# Analysis & Computation for the Semiclassical Limits of the Nonlinear Schrodinger Equations

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# Outline

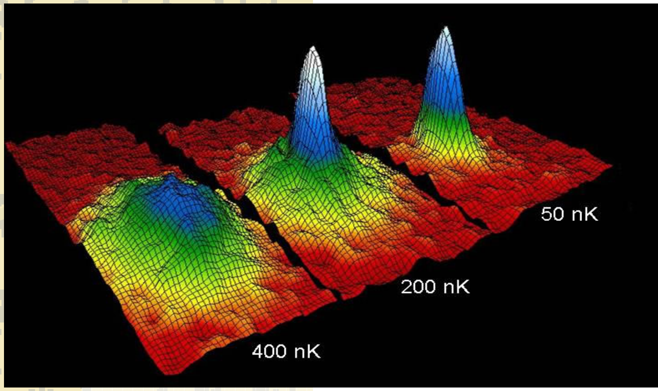
- Motivation
- Semiclassical limits of ground and excited states
  - Matched asymptotic approximations
  - Numerical results
- Semiclassical limits of the dynamics of NLS
  - Formal limits
  - Efficient computation
  - Caustics & vacuum
  - Difficulties in rotating frame and system
- Conclusions

# Motivation: NLS

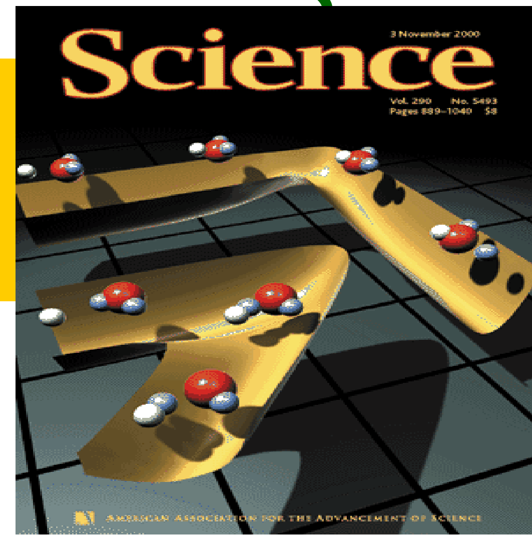
- The nonlinear Schrödinger (NLS) equation

$$i\varepsilon\,\partial_t\psi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi^\varepsilon + V(\vec{x})\psi^\varepsilon + \beta\,|\psi^\varepsilon|^2\,\psi^\varepsilon$$

  - t : time & $\vec{x}\ (\in \mathbb{R}^d)$ : spatial coordinate
  - $\psi(\vec{x},t)$ : complex-valued wave function
  - $V(\vec{x})$ : real-valued external potential
  - $\varepsilon\ (0<\varepsilon \ll 1)$ : scaled Planck constant
  - $\beta\ (=0,\pm 1)$ : interaction constant
    - =0: linear; =1: repulsive interaction
    - = -1: attractive interaction




# Motivation




- In quantum physics & nonlinear optics:
  - Interaction between particles with quantum effect
  - Bose-Einstein condensation (BEC): bosons at low temperature
  - Superfluids: liquid Helium,
  - Propagation of laser beams, …….
- In plasma physics; quantum chemistry; particle physics; biology; materials science; ….
- Conservation laws

$$N(\psi^\varepsilon) := \|\psi^\varepsilon\|^2 = \int_{\mathbb{R}^d} |\psi^\varepsilon(\vec{x},t)|^2 d\,\vec{x} \equiv \int_{\mathbb{R}^d} |\psi^\varepsilon(\vec{x},0)|^2 d\,\vec{x} = \int_{\mathbb{R}^d} |\psi_0^\varepsilon(\vec{x})|^2 d\,\vec{x} := N(\psi_0^\varepsilon) \quad (=1),$$

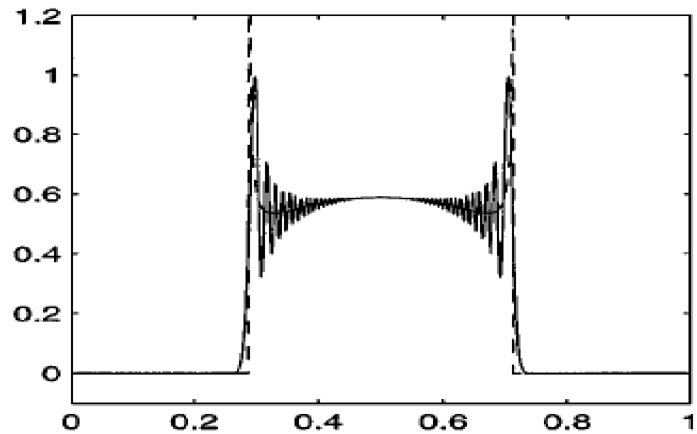
$$E(\psi^\varepsilon) := \int_{\mathbb{R}^d} \left[ \frac{\varepsilon^2}{2} |\nabla \psi^\varepsilon(\vec{x},t)|^2 + V(x)|\psi^\varepsilon(\vec{x},t)|^2 + \tfrac{\beta}{2}|\psi^\varepsilon(\vec{x},t)|^4 \right] d\,\vec{x} \equiv E(\psi_0^\varepsilon)$$

# Semiclassical limits

- Suppose initial data chosen as

$$\psi^{\varepsilon}(\vec{x},0) := \psi_0^{\varepsilon}(\vec{x}) = A_0^{\varepsilon}(\vec{x})\, e^{iS_0^{\varepsilon}(\vec{x})/\varepsilon} \Rightarrow \psi^{\varepsilon}(\vec{x},t) = A^{\varepsilon}(\vec{x},t)\, e^{iS^{\varepsilon}(\vec{x},t)/\varepsilon}$$

- Semiclassical limits: $\varepsilon \to 0$
  - Density: $\rho^{\varepsilon} := |\psi^{\varepsilon}|^2 \to ????$
  - Current: $\vec{J}^{\varepsilon} := \rho^{\varepsilon}\,\vec{v}^{\varepsilon} \to ???$ $\quad \vec{v}^{\varepsilon} := \nabla S^{\varepsilon} \to ???$
  - Other observable:
- Analysis: dispersive limits
  - WKB method vs Winger transform
- Efficient computation
  - Highly oscillatory wave in space & time



