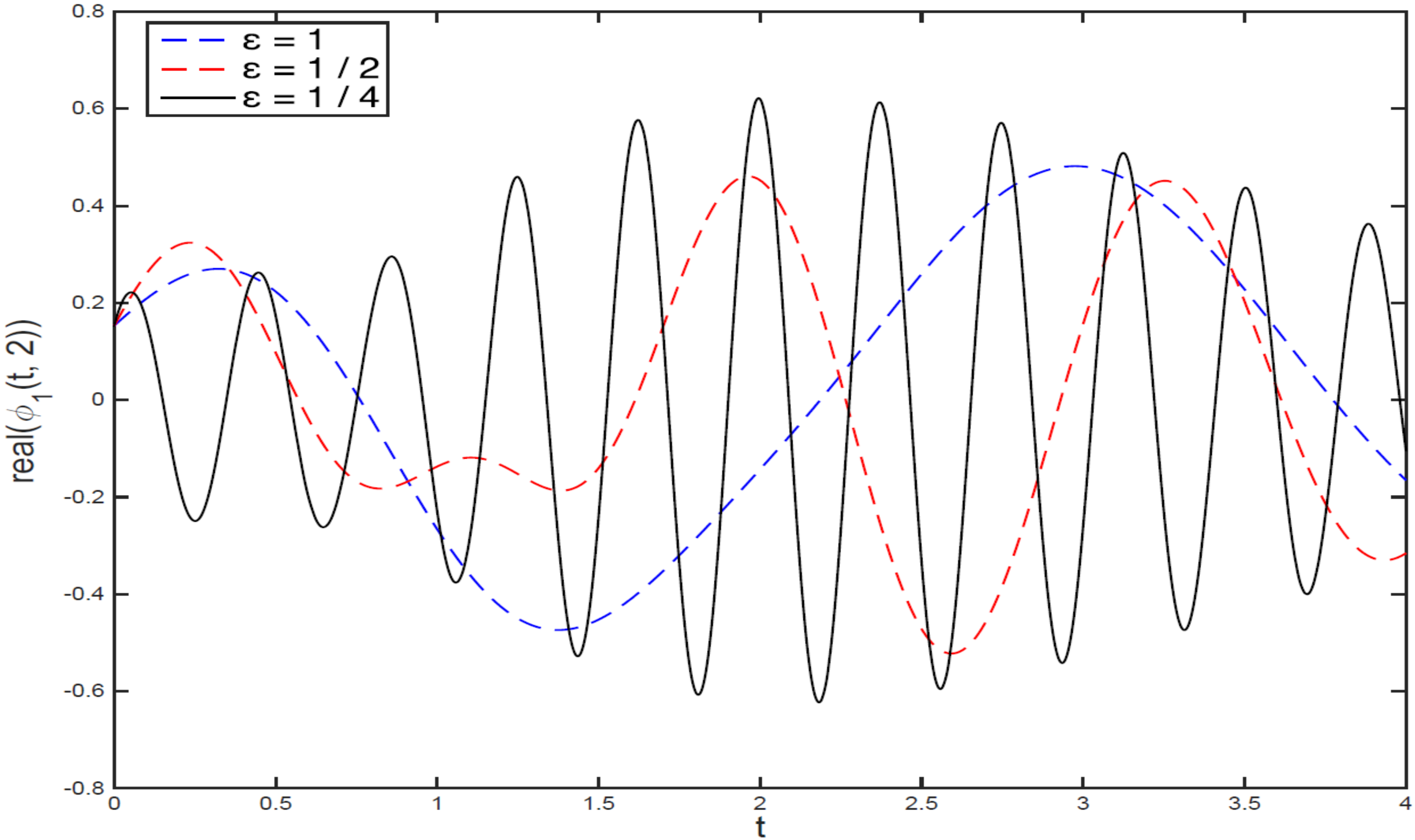
- Solution propagates waves with wavelength $O(\varepsilon^2)$ in time & $O(1)$ in space
  – Plane wave solutions $\Phi(t,\vec{x}) = \vec{B}\, e^{i(\vec{k}\cdot\vec{x}-\omega t)}$

$$\omega\vec{B} = \left(\sum_{j=1}^{d}\left(\frac{k_j}{\varepsilon} - A_j^0\right)\sigma_j + \frac{1}{\varepsilon^2}\sigma_3 + V^0 I_2\right)\vec{B}, \quad \vec{B}\in\mathbb{C}^2 \Rightarrow \omega = \varepsilon^{-2} + O(1)$$

Numerical results



Numerical results



Existing results in nonrelativistic regime

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\sigma_j\partial_j + \frac{1}{\varepsilon^2}\sigma_3 \right)\Phi + \left(V(\vec{x})I_2 - \sum_{j=1}^{d} A_j(\vec{x})\sigma_j \right)\Phi$$

– Asymptotic and rigorous results: Gross, 66'; Hunziker, 75'; Foldy & Wouthuysen, 78'; Schoene, 79'; Cirincione & Chernoff, 81'; Grigore, Nenciu & Purice, 89'; Najman, 92'; Gerad, Markowich, Mauser & Poupaud, 97'; Bechouche, Mauser & Poupaud, 98'; Bolte & Keppeler, 99'; Spohn, 00'; Kammerer, 04'; Bechouche, Mauser & Selberg, 05; ……

$$\Phi := \Phi^{\varepsilon} = e^{it/\varepsilon^2}\begin{pmatrix}\phi_+ \\ 0\end{pmatrix} + e^{-it/\varepsilon^2}\begin{pmatrix}0 \\ \phi_-\end{pmatrix} + O(\varepsilon), \quad \varepsilon \to 0$$

- The Schrodinger equation

$$i\partial_t \phi_\pm = \mp\frac{1}{2}\Delta\phi_\pm + V(\vec{x})\phi_\pm, \quad \vec{x} \in \mathbb{R}^d$$

- Semi-nonrelativistic limit: Bechouche, Mauser & Poupaud, 98

Highly oscillatory dispersive PDEs:

Numerical methods for Dirac equation

- Finite difference time domain (FDTD) methods

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon^2}\sigma_3 \right)\Phi + \big(V(t,x)I_2 - A_1(t,x)\sigma_1\big)\Phi, \quad x\in\Omega, \quad t>0$$

$$\Phi(a,t) = \Phi(b,t), \qquad t\ge 0; \qquad \Phi(x,0) = \Phi_0(x), \qquad x\in\overline{\Omega} = [a,b]$$

  - Mesh size $h := \Delta x = \frac{b-a}{M}, \quad x_j = a + jh, \quad j = 0,1,\ldots,M$
  - Time step $\tau := \Delta t > 0, \quad t_n = n\tau, \quad n = 0,1,\ldots$
  - Numerical approximation

$$\Phi(x_j, t_n) \approx \Phi_j^n, \quad j = 0,1,\ldots,M, \quad n = 0,1,\ldots$$

Numerical methods for Dirac equation

- Finite difference discretization operators

$$\delta_t^+ \Phi_j^n = \frac{\Phi_j^{n+1} - \Phi_j^n}{\tau}, \qquad \delta_t \Phi_j^n = \frac{\Phi_j^{n+1} - \Phi_j^{n-1}}{2\tau}, \qquad \delta_x \Phi_j^n = \frac{\Phi_{j+1}^n - \Phi_{j-1}^n}{2h}, \qquad \Phi_j^{n+\frac{1}{2}} = \frac{\Phi_j^{n+1} + \Phi_j^n}{2}.$$

