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

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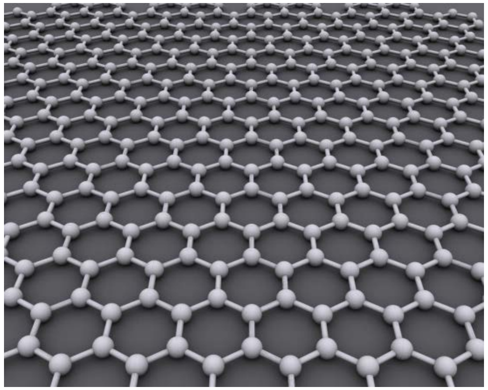

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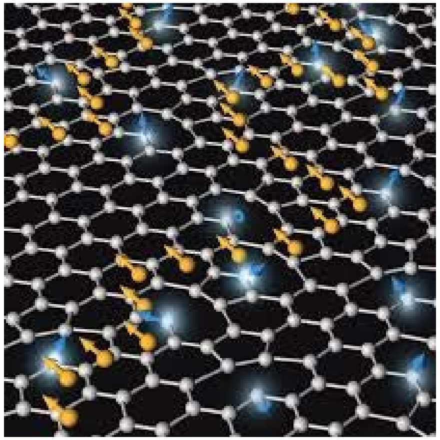
Outline

- 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 Dirac equation
- 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 $\gamma^0 = \beta, \quad \gamma^k = \gamma^0 \alpha_k, k = 1, 2, 3$
- 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 Relativistic

- Making the Schroedinger equation relativistic

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

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

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

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

$$\rho := \bar{\phi}\,\partial_t\phi - \phi\,\partial_t\bar{\phi}$$

$$J := \phi\nabla\bar{\phi} - \bar{\phi}\nabla\phi$$

$$\partial_t\rho + \nabla \bullet J = 0$$

Quantum Mechanics with Relativistic

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

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

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

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

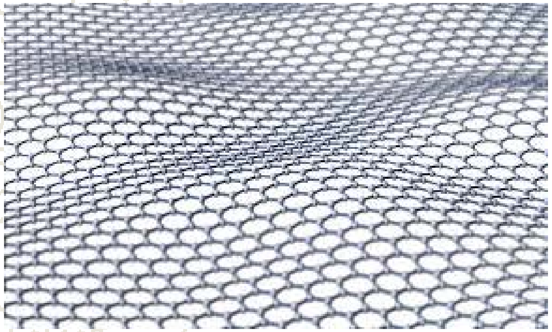
$$\Rightarrow A = i\beta\alpha_1, \quad B = i\beta\alpha_2, \quad C = i\beta\alpha_3, \quad D = \beta \Leftrightarrow \text{Clifford Algebra over 4d!!}$$

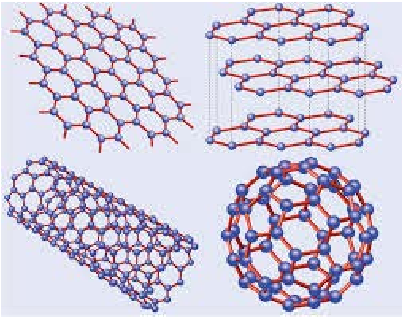
  - Dirac equation $\sqrt{\frac{E^2}{c^2} - \vec{p}^2} - mc = 0 \Rightarrow \left(A\partial_x + B\partial_y + C\partial_z + \frac{i}{c}D\partial_t - \frac{mc}{\hbar}\right)\psi = 0$

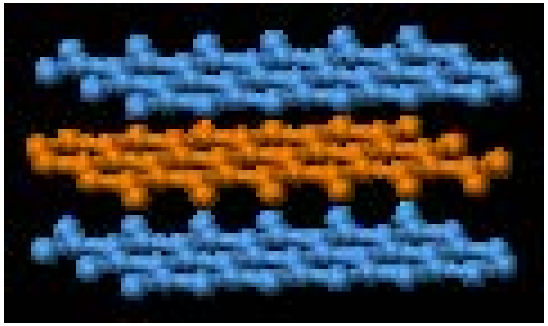
$$E = \sqrt{(\vec{p}c)^2 + (mc^2)^2} \overset{E\to i\hbar\partial_t;\ \vec{p}\to -i\hbar\nabla}{\Longrightarrow} i\hbar\partial_t\Psi = \left(-ic\hbar\sum_{j=1}^{3}\alpha_j\partial_j + mc^2\beta\right)\Psi$$

Typical Applications

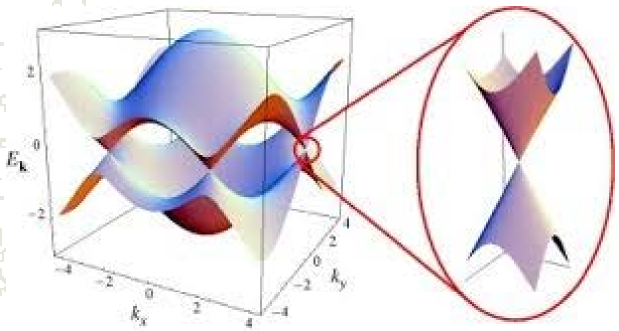
- Graphene/graphites and/or 2D materials – K. Novoselov, A. Geim, etc., Science, 2004; K. Novoselov, A. Geim , etc., Nature, 2005; K. Novoselov, …, A. Geim, Science, 2007; D.A. Abanin, etc., Science, 2011; A.H.C. Neto, etc., Rev. Mod. Phys., 2009, … (Nobel Prize in 2010!!!!)