# For ground & excited states

- For special initial data:

$$A_0^\varepsilon(\vec{x}) = \phi^\varepsilon(\vec{x}) \ \& \ S_0^\varepsilon(\vec{x}) = 0 \Rightarrow \psi^\varepsilon(\vec{x},t) = \phi^\varepsilon(\vec{x})\, e^{-i\,\mu^\varepsilon t/\varepsilon}$$

- Time-independent NLS: nonlinear eigenvalue problem

$$\mu^\varepsilon\,\phi^\varepsilon(\vec{x}) = -\frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon + V(\vec{x})\phi^\varepsilon + \beta\,|\phi^\varepsilon|^2\,\phi^\varepsilon, \quad \left\|\phi^\varepsilon\right\|^2 := \int_{R^d} \left|\phi^\varepsilon(\vec{x})\right|^2 d\,\vec{x} = 1$$

  – Eigenvalue (or chemical potential)

$$\mu^\varepsilon := \mu(\phi^\varepsilon) := \int_{\mathrm{R}^d}\left[\frac{\varepsilon^2}{2}\left|\nabla\phi^\varepsilon(\vec{x})\right|^2 + V(x)\left|\phi^\varepsilon(\vec{x})\right|^2 + \beta\left|\phi^\varepsilon(\vec{x})\right|^4\right] d\,\vec{x}$$

  – Eigenfunctions are
    - Orthogonal in linear case & Superposition is valid for dynamics!!
    - Not orthogonal in nonlinear case !!!! No superposition for dynamics!!!

# For ground & excited states

- Ground state: minimizer of the nonconvex minimization problem

$$E_g^\varepsilon := E(\phi_g^\varepsilon) = \min_{\phi^\varepsilon \in S} E(\phi^\varepsilon), \qquad S = \left\{\phi \mid \|\phi\| = 1,\ E(\phi) < \infty\right\}$$

  - Existence: $\beta \geq 0 \quad \& \quad \lim_{|\vec{x}| \to \infty} V(\vec{x}) = \infty$
  - Positive solution is unique

- Excited states: eigenfunctions with higher energy

$$\phi_1^\varepsilon, \phi_2^\varepsilon, \cdots, \phi_j^\varepsilon, \cdots \qquad E_j^\varepsilon := E(\phi_j^\varepsilon), \quad \mu_j^\varepsilon := \mu(\phi_j^\varepsilon)$$

- Semiclassical limits $\varepsilon \to 0$

$$\phi_g^\varepsilon \to ??? \quad E_g^\varepsilon \to ??? \quad \mu_g^\varepsilon := \mu(\phi_g^\varepsilon) \to ??? \quad \phi_j^\varepsilon \to ??? \quad E_j^\varepsilon \to ??? \quad \mu_j^\varepsilon \to ???$$

$$E_g^\varepsilon < E_1^\varepsilon < E_2^\varepsilon < \cdots < E_j^\varepsilon < \cdots \Rightarrow \mu_g^\varepsilon < \mu_1^\varepsilon < \mu_2^\varepsilon < \cdots < \mu_j^\varepsilon < \cdots ?????$$

# For ground state: Box Potential in 1D

- The potential: $V(x)=\begin{cases}0, & 0\le x\le 1,\\ \infty, & \text{otherwise.}\end{cases}$ $\quad d=1,\quad \beta=1$
- The nonlinear eigenvalue problem (Bao,Lim,Zhang,Bull. Inst. Math., 05')

$$\mu^\varepsilon\ \phi^\varepsilon(x)=-\frac{\varepsilon^2}{2}(\phi^\varepsilon)''(x)+|\phi^\varepsilon(x)|^2\ \phi^\varepsilon(x),\qquad 0<x<1,$$

$$\phi^\varepsilon(0)=\phi^\varepsilon(1)=0\qquad \text{with}\qquad \int_0^1|\phi^\varepsilon(x)|^2dx=1$$

- Leading order approximation, i.e. drop the diffusion term $0<\varepsilon \ll 1$

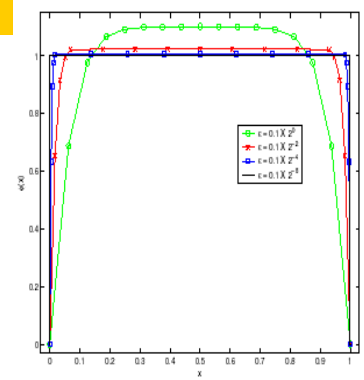
$$\mu_g^{\mathrm{TF}}\ \phi_g^{\mathrm{TF}}(x)=|\phi_g^{\mathrm{TF}}(x)|^2\ \phi_g^{\mathrm{TF}}(x),\qquad 0<x<1,\qquad \Rightarrow\quad \phi_g^{\mathrm{TF}}(x)=\sqrt{\mu_g^{\mathrm{TF}}}$$

$$\Downarrow\ \int_0^1|\phi_g^{\mathrm{TF}}(x)|^2\ dx=1$$

$$\phi_g^\varepsilon(x)\approx\phi_g^{\mathrm{TF}}(x)=1,\qquad \mu_g^\varepsilon\approx\mu_g^{\mathrm{TF}}=1,\qquad \mathrm{E}_g^\varepsilon\approx\mathrm{E}_g^{\mathrm{TF}}=\frac{1}{2}$$

  - Boundary condition is NOT satisfied, i.e. $\phi_g^{\mathrm{TF}}(0)=\phi_g^{\mathrm{TF}}(1)=1\neq 0$
  - Boundary layer near the boundary

# For ground state: Box Potential in 1D



- Matched asymptotic approximation
  - Consider near x=0, rescale $x = \frac{\varepsilon}{\sqrt{\mu_g^\varepsilon}} X, \quad \phi_g^\varepsilon(x) = \sqrt{\mu_g^\varepsilon}\,\Phi(x)$
  - We get

$$\Phi(X) = -\frac{1}{2}\Phi''(X) + \Phi^3(X), \quad 0 \le X < \infty; \qquad \Phi(0) = 0, \quad \lim_{X\to\infty}\Phi(X) = 1$$

  - The inner solution

$$\Phi(X) = \tanh(X), \quad 0 \le X < \infty \qquad \Rightarrow \quad \phi_g^\varepsilon(x) \approx \sqrt{\mu_g}\,\tanh(\frac{\sqrt{\mu_g}}{\varepsilon}x), \quad 0 \le x = o(1)$$