- Leap-frog finite difference (LFFD) method

$$i\delta_t \Phi_j^n = \left[-\frac{i}{\varepsilon}\sigma_1 \delta_x + \frac{1}{\varepsilon^2}\sigma_3\right]\Phi_j^n + \left[V_j^n I_2 - A_{1,j}^n \sigma_1\right]\Phi_j^n, \quad n \geq 1.$$

- Semi-implicit finite difference (SIFD1) method

$$i\delta_t \Phi_j^n = -\frac{i}{\varepsilon}\sigma_1 \delta_x \Phi_j^n + \frac{1}{\varepsilon^2}\sigma_3 \frac{\Phi_j^{n+1} + \Phi_j^{n-1}}{2} + \left[V_j^n I_2 - A_{1,j}^n \sigma_1\right]\frac{\Phi_j^{n+1} + \Phi_j^{n-1}}{2},$$

Numerical methods for Dirac equation

- Semi-implicit finite difference (SIFD2) method

$$i\delta_t \Phi_j^n = \left[-\frac{i}{\varepsilon}\sigma_1\delta_x + \frac{1}{\varepsilon^2}\sigma_3\right]\frac{\Phi_j^{n+1}+\Phi_j^{n-1}}{2} + \left[V_j^n I_2 - A_{1,j}^n\sigma_1\right]\Phi_j^n,$$

- Energy conservative finite difference (CNFD) method

$$i\delta_t^+ \Phi_j^n = \left[-\frac{i}{\varepsilon}\sigma_1\delta_x + \frac{1}{\varepsilon^2}\sigma_3\right]\Phi_j^{n+1/2} + \left[V_j^{n+1/2} I_2 - A_{1,j}^{n+1/2}\sigma_1\right]\Phi_j^{n+1/2},$$

  – Initial and boundary data

$$\Phi_M^{n+1} = \Phi_0^{n+1}, \quad \Phi_{-1}^{n+1} = \Phi_{M-1}^{n+1}, \quad n \geq 0, \qquad \Phi_j^0 = \Phi_0(x_j), \quad j = 0, 1, ..., M.$$

  – First step for LFFD, SIFD1 &SIFD2

$$\Phi_j^1 = \Phi_j^0 + \tau\left[-\frac{1}{\varepsilon}\sigma_1\Phi_0'(x_j) - i\left(\frac{1}{\varepsilon^2}\sigma_3 + V_j^0 I_2 - A_{1,j}^0\sigma_1\right)\Phi_j^0\right],$$

Properties of FDTD methods

- Time symmetric, unchanged if $n+1 \leftrightarrow n-1 \quad \& \quad \tau \leftrightarrow -\tau$
- Stability
  - CNFD is unconditionally stable
  - LFFD, SIFD1 & SIFD2 are conditionally stable
- Energy conservation: CNFD conserves mass & energy vs others not
- Computational cost
  - CNFD needs solve a linear coupled system per time step!! LFFD is explicit!
  - SIFD1 & SIFD2 can be solved very almost explicit !!
- Resolution in nonrelativistic regime

$$h = O(\varepsilon^{?}) \quad \& \quad \tau = O(\varepsilon^{?}), \quad 0 < \varepsilon \ll 1$$

Error estimates for FDTD methods

- Define `error' function

$$\mathbf{e}_j^n = \Phi(t_n, x_j) - \Phi_j^n, \qquad j = 0, 1, \ldots, M, \quad n \geq 0,$$

- Assumptions
  - For the solution of the Dirac equation --- (A)

$$\left\| \frac{\partial^{r+s}}{\partial t^r \partial x^s} \Phi \right\|_{L^\infty([0,T];(L^\infty(\Omega))^2)} \lesssim \frac{1}{\varepsilon^{2r}}, \quad 0 \leq r \leq 3,\ 0 \leq r+s \leq 3, \qquad 0 < \varepsilon \leq 1,$$

  - For the electronic & magnetic potentials – (B)

$$V_{\max} := \max_{(t,x)\in\overline{\Omega}_T} |V(t,x)|, \qquad A_{1,\max} := \max_{(t,x)\in\overline{\Omega}_T} |A_1(t,x)|.$$

Error estimates for FDTD methods

- Theorem Under some stability conditions, we have error estimates for LFFD, SIFD1, SIFD2 & CNFD as

$$\|\mathrm{e}^n\|_{l^2} \lesssim \frac{h^2}{\varepsilon} + \frac{\tau^2}{\varepsilon^6}, \qquad 0 \le n \le \frac{T}{\tau}.$$

  – Resolution ---- (under resolution)

$$\tau = O\left(\varepsilon^3\sqrt{\delta}\right) = O(\varepsilon^3), \qquad h = O\left(\sqrt{\delta\varepsilon}\right) = O\left(\sqrt{\varepsilon}\right), \qquad 0 < \varepsilon \ll 1.$$

W. Bao, Y. Cai, X. Jia and Q. Tang, Numerical methods and comparison for the Dirac equation in the nonrelativistic limit regime, J. Sci. Comput., Vol. 71 (2017), pp. 1094-1134.

EWI-FP method

- Apply Fourier spectral method for spatial derivatives

$$i\partial_t \Phi_M(t,x) = \left[-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon^2}\sigma_3\right]\Phi_M(t,x) + P_M(V\Phi_M)(t,x) - \sigma_1 P_M(A_1\Phi_M)(t,x).$$

  – with

$$\Phi_M(t,x) = \sum_{l=-M/2}^{M/2-1} \widehat{(\Phi_M)}_l(t)\, e^{i\mu_l(x-a)}, \qquad a \le x \le b, \qquad t \ge 0,$$

- Take Fourier transform, we get ODEs for *l=-M/2,…,M/2-1*

$$i\frac{d}{dt}\widehat{(\Phi_M)}_l(t) = \left[\frac{\mu_l}{\varepsilon}\sigma_1 + \frac{1}{\varepsilon^2}\sigma_3\right]\widehat{(\Phi_M)}_l(t) + \widehat{(V\Phi_M)}_l(t) - \sigma_1\widehat{(A_1\Phi_M)}_l(t) = 0,$$

$$i\frac{d}{ds}\widehat{(\Phi_M)}_l(t_n+s) = \frac{1}{\varepsilon^2}\Gamma_l\,\widehat{(\Phi_M)}_l(t_n+s) + \widehat{F}_l^n(s), \qquad s \in \mathbb{R},$$

Exponential wave integrator (EWI) for 1st ODEs

$$\widehat{(\Phi_M)}_l(t_n+s) = e^{-is\Gamma_l/\varepsilon^2}\widehat{(\Phi_M)}_l(t_n) - i\int_0^s e^{i(w-s)\Gamma_l/\varepsilon^2}\widehat{F}_l^n(w)\,dw,$$

- Take $s=\tau$ and approximate the integral --W. Gautschi (61'); P. Deuflhard (79'); E. Hairer, Ch. Lubich, G. Wanner, A. Iserles, V. Grimm, M. Hochbruck, D. Cohen, …..