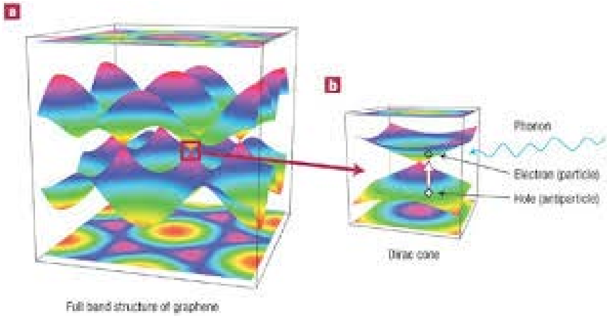






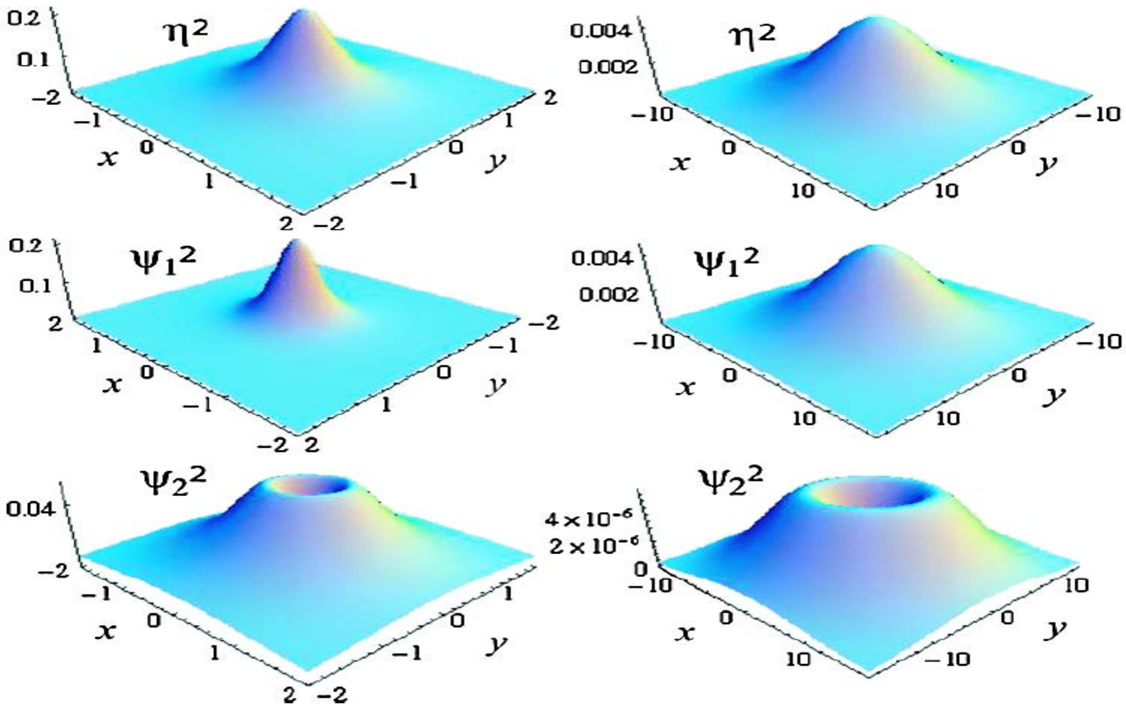
  - Same dispersion relation at Dirac cone





Typical Applications

- 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

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

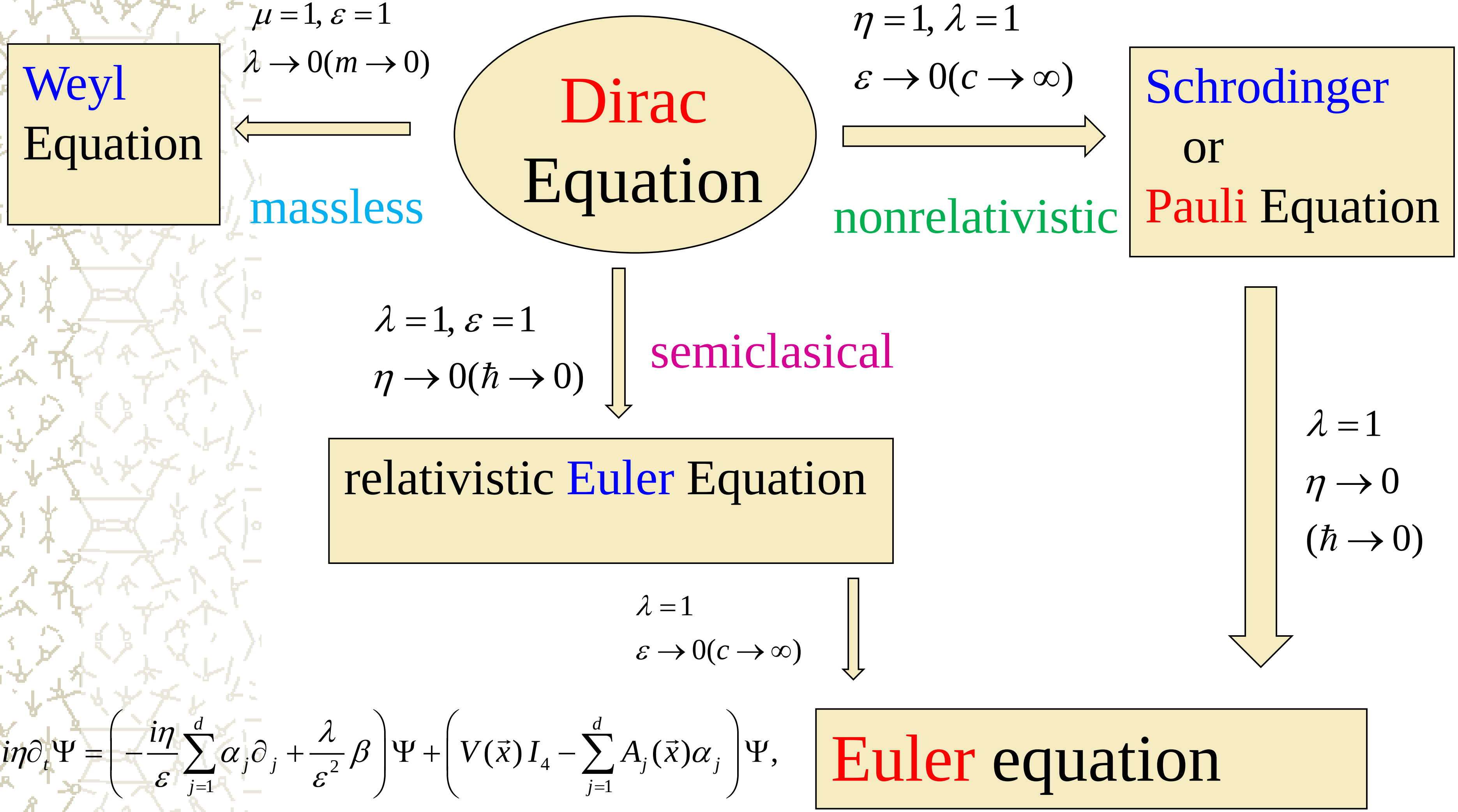
- Dimensionless Dirac equation in *d*-dimension (d=3,2,1)

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

$$0<\varepsilon := \frac{x_s}{t_s c} = \frac{v}{c} \le 1; \quad 0<\eta := \frac{\hbar\kappa_0 v}{e^2} \le 1; \quad 0<\lambda := \frac{m}{m_0} \le 1$$

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

Different limits of the Dirac 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

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

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

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

- Energy (or Hamiltonian) conservation

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

The Dirac equation

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

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

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

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

- 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

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

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

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

- Energy (or Hamiltonian) conservation

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

Two typical regimes & results

- Standard regime $v = O(c) \Leftrightarrow \varepsilon = 1$
  - 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 limit regime