  - Matched asymptotic approximation for ground state

$$\phi_g^\varepsilon(x) \approx \phi_g^{\mathrm{MA}}(x) = \sqrt{\mu_g^{\mathrm{MA}}}\left[\tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon}x) + \tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon}(1-x)) - \tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon})\right], \quad 0 \le x \le 1$$

$$1 = \int_0^1 |\phi_g^{\mathrm{MA}}(x)|^2 dx \quad \Rightarrow \quad \mu_g^\varepsilon \approx \mu_g^{\mathrm{MA}} = 1 + 2\varepsilon\sqrt{1+\varepsilon^2} + 2\varepsilon^2 = \mu_g^{\mathrm{TF}} + 2\varepsilon\sqrt{1+\varepsilon^2} + 2\varepsilon^2, \quad 0 < \varepsilon \ll 1.$$

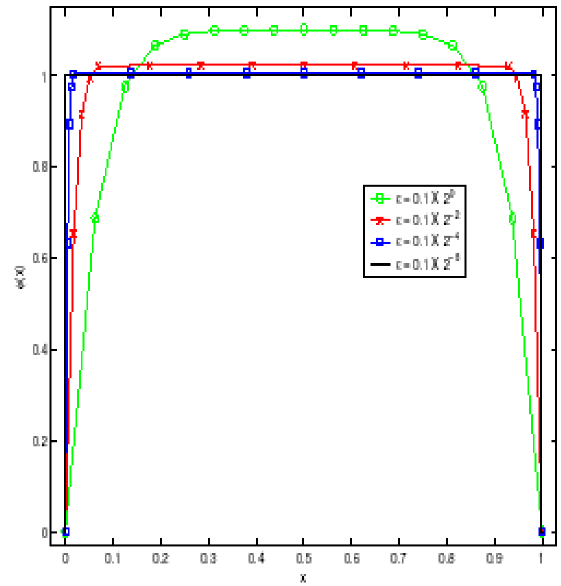
# For ground state: Box Potential in 1D

- Approximate energy

$$E_g^\varepsilon \approx E_g^{\mathrm{MA}} = \frac{1}{2} + \frac{4}{3}\varepsilon\sqrt{1+\varepsilon^2} + 2\varepsilon^2$$

- Asymptotic ratios: $\lim_{\varepsilon \to 0} \frac{E_g^\varepsilon}{\mu_g^\varepsilon} = \frac{1}{2},$

- Width of the boundary layer: $O(\varepsilon)$




## Semiclassical limits $\varepsilon \to 0$

$$\phi_g^\varepsilon \to \phi_g^0(x) = \begin{cases} 1 & 0 < x < 1 \\ 0 & x = 0,1 \end{cases} \qquad E_g^\varepsilon \to \frac{1}{2} \qquad \mu_g^\varepsilon \to 1$$

# For excited states: Box Potential in 1D

- Matched asymptotic approximation for excited states

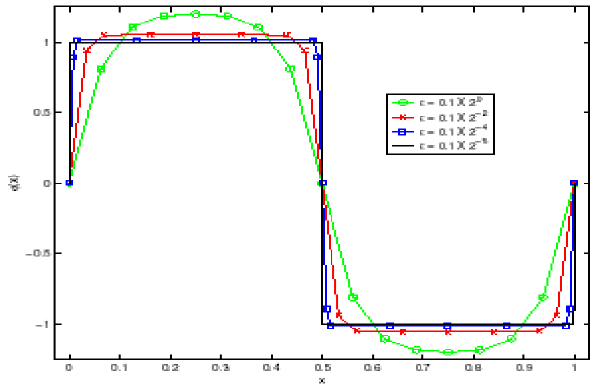
$$\phi_j^\varepsilon(x) \approx \phi_j^{\mathrm{MA}}(x) = \sqrt{\mu_j^{\mathrm{MA}}} \quad [\sum_{l=0}^{[(j+1)/2]} \tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon}(x - \frac{2l}{j+1})) + \sum_{l=0}^{[j/2]} \tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon}(\frac{2l+1}{j+1} - x)) - C_j \tanh(\frac{\sqrt{\mu_g^{\mathrm{MA}}}}{\varepsilon})]$$

  – Approximate chemical potential & energy

$$\mu_j^\varepsilon \approx \mu_j^{\mathrm{MA}} = 1 + 2(j+1)\varepsilon\sqrt{1+(j+1)^2\varepsilon^2} + 2(j+1)^2\varepsilon^2,$$

$$E_j^\varepsilon \approx E_j^{\mathrm{MA}} = \frac{1}{2} + \frac{4}{3}(j+1)\varepsilon\sqrt{1+(j+1)^2\varepsilon^2} + 2(j+1)^2\varepsilon^2,$$

  – Boundary & interior layers $O(\varepsilon)$

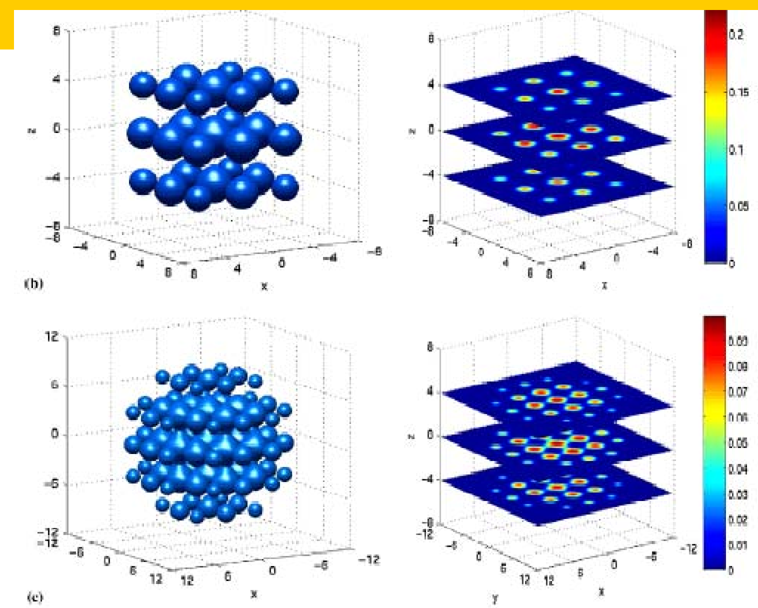



- Semiclassical limits $\varepsilon \to 0$

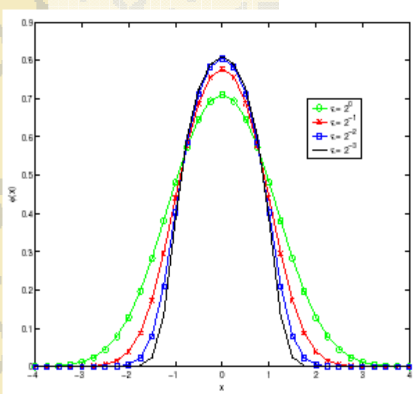
$$\phi_j^\varepsilon \to \phi_j^0(x) = \begin{cases} \pm 1 & x \neq l/(j+1) \\ 0 & x = l/(j+1) \end{cases} \qquad E_j^\varepsilon \to \frac{1}{2} \qquad \mu_j^\varepsilon \to 1$$

