Multiscale Methods & Analysis for Nonlinear Klein-Gordon Equation in Nonrelativistic Limit Regime

Weizhu Bao

Department of Mathematics

National University of Singapore

Email: matbaowz@nus.edu.sg

URL: http://www.math.nus.edu.sg/~bao

&

Beijing Computational Science Research Center (CSRC)

URL: http://www.csrc.ac.cn

Collaborators: Yongyong Cai (postdoc, Purdue), Xuanchun Dong, Xiaofei Zhao (postdoc, Rennes)

Outline

- Nonlinear Klein-Gordon (KG) equation
- Numerical methods and error estimates
  - Finite difference time domain (FDTD) methods
  - Exponential wave integrator (EWI) spectral method
- Nonlinear Schrodinger (NLS) equation with wave operator
  - FDTD methods and uniform error estimates
  - EWI spectral method and uniform & optimal error estimate
- A multiscale method for nonlinear KG equation
- Conclusion & future challenges

Motivation

- The nonlinear Klein-Gordon (KG) equation

$$\varepsilon^2\partial_{tt}u(\vec{x},t)-\Delta u+\frac{1}{\varepsilon^2}u+f(u)=0 \qquad \vec{x}\in\mathbb{R}^d, \quad t>0$$

  - With initial conditions

$$u(\vec{x},0)=\phi(\vec{x}), \quad \partial_t u(\vec{x},0)=\frac{1}{\varepsilon^2}\gamma(\vec{x}), \quad \vec{x}\in\mathbb{R}^d$$

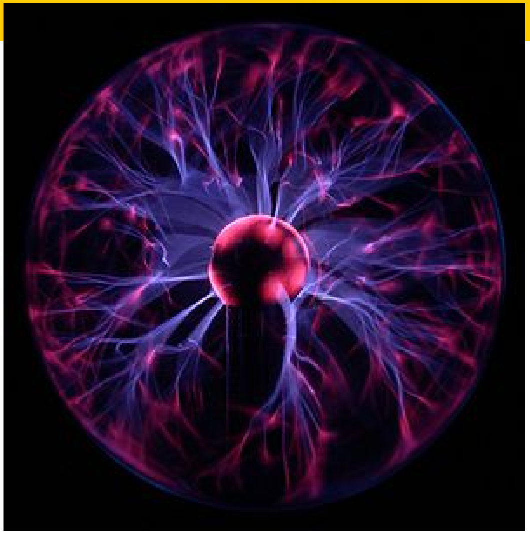
  - $u=u(\vec{x},t)$ real (complex)-valued field (order parameter)
  - $0<\varepsilon\le 1$ dimensionless parameter, e.g. $\sim 1/c$
  - $f(u)$ real-valued function (or $f(u)=g(|u|^2)u$ if u is complex)
  - $\phi\,\&\,\gamma$ given dimensionless real (or complex) functions

The (linear) Klein-Gordon (KG) equation

$$\frac{\hbar^2}{mc^2}\partial_{tt}u - \frac{\hbar^2}{m}\Delta u + mc^2 u = 0$$

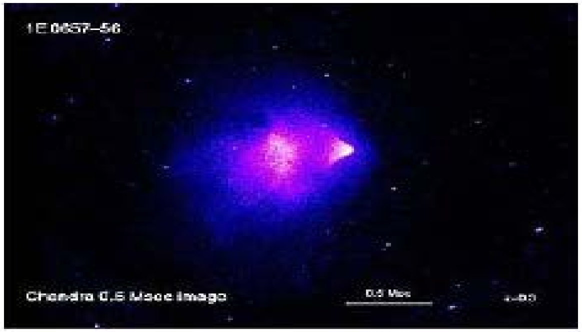
- Proposed in 1927 by physicists Oskar Klein & Walter Gordon
  - To describe relativistic electrons (correct for spinless pion)
  - It is a relativistic version of the Schrodinger equation which suffers from not being relativistically covariant or not take into account Einstein's special relativity
  - An equation of motion of a quantum scalar field for spinless particles
  - With appropriate interpretation, it does describe the quantum amplitude for finding a point particle in various places, but particle propagates both forwards and backwards in time!!

The (nonlinear) Klein-Gordon (KG) equation

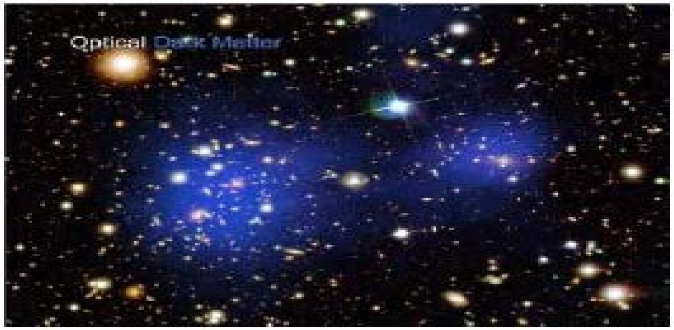


Plasma lamp

- Applications in other areas
  - Plasma, e.g. interaction between langmuir & ion sound waves (Klein-Gordon-Zakharv)
    - P.M. Bellan, Fundamental of Plasma Physics, 2006
    - R. O. Dendy, Plasma Dynamics, 1990
  - Universe & Cosmology, e.g. dark matter or black-hole evaporation (Huang, 10')



Overall view



Dark matter

Properties of KG equation

- Time symmetric, i.e. unchanged if $t \to -t$
- Hamiltonian (or energy) conservation

$$F(u) = 2\int_0^u f(s)\,ds$$

$$E(t) = \int_{\mathbb{R}^d} \left[\varepsilon^2 |\partial_t u|^2 + |\nabla u|^2 + \frac{1}{\varepsilon^2}|u|^2 + F(u) \right] d\vec{x}$$

$$\equiv \int_{\mathbb{R}^d} \left[\frac{1}{\varepsilon^2}|\gamma|^2 + |\nabla \phi|^2 + \frac{1}{\varepsilon^2}|\phi|^2 + F(\phi) \right] d\vec{x} := E(0), \quad t \ge 0$$

- Two different regimes
  - O(1)-wave regime, e.g. $\varepsilon = 1$
  - Nonrelativistic limit regime, $0 < \varepsilon \ll 1$

Existing results in O(1)-wave regime

- Analytical results for Cauchy problem: Browder, 62'; Segal, 63'; Strauss, 68'; Morawetz & Strauss, 72'; Glassey, 73' &82'; Ablowitz, Kruskal & Ladik, 79'; Shatah, 85'; Ginibre & Velo, 85'&89'; Klainerman & Machedon, 93'; Adomian, 96'; Nakmura & Ozawa, 01'; Tao, 01'; Ibrahim, Majdoub & Masmoudi, 06'; ……
  - Existence, uniqueness & regularity for defocusing case $F(u) \geq 0$
  - Finite time blow-up for focusing case $F(u) \leq 0$
- Numerical methods
  - Finite difference time domain (FDTD) methods: Strauss & Vazquez, 78'; Jimenez & Vazquez, 90'; Tourigny, 90'; Li & Vu-Quoc, 95'; Duncan, 97'; Cohen, Hairer & Lubich, 08';……
    - Conservative vs non-conservative
    - Implicit vs explicit
  - Spectral methods: Cao& Guo, 93'; ……..