- EWI-FP method

$$\Phi_M^{n+1}(x) = \sum_{l=-M/2}^{M/2-1} \widehat{(\Phi_M^{n+1})}_l\, e^{i\mu_l(x-a)},$$

$$\widehat{(\Phi_M^{n+1})}_l = \begin{cases} e^{-i\tau\Gamma_l/\varepsilon^2}\widehat{(\Phi_M^0)}_l - i\varepsilon^2\Gamma_l^{-1}\left[I_2 - e^{-\frac{i\tau}{\varepsilon^2}\Gamma_l}\right]\widehat{(G(t_0)\Phi_M^0)}_l, & n=0,\\ e^{-i\tau\Gamma_l/\varepsilon^2}\widehat{(\Phi_M^n)}_l - iQ_l^{(1)}(\tau)\,\widehat{(G(t_n)\Phi_M^n)}_l - iQ_l^{(2)}(\tau)\delta_t^-\widehat{(G(t_n)\Phi_M^n)}_l, & n\geq 1,\end{cases}$$

$$Q_l^{(1)}(\tau) = -i\varepsilon^2\Gamma_l^{-1}\left[I - e^{-\frac{i\tau}{\varepsilon^2}\Gamma_l}\right], \quad Q_l^{(2)}(\tau) = -i\varepsilon^2\tau\Gamma_l^{-1} + \varepsilon^4\Gamma_l^{-2}\left(I - e^{-\frac{i\tau}{\varepsilon^2}\Gamma_l}\right).$$

Error estimates for EWI-FP method

- **Theorem** Under some stability conditions, we have error estimates for EWI-FP and sEWI-FP as

$$\|\Phi(t_n,x)-\Phi_M^n(x)\|_{L^2} \lesssim \frac{\tau^2}{\varepsilon^4}+h^{m_0}, \quad 0\le n\le \frac{T}{\tau}.$$

  – Resolution --- (optimal resolution)

$$\tau = O(\varepsilon^2\sqrt{\delta}) = O(\varepsilon^2), \quad h = O(\delta^{1/m_0}) = O(1), \quad 0<\varepsilon\ll 1$$

W. Bao, Y. Cai, X. Jia and Q. Tang, Numerical methods and comparison for the Dirac equation in the nonrelativistic limit regime, J. Sci. Comput., Vol. 71 (2017), pp. 1094-1134.

Time-splitting Fourier spectral (TSFP) method

- From $[t_n, t_{n+1}]$, apply time splitting technique
  - Step 1

$$i\partial_t \Phi(t,x) = \left[-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon^2}\sigma_3\right]\Phi(t,x),$$

  - Step 2

$$i\partial_t \Phi(t,x) = \left[-A_1(t,x)\sigma_1 + V(t,x)I_2\right]\Phi(t,x), \quad x \in \Omega,$$

- Thm. Under proper assumptions, we have

$$\|\Phi(t_n,x) - I_M(\Phi^n)\|_{L^2} \lesssim h^{m_0} + \frac{\tau^2}{\varepsilon^4}, \qquad 0 \le n \le \frac{T}{\tau},$$

  - Resolution --- (optimal resolution)

$$\tau = O(\varepsilon^2\sqrt{\delta}) = O(\varepsilon^2), \quad h = O(\delta^{1/m_0}) = O(1), \quad 0 < \varepsilon \ll 1$$

W. Bao, Y. Cai, X. Jia and Q. Tang, Numerical methods and comparison for the Dirac equation in the nonrelativistic limit regime, J. Sci. Comput., Vol. 71 (2017), pp. 1094-1134.

Spatial Errors of TSFP

Spatial Errors	$h_0 = 2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0 = 1$	1.10	2.43E-1	2.99E-3	2.79E-6	9.45E-9
$\varepsilon_0/2$	1.06	1.46E-1	1.34E-3	9.61E-7	5.57E-9
$\varepsilon_0/2^2$	1.11	1.43E-1	9.40E-4	5.10E-7	6.50E-9
$\varepsilon_0/2^3$	1.15	1.44E-1	7.89E-4	3.62E-7	6.84E-9
$\varepsilon_0/2^4$	1.18	1.45E-1	7.62E-4	2.88E-7	7.49E-9
$\varepsilon_0/2^5$	1.19	1.46E-1	7.53E-4	2.59E-7	7.96E-9
$\varepsilon_0/2^6$	1.20	1.47E-1	7.49E-4	2.63E-7	6.90E-9

Temporal Errors of TSFP

Temporal Errors	τ_0=0.4	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$	$\tau_0/4^6$
$\varepsilon_0 = 1$	**2.17E-1**	1.32E-2	8.22E-4	5.13E-5	3.21E-6	2.01E-7	1.26E-8
order	–	2.02	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	1.32	**6.60E-2**	4.07E-3	2.54E-4	1.59E-5	9.92E-7	6.20E-8
order	–	**2.16**	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	2.50	3.33E-1	**1.68E-2**	1.04E-3	6.49E-5	4.06E-6	2.54E-7
order	–	1.45	**2.15**	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	1.79	1.97	8.15E-2	**4.15E-3**	2.57E-4	1.60E-5	1.00E-6
order	–	-0.07	2.30	**2.14**	2.01	2.00	2.00
$\varepsilon_0/2^4$	1.35	8.27E-1	8.85E-1	2.01E-2	**1.03E-3**	6.35E-5	3.97E-6
order	–	0.35	-0.05	2.73	**2.14**	2.01	2.00
$\varepsilon_0/2^5$	8.73E-1	2.25E-1	2.33E-1	2.49E-1	4.98E-3	**2.55E-4**	1.58E-5
order	–	0.98	-0.03	-0.05	2.82	**2.14**	2.01

$$\tau \le C\varepsilon^2 \Rightarrow \quad \|\Phi(t_n,\cdot) - I_M(\Phi^n)\|_{L^2} \lesssim h^{m_0} + \frac{\tau^2}{\varepsilon^2}, \qquad 0 \le n \le \frac{T}{\tau},$$

- Thm. If time step satisfies $\tau = 2\pi\varepsilon^2 / N$

$$\|\Phi(t_n,x) - (I_M\Phi^n)(x)\|_{H^s} \lesssim \frac{\tau^2}{\varepsilon^2} + h^{m_0-s} + N^{-m^*}$$

W. Bao, Y.Cai, X. Jia and Y. Jia, Error estimates of numerical methods for the nonlinear Dirac equation in the nonrelativistic limit regime, Sci. China Math., Vol. 59 (2016), pp. 1461-1494.

Super-resolution of TSFP

(without magnetic potential)

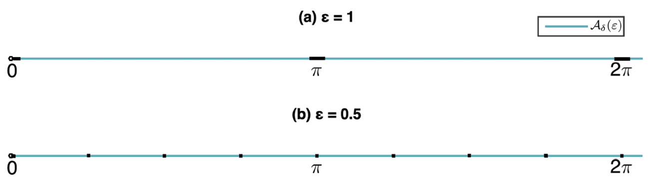
- For 1st-order Lie-Trotter splitting $i\partial_t\Phi = \left(-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon^2}\sigma_3\right)\Phi + V(t,x)\Phi$
  - For any time step

$$\|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau+\varepsilon, \quad \|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau+\tau/\varepsilon,$$

$$\left\|\Phi(t_n,.)-\Phi^n(\bullet)\right\|_{L^2} \le \tau + \max_{0<\varepsilon\le 1}\min\left\{\varepsilon,\frac{\tau}{\varepsilon}\right\} \le \sqrt{\tau}$$

  - For non-resonant time steps $\mathcal{S}_{\varepsilon}^{(\delta_0)} := \{\tau \,|\, |\tau - k\pi\varepsilon^2| \ge \delta_0, \quad k\in\mathbb{N}^*\}$

$$\|\Phi(t_n,x)-\Phi^n(x)\|_{L^2} \lesssim \tau$$



- Extension to high order TSFP & nonlinear Dirac

W. Bao, Y. Cai and J. Yin, Super-resolution of time-splitting methods for the Dirac equation in the nonrelativistic regime, Math. Comp., Vol. 89 (2020), 2141-2173.
W. Bao, Y. Cai and J. Yin, Uniform error bounds of time-splitting methods for the nonlinear Dirac equation in the nonrelativistic regime without magnetic potential, SIAM J. Numer. Anal., Vol. 59 (2021), pp. 1040-1066.