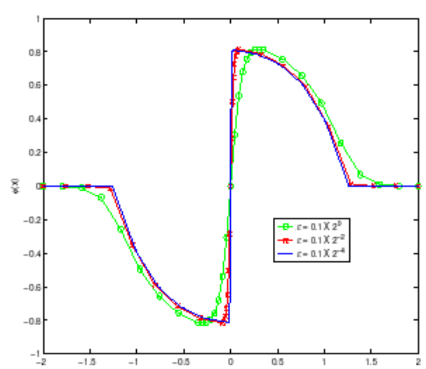
$$E_g^\varepsilon < E_1^\varepsilon < E_2^\varepsilon < \cdots < E_j^\varepsilon < \cdots \Rightarrow \mu_g^\varepsilon < \mu_1^\varepsilon < \mu_2^\varepsilon < \cdots < \mu_j^\varepsilon < \cdots$$

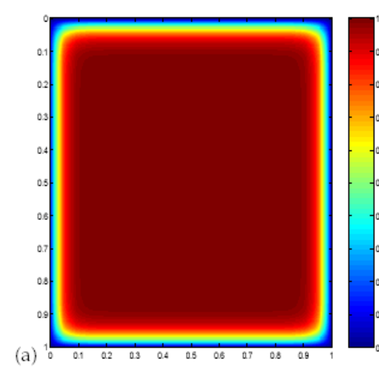
# Extension & numerical computation

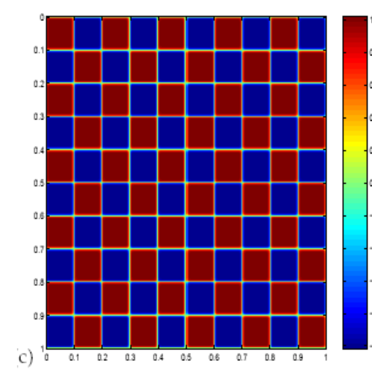


- Extension
  - High dimension
  - Nonzero external potential
- Numerical method & results
  - Normalized gradient flow
  - Backward Euler finite difference method









# For dynamics: Formal limits

- WKB analysis

$$i\varepsilon\,\partial_t \psi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi^\varepsilon + V(\vec{x})\psi^\varepsilon + \beta\,|\psi^\varepsilon|^2\,\psi^\varepsilon$$

$$\psi^\varepsilon(\vec{x},0) := \psi_0^\varepsilon(\vec{x}) = \sqrt{\rho_0^\varepsilon(\vec{x})}\; e^{iS_0^\varepsilon(\vec{x})/\varepsilon}$$

- – Formally assume

$$\psi^\varepsilon = \sqrt{\rho^\varepsilon}\; e^{iS^\varepsilon/\varepsilon}, \quad \vec{v}^\varepsilon = \nabla S^\varepsilon, \quad \vec{J}^\varepsilon = \rho^\varepsilon \vec{v}^\varepsilon$$

- – Geometrical Optics: Transport + Hamilton-Jacobi

$$\partial_t\,\rho^\varepsilon + \nabla \bullet (\rho^\varepsilon\,\nabla S^\varepsilon) = 0,$$

$$\partial_t S^\varepsilon + \frac{1}{2}\left|\nabla S^\varepsilon\right|^2 + V_d(\vec{x}) + \beta\,\rho^\varepsilon = \frac{\varepsilon^2}{2}\frac{1}{\sqrt{\rho^\varepsilon}}\Delta\sqrt{\rho^\varepsilon}$$

# For dynamics: Formal limits

- Quantum Hydrodynamics (QHD): Euler +3rd dispersion

$$\partial_t \rho^\varepsilon + \nabla \bullet (\rho^\varepsilon \vec{v}^\varepsilon) = 0 \qquad P(\rho) = \beta \rho^2 / 2$$

$$\partial_t(\vec{J}^\varepsilon) + \nabla \bullet \left(\frac{\vec{J}^\varepsilon \otimes \vec{J}^\varepsilon}{\rho^\varepsilon}\right) + \nabla P(\rho^\varepsilon) + \rho^\varepsilon \nabla V = \frac{\varepsilon^2}{4} \nabla(\rho^\varepsilon \Delta \ln \rho^\varepsilon)$$

- Formal Limits

$$\partial_t \rho^0 + \nabla \bullet (\rho^0 \vec{v}^0) = 0 \qquad P(\rho) = \beta \rho^2 / 2$$

$$\partial_t(\vec{J}^0) + \nabla \bullet \left(\frac{\vec{J}^0 \otimes \vec{J}^0}{\rho^0}\right) + \nabla P(\rho^0) + \rho^0 \nabla V = 0$$

- Mathematical justification: G. B. Whitman, E. Madelung, E. Wigner, P.L. Lious, P. A. Markowich, F.-H. Lin, P. Degond, C. D. Levermore, D. W. McLaughlin, E. Grenier, F. Poupaud, C. Ringhofer, N. J. Mauser, P. Gerand, R. Carles, P. Zhang, P. Marcati, J. Jungel, C. Gardner, S. Kerranni, H.L. Li, C.-K. Lin, C. Sparber, …..
  - Linear case
  - NLS before caustics

# Efficient Computation

- Solve the limiting QHD system with multi-values
  - Level set method: S. Osher, S. Jin, H.L. Liu, L.T. Cheng, ….
  - K-branch method: L. Goss, P.A. Markowich, …..
- Solve the Liouville equation (obtained by Wigner transform): S. Jin, X. Wen, ……..
- Directly solve NLS: J.C. Bronksi, D.W. McLaughlin, P.A. Markowich, P. Pietra, C. Pohl, P.D. Miller, S. Kamvissis, H.D. Ceniceros, F.R. Tian, W. Bao, S. Jin, P. Degond, N. J. Mauser, H. P. Stimming, …….
  - $\varepsilon$ is small but finite, e.g. 0.01 to 0.1 in typical BEC setups
  - Provide benchmark results for other approaches
  - Hints for analysis after caustics and/or with vacuum