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

Existing results in nonrelativistic limit regime

- 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; ……

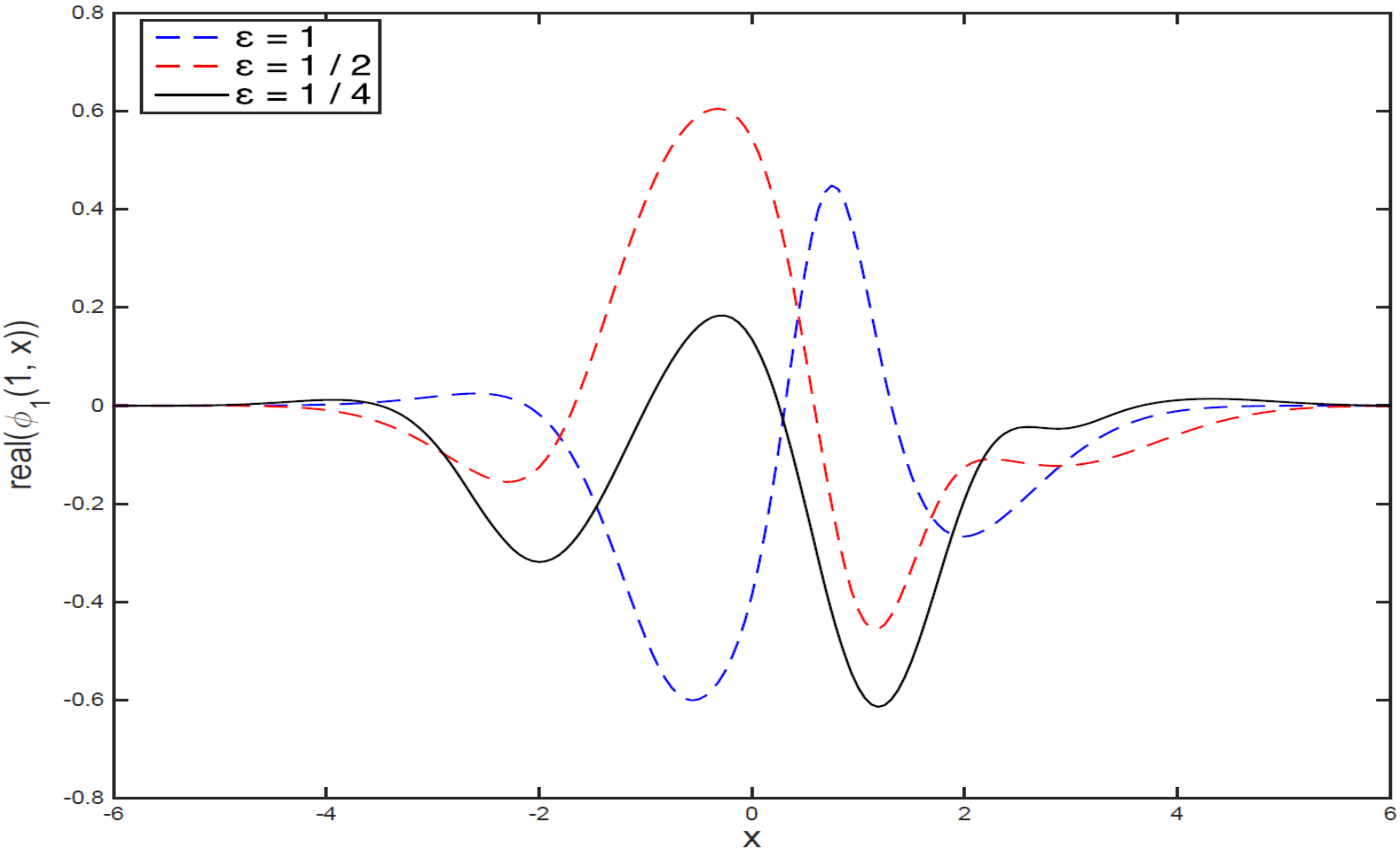
$$\Psi := \Psi^{\varepsilon} \quad (\text{or } \Phi := \Phi^{\varepsilon}) \to ??? \quad \text{when} \quad \varepsilon \to 0$$

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

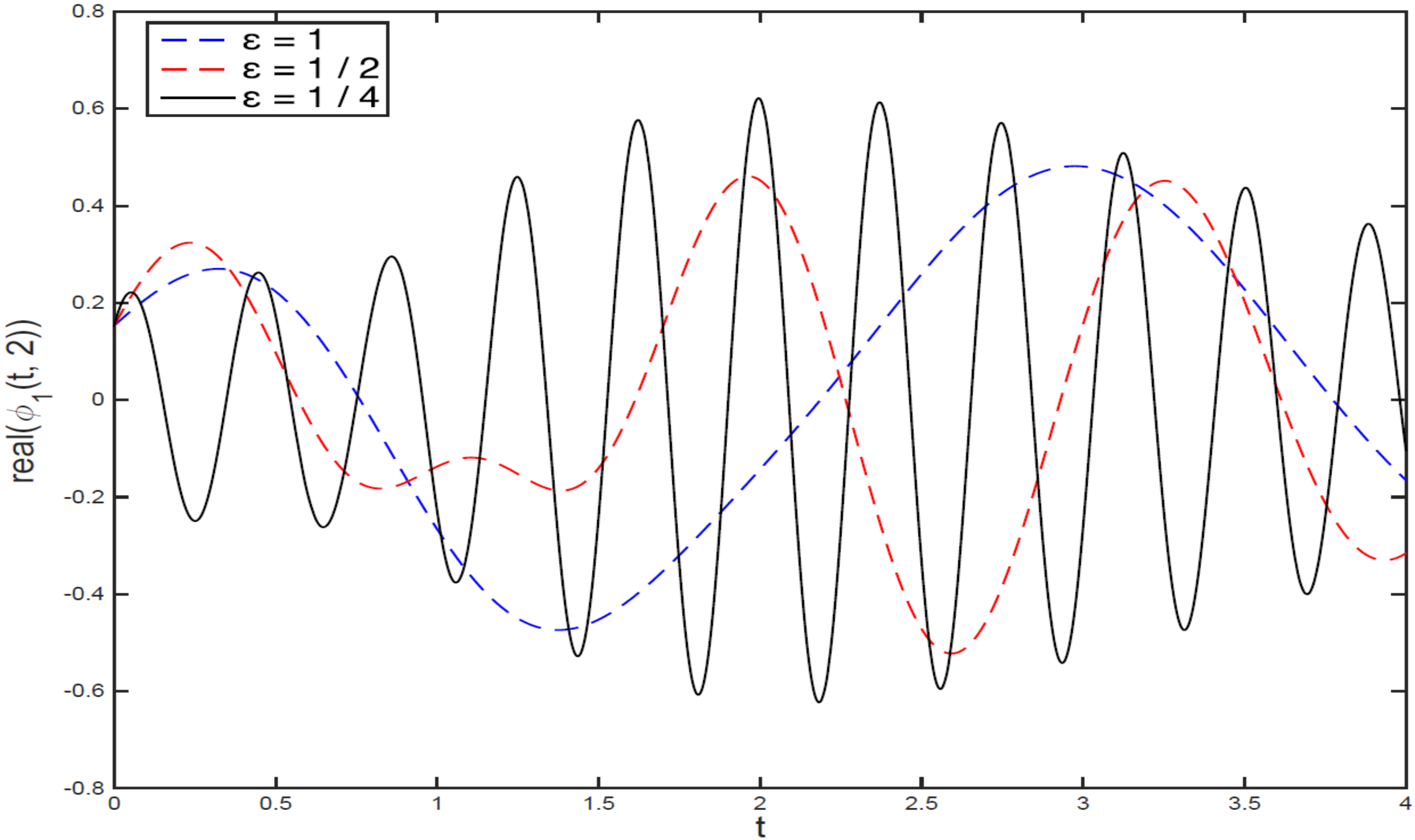
- Solution propagates waves with wavelength $O(\varepsilon^2)$ in time & $O(1)$ in space
  – Plane wave solutions $\Phi(t,\vec{x}) = \vec{B}\, e^{i(\vec{k}\cdot\vec{x}-\omega t)}$