Relative temporal errors $e^r(t = 2\pi)$ for the wave function with resonance time step size, S_1 method.

	$\tau_0 = \pi/4$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$
$\varepsilon_0 = 1$	2.57E-1	6.73E-2	1.70E-2	4.26E-3	1.07E-3	2.67E-4
order	–	0.98	0.99	1.00	1.00	1.00
$\varepsilon_0/2$	3.61E-1	**6.44E-2**	1.64E-2	4.13E-3	1.03E-3	2.59E-4
order	–	**0.98**	0.99	1.00	1.00	1.00
$\varepsilon_0/2^2$	3.07E-1	1.44E-1	**1.63E-2**	4.12E-3	1.03E-3	2.59E-4
order	–	0.41	**0.98**	1.00	1.00	1.00
$\varepsilon_0/2^3$	2.83E-1	9.83E-2	6.44E-2	**4.12E-3**	1.03E-3	2.59E-4
order	–	0.66	0.20	**0.99**	1.00	1.00
$\varepsilon_0/2^4$	2.73E-1	7.87E-2	3.73E-2	3.06E-2	**1.03E-3**	2.59E-4
order	–	0.84	0.41	0.08	**0.99**	1.00
$\varepsilon_0/2^5$	2.68E-1	**7.10E-2**	2.49E-2	1.63E-2	1.50E-2	**2.59E-4**
order	–	**0.92**	0.67	0.20	0.04	**1.00**
$\varepsilon_0/2^7$	2.65E-1	6.66E-2	**1.79E-2**	6.26E-3	4.08E-3	3.74E-3
order	–	0.98	**0.93**	0.67	0.20	0.04
$\varepsilon_0/2^9$	2.64E-1	6.57E-2	1.68E-2	**4.49E-3**	1.57E-3	1.02E-3
order	–	0.99	0.98	**0.94**	0.67	0.20
$\varepsilon_0/2^{11}$	2.64E-1	6.55E-2	1.66E-2	4.22E-3	**1.12E-3**	3.91E-4
order	–	0.99	0.99	0.99	**0.94**	0.67
max	3.61E-1	1.44E-1	6.44E-2	3.06E-2	1.50E-2	7.40E-3
order	–	0.66	0.58	0.54	0.52	0.51

Relative temporal errors $e^r(t=4)$ for the wave function with non-resonance time step size, S_1 method.

	$\tau_0=1$	$\tau_0/2$	$\tau_0/2^2$	$\tau_0/2^3$	$\tau_0/2^4$	$\tau_0/2^5$	$\tau_0/2^6$	$\tau_0/2^7$
$\varepsilon_0=1$	3.66E-1	1.86E-1	9.45E-2	4.76E-2	2.39E-2	1.20E-2	5.99E-3	2.99E-3
order	–	0.98	0.98	0.99	0.99	1.00	1.00	1.00
$\varepsilon_0/2$	3.46E-1	1.87E-1	8.75E-2	4.43E-2	2.23E-2	1.12E-2	5.60E-3	2.80E-3
order	–	0.89	1.10	0.98	0.99	1.00	1.00	1.00
$\varepsilon_0/2^2$	3.60E-1	1.72E-1	8.70E-2	4.27E-2	2.16E-2	1.09E-2	5.46E-3	2.74E-3
order	–	1.06	0.99	1.03	0.98	0.99	1.00	1.00
$\varepsilon_0/2^3$	3.41E-1	1.72E-1	8.95E-2	4.30E-2	2.19E-2	1.08E-2	5.43E-3	2.72E-3
order	–	0.99	0.94	1.06	0.97	1.03	0.99	0.99
$\varepsilon_0/2^4$	3.40E-1	1.66E-1	8.57E-2	4.38E-2	2.24E-2	1.09E-2	5.49E-3	2.71E-3
order	–	1.04	0.95	0.97	0.97	1.04	0.99	1.02
$\varepsilon_0/2^5$	3.45E-1	1.73E-1	8.54E-2	4.30E-2	2.18E-2	1.10E-2	5.54E-3	2.73E-3
order	–	1.00	1.02	0.99	0.98	0.99	0.98	1.02
$\varepsilon_0/2^6$	3.42E-1	1.70E-1	8.64E-2	4.48E-2	2.17E-2	1.09E-2	5.46E-3	2.74E-3
order	–	1.01	0.97	0.95	1.04	1.00	0.99	0.99
$\varepsilon_0/2^7$	3.43E-1	1.69E-1	8.52E-2	4.30E-2	2.16E-2	1.09E-2	5.46E-3	2.73E-3
order	–	1.02	0.99	0.99	0.99	0.99	0.99	1.00

A uniformly accurate (UA) method

$$i\partial_t \Phi = \frac{1}{\varepsilon^2} T\Phi + W(t,x)\Phi, \quad x \in \mathbb{R}, \quad t > 0$$

$$T = -i\varepsilon\sigma_1\partial_x + \sigma_3, \quad W(t,x) = V(t,x) I_2 - A_1(t,x)\sigma_1$$

$$\Phi(0,x) = \Phi_0(x), \qquad x \in \mathbb{R}$$

- *T* can be diagonalizable (Bechouche, Mauser & Poupaud, 98')

$$T = \sqrt{1-\varepsilon^2\Delta}\,\Pi_+ - \sqrt{1-\varepsilon^2\Delta}\,\Pi_-$$

  – With

$$\Pi_+ = \frac{1}{2}\left[I_2 + \left(1-\varepsilon^2\Delta\right)^{-1/2} T\right], \qquad \Pi_- = \frac{1}{2}\left[I_2 - \left(1-\varepsilon^2\Delta\right)^{-1/2} T\right]$$

  – Satisfying

$$\Pi_+ + \Pi_- = I_2, \quad \Pi_+\Pi_- = \Pi_-\Pi_+ = 0, \quad \Pi_\pm^2 = \Pi_\pm$$

A uniformly accurate (UA) method

- Given initial data at $t = t_n$: $\Phi(t_n, x) = \Phi_n(x), \quad x \in \mathbb{R}$
- Multiscale decomposition by frequency (MDF) :(Bechouche, Mauser & Poupaud, 98')

$$\Phi(t_n + s, x) = e^{is/\varepsilon^2}\left[\Psi_+^{1,n} + \Psi_-^{1,n}\right](s,x) + e^{-is/\varepsilon^2}\left[\Psi_+^{2,n} + \Psi_-^{2,n}\right](s,x), \quad 0 \le s \le \tau$$