# NLS and its properties

$$i\varepsilon\, \partial_t \psi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi^\varepsilon + V(\vec{x})\psi^\varepsilon + \beta\,|\psi^\varepsilon|^2\,\psi^\varepsilon$$

$$\psi^\varepsilon(\vec{x},0) = \psi_0^\varepsilon(\vec{x}) = A_0^\varepsilon(\vec{x})\, e^{iS_0^\varepsilon(\vec{x})/\varepsilon}$$

- Time reversible
- Time transverse invariant (gauge invariant)

$$V(\vec{x}) \to V(\vec{x}) + \alpha \Rightarrow \psi^\varepsilon \to \psi^\varepsilon\, e^{-it\alpha/\varepsilon} \Rightarrow |\psi^\varepsilon| \quad \text{unchanged}$$

- Mass (wave energy) conservation

$$N_\psi(t) := \int_{\mathbb{R}^d} \left|\psi^\varepsilon(\vec{x},t)\right|^2 d\vec{x} \equiv N_\psi(0) := \int_{\mathbb{R}^d} \left|\psi^\varepsilon(\vec{x},0)\right|^2 d\vec{x} = \int_{\mathbb{R}^d} \left|\psi_0^\varepsilon(\vec{x})\right|^2 d\vec{x}, \qquad t \ge 0$$

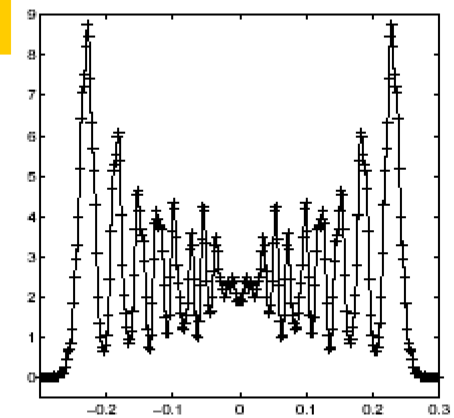
- Energy ( or Hamiltonian) conservation

$$E_\psi(t) := \int_{\mathbb{R}^d} \left[\frac{\varepsilon^2}{2}\left|\nabla\psi^\varepsilon(\vec{x},t)\right|^2 + V(x)\left|\psi^\varepsilon(\vec{x},t)\right|^2 + \tfrac{\beta}{2}\left|\psi^\varepsilon(\vec{x},t)\right|^4\right] d\vec{x} \equiv E_\psi(0), \quad t \ge 0$$

- Dispersion relation without external potential

$$\psi^\varepsilon(x,t) = a\, e^{i(kx-\omega t)} \ \text{(plane wave solution)} \Rightarrow \omega = \frac{\varepsilon^2}{2}k^2 + \beta\,|a|^2$$

# Numerical difficulties




- Explicit vs implicit (or computation cost)
- Spatial/temporal accuracy
- Stability
- Keep the properties of NLS in the discretized level
  - Time reversible & time transverse invariant
  - Mass & energy conservation
  - Dispersion conservation
- Resolution in the semiclassical regime: $0 < \varepsilon \ll 1$

$$\psi^{\varepsilon} = A^{\varepsilon}\, e^{i S^{\varepsilon}/\varepsilon} \quad \text{(solution has wavelength of } O(\varepsilon))$$

# Time-splitting spectral method (TSSP)

- For $[t_n, t_{n+1}]$ , apply time-splitting technique
  - Step 1: Discretize by spectral method & integrate in phase space exactly

$$i\,\varepsilon\,\partial_t \psi^{\varepsilon}(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2 \psi^{\varepsilon}$$

  - Step 2: solve the nonlinear ODE analytically

$$i\,\varepsilon\,\partial_t \psi^{\varepsilon}(\vec{x},t) = V(\vec{x})\psi^{\varepsilon}(\vec{x},t) + \beta\,|\psi^{\varepsilon}(\vec{x},t)|^2\,\psi^{\varepsilon}(\vec{x},t)$$

$$\Downarrow \partial_t(|\psi^{\varepsilon}(\vec{x},t)|^2) = 0 \Rightarrow |\psi^{\varepsilon}(\vec{x},t)| = |\psi^{\varepsilon}(\vec{x},t_n)|$$

$$i\,\varepsilon\,\partial_t \psi^{\varepsilon}(\vec{x},t) = V(\vec{x})\psi^{\varepsilon}(\vec{x},t) + \beta\,|\psi^{\varepsilon}(\vec{x},t_n)|^2\,\psi^{\varepsilon}(\vec{x},t)$$

$$\Rightarrow \psi^{\varepsilon}(\vec{x},t) = e^{-i\,(t-t_n)[V(x)+\beta|\psi^{\varepsilon}(\vec{x},t_n)|^2]/\varepsilon}\,\psi^{\varepsilon}(\vec{x},t_n)$$

- Use 2nd order Strang splitting (or 4th order time-splitting)

# An algorithm in 1D for NLS

- Choose time step: $k = \Delta t$ ; set $t_n = n\,k,\ n = 0,1,\cdots$
- Choose mesh size $h = \Delta x = \frac{b-a}{M}$; set $x_j = a + j\,h$ & $\psi_j^n \approx \psi(x_j, t_n)$
- The algorithm (10 lines code in Matlab!!!) (Bao,Jin,Markowich, JCP,02')

$$\psi_j^{(1)} = e^{-i\,k[V(x_j)+\beta|\psi_j^n|^2]/2\varepsilon}\ \psi_j^n$$

$$\psi_j^{(2)} = \frac{1}{M}\sum_{l=-M/2}^{M/2-1} e^{-i\,\varepsilon\,k\,\mu_l^2/2}\ \hat{\psi}_j^{(1)}\ e^{i\,\mu_l\,(x_j-a)}, \quad j = 0,1,\cdots,M-1$$

$$\psi_j^{n+1} = e^{-i\,k[V(x_j)+\beta|\psi_j^{(2)}|^2]/2\varepsilon}\ \psi_j^{(2)}$$

  – with

$$\mu_l = \frac{l\,\pi}{(b-a)}, \quad \hat{\psi}_l^{(1)} = \sum_{j=0}^{M-1}\psi_j^{(1)}\ e^{-i\,\mu_l\,(x_j-a)}, \quad l = -\frac{M}{2}, -\frac{M}{2}+1, \cdots, \frac{M}{2}-1$$

# Properties of the method

- Explicit & computational cost per time step: $O(M \ln M)$
- Time reversible: yes

$$n+1 \leftrightarrow n \quad \& \quad \psi_j^n \leftrightarrow \psi_j^{n+1} \Rightarrow \quad \text{scheme unchanged!!}$$