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

Numerical results



Numerical results



Existing results in nonrelativistic limit regime

– 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

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

$$\Phi(a,t)=\Phi(b,t),\qquad \partial_x\Phi(a,t)=\partial_x\Phi(b,t),\qquad t\ge 0;$$

$$\Phi(x,0)=\Phi_0(x),\qquad x\in\bar{\Omega}=[a,b]$$

  - 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 limit 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 (Bao, Cai , Jia & Tang, JSC, 16')

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

  – Resolution ---- (under resolution)

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

Spatial Errors of CNFD

Spatial Errors	h_0=1/8	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^3$
$\varepsilon_0 = 1$	1.06E-1	2.65E-2	6.58E-3	1.64E-3	4.10E-4
order	–	2.00	2.01	2.00	2.00
$\varepsilon_0/2$	9.06E-2	2.26E-2	5.64E-3	1.41E-3	3.51E-4
order	–	2.00	2.00	2.00	2.00
$\varepsilon_0/2^2$	8.03E-2	2.02E-2	5.04E-3	1.25E-3	3.05E-4
order	–	1.99	2.00	2.01	2.02
$\varepsilon_0/2^3$	9.89E-2	2.47E-2	6.17E-3	1.54E-3	3.85E-4
order	–	2.00	2.00	2.00	2.00
$\varepsilon_0/2^4$	9.87E-2	2.48E-2	6.18E-3	1.54E-3	3.83E-4
order	–	1.99	2.00	2.00	2.01

Temporal Errors of CNFD

Temporal Errors	τ_0=0.1	$\tau_0/8$	$\tau_0/8^2$	$\tau_0/8^3$	$\tau_0/8^4$
$\varepsilon_0 = 1$	**5.48E-2**	8.56E-4	1.34E-5	2.09E-7	3.27E-9
order	–	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	3.90E-1	**6.63E-3**	1.77E-4	2.77E-6	4.32E-8
order	–	**1.96**	1.74	2.00	2.00
$\varepsilon_0/2^2$	1.79	2.27E-1	**3.55E-3**	1.56E-5	2.44E-7
order	–	0.99	**2.00**	2.61	2.00
$\varepsilon_0/2^3$	3.10	4.69E-1	2.06E-1	**3.22E-3**	5.03E-5
order	–	0.91	0.40	**2.00**	2.00
$\varepsilon_0/2^4$	2.34	1.83	8.05E-1	2.04E-1	**3.19E-3**
order	–	0.12	0.39	0.66	**2.00**

Spatial Errors of CNFD

ε	$\varepsilon_0 = 1$	$\varepsilon_0/2$	$\varepsilon_0/2^2$	$\varepsilon_0/2^3$	$\varepsilon_0/2^4$
$h_0 = 1/256$	1.61E-1	3.21E-1	6.35E-1	1.21	2.07
$h_0/2$	4.03E-2	8.05E-2	1.59E-1	3.07E-1	5.43E-1
$h_0/2^2$	1.01E-2	2.01E-2	3.99E-2	7.69E-2	1.36E-1
$h_0/2^3$	2.52E-3	5.03E-3	9.97E-3	1.92E-2	3.41E-2
$h_0/2^4$	6.30E-4	1.26E-3	2.47E-3	4.95E-3	8.64E-3

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

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

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

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

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

Symmetric Exponential wave integrator (sEWI)

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

- Take $s = \pm\tau$ and approximate the integral

$$\begin{aligned}\widehat{(\Phi_M)}_l(t_{n+1}) =& \widehat{(\Phi_M)}_l(t_{n-1}) - 2i\sin(\tau\Gamma_l/\varepsilon^2)\widehat{(\Phi_M)}_l(t_n)\\ & - i\int_0^\tau \cos\left(\frac{(w-\tau)\delta_l}{\varepsilon^2}\right)\left(\widehat{F}_l^n(w)+\widehat{F}_l^n(-w)\right)dw\\ & + \int_0^\tau \sin\left(\frac{(w-\tau)\Gamma_l}{\varepsilon^2}\right)\left(\widehat{F}_l^n(w)-\widehat{F}_l^n(-w)\right)dw,\end{aligned}$$

- sEWI-FP method

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

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

Error estimates for EWI-FP method

- Theorem Under some stability conditions, we have error estimates for EWI-FP and sEWI-FP as (Bao, Cai, Jia & Tang, JSC,16')

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

  – Resolution --- (optimal resolution)

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

Spatial Errors of EWI-FP

Spatial Errors	$h_0=2$	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0 = 1$	8.79E-1	3.07E-1	3.73E-2	4.35E-5	4.12E-10
$\varepsilon_0/2$	7.68E-1	1.89E-1	4.36E-3	3.83E-6	4.17E-10
$\varepsilon_0/2^2$	6.35E-1	1.23E-1	1.28E-3	8.18E-7	3.98E-10
$\varepsilon_0/2^3$	6.39E-1	1.17E-1	8.12E-4	3.62E-7	3.87E-10
$\varepsilon_0/2^4$	6.28E-1	1.18E-1	7.36E-4	2.82E-7	6.18E-9

Temporal Errors of EWI-FP

Temporal Errors	τ_0=0.1	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$
$\varepsilon_0 = 1$	$\underline{1.40E-1}$	8.51E-3	5.33E-4	3.34E-5	2.09E-6
order	–	2.02	2.00	2.00	2.00
$\varepsilon_0/2$	4.11E-1	$\underline{2.37E-2}$	1.49E-3	9.29E-5	5.81E-6
order	–	2.06	2.00	2.00	2.00
$\varepsilon_0/2^2$	6.03	1.88E-1	$\underline{1.18E-2}$	7.38E-4	4.62E-5
order	–	2.50	2.00	2.00	2.00
$\varepsilon_0/2^3$	2.21	3.98	1.60E-1	$\underline{1.01E-2}$	6.31E-4
order	–	-0.42	2.32	2.00	2.00
$\varepsilon_0/2^4$	2.16	2.09	3.58	1.53E-1	$\underline{9.69E-3}$
order	–	0.02	-0.39	2.27	1.99

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)

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

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 $\tau = 2\pi\varepsilon^2 / N$ (Bao, Cai, Jia&Yin, SCM, 16')

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

  – P. Chartier,F. Mehats,M. Thalhammer &Y. Zhang, superconvergnnce for TSSP for NLSE, 14'