Existing results in nonrelativistic limit regime

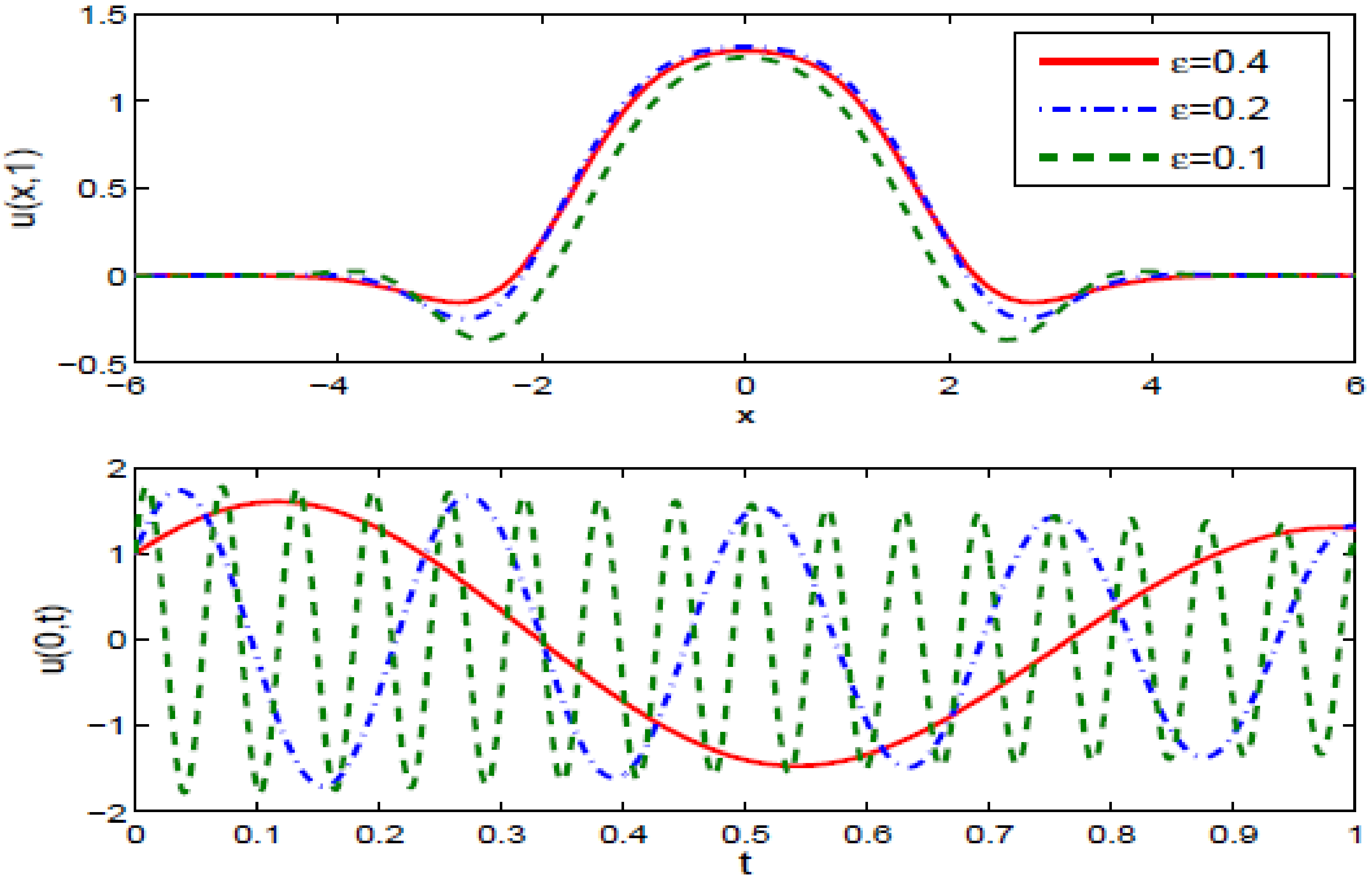
- Nonrelativistic limits: Tsutsumi, 84'; Najman, 89' & 90'; Machiara, 01'; Masmoudi, Nakanishi, 02'; Machihara, Nakanishi & Ozawa, 02'; Bechouche, Mauser & Selberg, 03'; Masmoudi & Nakaishi, Invent. Math. 08';...

$$u := u^{\varepsilon} \to ??? \quad \text{when} \quad \varepsilon \to 0$$

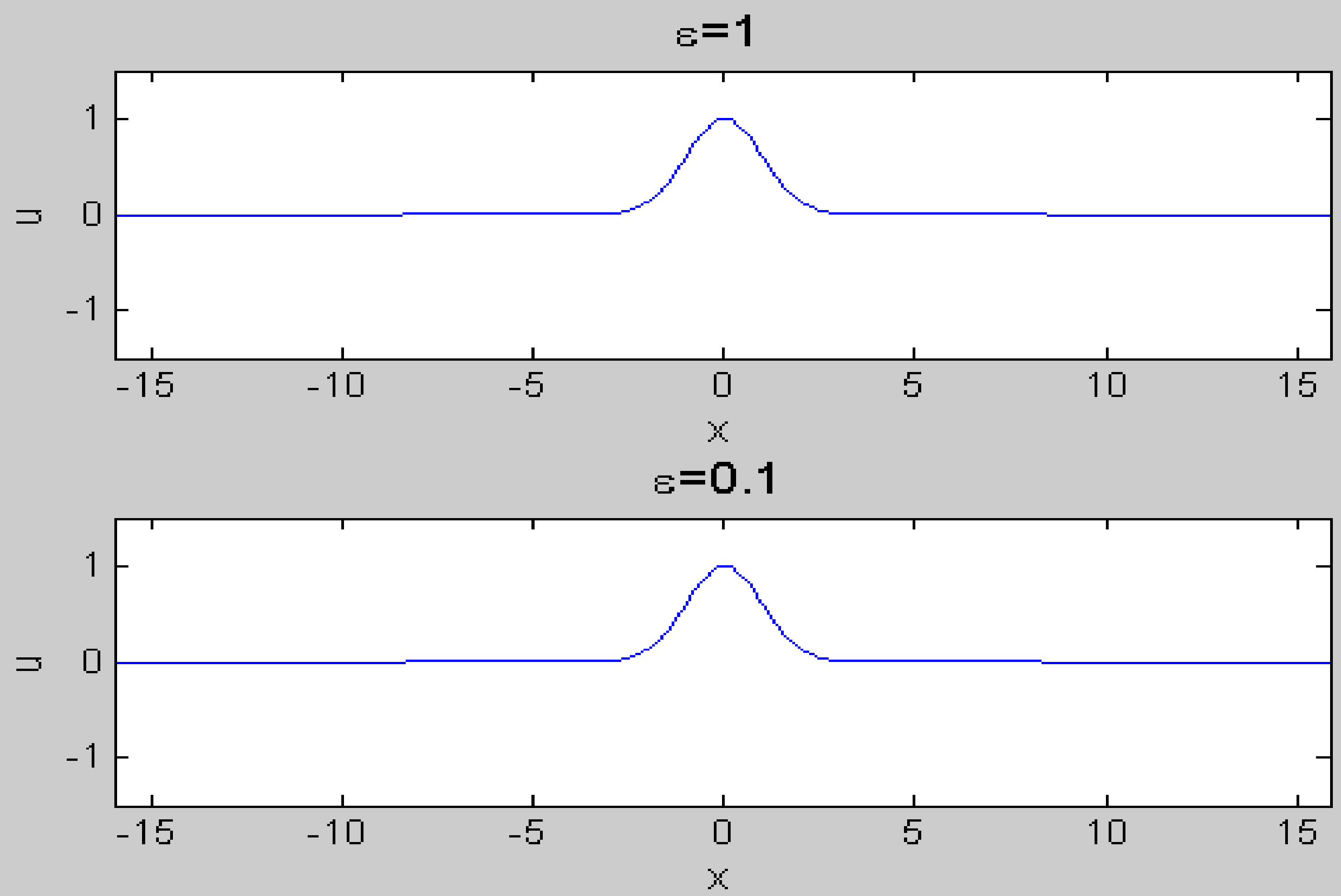
  - Main difficulty: $E(t)$ is unbounded when $\varepsilon \to 0$!!!
- Solution propagates waves with wavelength $O(\varepsilon^2)$ in time & $O(1)$ in space
  - Plane wave solutions $f(u) = \lambda |u|^p u$

$$u(\vec{x},t) = Ae^{i(\vec{k}\bullet\vec{x}+\omega t)} \quad \text{with} \quad \omega_{\pm} = \frac{\pm 1}{\varepsilon^2}\sqrt{1+\varepsilon^2(|\vec{k}|^2 + \lambda A^p)} = O\left(\frac{1}{\varepsilon^2}\right)$$

Numerical results



Numerical results



Existing results in nonrelativistic limit regime

– Asymptotic and rigorous results: Masmoudi, Nakanishi, Math Ann., 02'; Machihara, Nakanishi & Ozawa, Math. Ann., 02'; ….

$$u := u^{\varepsilon} \to e^{it/\varepsilon^2}\psi + e^{-it/\varepsilon^2}\bar{\psi}, \quad \varepsilon \to 0$$

- Nonlinear Schrodinger equation with wave operator (NLSW)

$$2i\partial_t\psi + \varepsilon^2\partial_{tt}\psi - \Delta\psi + F(\psi) = 0$$

- Nonlinear Schrodinger equation (NLSE)

$$2i\partial_t\psi - \Delta\psi + F(\psi) = 0 \qquad F(\psi) := \frac{1}{2\pi}\int_0^{2\pi} f(e^{i\theta}\psi + e^{-i\theta}\bar{\psi})e^{-i\theta}\,d\theta$$