- Two sub-problems $\Psi_+^{1,n} = O(1), \quad \Psi_-^{1,n} = O(\varepsilon^2)$

$$i\partial_s \Psi_+^{1,n}(s,x) = \frac{1}{\varepsilon^2}\left(\sqrt{1-\varepsilon^2\Delta} - 1\right)\Psi_+^{1,n}(s,x) + \Pi_+\left(W\Psi_+^{1,n}(s,x) + W\Psi_-^{1,n}(s,x)\right)$$

$$i\partial_s \Psi_-^{1,n}(s,x) = \frac{1}{\varepsilon^2}\left(-\sqrt{1-\varepsilon^2\Delta} - 1\right)\Psi_-^{1,n}(s,x) + \Pi_-\left(W\Psi_+^{1,n}(s,x) + W\Psi_-^{1,n}(s,x)\right)$$

$$\Psi_+^{1,n}(0,x) = \Pi_+\Phi_n(x), \qquad \Psi_-^{1,n}(0,x) = 0, \qquad \text{with} \quad W := W(t_n + s, x)$$

A uniformly accurate (UA) method

- Two sub-problems $\Psi_+^{2,n} = O(\varepsilon^2), \quad \Psi_-^{2,n} = O(1)$

$$i\partial_s \Psi_+^{2,n}(s,x) = \frac{1}{\varepsilon^2}\left(\sqrt{1-\varepsilon^2\Delta}+1\right)\Psi_+^{2,n}(s,x) + \Pi_+\left(W\Psi_+^{2,n}(s,x) + W\Psi_-^{2,n}(s,x)\right)$$

$$i\partial_s \Psi_-^{2,n}(s,x) = \frac{-1}{\varepsilon^2}\left(\sqrt{1-\varepsilon^2\Delta}-1\right)\Psi_-^{2,n}(s,x) + \Pi_-\left(W\Psi_+^{2,n}(s,x) + W\Psi_-^{2,n}(s,x)\right)$$

$$\Psi_+^{2,n}(0,x) = 0, \qquad \Psi_-^{2,n}(0,x) = \Pi_-\Phi_n(x), \qquad \text{with} \quad W := W(t_n + s, x)$$

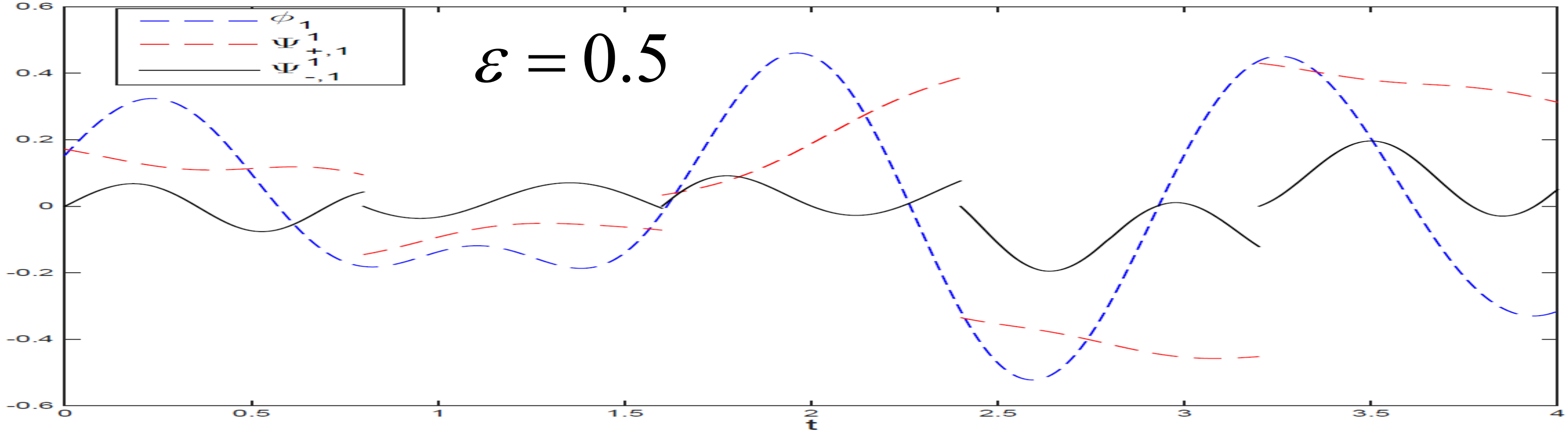
- Solve the two sub-problems via EW-FP

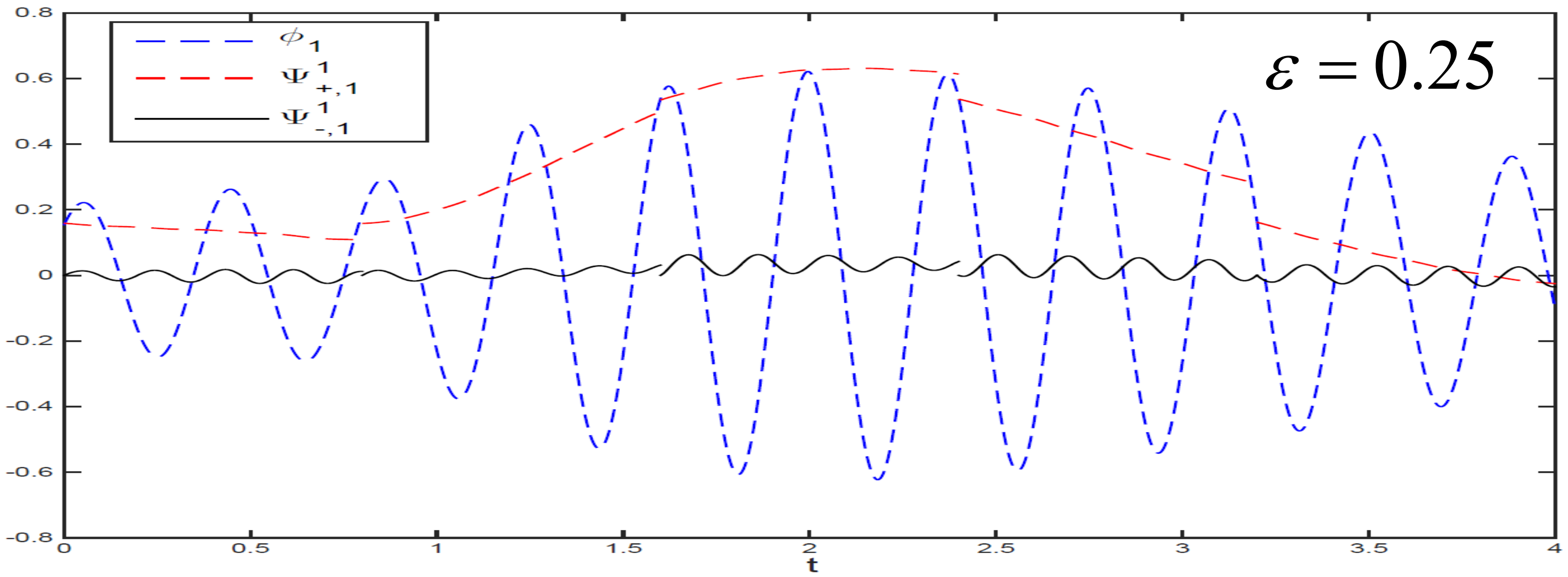
$$\Psi_\pm^{1,n}(\tau,x) \quad \& \quad \Psi_\pm^{2,n}(\tau,x)$$