Comparison

$\tau = O(\varepsilon^3)$ $\tau = O(h)$	$\varepsilon_0 = 0.4$ $h_0 = 1/8$ $\tau_0 = 0.04$	$\varepsilon_0/2$ $h_0/8$ $\tau_0/8$	$\varepsilon_0/2^2$ $h_0/8^2$ $\tau_0/8^2$	$\varepsilon_0/2^3$ $h_0/8^3$ $\tau_0/8^3$
LFFD	3.57E-1	2.47E-1	2.44E-1	2.30E-1
SIFD1	2.43E-1	2.30E-1	2.35E-1	2.38E-1
$\tau = O(\varepsilon^3)$	$\varepsilon_0 = 0.4$ $\tau_0 = 0.04$	$\varepsilon_0/2$ $\tau_0/8$	$\varepsilon_0/2^2$ $\tau_0/8^2$	$\varepsilon_0/2^3$ $\tau_0/8^3$
SIFD2	6.88E-1	5.54E-1	4.96E-1	4.91E-1
CNFD	1.82E-1	1.32E-1	1.25E-1	1.23E-1
$\tau = O(\varepsilon^2)$	$\varepsilon_0 = 0.4$ $\tau_0 = 0.04$	$\varepsilon_0/2$ $\tau_0/4$	$\varepsilon_0/2^2$ $\tau_0/4^2$	$\varepsilon_0/2^3$ $\tau_0/4^3$
EWI-FP	1.05E-1	6.79E-2	6.17E-2	6.00E-2
TSFP	1.62E-2	4.09E-3	1.04E-3	2.59E-5

Comparison

Method	LFFD	SIFD1	SIFD2	CNFD	EWI-FP	TSFP
Time symmetric	Yes	Yes	Yes	Yes	No	Yes
Mass conservation	No	No	No	Yes	No	Yes
Energy conservation	No	No	No	Yes	No	No
Dispersion Relation	No	No	No	No	No	Yes
Unconditionally stable	No	No	No	Yes	No	Yes
Explicit scheme	Yes	No	No	No	Yes	Yes
Temporal accuracy	2nd	2nd	2nd	2nd	2nd	2nd
Spatial accuracy	2nd	2nd	2nd	2nd	Spectral	Spectral
Memory cost	$O(M)$	$O(M)$	$O(M)$	$O(M)$	$O(M)$	$O(M)$
Computational cost	$O(M)$	$O(M)$	$O(M\ln M)$	$\gg O(M)$	$O(M\ln M)$	$O(M\ln M)$
Resolution when $0<\varepsilon\ll 1$	$h=O(\sqrt{\varepsilon})$ $\tau=O(\varepsilon^3)$	$h=O(\sqrt{\varepsilon})$ $\tau=O(\varepsilon^3)$	$h=O(\sqrt{\varepsilon})$ $\tau=O(\varepsilon^3)$	$h=O(\sqrt{\varepsilon})$ $\tau=O(\varepsilon^3)$	$h=O(1)$ $\tau=O(\varepsilon^2)$	$h=O(1)$ $\tau=O(\varepsilon^2)$