- Highly oscillatory dispersive PDE

Numerical methods in nonrelativistic limit

$$0 < \varepsilon \le 1 \quad (0 < \varepsilon \ll 1)$$

- FDTD--Finite difference time domain– methods: Bao& Dong, Numer. Math., 11'
  - CNFD, SIFD or LPFD: $O(h^2 + \tau^2/\varepsilon^6)$
- EWI–exponential wave integrator– methods: Bao & Dong, Numer. Math., 11'
  - EWI-SP, EWI-FD: $O(h^2 + \tau^2/\varepsilon^4)$
- MTI–multiscale time integrator– methods: Bao, Cai& Zhao, 14'
  - MTI-SP, MTI-FD: $O\left(h^m + \min(\varepsilon^2, \tau^2/\varepsilon^2)\right) \le O\left(h^m + \tau\right)$
- AP–Asymptotic preserving –methods: Faou&Schratz, Numer. Math, 14'
  - AP-SP, AP-FD: $O(h^2 + \tau^2 + \varepsilon^2)$
- A two-scale method: Chartier, Crouseilles, Lemou, Mehats, 14'

Numerical methods for KG equation

- Finite difference time domain (FDTD) methods

$$\varepsilon^2 \partial_{tt} u(x,t) - \partial_{xx} u + \frac{1}{\varepsilon^2} u + f(u) = 0 \qquad \vec{x} \in \Omega = (a,b), \quad t > 0$$

$$u(a,t) = u(b,t) = 0, \qquad t \geq 0$$

$$u(x,0) = \phi(x), \quad \partial_t u(x,0) = \frac{1}{\varepsilon^2} \gamma(x), \qquad a \leq x \leq b$$

  - 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

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

Numerical methods for KG equation

- Finite difference discretization operators

$$\delta_t^+ u_j^n = \frac{u_j^{n+1} - u_j^n}{\tau}, \quad \delta_t^- u_j^n = \frac{u_j^n - u_j^{n-1}}{\tau}, \quad \delta_t^2 u_j^n = \frac{u_j^{n+1} - 2u_j^n + u_j^{n-1}}{\tau^2},$$

$$\delta_x^+ u_j^n = \frac{u_{j+1}^n - u_j^n}{h}, \quad \delta_x^- u_j^n = \frac{u_j^n - u_{j-1}^n}{h}, \quad \delta_x^2 u_j^n = \frac{u_{j+1}^n - 2u_j^n + u_{j-1}^n}{h^2}.$$

- Energy conservative finite difference (CNFD) method

$$\varepsilon^2 \delta_t^2 u_j^n - \frac{1}{2}\delta_x^2 \left(u_j^{n+1} + u_j^{n-1}\right) + \frac{1}{2\varepsilon^2}\left(u_j^{n+1} + u_j^{n-1}\right) + G\left(u_j^{n+1}, u_j^{n-1}\right) = 0;$$

$$G(v, w) = \int_0^1 f\left(\theta v + (1-\theta) w\right)\, d\theta = \frac{F(v) - F(w)}{2(v-w)}, \quad \forall\, v, w \in \mathbb{R},$$

- Semi-implicit finite difference (SIFD) method

$$\varepsilon^2 \delta_t^2 u_j^n - \frac{1}{2}\delta_x^2 \left(u_j^{n+1} + u_j^{n-1}\right) + \frac{1}{2\varepsilon^2}\left(u_j^{n+1} + u_j^{n-1}\right) + f(u_j^n) = 0;$$

Properties of FDTD methods

- Time symmetric, unchanged if $n+1 \leftrightarrow n-1 \quad \& \quad \tau \leftrightarrow -\tau$
- Stability
  - CNFD is unconditionally stable
  - SIFD is unconditionally stable when it is wave type
- Energy conservation: CNFD conserves energy vs SIFD not
- Computational cost
  - CNFD needs solve a nonlinear coupled system per time step!!
  - SIFD needs solve a linear coupled system via fast solver!!
- Resolution in nonrelativistic limit regime

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

Error estimates for FDTD methods

$$e_j^n = u(x_j, t^n) - e_j^n, \quad j = 0,1,\ldots,M, \quad n \ge 0$$

$$\left\| \frac{\partial^{m+n} u}{\partial t^m \partial x^n} \right\|_{L^\infty} \le \frac{1}{\varepsilon^{2m}}, \quad m \ge 0, \quad n \ge 0$$

- For CNFD (Bao& Dong, Numer. Math., 11')

Theorem 2 *Assume $\tau \lesssim h$ and under assumptions (A) and (B2), there exist constants $\tau_0 > 0$ and $h_0 > 0$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \le 1$, when $0 < \tau \le \tau_0$ and $0 < h \le h_0$, we have the following error estimate for the method Impt-EC-FD (2.2) with (2.7) and (2.8)*

$$\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim h^2 + \frac{\tau^2}{\varepsilon^6}, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.25}$$

- For SIFD (Bao& Dong, Numer. Math., 11')

Theorem 5 *Assume $\tau \lesssim h$ and under assumptions (A) and (B1), there exist constants $\tau_0 > 0$ and $h_0 > 0$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \le 1$, when $0 < \tau \le \tau_0$ and $0 < h \le h_0$, we have the following error estimate for the method SImpt-FD (2.4) with (2.7) and (2.8)*

$$\|e^n\|_{l^2} + \|\delta_x^+ e^n\|_{l^2} \lesssim h^2 + \frac{\tau^2}{\varepsilon^6}, \quad 0 \le n \le \frac{T}{\tau}. \tag{2.29}$$

Exponential wave integrator (EWI) spectral method

- Apply sine spectral method for spatial derivatives

$$\varepsilon^2 \partial_{tt} u_M(x,t) - \Delta u_M + \frac{1}{\varepsilon^2} u_M + P_M f(u_M) = 0, \quad a \le x \le b, \quad t \ge 0.$$

  – with

$$u_M(x,t) = \sum_{l=1}^{M-1} \widehat{u}_l(t) \sin(\mu_l(x-a)), \quad a \le x \le b, \quad \mu_l = \frac{l\pi}{b-a}, \quad l = 1,2,\dots,M-1$$

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

$$\varepsilon^2 \frac{\mathrm{d}^2}{\mathrm{d}t^2} \widehat{u}_l(t) + \frac{1+\varepsilon^2\mu_l^2}{\varepsilon^2} \widehat{u}_l(t) + \widehat{f(u_M)}_l(t) = 0,$$

Oscillatory Differential Equations

- Gautschi-type method: W. Gautschi (61'); P. Deuflhard (79'); E. Hairer, Ch. Lubich, G. Wanner, V. Grimm, M. Hochbruck, D. Cohen, ...
- Modulated impulse method: J.M. Sanz-Serna (98'), B. Garcia-Archilla, R.D. Skeel, ……
- Modulated Fourier expansion: D. Cohen, E. Hairer & Ch. Lubich (03'), D. Cohen, J. M. Sanz-Serna, …
- HMM (Heterogeneous multiscale method): W. E (03'), B. Engquist (03'), X. Li, W. Ren, E. Vanden-Eijnden, G. Ariel, R. Tsai, R. Sharp, ……
- SAM (stroboscopic averaging method): U. Kirchgraber, M.P. Calvo, Ph. Chartier, A. Murua, J. M. Sanz-Serna, F. Castella, F. Mehats, ….
- Many other techniques: L.R. Petzold, A. Iserles, S. Reich, M. Condon, …….