- Time transverse invariant: yes

$$V(x) \to V(x) + \alpha \quad (0 \le j \le M) \Rightarrow \psi_j^n \to \psi_j^n \, e^{-ink\alpha/\varepsilon} \Rightarrow |\psi_j^n| \ \text{unchanged!!!}$$

- Mass conservation: yes

$$\|\psi^n\|_{l^2} := h\sum_{j=0}^{M-1} |\psi_j^n|^2 \equiv \|\psi^0\|_{l^2} = \|\psi_0\|_{l^2} := h\sum_{j=0}^{M-1} |\psi_0(x_j)|^2, \quad n = 0,1,\cdots \quad \text{for any } h \,\&\, k$$

- Stability: yes

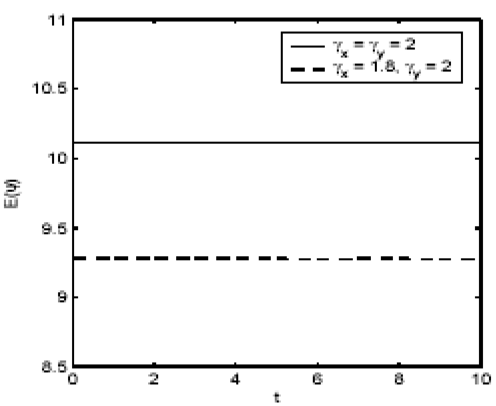
# Properties of the method

- Dispersion relation without potential: yes

$$\psi_j^0 = a\, e^{i k x_j} \ (0 \le j \le M) \Rightarrow \psi_j^n = a\, e^{i(k x_j - \omega t_n)} \ (0 \le j \le M \ \&\ n \ge 0)$$

$$\text{with } \omega = \frac{\varepsilon^2}{2} k^2 + \beta |a|^2 \quad \text{if} \quad M > k$$

  - Exact for plane wave solution
- Energy conservation (Bao, Jin & Markowich, JCP, 02'):
  - cannot prove analytically
  - Conserved very well in computation



# Properties of the method

- Accuracy
  - Spatial: spectral order
  - Temporal: 2nd or 4th order
- Resolution in semiclassical regime (Bao, Jin & Markowich, JCP, 02')
  - Linear case: $\beta = 0$

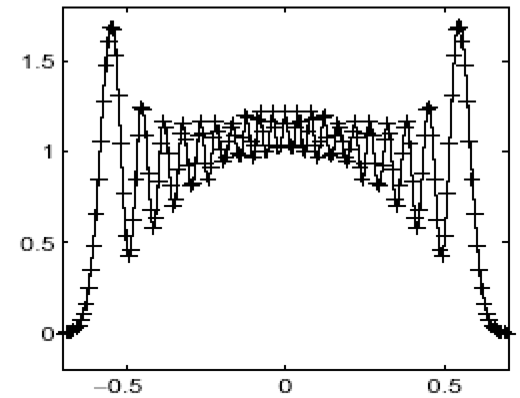
$$h = O(\varepsilon) \quad \& \quad k - \text{independent of } \varepsilon$$

  - Weakly nonlinear case: $\beta = O(\varepsilon)$

$$h = O(\varepsilon) \quad \& \quad k - \text{independent of } \varepsilon$$

  - Strongly repulsive case: $0 < \beta = O(1)$

$$h = O(\varepsilon) \quad \& \quad k = O(\varepsilon)$$

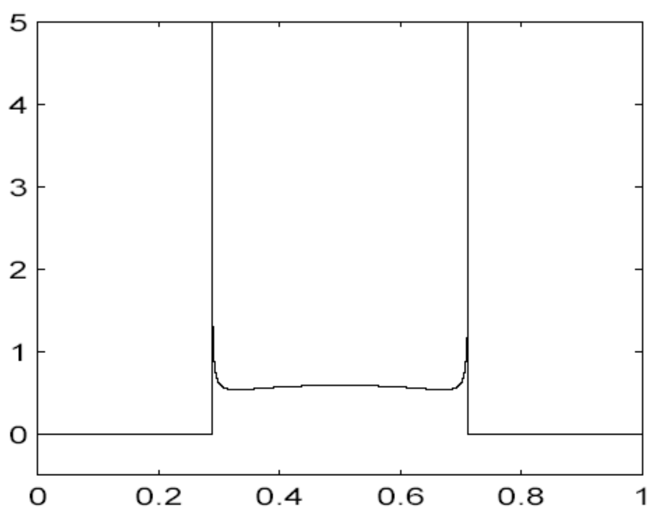



- Error estimate: not available yet!!

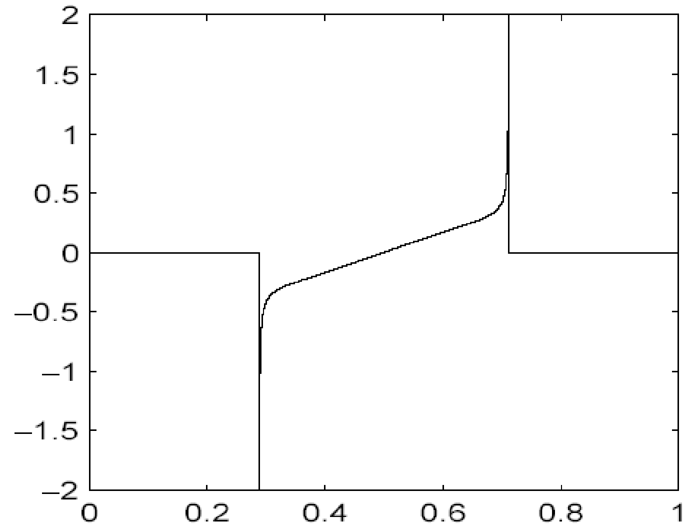
# Numerical Results

- Example 1. Linear Schrodinger equation

$$\beta=0, V(x)=10, A_0(x)=e^{-25(x-0.5)^2}, S_0(x)=-\frac{1}{5}\ln[e^{5(x-0.5)}+e^{-5(x-0.5)}]$$