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

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

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

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

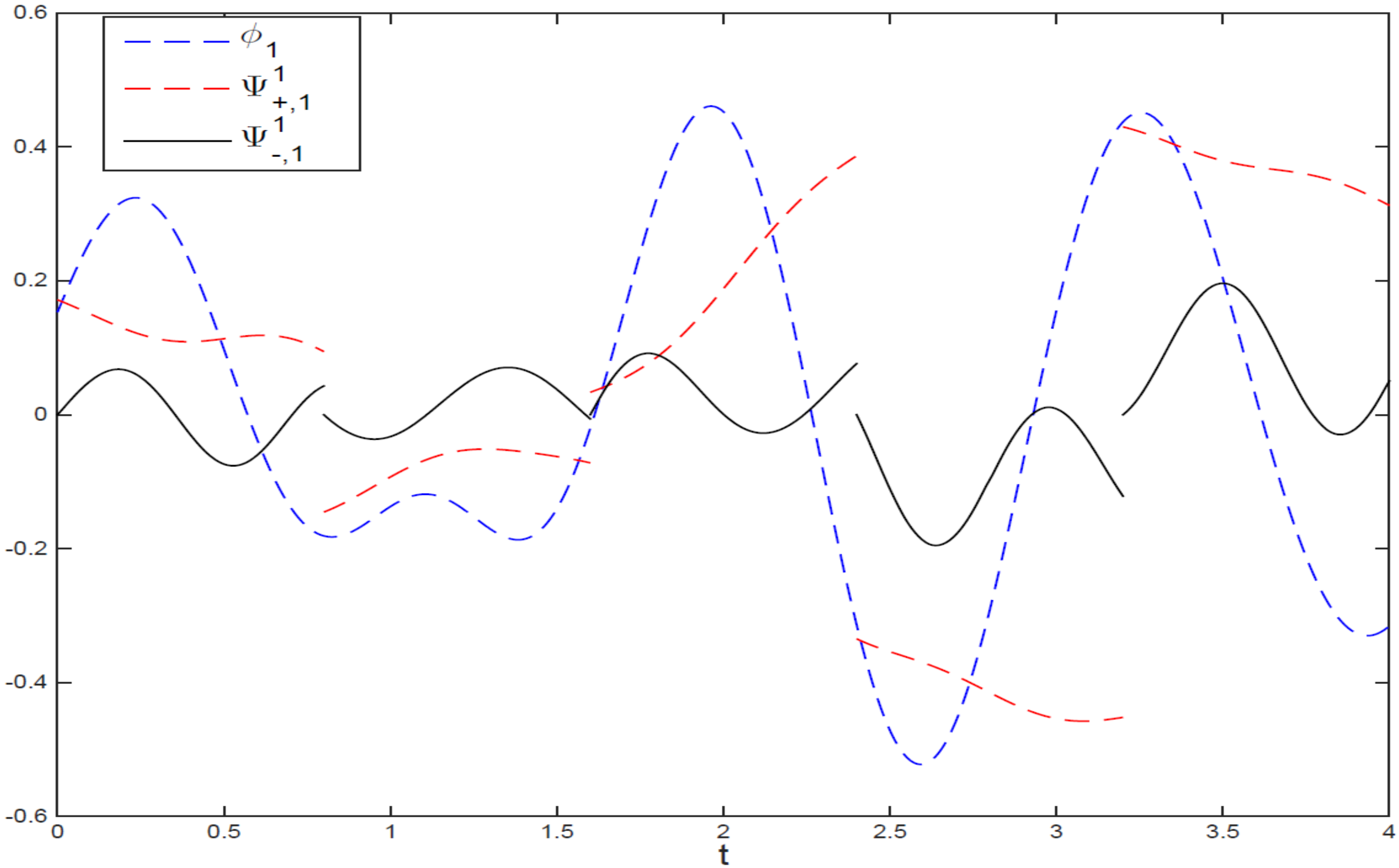
- Solve the two sub-problems via EW-FP

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

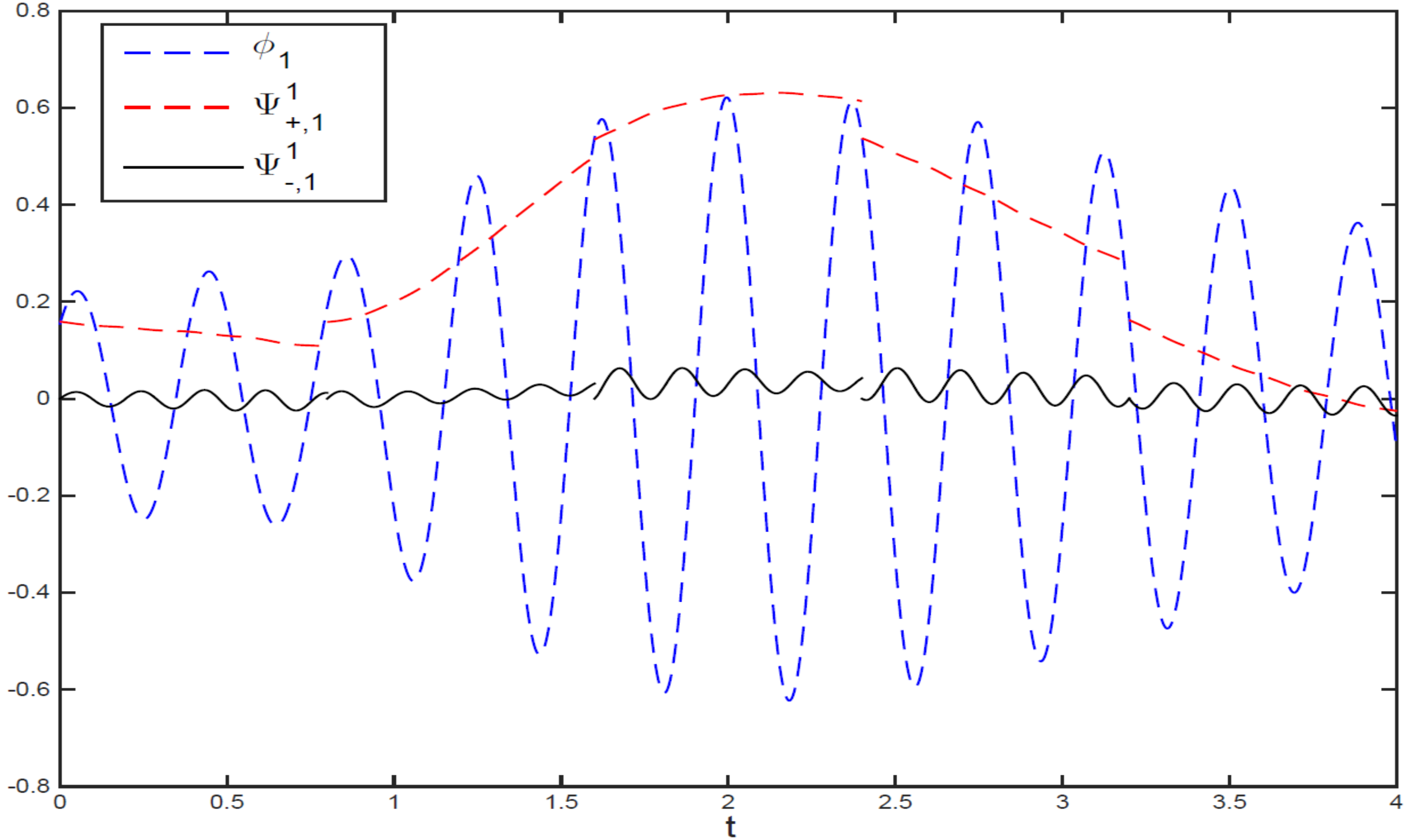
- Reconstruct the solution at $t = t_{n+1}$

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

Multiscale Decomposition $\varepsilon = 0.5$



Multiscale Decomposition $\varepsilon = 0.25$



Error estimates for MTI-FP method

- Theorem Under proper assumptions on the solution, we have error estimates for the MTI-FP method (Bao, Cai, Jia & Tang, SINUM 15')

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

  – Which yields a uniform error bound

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

  – Resolution ---- (super resolution)

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

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

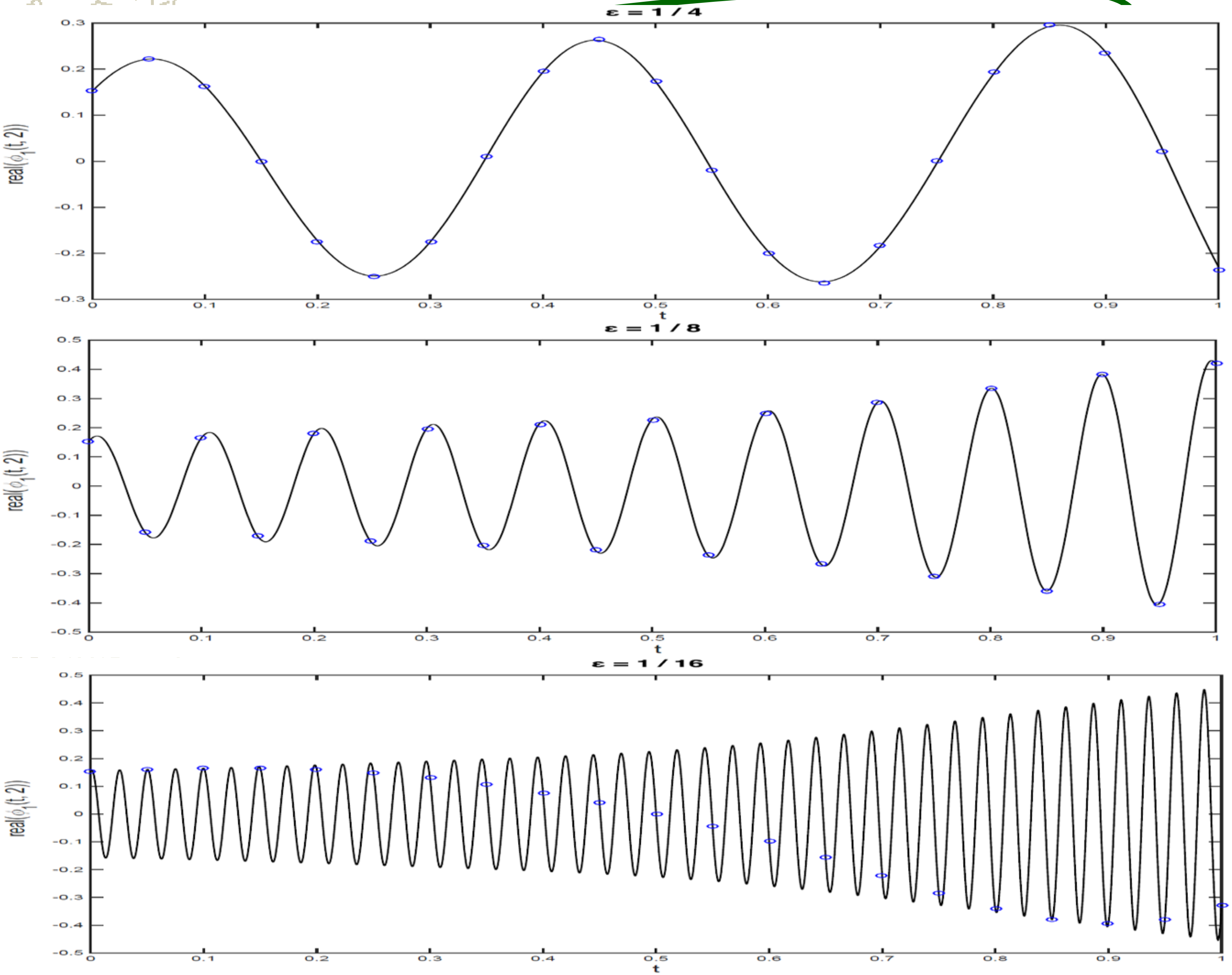
$$\left\|\Phi(t_n,.)-\Phi_I^n(\bullet)\right\|_{L^2} \le h^{m_0}+\tau^2+\min\left\{\varepsilon^2,\frac{\tau^2}{\varepsilon^2}\right\} \le h^{m_0}+\tau, \quad 0<\varepsilon\le 1$$