Exponential wave integrator (EWI) for 2nd ODE

- Second-order wave-type ODE

$$y''(t)+\lambda^2 y(t)+f(y)=0,\quad t>0,$$

$$y(0)=y_0,\quad y'(0)=y_1 \qquad \text{with} \quad \lambda>0\ \&\ f(0)=0$$

- Notations $\tau=\Delta t>0,\quad t_n=n\tau,\quad n=0,1,2,\ldots \quad y^n\approx y(t_n)$
- Analytical solution near $t=t_n$

$$y(t_n+s)=y(t_n)\cos(\omega s)+y'(t_n)\frac{\sin(\omega s)}{\omega}-\frac{1}{\omega}\int_0^s g(y(t_n+w))\sin(\omega(s-w))dw$$

$$\omega=\sqrt{\lambda^2+a},\quad a=f'(0),\quad g(y)=f(y)-a\,y,\quad s\in\mathbb{R}$$

Exponential wave integrator (EWI) for 2nd ODE

- Take $s=\tau$ or $s=-\tau$

$$y(t_n+\tau)=y(t_n)\cos(\omega\tau)+y'(t_n)\frac{\sin(\omega\tau)}{\omega}-\frac{1}{\omega}\int_0^{\tau}g(y(t_n+w))\sin(\omega(\tau-w))dw$$

$$y(t_n-\tau)=y(t_n)\cos(-\omega\tau)+y'(t_n)\frac{\sin(-\omega\tau)}{\omega}-\frac{1}{\omega}\int_0^{-\tau}g(y(t_n+w))\sin(\omega(-\tau-w))dw$$

$$=y(t_n)\cos(\omega\tau)-y'(t_n)\frac{\sin(\omega\tau)}{\omega}-\frac{1}{\omega}\int_0^{\tau}g(y(t_n-w))\sin(\omega(\tau-w))dw$$

- Sum together

$$y(t_{n+1})=2y(t_n)\cos(\omega\tau)-y(t_{n-1})-\frac{1}{\omega}\int_0^{\tau}[g(y(t_n+w))+g(y(t_n-w))]\sin(\omega(\tau-w))dw$$

Approximate integral via quadratures

– Exponential wave integrator (EWI) in Gautschi-type :
  Gautschi, 68'; Hochbruck & Lubich, 99'; Hochbruck & Ostermann, 00'; Hairer, Lubich & Wanner, 02'; Grim, 05' & 06'; ….

$$y^{n+1} = 2\cos(\omega\tau)y^n - y^{n-1} - 2\frac{1-\cos(\omega\tau)}{\omega^2}g(y^n), \quad n \ge 1$$

$$y^0 = y_0, \quad y^1 = y_0\cos(\omega\tau) + y_1\frac{\sin(\omega\tau)}{\omega} - \frac{1-\cos(\omega\tau)}{\omega^2}g(y_0)$$

– Via trapezoidal rule: Deuflhart, 79', ……

$$y^{n+1} = 2\cos(\omega\tau)y^n - y^{n-1} - \frac{\sin(\omega\tau)}{\omega}g(y^n), \quad n \ge 1$$

$$y^0 = y_0, \quad y^1 = y_0\cos(\omega\tau) + y_1\frac{\sin(\omega\tau)}{\omega} - \frac{\sin(\omega\tau)}{2\omega}g(y_0)$$

Approximate first-order derivative

- Take derivative & subtract: Hochbruck & Lubich, Numer. Math., 99'

$$y'(t_n+\tau)-y'(t_n-\tau)=-2\sin(\omega\tau)y(t_n)$$
$$-\int_0^\tau [g(y(t_n+w))+g(y(t_n-w))]\cos(\omega(\tau-w))dw$$

- Approximate by Gautschi-type rule

$$y'(t_{n+1})\approx y'(t_{n-1})-2\sin(\omega\tau)y^n-\frac{2\sin(\omega\tau)}{\omega}g(y^n),\quad n\geq 1$$

EWI-SP method for KG equation

- EWI spectral (EWI-SP) method (Bao & Dong, Numer. Math. 11)
  - Spectral method for spatial derivatives
  - Exponential wave integrators (EWI) for second-order ODEs
- Properties
  - Explicit –no need to solve any linear system
  - Easy to extend to 2D or 3D
  - Conditionally stable with $\tau \varepsilon^2 \le C$, but it can be unconditionally stable by adding a proper linear stabilizing term!!
  - Give exact solutions for linear case, i.e. *f(u)=a u*

Error Estimate of EWI-SP (Bao & Dong, Numer. Math., 11')

Theorem 9 *Let $u_M^n(x)$ be the approximation obtained from the Gautschi-FP method (3.10) with (3.16). Assume $\tau \lesssim \varepsilon^2\sqrt{C_d(h)}$ and $f(\cdot) \in C^3(\mathbb{R})$, under the assumption (C), there exist $h_0 > 0$ and $\tau_0 > 0$ sufficiently small and independent of ε such that, for any $0 < \varepsilon \le 1$, when $0 < h \le h_0$ and $0 < \tau \le \tau_0$ and under the condition (3.31), we have the following error estimate*

$$\|u(x,t_n) - u_M^n(x)\|_{L^2} \lesssim \frac{\tau^2}{\varepsilon^4} + h^{m_0}, \quad \|u_M^n(x)\|_{L^\infty} \le 1 + M_1, \tag{3.32a}$$

$$\|\nabla[u(x,t_n) - u_M^n(x)]\|_{L^2} \lesssim \frac{\tau^2}{\varepsilon^4} + h^{m_0-1}, \quad 0 \le n \le \frac{T}{\tau}. \tag{3.32b}$$

- Resolution in nonrelativistic limit regime
  - Linear case $h = O(1) \quad \tau = O(1)$
  - Nonlinear case $h = O(1) \quad \tau = O(\varepsilon^2)$

NLS equation with wave operator (NLSW)

$$\begin{cases} i\partial_t u^\varepsilon(\mathbf{x},t) - \varepsilon^2 \partial_{tt} u^\varepsilon(\mathbf{x},t) + \nabla^2 u^\varepsilon(\mathbf{x},t) + f(|u^\varepsilon|^2) u^\varepsilon(\mathbf{x},t) = 0, & \mathbf{x} \in \mathbb{R}^d, \ t > 0, \\ u^\varepsilon(\mathbf{x},0) = u_0(\mathbf{x}), \qquad \partial_t u^\varepsilon(\mathbf{x},0) = u_1^\varepsilon(\mathbf{x}), & \mathbf{x} \in \mathbb{R}^d, \end{cases}$$

- Arising in many applications
  - Nonrelativistic limits of nonlinear KG equation: Masmoudi, Nakanishi, Math Ann., 02'; Machihara, Nakanishi & Ozawa, Math. Ann., 02'; ….
  - Langmuir wave envelope approximation in plasma: Berge & Colin, 95'; Colin & Fabrie, 98'; ….
  - Modulated pulse approximation of sine-Gordon equation for light bullets: Xin, 00'; Bao, Dong & Xin, 10'; ….

Properties of NLSW

$$\|u^\varepsilon - u\|_{L^\infty([0,T];H^2)} \le C\varepsilon^2.$$

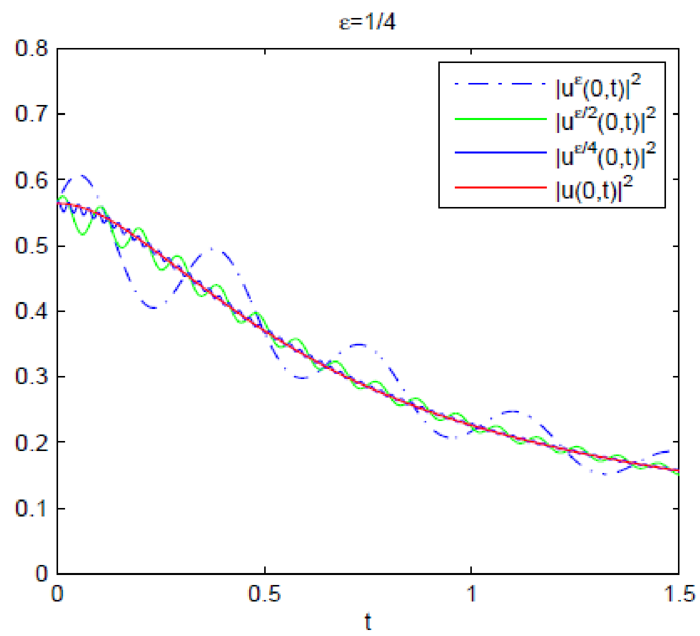
- Converge to NLS at rate: Berge & Colin, 95
- Initial data $u_1^\varepsilon(\mathbf{x}) = i\left(\nabla^2 u_0(\mathbf{x}) + f(|u_0(\mathbf{x})|^2)u_0(\mathbf{x})\right) + \varepsilon^\alpha w(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \qquad \alpha \ge 0,$
  - Well-prepared $\alpha \ge 2$
  - ill-prepared $0 \le \alpha < 2$
- Plane wave solution $f(\rho) = -\lambda\,\rho^p$

$$u^\varepsilon(\vec{x},t) = Ae^{i(\vec{k}\cdot\vec{x}+\omega t)} \text{ with } \omega_\pm = \frac{1 \pm \sqrt{1+4\varepsilon^2(|\vec{k}|^2 + \lambda A^{2p})}}{2\varepsilon^2} = O(1) \quad \& \quad O\left(\frac{1}{\varepsilon^2}\right)$$