Density at t=0.54

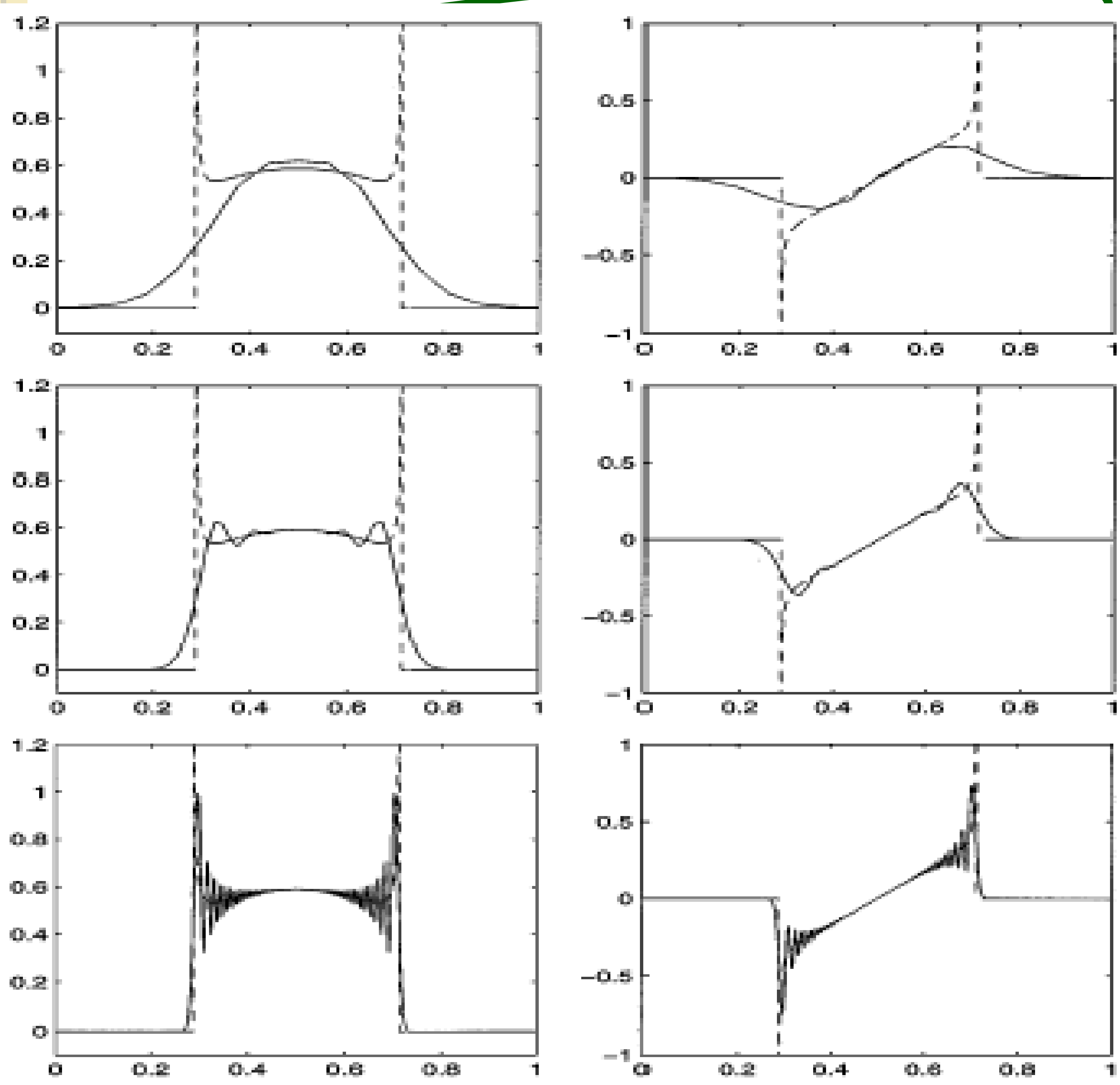


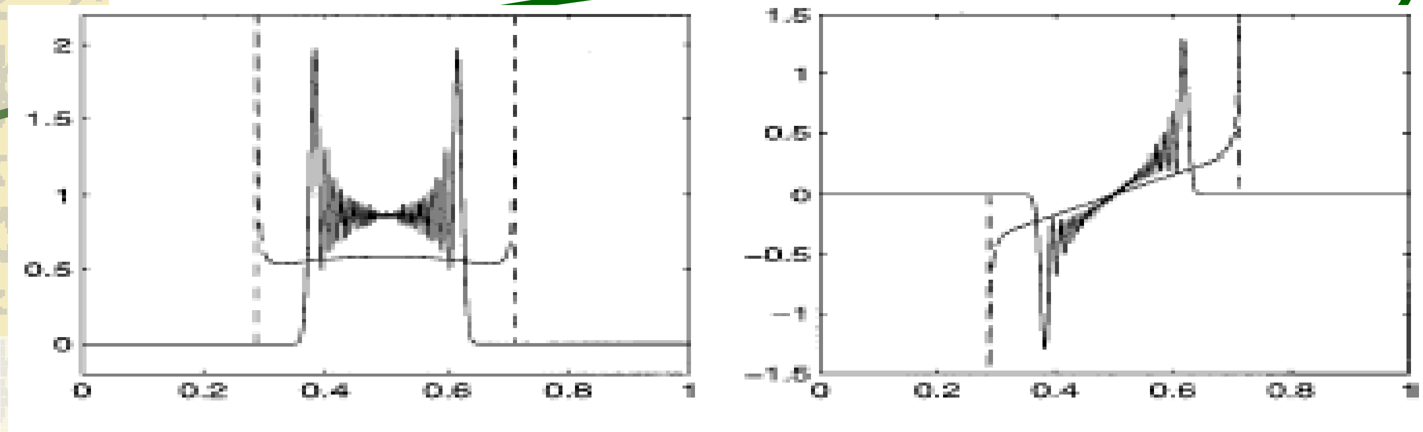

Current at t=0.54

$\varepsilon = 0.0256$

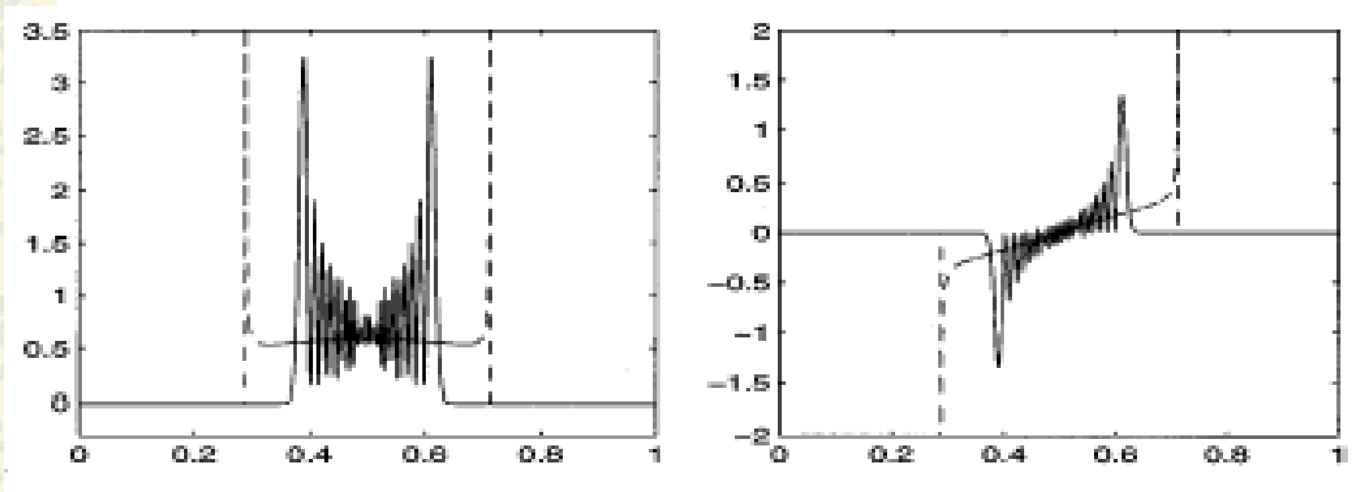
$\varepsilon = 0.0064$

$\varepsilon = 0.0008$






Crank-Nicolson finite difference method

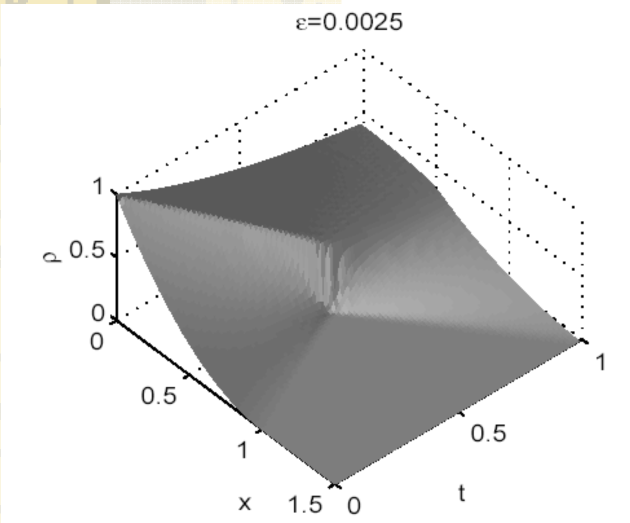