- Reconstruct the solution at $t = t_{n+1}$

$$\Phi(t_{n+1},x) = e^{i\tau/\varepsilon^2}\left[\Psi_+^{1,n} + \Psi_-^{1,n}\right](\tau,x) + e^{-i\tau/\varepsilon^2}\left[\Psi_+^{2,n} + \Psi_-^{2,n}\right](\tau,x)$$

Multiscale Decomposition





Error estimates for MTI-FP method

- **Theorem** Under proper assumptions on the solution, we have error estimates for the MTI-FP method

$$\|\Phi(t_n,\cdot)-\Phi_I^n(\cdot)\|_{L^2} \lesssim h^{m_0}+\frac{\tau^2}{\varepsilon^2}, \quad \|\Phi(t_n,\cdot)-\Phi_I^n(\cdot)\|_{L^2} \lesssim h^{m_0}+\tau^2+\varepsilon^2$$

  - Which yields a uniform error bound

$$\left\|\Phi(t_n,\bullet)-\Phi_I^n(\bullet)\right\|_{L^2} \le h^{m_0} + \max_{0<\varepsilon\le 1} \min\{\frac{\tau^2}{\varepsilon^2}, \tau^2+\varepsilon^2\} \le h^{m_0}+\tau$$

  - Resolution ---- (super resolution)

$$\tau = O(\delta) = O(1), \quad h = O(\delta^{1/m_0}) = O(1), \quad 0<\varepsilon \ll 1$$

W. Bao, Y. Cai, X. Jia and Q. Tang, A uniformly accurate multiscale time integrator pseudospectral method for the Dirac equation in the nonrelativistic limit regime, SIAM J. Numer. Anal., Vol. 54 (2016), pp. 1785-1812.

Key Steps in the Proof

- Step 1. Some properties of micro variables

$$\left\|\Psi_+^{1,n}\right\| + \left\|\Psi_-^{2,n}\right\| + \left\|\partial_s \Psi_+^{1,n}\right\| + \left\|\partial_s \Psi_-^{2,n}\right\| + \left\|\partial_{ss} \Psi_+^{1,n}\right\| + \left\|\partial_{ss} \Psi_-^{2,n}\right\| \le O(1)$$

$$\left\|\Psi_-^{1,n}\right\| + \left\|\Psi_+^{2,n}\right\| \le O(\varepsilon^2), \quad \left\|\partial_s \Psi_-^{1,n}\right\| + \left\|\partial_s \Psi_+^{2,n}\right\| \le O(1), \quad \left\|\partial_{ss} \Psi_-^{1,n}\right\| + \left\|\partial_{ss} \Psi_+^{2,n}\right\| \le O(\frac{1}{\varepsilon^2})$$

- Step 2. Local error bounds for micro variables

$$\left\|\Psi_+^{1,n} - \Psi_{+,h}^{1,n}\right\|_{L^2} \le \left\|\Phi(t_{n-1},.) - \Phi_I^{n-1}(\bullet)\right\|_{L^2} + \tau(h^{m_0} + \tau^2),$$

$$\left\|\Psi_-^{2,n} - \Psi_{-,h}^{2,n}\right\|_{L^2} \le \left\|\Phi(t_{n-1},.) - \Phi_I^{n-1}(\bullet)\right\|_{L^2} + \tau(h^{m_0} + \tau^2),$$

$$\left\|\Psi_-^{1,n} - \Psi_{-,h}^{1,n}\right\|_{L^2} \le \tau(h^{m_0} + \varepsilon^2), \quad \left\|\Psi_-^{1,n} - \Psi_{-,h}^{1,n}\right\|_{L^2} \le \tau(h^{m_0} + \tau^2/\varepsilon^2),$$

$$\left\|\Psi_+^{2,n} - \Psi_{+,h}^{2,n}\right\|_{L^2} \le \tau(h^{m_0} + \varepsilon^2), \quad \left\|\Psi_+^{2,n} - \Psi_{+,h}^{2,n}\right\|_{L^2} \le \tau(h^{m_0} + \tau^2/\varepsilon^2)$$

Key Steps in the Proof

- Step 3. Local error bounds for macro variables

$$\left\|\Phi(t_n,.)-\Phi_I^n(\bullet)\right\|_{L^2}\le\left\|\Psi_+^{1,n}-\Psi_{+,h}^{1,n}\right\|_{L^2}+\left\|\Psi_-^{2,n}-\Psi_{-,h}^{2,n}\right\|_{L^2}+\left\|\Psi_-^{1,n}-\Psi_{-,h}^{1,n}\right\|_{L^2}+\left\|\Psi_+^{2,n}-\Psi_{+,h}^{2,n}\right\|_{L^2}$$

$$\le\left\|\Phi(t_{n-1},.)-\Phi_I^{n-1}(\bullet)\right\|_{L^2}+\tau(h^{m_0}+\tau^2+\frac{\tau^2}{\varepsilon^2})$$

$$\left\|\Phi(t_n,.)-\Phi_I^n(\bullet)\right\|_{L^2}\le\left\|\Phi(t_{n-1},.)-\Phi_I^{n-1}(\bullet)\right\|_{L^2}+\tau(h^{m_0}+\tau^2+\varepsilon^2)$$

- Step 4. The energy method via discrete Gronwall's inequality
- Step 5. Uniform error bound

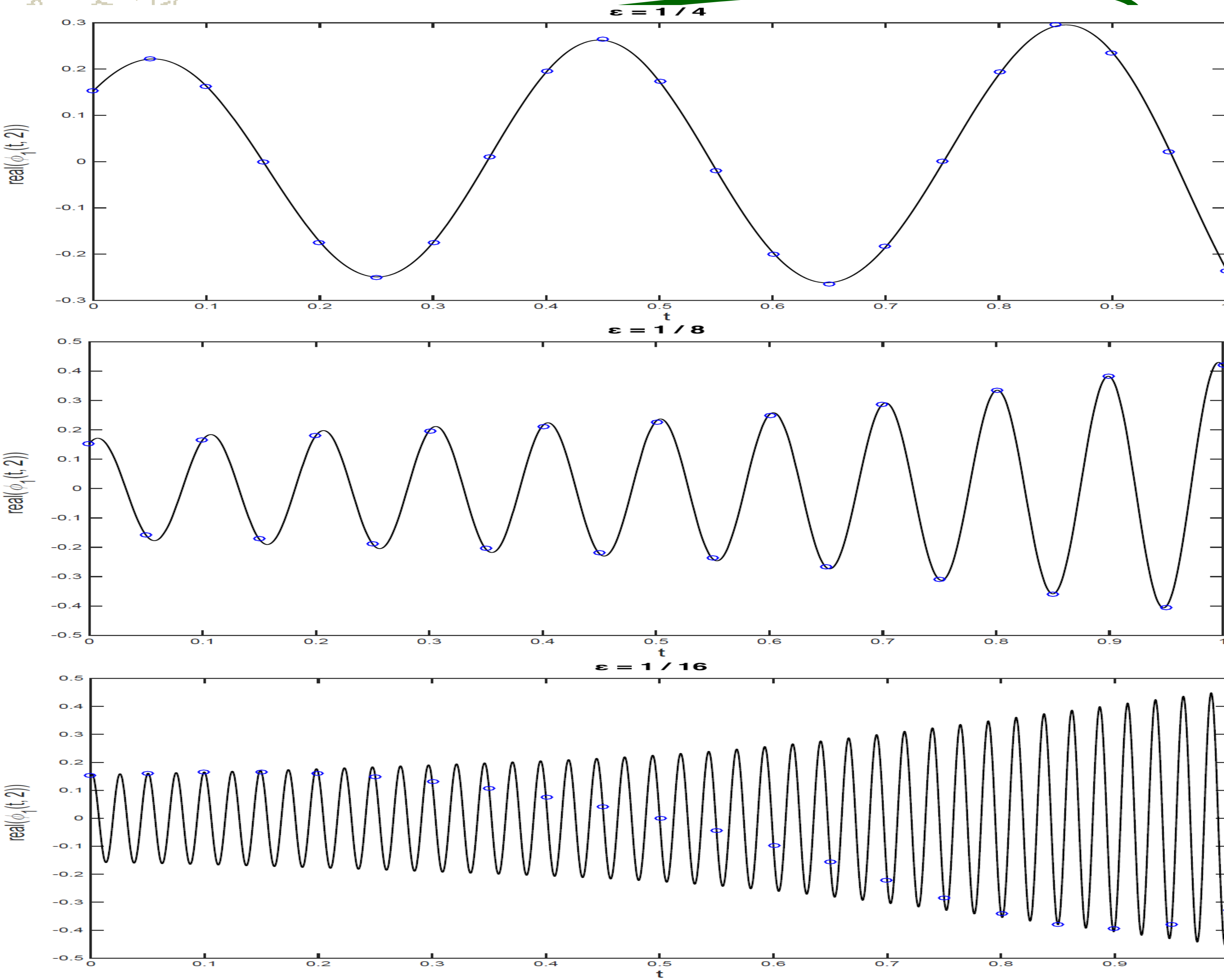
$$\left\|\Phi(t_n,.)-\Phi_I^n(\bullet)\right\|_{L^2}\le h^{m_0}+\tau^2+\max_{0<\varepsilon\le 1}\min\left\{\varepsilon^2,\frac{\tau^2}{\varepsilon^2}\right\}\le h^{m_0}+\tau$$