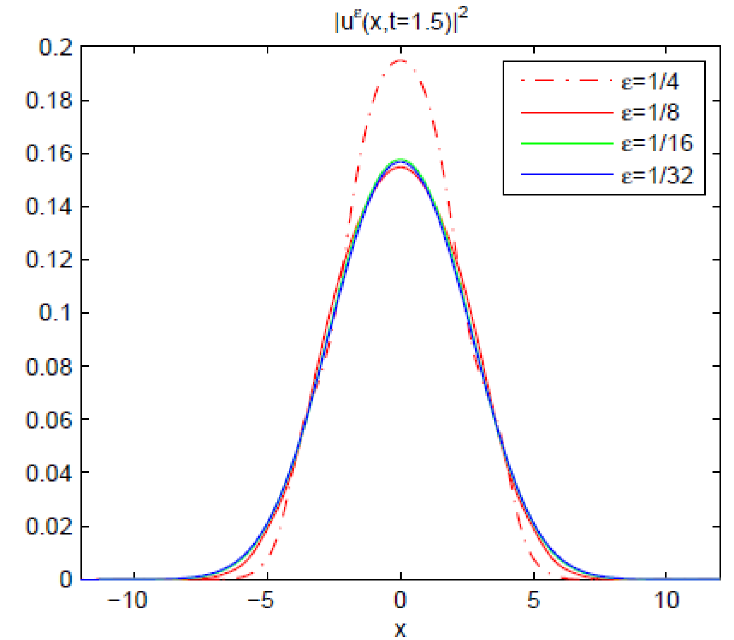
- Fast-slow wave decomposition (FSWD)

$$u^\varepsilon(\mathbf{x},t) = u(\mathbf{x},t) + \varepsilon^2\{\text{terms without oscillation}\}$$
$$+\varepsilon^{2+\min\{\alpha,2\}}v(\mathbf{x},t/\varepsilon^2) + \text{higher order terms with oscillation},$$

Oscillatory structure of NLSW $0<\varepsilon\ll 1$



Time dynamics for ε



Spatial dynamics for ε

- **Observations:** Solution propagates waves with wavelength
  - In space at *O(1)*; in time at $O(\varepsilon^2)$ with amplitude $O(\varepsilon^4)$ for well-prepared initial data & $O(\varepsilon^{2+\alpha})$ for ill-prepared initial data

EWI-SP method for NLSW

- EWI spectral (EWI-SP) method (Bao & Cai, SINUM, 13')
  - Spectral method for spatial derivatives
  - Exponential wave integrators (EWI) for time derivatives
- Properties
  - Explicit –no need to solve any linear system
  - Easy to extend to 2D or 3D
  - Unconditionally stable
  - Give exact solutions for linear case, i.e. $f(v)=a\,v$

Error Estimates of EWI-SP (Bao & Cai, SINUM, 13')

- For well-prepared initial data (Bao & Cai, SINUM, 13')

THEOREM 2.1. *(Well-prepared initial data) Let $\psi^n \in Y_M$ and $\psi_I^n(x) = I_M(\psi^n)$ $(n \geq 0)$ be the numerical approximation obtained from (2.27)-(2.28). Assume $f(s) \in C^k([0, +\infty))$ $(k \geq 3)$, under assumptions (A) and (B), there exist constants $0 < \tau_0, h_0 \leq 1$ independent of ε, if $h \leq h_0$ and $\tau \leq \tau_0$, we have for $\alpha \geq 2$, i.e. the well-prepared initial data case,*

$$\begin{aligned}
&\|\psi(x,t_n) - \psi_I^n(x)\|_{L^2} \lesssim h^m + \tau^2, \qquad \|\psi^n\|_{l^\infty} \leq M_1 + 1, \\
&\|\nabla(\psi(x,t_n) - \psi_I^n(x))\|_{L^2} \lesssim h^{m-1} + \tau^2, \qquad 0 \leq n \leq \frac{T}{\tau},
\end{aligned} \tag{2.34}$$

- Observations
  - Spectral accuracy in space
  - 2nd order accuracy in time: uniform & optimal for $0 \leq \varepsilon \leq 1$

A multiscale method for KG equation

$$\varepsilon^2\partial_{tt}u(\vec{x},t)-\Delta u+\frac{1}{\varepsilon^2}u+f(u)=0,\qquad \vec{x}\in\mathbb{R}^d,\quad t>0$$

$$u(\vec{x},0)=\phi(\vec{x}),\quad \partial_t u(\vec{x},0)=\frac{1}{\varepsilon^2}\gamma(\vec{x}),\quad \vec{x}\in\mathbb{R}^d$$

- For time interval $[t_n, t_{n+1}]$: (Bao, Cai & Zhao, SINUM, 14')
  - Given initial data

$$u(\vec{x},t_n)=\phi_n(\vec{x})\quad \&\quad \partial_t u(\vec{x},t_n)=\frac{1}{\varepsilon^2}\gamma_n(\vec{x}),\quad \vec{x}\in\Omega$$

  - Multiscale decomposition in frequency (MDF)

$$u(\vec{x},t_n+s)=e^{is/\varepsilon^2}\,z^n(\vec{x},s)+e^{-is/\varepsilon^2}\,\overline{z}^n(\vec{x},s)+r^n(\vec{x},s),\quad \vec{x}\in\Omega,\quad 0\le s\le\tau$$

Multiscale decomposition of KG

– NLSW for z^n with well-prepared initial data ($\varepsilon^2 -$)

$$2i\partial_s z^n(\vec{x},s) + \varepsilon^2 \partial_{ss} z^n - \Delta z^n + F(z^n) = 0, \quad \vec{x} \in \Omega, 0 \le s \le \tau$$

– Nonlinear KG-type equation for r^n with small data (rest)

$$\varepsilon^2 \partial_{ss} r^n(\vec{x},s) - \Delta r^n + \frac{1}{\varepsilon^2} r^n + G(r^n, s; z^n) = 0, \quad \vec{x} \in \Omega, \quad 0 \le s \le \tau$$

- with

$$G(r,s;z) := f(ze^{is/\varepsilon^2} + \overline{z}e^{-is/\varepsilon^2} + r) - F(z)e^{is/\varepsilon^2} - F(\overline{z})e^{-is/\varepsilon^2}, \quad 0 \le s \le \tau$$

Multiscale decomposion of initial data

$$t = t_n \Leftrightarrow s = 0$$

$$u(\vec{x}, t_n) = z^n(\vec{x}, 0) + \overline{z}^n(\vec{x}, 0) + r^n(\vec{x}, 0) = \phi_n(\vec{x})$$

$$\partial_t u(\vec{x}, t_n) = \frac{i}{\varepsilon^2}\left[z^n(\vec{x}, 0) - \overline{z}^n(\vec{x}, 0)\right] + \partial_s z^n(\vec{x}, 0) + \partial_s \overline{z}^n(\vec{x}, 0) + \partial_s r^n(\vec{x}, 0) = \frac{1}{\varepsilon^2}\gamma_n(\vec{x})$$

- Small data for r^n :

$$r^n(\vec{x}, 0) = 0 \quad \& \quad z^n(\vec{x}, 0) + \overline{z}^n(\vec{x}, 0) = \phi_n(\vec{x})$$

- Well-prepared data for z^n

$$\partial_s z^n(\vec{x}, 0) = \frac{-i}{2}[\Delta z^n - F(z^n)]_{s=0}$$

- Equate *O(1)* and $O(1/\varepsilon^2)$

$$z^n(\vec{x}, 0) - \overline{z}^n(\vec{x}, 0) = -i\gamma_n(\vec{x}) \quad \& \quad \partial_s r^n(\vec{x}, 0) = -\partial_s z^n(\vec{x}, 0) - \partial_s \overline{z}^n(\vec{x}, 0), \quad \vec{x} \in \overline{\Omega}$$

- Solve and get

$$z^n(\vec{x}, 0) = \frac{1}{2}[\phi_n(\vec{x}) - i\gamma_n(\vec{x})], \quad \vec{x} \in \overline{\Omega}$$