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

The nonlinear Dirac equation (NLDE)

$$0 < \varepsilon := v / c \le 1$$

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

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

  - Initial data $\Psi(0,\vec{x}) = \Psi_0(\vec{x}), \quad \vec{x} \in \mathbb{R}^d$
  - Dispersive PDEs & time symmetric
  - Soliton solution in 1D when $\varepsilon = 1$
  - Mass & energy conservation

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

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

The nonlinear Dirac equation

$$\Phi = (\phi_1, \phi_2)^T \quad \text{with} \quad \Phi=(\psi_1,\psi_4)^T \quad \text{or} \quad (\psi_2,\psi_3)^T$$

- In 2D/1D (d=2,1):

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

  - Initial data $\quad \Phi(0,\vec{x}) = \Phi_0(\vec{x}), \quad \vec{x} \in \mathbb{R}^d$
  - Dispersive PDEs & time symmetric
  - Soliton solution in 1D when $\varepsilon = 1$
  - Mass & energy conservation

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

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

Extension to nonlinear Dirac equation

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sigma_1\partial_x + \frac{1}{\varepsilon^2}\sigma_3\right)\Phi + \left(V(t,x)I_2 - A_1(t,x)\sigma_1\right)\Phi + \delta\left(\Phi^*\sigma_3\Phi\right)\sigma_3\Phi$$

- FDTD methods
  - LFFD

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

  - SIFD1

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

  - SIFD2

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

  - CNFD ---- mass & energy conservation!!

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

Error estimates of FDTD for NLDE

- Thm. Under some stability conditions and $\tau \le C\varepsilon^3 h^{1/4}$ & $h \le C\varepsilon^{2/3}$ we have error estimates for LFFD, SIFD1, SIFD2 & CNFD as (Bao, Cai, Jia & Yin, SCM,16')

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

– Resolution

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

Extension to nonlinear Dirac equation

$$i\partial_t \Phi = \left(-\frac{i}{\varepsilon}\sigma_1 \partial_x + \frac{1}{\varepsilon^2}\sigma_3 \right)\Phi + \left(V(t,x) I_2 - A_1(t,x)\sigma_1 \right)\Phi + \delta\left(\Phi^* \sigma_3 \Phi \right)\sigma_3 \Phi$$

- EWI-FP method
- TSFP method

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

  - Step 1
  - Step 2

$$i\partial_t \Phi(t,\vec{x}) = \left(V(\vec{x}) I_2 - \sum_{j=1}^{d} A_j(\vec{x})\sigma_j \right)\Phi(t,\vec{x}) + \delta\left(\Phi^* \sigma_3 \Phi \right)(t,\vec{x})\sigma_3 \Phi(t,\vec{x})$$

$$\Rightarrow \left(\Phi^* \sigma_3 \Phi \right)(t,\vec{x}) = \left(\Phi^* \sigma_3 \Phi \right)(t_n,\vec{x}), \quad t \ge t_n$$

$$i\partial_t \Phi(t,\vec{x}) = \left(V(\vec{x}) I_2 - \sum_{j=1}^{d} A_j(\vec{x})\sigma_j \right)\Phi(t,\vec{x}) + \delta\left(\Phi^* \sigma_3 \Phi \right)(t_n,\vec{x})\sigma_3 \Phi(t,\vec{x})$$

  - Time symmetric, dispersive relation, mass conservation!

Error estimates of EWI-FP for NLDE

- Theorem Under some stability conditions and $\tau \le C\varepsilon^2 h^{1/4}$, we have error estimates for EWI-FP as (Bao, Cai, Jia & Yin, SCM, 16')

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

  – Resolution

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

Error estimates of TSFP for NLDE

- Thm. Under some stability conditions and $\tau \le C\varepsilon^2$, we have error estimates for TSFP as (Bao, Cai, Jia & Yin, SCM, 16')

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

  – Resolution

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

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

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

Spatial Errors of TSFP for NLDE

$e_{h,\tau_e}(t=2)$	h_0=2	$h_0/2$	$h_0/2^2$	$h_0/2^3$	$h_0/2^4$
$\varepsilon_0 = 1$	1.68	4.92E-1	4.78E-2	1.40E-4	2.15E-9
$\varepsilon_0/2$	1.48	3.75E-1	1.57E-2	4.24E-5	6.60E-10
$\varepsilon_0/2^2$	1.21	2.90E-1	4.66E-3	4.91E-6	6.45E-10
$\varepsilon_0/2^3$	1.37	2.68E-1	2.40E-3	6.00E-7	6.34E-10
$\varepsilon_0/2^4$	1.41	2.75E-1	1.84E-3	3.06E-7	6.13E-10
$\varepsilon_0/2^5$	1.45	2.76E-1	1.74E-3	2.37E-7	5.98E-10

Temporal Errors of TSFP for NLDE

$e_{h_\varepsilon,\tau}(t=2)$	τ_0=0.4	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$
$\varepsilon_0=1$	1.60E-1	9.56E-3	5.95E-4	3.72E-5	2.32E-6	1.46E-7
order	-	2.03	2.00	2.00	2.00	2.00
$\varepsilon_0/2$	8.94E-1	3.91E-2	2.40E-3	1.50E-4	9.36E-6	5.87E-7
order	-	2.26	2.01	2.00	2.00	2.00
$\varepsilon_0/2^2$	2.60	2.18E-1	1.06E-2	6.56E-4	4.09E-5	2.56E-6
order	-	1.79	2.18	2.01	2.00	2.00
$\varepsilon_0/2^3$	2.28	2.33	4.84E-2	2.58E-3	1.60E-4	9.98E-6
order	-	-0.02	2.79	2.11	2.01	2.00
$\varepsilon_0/2^4$	1.46	1.28	1.30	1.15E-2	6.19E-4	3.84E-5
order	-	0.10	-0.01	3.41	2.11	2.01
$\varepsilon_0/2^5$	1.53	3.27E-1	4.06E-1	4.13E-1	2.83E-3	1.53E-4
order	-	1.11	-0.16	-0.01	3.59	2.10