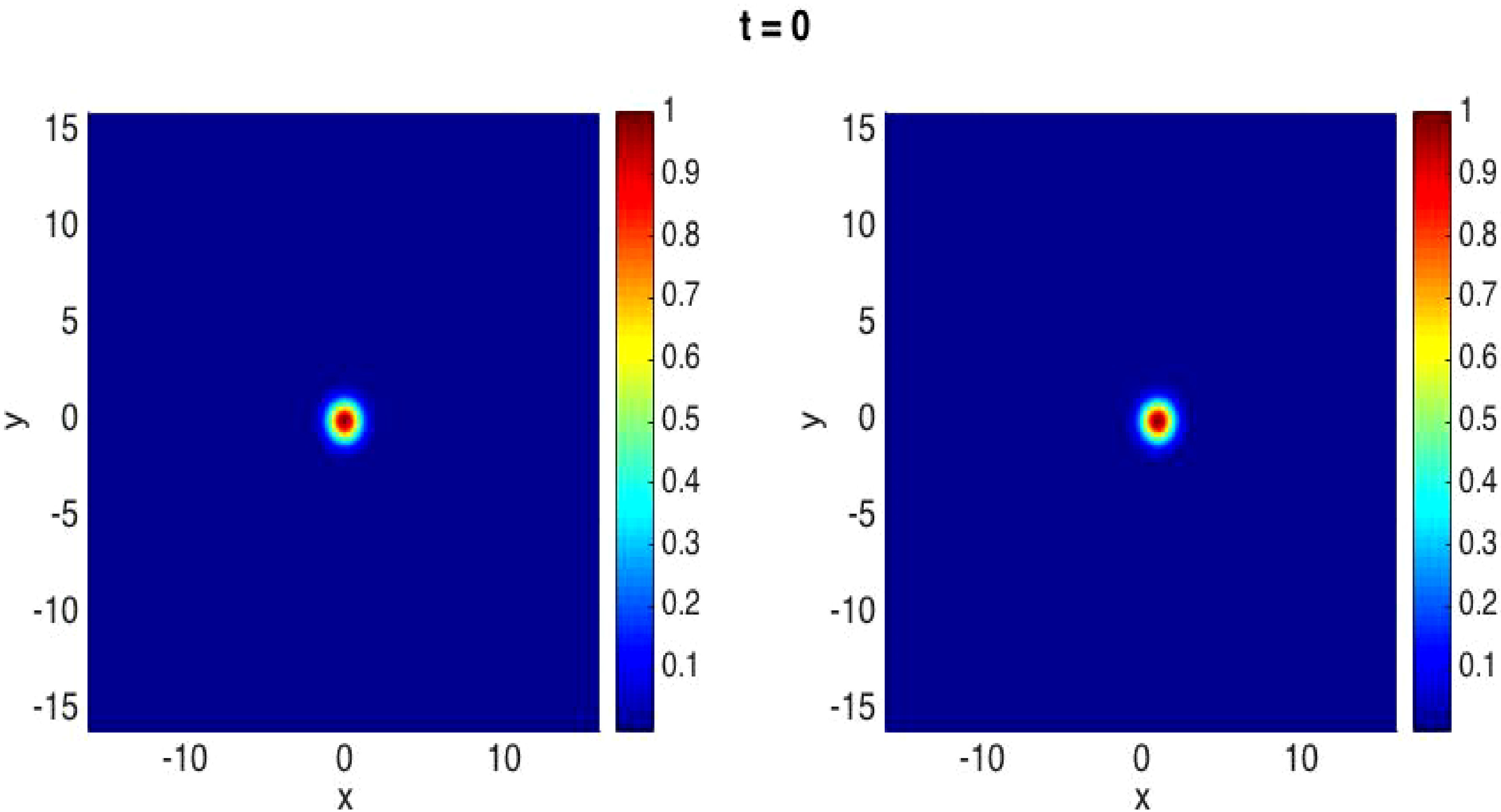
Spatial Errors of MTI-FP

$e_{h,\tau}(2.0)$	$h_0 = 2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0 = 1$	1.65	5.74E-1	7.08E-2	7.00E-5	8.53E-10
$\varepsilon_0/2$	1.39	3.45E-1	7.06E-3	6.67E-6	9.71E-10
$\varepsilon_0/2^2$	1.18	1.67E-1	1.71E-3	1.43E-6	1.10E-9
$\varepsilon_0/2^3$	1.13	1.46E-1	1.03E-3	6.77E-7	9.16E-10
$\varepsilon_0/2^4$	1.15	1.45E-1	8.52E-4	4.86E-7	1.33E-9