Two subproblems

– NLSW for z^n with well-prepared initial data

$$2i\partial_s z^n(\vec{x},s)+\varepsilon^2\partial_{ss}z^n-\Delta z^n+F(z^n)=0,\quad \vec{x}\in\Omega, 0\le s\le\tau$$

- with

$$z^n(\vec{x},0)=\frac{1}{2}[\phi_n(\vec{x})-i\gamma_n(\vec{x})],\quad \partial_s z^n(\vec{x},0)=\frac{-i}{2}[\Delta z^n-F(z^n)]_{s=0},\qquad \vec{x}\in\overline{\Omega}$$

– Nonlinear KG-type equation for *w* with small data

$$\varepsilon^2\partial_{ss}r^n(\vec{x},s)-\Delta r^n+\frac{1}{\varepsilon^2}r^n+G(r^n,s;z^n)=0,\quad \vec{x}\in\Omega,\quad 0\le s\le\tau$$

$$r^n(\vec{x},0)=0,\quad \partial_s r^n(\vec{x},0)=-\partial_s z^n(\vec{x},0)-\partial_s\overline{z}^n(\vec{x},0),\quad \vec{x}\in\overline{\Omega}$$

Reconstruction at $t = t_{n+1}$

- Solve the NLSW for z^n by EWI-SP method to obtain

$$z^n(x,\tau), \quad \partial_s z^n(x,\tau), \quad \vec{x} \in \Omega$$

- Solve the KG-type equation for *w* by EWI-SP to obtain

$$r^n(x,\tau), \quad \partial_s r^n(x,\tau), \quad \vec{x} \in \Omega$$

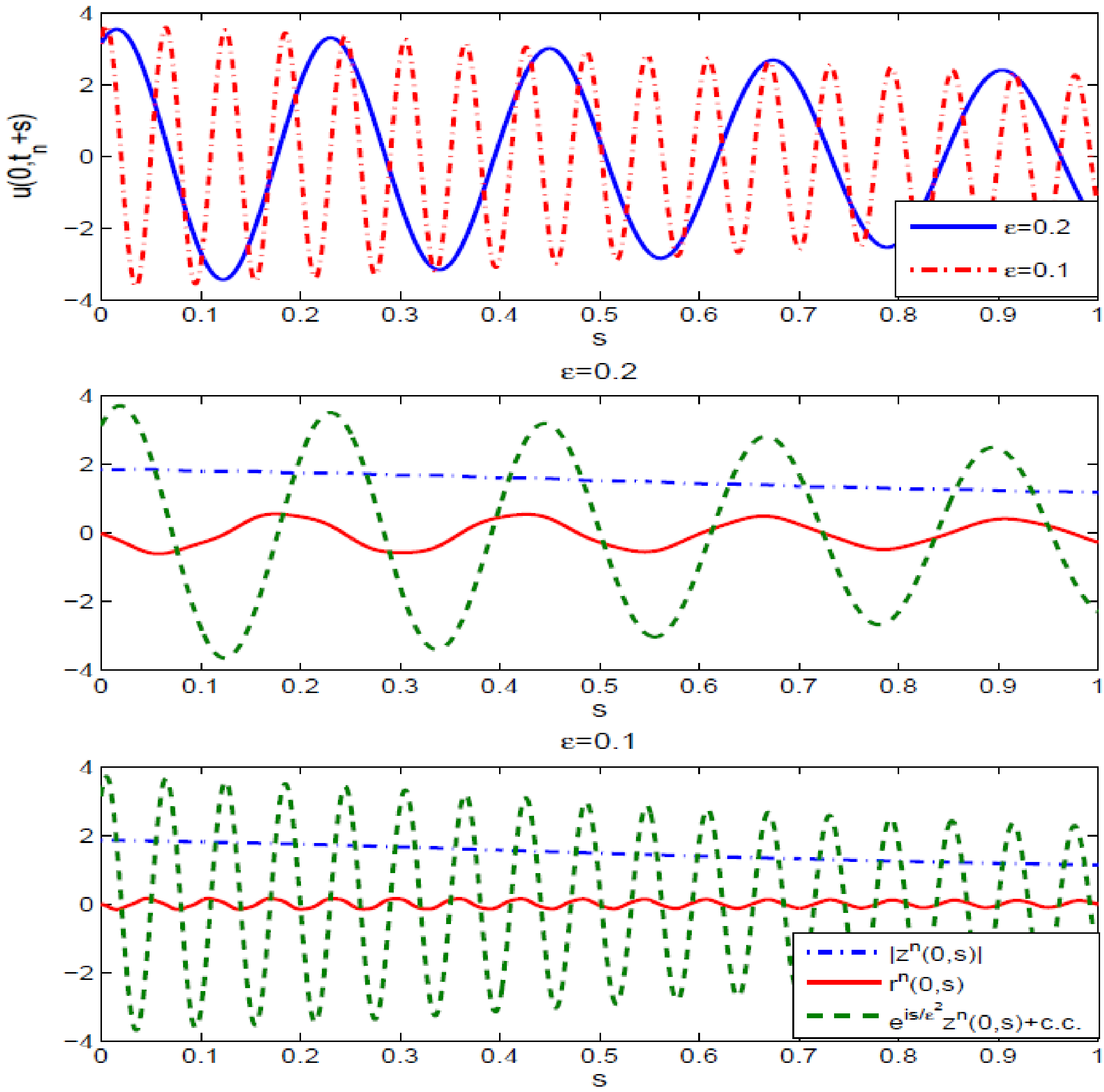
- Construct solution at $t = t_{n+1}$ based on the decomposition

$$u(x,t_{n+1}) := e^{i\tau/\varepsilon^2} z^n(\vec{x},\tau) + e^{-i\tau/\varepsilon^2} \overline{z}^n(\vec{x},\tau) + r^n(\vec{x},\tau) := \phi_{n+1}(\vec{x}), \quad \vec{x} \in \Omega$$

$$\partial_t u(x,t_{n+1}) := e^{i\tau/\varepsilon^2} \partial_s z^n(\vec{x},\tau) + e^{-i\tau/\varepsilon^2} \partial_s \overline{z}^n(\vec{x},\tau) + \partial_s r^n(\vec{x},\tau) + \frac{i}{\varepsilon^2}[z^n(\vec{x},\tau) - \overline{z}^n(\vec{x},\tau)]$$

$$\Rightarrow \gamma_{n+1}(\vec{x}) = i[z^n(\vec{x},\tau) - \overline{z}^n(\vec{x},\tau)] + \varepsilon^2[e^{i\tau/\varepsilon^2} \partial_s z^n(\vec{x},\tau) + e^{-i\tau/\varepsilon^2} \partial_s \overline{z}^n(\vec{x},\tau) + \partial_s r^n(\vec{x},\tau)]$$

$$u(\vec{x}, t_n + s) = e^{is/\varepsilon^2} z^n(\vec{x}, s) + \text{c.c.} + r^n(\vec{x}, s)$$



z^n is smooth & no oscillation!

r^n is oscillating, but its amplitude is small! Also, r^n(.,0)=0!!, no numerical error be accumulated between different time interval

Properties of the multiscale method

- Explicit & unconditionally stable
- Easy to extend to 2D & 3D
- Accuracy
  - Spectral accuracy in space
  - Uniform convergence in time for $0 < \varepsilon \leq 1$
- Resolution in nonrelativistic limit regime

$$h = O(1) \quad \& \quad \tau = O(1)$$

Error bounds for the multiscale method

- Theorem (Bao Cai &Zhao, SINUM,14') Under some reasonable and proper assumptions, for $0<\varepsilon\le 1$, we can establish the following two independent error estimates for

$$\|u(x,t_n)-u_M^n(x)\|_{L^2}\le\frac{\tau^2}{\varepsilon^2}+h^{m_0},\quad \|\nabla(u(x,t_n)-u_M^n(x))\|_{L^2}\le\frac{\tau^2}{\varepsilon^2}+h^{m_0-1},\quad 0\le n\le\frac{T}{\tau},$$