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

TSFP for Dirac without magnetic potential

Temporal Errors	$\tau_0 = 0.4$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$	$\tau_0/4^6$
$\varepsilon_0 = 1$	1.20E-2	7.34E-4	4.58E-5	2.86E-6	1.79E-7	1.15E-8	**6.94E-10**
order	-	2.01	2.00	2.00	2.00	1.98	2.02
$\varepsilon_0/2$	3.48E-2	1.42E-3	8.78E-5	5.49E-6	3.43E-7	2.17E-8	**1.33E-9**
order	-	2.31	2.01	2.00	2.00	1.99	2.01
$\varepsilon_0/2^2$	7.98E-2	4.09E-3	2.06E-4	1.27E-5	7.96E-7	5.00E-8	**3.09E-9**
order	-	2.14	2.16	2.01	2.00	2.00	2.01
$\varepsilon_0/2^3$	2.18E-2	1.15E-2	3.86E-4	1.97E-5	1.22E-6	7.65E-8	4.73E-9
order	-	0.46	2.45	2.15	2.01	2.00	2.01
$\varepsilon_0/2^4$	2.30E-2	2.42E-3	2.40E-3	5.70E-5	2.93E-6	1.81E-7	**1.16E-8**
order	-	1.62	0.01	2.70	2.14	2.01	1.99
$\varepsilon_0/2^5$	2.07E-2	1.03E-3	3.07E-4	3.21E-4	6.69E-6	3.44E-7	**2.15E-8**
order	-	2.16	0.88	-0.03	2.79	2.14	2.00
$\varepsilon_0/2^6$	2.06E-2	9.66E-4	6.36E-5	3.63E-5	3.87E-5	7.70E-7	**4.00E-8**
order	-	2.21	1.96	0.40	-0.05	2.83	2.13
$\varepsilon_0/2^8$	2.06E-2	1.00E-3	5.93E-5	4.26E-6	4.53E-7	6.08E-7	6.54E-7
order	-	2.18	2.04	1.90	1.62	-0.21	-0.05
$\varepsilon_0/2^{10}$	2.06E-2	9.57E-4	5.97E-5	7.18E-6	2.32E-7	4.00E-8	7.97E-9
order	-	2.21	2.00	1.53	2.47	1.27	1.16
$\varepsilon_0/2^{12}$	2.06E-2	9.56E-4	5.94E-5	3.75E-6	2.42E-7	8.81E-8	4.40E-9
order	-	2.21	2.00	1.99	1.98	0.73	2.16
max	7.98E-2	1.15E-2	2.40E-3	3.21E-4	3.87E-5	5.83E-6	6.54E-7
order	-	1.40	1.13	1.45	1.53	1.37	1.58

$$\left\|\Phi(t_n,\bullet)-I_M(\Phi^n)\right\|_{L^2} \le h^{m_0}+\frac{\tau^2}{\varepsilon}; \quad \left\|\Phi(t_n,\bullet)-I_M(\Phi^n)\right\|_{L^2} \le h^{m_0}+\tau^2+\varepsilon^2 \Rightarrow \text{uniform accurate}$$

TSFP for NLDE without magnetic potential

Temporal Errors	$\tau_0=0.4$	$\tau_0/4$	$\tau_0/4^2$	$\tau_0/4^3$	$\tau_0/4^4$	$\tau_0/4^5$	$\tau_0/4^6$
$\varepsilon_0=1$	1.00E-1	2.06E-3	1.25E-4	7.78E-6	4.86E-7	3.04E-8	**1.93E-9**
order	-	2.80	2.02	2.00	2.00	2.00	1.99
$\varepsilon_0/2$	1.30E-1	4.25E-3	2.19E-4	1.36E-5	8.49E-7	5.31E-8	**3.36E-9**
order	-	2.47	2.14	2.01	2.00	2.00	1.99
$\varepsilon_0/2^2$	1.21E-1	3.10E-2	4.47E-4	2.65E-5	1.65E-6	1.03E-7	**6.47E-9**
order	-	0.98	3.06	2.04	2.00	2.00	2.00
$\varepsilon_0/2^3$	1.43E-1	2.28E-2	1.63E-3	5.32E-5	3.23E-6	2.02E-7	**1.26E-8**
order	-	1.32	1.90	2.47	2.02	2.00	2.00
$\varepsilon_0/2^4$	1.49E-1	1.08E-2	6.13E-3	2.15E-4	6.42E-6	3.93E-7	**2.45E-8**
order	-	1.89	0.41	2.42	2.53	2.02	2.00
$\varepsilon_0/2^5$	1.53E-1	1.19E-2	1.14E-3	1.07E-3	2.25E-5	7.87E-7	**4.83E-8**
order	-	1.84	1.69	0.05	2.78	2.42	2.01
$\varepsilon_0/2^6$	1.58E-1	8.34E-3	5.64E-4	1.73E-4	1.66E-4	2.28E-6	**9.75E-8**
order	-	2.12	1.94	0.85	0.03	3.09	2.27
$\varepsilon_0/2^8$	1.57E-1	7.77E-3	2.82E-4	2.68E-5	5.89E-6	3.06E-6	2.96E-6
order	-	2.17	2.39	1.70	1.09	0.47	0.02
$\varepsilon_0/2^{10}$	1.58E-1	7.89E-3	2.48E-4	2.30E-5	1.81E-6	3.78E-7	9.13E-8
order	-	2.16	2.49	1.72	1.83	1.13	1.02
$\varepsilon_0/2^{12}$	1.58E-1	7.87E-3	2.56E-4	1.58E-5	1.01E-6	3.67E-7	2.44E-8
order	-	2.16	2.47	2.01	1.99	0.73	1.96
max	1.58E-1	3.10E-2	6.13E-3	1.07E-3	1.66E-4	2.29E-5	2.96E-6
order	-	1.17	1.17	1.26	1.34	1.43	1.48

$\left\|\Phi(t_n,\bullet)-I_M(\Phi^n)\right\|_{L^2} \le h^{m_0}+\frac{\tau^2}{\varepsilon}$; $\left\|\Phi(t_n,\bullet)-I_M(\Phi^n)\right\|_{L^2} \le h^{m_0}+\tau^2+\varepsilon^2 \Rightarrow$ uniform accurate

Conclusion & future challenges

- Conclusion
  - For Dirac equation in nonrelativistic limit regime
    - FDTD methods: $O\left(h^2/\varepsilon + \tau^2/\varepsilon^6\right) \quad \Rightarrow \quad h = O(\sqrt{\varepsilon})\ \&\ \tau = O(\varepsilon^3)$
    - An EWI-FP method: $O\left(h^m + \tau^2/\varepsilon^4\right) \quad \Rightarrow \quad h = O(1)\ \&\ \tau = O(\varepsilon^2)$
    - A TSFP method : $\tau \le \varepsilon^2 \Rightarrow O\left(h^m + \tau^2/\varepsilon^2\right) \Rightarrow h = O(1)\ \&\ \tau = O(\varepsilon^2)$
  - A uniformly accurate (UA) method
- Future challenges $h^m + \max_{0<\varepsilon\le 1} \min\left\{\frac{\tau^2}{\varepsilon^2}, \varepsilon^2\right\} = O\left(h^m + \tau\right) \quad \Rightarrow \quad h = O(1)\ \&\ \tau = O(1)$
  - Extension of the UA method to nonlinear Dirac equation (Y. Cai & Y.Wang, 17')
  - For coupled systems – Klein-Gordon-Dirac, Maxwell-Dirac, …
  - For other parameter limit regimes