Temporal Errors of MTI-FP

$e_{h,\tau}(2.0)$	$\tau_0 = 0.1$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0 = 1$	**3.69E-2**	2.29E-3	1.43E-4	8.94E-6	5.59E-7	3.49E-8	2.21E-9
order	-	2.00	2.00	2.00	2.00	2.00	1.99
$\varepsilon_0/2$	5.98E-2	**3.77E-3**	2.36E-4	1.48E-5	9.23E-7	5.77E-8	3.60E-9
order	-	**1.99**	2.00	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	1.91E-1	1.48E-2	**9.39E-4**	5.87E-5	3.67E-6	2.30E-7	1.43E-8
order	-	1.85	**1.99**	2.00	2.00	2.00	2.00
$\varepsilon_0/2^3$	7.12E-2	4.90E-2	3.89E-3	**2.47E-4**	1.54E-5	9.64E-7	6.02E-8
order	-	0.27	1.83	**1.99**	2.00	2.00	2.00
$\varepsilon_0/2^4$	1.78E-2	1.80E-2	1.22E-2	9.79E-4	**6.21E-5**	3.89E-6	2.43E-7
order	-	-0.01	0.28	1.82	**1.99**	2.00	2.00
$\varepsilon_0/2^5$	*7.11E-3*	4.07E-3	4.53E-3	3.05E-3	2.45E-4	**1.55E-5**	9.69E-7
order	-	0.40	-0.08	0.29	1.82	**1.99**	2.00
$\varepsilon_0/2^6$	7.19E-3	5.10E-4	1.02E-3	1.13E-3	7.61E-4	6.10E-5	**3.87E-6**
order	-	1.91	-0.50	-0.08	0.29	1.82	**1.99**
$\varepsilon_0/2^7$	7.07E-3	*4.49E-4*	8.81E-5	2.54E-4	2.83E-4	1.90E-4	1.52E-5
order	-	*1.99*	1.17	-0.76	-0.08	0.29	1.82
$\varepsilon_0/2^9$	7.05E-3	4.22E-4	*2.60E-5*	7.22E-6	5.52E-6	1.63E-5	1.81E-5
order	-	2.03	*2.01*	0.92	0.19	-0.78	-0.08
$\varepsilon_0/2^{11}$	7.04E-3	4.23E-4	2.62E-5	*1.78E-6*	3.92E-7	1.08E-7	6.16E-7
order	-	2.03	2.01	*1.94*	1.09	0.93	-1.26
$\varepsilon_0/2^{13}$	7.04E-3	4.23E-4	2.62E-5	1.64E-6	*1.15E-7*	4.76E-8	5.55E-8
order	-	2.03	2.01	2.00	*1.92*	0.64	-0.11
$e^{\infty}_{h,\tau}(2.0)$	1.91E-1	4.90E-2	1.22E-2	3.05E-3	7.61E-4	1.90e-4	4.75e-5
order	-	0.98	1.00	1.00	1.00	1.00	1.00


ε = 1 / 4
ε = 1 / 8
ε = 1 / 16
real(φ1(t, 2))
t



$$\varepsilon = \begin{cases} 0.001 & 0 \le t \le 5 \\ 1 & t > 5 \end{cases} \qquad V = \begin{cases} \text{honeycomb} & 0 \le t \le 5 \\ 0 & t > 5 \end{cases} \qquad \tau = 0.01$$

Schrodinger dynamics (t<5) + relativistic QM (t>5): density fluctuate in the Zitterbewegung form

Extensions

- Nonlinear Dirac equation

$$i\partial_t\Phi=\left(-\frac{i}{\varepsilon}\sum_{j=1}^{d}\sigma_j\partial_j+\frac{1}{\varepsilon^2}\sigma_3\right)\Phi+\left(V(\vec{x})I_2-\sum_{j=1}^{d}A_j(\vec{x})\sigma_j\right)\Phi+[\lambda_1\Phi^*\sigma_3\Phi+\lambda_1|\Phi|^2I_2]\Phi,\quad \vec{x}\in\mathbb{R}^d$$

- Long-time dynamics of the Dirac equation with small electromagnetic potential

$$i\partial_t\Phi=\left(-i\sum_{j=1}^{d}\sigma_j\partial_j+\sigma_3\right)\Phi+\varepsilon\left(V(\vec{x})I_2-\sum_{j=1}^{d}A_j(\vec{x})\sigma_j\right)\Phi,\quad \vec{x}\in\mathbb{R}^d,\quad 0<t<\frac{T}{\varepsilon}$$

  - FDTD methods – non-uniform $\left\|\Phi(\bullet,t_n)-\Phi_{h,\tau}^n\right\|_{l^2}\le C\left[\frac{h^2}{\varepsilon}+\frac{\tau^2}{\varepsilon}\right],\quad 0\le n\le\frac{T_\varepsilon}{\tau}=\frac{T}{\varepsilon\tau}\Leftrightarrow n\tau=O(\varepsilon^{-1})\overset{0<\varepsilon\ll 1}{\gg}1$
  - 2nd order time-splitting method -- (improved) uniform error bounds

$$\left\|\Phi(\bullet,t_n)-\Phi_{h,\tau}^n\right\|_{L^2}\le(C_0+C_1t_n)\left[h^{m_0}+\tau^2\right],\quad \left\|\Phi(\bullet,t_n)-\Phi_{h,\tau}^n\right\|_{L^2}\le C\left[h^{m_0}+\varepsilon\tau^2\right],\quad 0\le n\le\frac{T_\varepsilon}{\tau}=\frac{T}{\varepsilon\tau}\Leftrightarrow n\tau=O(\varepsilon^{-1})\overset{0<\varepsilon\ll 1}{\gg}1$$

- Long-time dynamics of nonlinear Dirac equation with weak nonlinearity

$$i\partial_t\Phi=\left(-i\sum_{j=1}^{d}\sigma_j\partial_j+\sigma_3\right)\Phi+\varepsilon^2[\lambda_1\Phi^*\sigma_3\Phi+\lambda_1|\Phi|^2I_2]\Phi,\quad \vec{x}\in\mathbb{R}^d,0<t<\frac{T}{\varepsilon^2}$$

$$\left\|\Phi(\bullet,t_n)-\Phi_{h,\tau}^n\right\|_{L^2}\le C\left[h^{m_0}+\varepsilon^2\tau^2\right],\quad 0\le n\le\frac{T_\varepsilon}{\tau}=\frac{T}{\varepsilon^2\tau}\Leftrightarrow n\tau=O(\varepsilon^{-2})\overset{0<\varepsilon\ll 1}{\gg}1$$

W. Bao, Y. Cai, X. Jia and J. Yin, Error estimates of numerical methods for the nonlinear Dirac equation in the nonrelativistic limit regime, Sci. China Math., Vol. 59 (2016), pp. 1461-1494.

W. Bao, Y. Feng and J. Yin, Improved uniform error bounds on time splitting methods for the long-time dynamics of the Dirac equation with small potentials, in preparation.

Conclusion & future challenges

Conclusion

- For Dirac equation in nonrelativistic regime
  - FDTD methods -- (under-resolution) $O\left(h^2/\varepsilon+\tau^2/\varepsilon^6\right) \Rightarrow h=O(\sqrt{\varepsilon})\ \&\ \tau=O(\varepsilon^3)$
  - EWI-FP methods – (optimal-resolution) $O\left(h^m+\tau^2/\varepsilon^4\right) \Rightarrow h=O(1)\ \&\ \tau=O(\varepsilon^2)$
  - TSFP methods – (optimal-resolution & super-resolution no magnetic)

$$O\left(h^m+\tau^2/\varepsilon^4\right) \Rightarrow h=O(1)\ \&\ \tau=O(\varepsilon^2), \quad \text{when } \tau\le\varepsilon^2 \Rightarrow O\left(h^m+\tau^2/\varepsilon^2\right)$$

- A uniformly accurate (UA) method --- (super-resolution)

$$h^m+\max_{0<\varepsilon\le 1}\min\left\{\frac{\tau^2}{\varepsilon^2},\varepsilon^2\right\}=O\left(h^m+\tau\right) \Rightarrow h=O(1)\ \&\ \tau=O(1)$$

Future challenges

- For other parameter regimes
- For other coupled systems
- Emerging applications