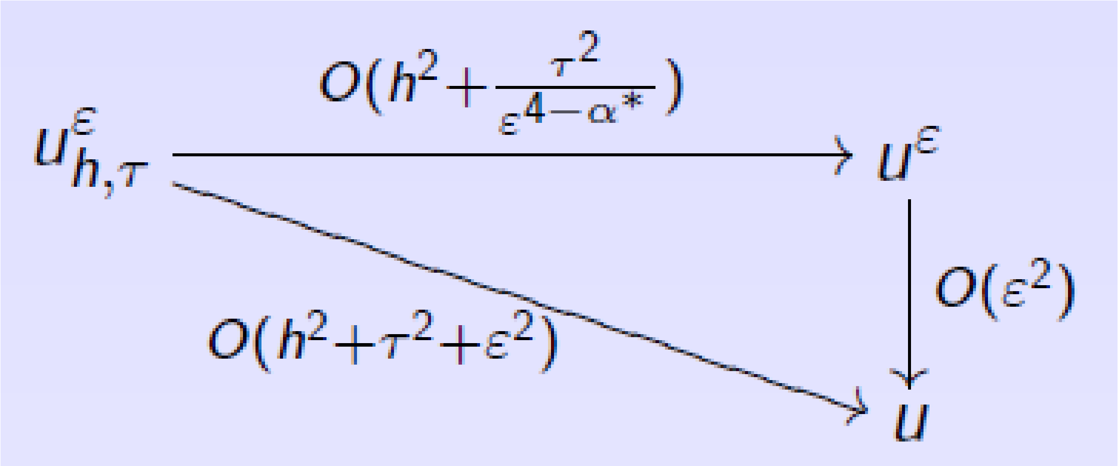
$$\|u(x,t_n)-u_M^n(x)\|_{L^2}\le\tau^2+\varepsilon^2+h^{m_0},\quad \|\nabla(u(x,t_n)-u_M^n(x))\|_{L^2}\le\tau^2+\varepsilon^2+h^{m_0-1}.$$

By taking the minimum, we get error bound uniformly for $0<\varepsilon\le 1$ as:

$$\|u(x,t_n)-u_M^n(x)\|_{L^2}\le\tau+h^{m_0},\quad \|\nabla(u(x,t_n)-u_M^n(x))\|_{L^2}\le\tau+h^{m_0-1},\quad 0\le n\le\frac{T}{\tau}.$$

Ingredients of the proof

– Energy method
– Inverse inequality & either mathematical induction or bots-trap technique to bound numerical solution u^n
– Asymptotic behavior of the exact solution u
– Use the limit equation: Jin, SISC, 99'; Degond, Liu & Vignal, 08', ….



Numerical results (Bao,Cai & Zhao, SINUM,14')

$$\varepsilon^2\partial_{tt}u(x,t)-\partial_{xx}u+\frac{1}{\varepsilon^2}u+|u|^2u=0 \qquad x\in\mathbb{R},\quad t>0$$

$$u(x,0)=\phi(x)=(1+i)e^{-x^2/2},\quad \partial_t u(x,0)=\frac{3\phi(x)}{2\varepsilon^2},\quad \vec{x}\in\mathbb{R}$$

$e_\varepsilon^{\tau,h}(T)$	$h_0=1$	$h_0/2$	$h_0/4$	$h_0/8$
$\varepsilon_0=0.5$	1.65E−1	3.60E−3	1.03E−6	7.34E−11
$\varepsilon_0/2^1$	2.65E−1	9.70E−3	9.07E−7	5.03E−11
$\varepsilon_0/2^2$	9.02E−1	1.34E−2	1.73E−7	4.60E−11
$\varepsilon_0/2^3$	1.13E+0	2.98E−2	2.25E−7	4.10E−11
$\varepsilon_0/2^4$	4.67E−1	3.14E−2	1.79E−7	4.78E−11
$\varepsilon_0/2^5$	7.41E−1	2.73E−2	2.50E−7	5.49E−11
$\varepsilon_0/2^7$	7.41E−1	2.62E−2	2.12E−7	4.96E−11
$\varepsilon_0/2^9$	6.33E−1	3.57E−2	1.92E−7	5.04E−11
$\varepsilon_0/2^{11}$	9.19E−1	2.44E−2	2.19E−7	6.18E−11
$\varepsilon_0/2^{13}$	1.18E+0	2.38E−2	2.59E−7	5.86E−11

Observation: spectral order in time & uniform convergence in ε !!!!

Numerical results (Bao, Cai & Zhao, SINUM, 14')

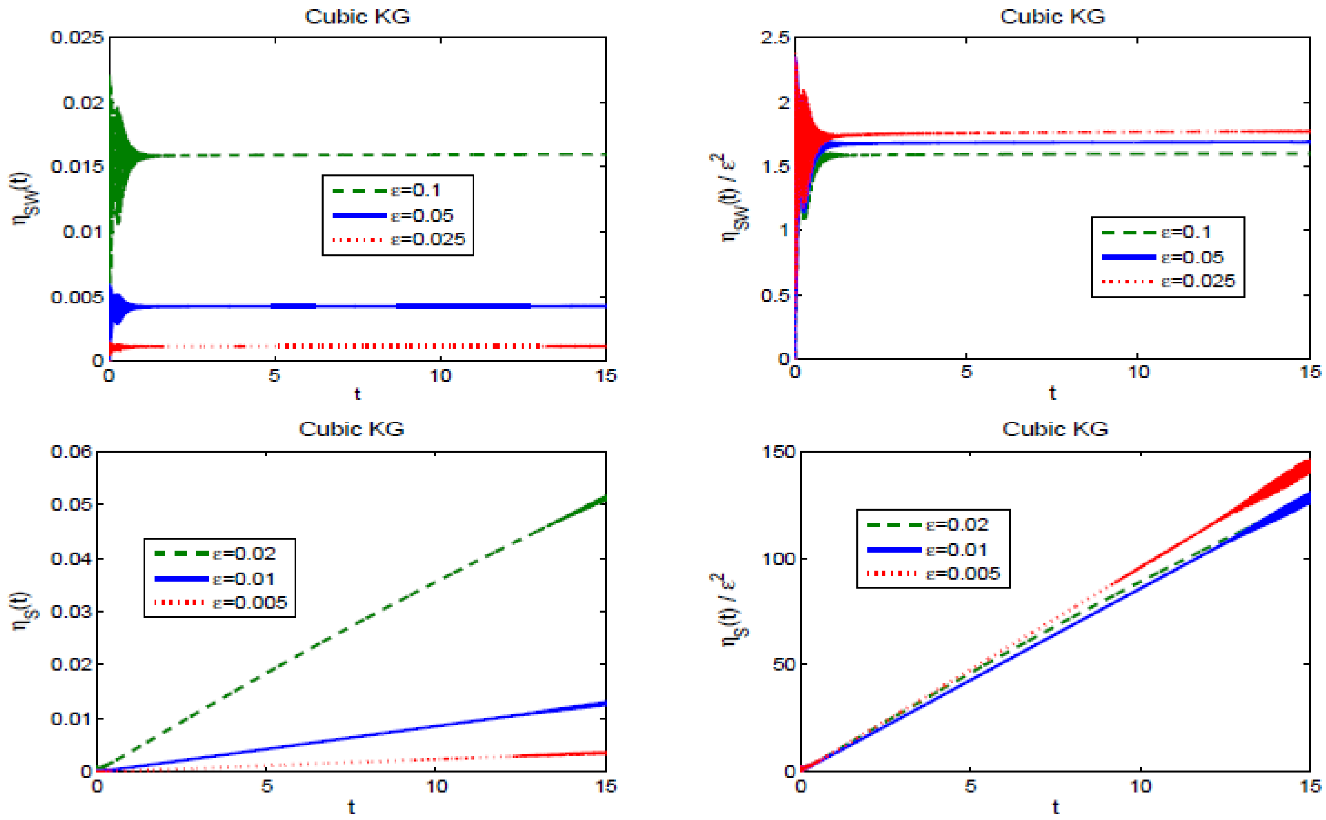
$e_\varepsilon^{\tau,h}(T)$	$\tau_0=0.2$	$\tau_0/2^2$	$\tau_0/2^4$	$\tau_0/2^6$	$\tau_0/2^8$	$\tau_0/2^{10}$	$\tau_0/2^{12}$
$\varepsilon_0=0.5$	7.04E-1	5.73E-2	3.50E-3	2.14E-4	1.33E-5	8.14E-7	3.67E-8
rate	—	1.81	2.02	2.01	2.00	2.01	2.20
$\varepsilon_0/2^1$	4.92E-1	1.58E-1	1.12E-2	6.74E-4	4.15E-5	2.54E-6	1.18E-7
rate	—	0.82	1.91	2.02	2.01	2.01	2.21
$\varepsilon_0/2^2$	4.55E-1	1.47E-1	3.70E-2	2.70E-3	1.62E-4	9.87E-6	4.62E-7
rate	—	0.82	0.99	1.90	2.02	2.01	2.20
$\varepsilon_0/2^3$	5.46E-1	6.11E-2	4.13E-2	8.90E-3	6.51E-4	3.92E-5	1.82E-6
rate	—	1.58	0.28	1.11	1.89	2.02	2.21
$\varepsilon_0/2^4$	5.20E-1	2.83E-2	1.16E-2	1.05E-2	2.20E-3	1.60E-4	7.41E-6
rate	—	2.09	0.64	0.07	1.13	1.89	2.21
$\varepsilon_0/2^5$	5.23E-1	2.83E-2	2.50E-3	2.70E-3	2.60E-3	5.26E-4	2.98E-5
rate	—	2.10	1.75	-0.06	0.01	1.17	2.07
$\varepsilon_0/2^7$	5.21E-1	2.74E-2	1.76E-3	2.37E-4	1.37E-4	1.96E-4	1.91E-4
rate	—	2.12	1.98	1.45	0.40	-0.26	0.02
$\varepsilon_0/2^9$	5.21E-1	2.73E-2	1.69E-3	1.12E-4	1.09E-5	5.51E-6	1.69E-6
rate	—	2.12	2.00	1.96	1.68	0.49	0.85
$\varepsilon_0/2^{11}$	5.21E-1	2.73E-2	1.69E-3	1.05E-4	6.95E-6	9.97E-7	3.38E-7
rate	—	2.12	2.00	2.00	1.96	1.40	0.78
$\varepsilon_0/2^{13}$	5.25E-1	2.76E-2	1.70E-3	1.06E-4	6.61E-6	3.94E-7	2.38E-8
rate	—	2.12	2.00	2.00	2.00	2.03	2.02
$e_\infty^{\tau,h}(T)$	7.04E-1	1.58E-1	4.13E-2	1.05E-2	2.60E-3	5.26E-4	1.91E-4
rate	—	1.07	0.97	0.99	1.00	1.15	0.74

Observation: 2nd order in time & uniform convergence in ε !!!!

Convergence rates from NKG to NLSW & NLSE

$$u_{\mathrm{sw}} = e^{it/\varepsilon^2}\psi_{\mathrm{sw}} + e^{-it/\varepsilon^2}\overline{\psi}_{\mathrm{sw}}$$

$$u_{\mathrm{s}} = e^{it/\varepsilon^2}\psi_{\mathrm{s}} + e^{-it/\varepsilon^2}\overline{\psi}_{\mathrm{s}}$$

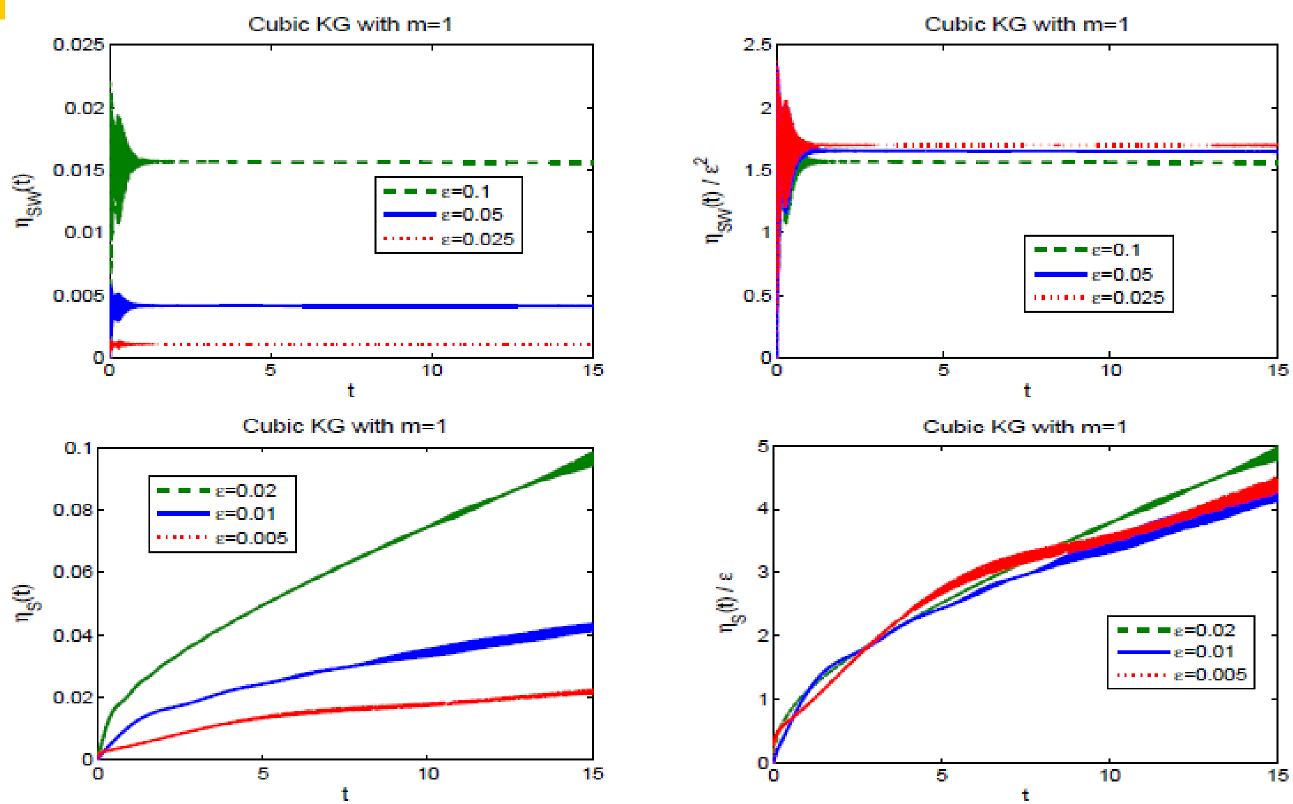


$$\phi(\vec{x}) \in H^3$$

$$\gamma(\vec{x}) \in H^3 \Rightarrow \quad \eta_{\mathrm{sw}}(t) = \left\| u(\cdot,t) - u_{\mathrm{sw}}(\cdot,t) \right\|_{H^1} \le C_0 \varepsilon^2, \quad 0 \le t < T^*$$

$$\eta_{\mathrm{s}}(t) = \left\| u(\cdot,t) - u_{\mathrm{s}}(\cdot,t) \right\|_{H^1} \le (C_1 + C_2 T)\varepsilon^2, \quad 0 \le t \le T$$

Convergence rates from NKG to NLSW & NLSE



$$\phi(\vec{x}) \in H^2$$

$$\gamma(\vec{x}) \in H^2 \Rightarrow$$

$$\eta_{sw}(t) = \left\| u(\cdot,t) - u_{sw}(\cdot,t) \right\|_{H^1} \le C_0 \varepsilon^2, \quad 0 \le t < T^*$$

$$\eta_s(t) = \left\| u(\cdot,t) - u_s(\cdot,t) \right\|_{H^1} \le (C_1 + C_2 T)\varepsilon, \quad 0 \le t \le T$$

Conclusion & future challenges

- Conclusion
  - For nonlinear KG equation in nonrelativistic limit regime
    - FDTD methods $O\left(h^2+\tau^2/\varepsilon^6\right) \Rightarrow h=O(1)\ \&\ \tau=O(\varepsilon^3)$
    - An EWI spectral method $O\left(h^m+\tau^2/\varepsilon^4\right) \Rightarrow h=O(1)\ \&\ \tau=O(\varepsilon^2)$
    - A multiscale method $O\left(h^m+\min(\varepsilon^2,\frac{\tau^2}{\varepsilon^2})\right)\le O\left(h^m+\tau\right)\Rightarrow h=O(1)\ \&\ \tau=O(1)$
  - For NLS perturbed by wave operator
    - FDTD methods $O\left(h^2+\tau\right) \Rightarrow h=O(1)\ \&\ \tau=O(1)$
    - An EWI spectral method $O\left(h^m+\tau^2\right) \Rightarrow h=O(1)\ \&\ \tau=O(1)$
- Extension to oscillatory dispersive PDEs
  - Dirac equation & Klein-Gordon-Schrodinger in nonrelativisitic limit regime
  - Zakharov system in subsonic limit regime, …..