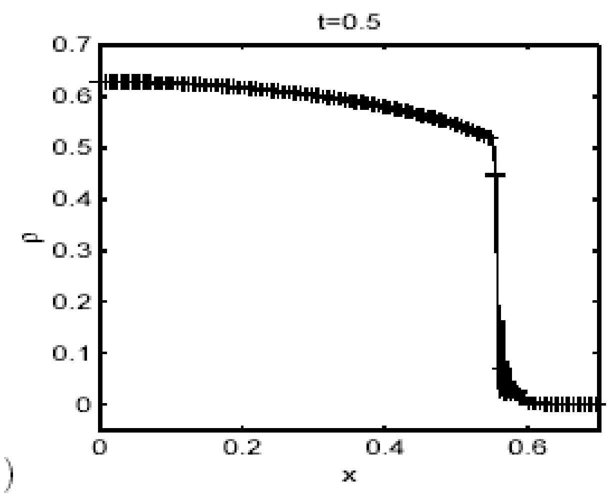

Crank-Nicolson spectral method

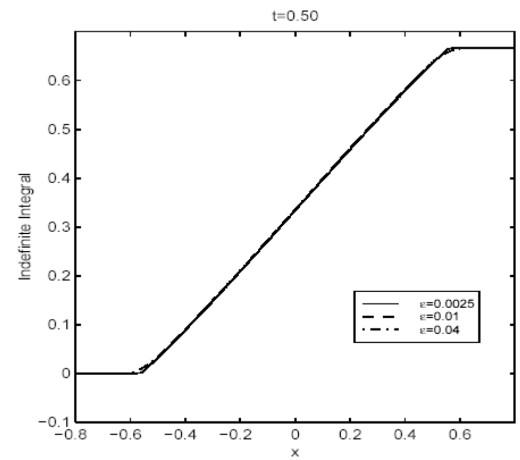
# Numerical Results

- Example 2. NLS with defocusing nonlinearity

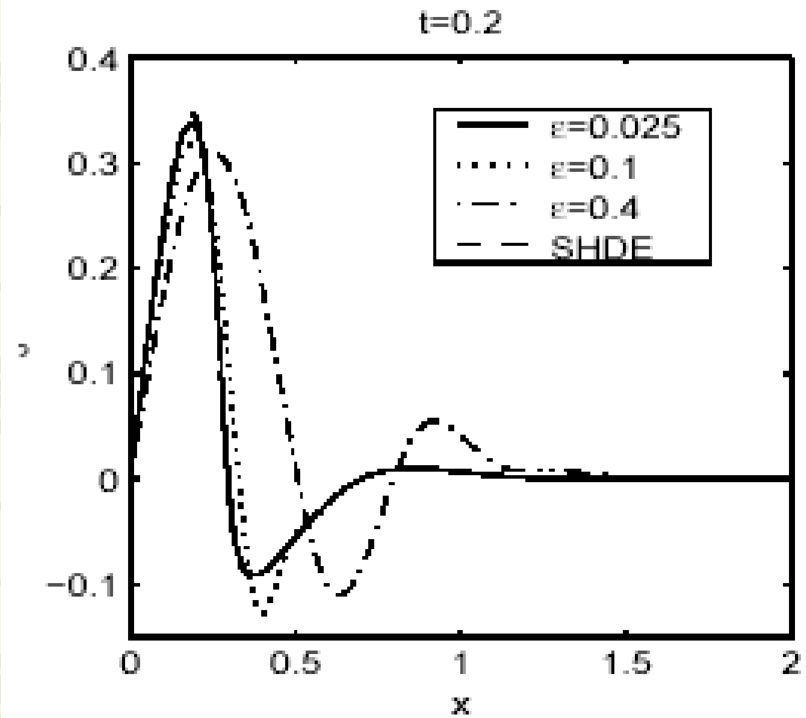
$$\beta = 1, V(x) = 0, A_0(x) = \begin{cases} 1 - |x| & |x| < 1 \\ 0 & \text{otherwise} \end{cases}, S_0(x) = -\ln[e^x + e^{-x}]$$



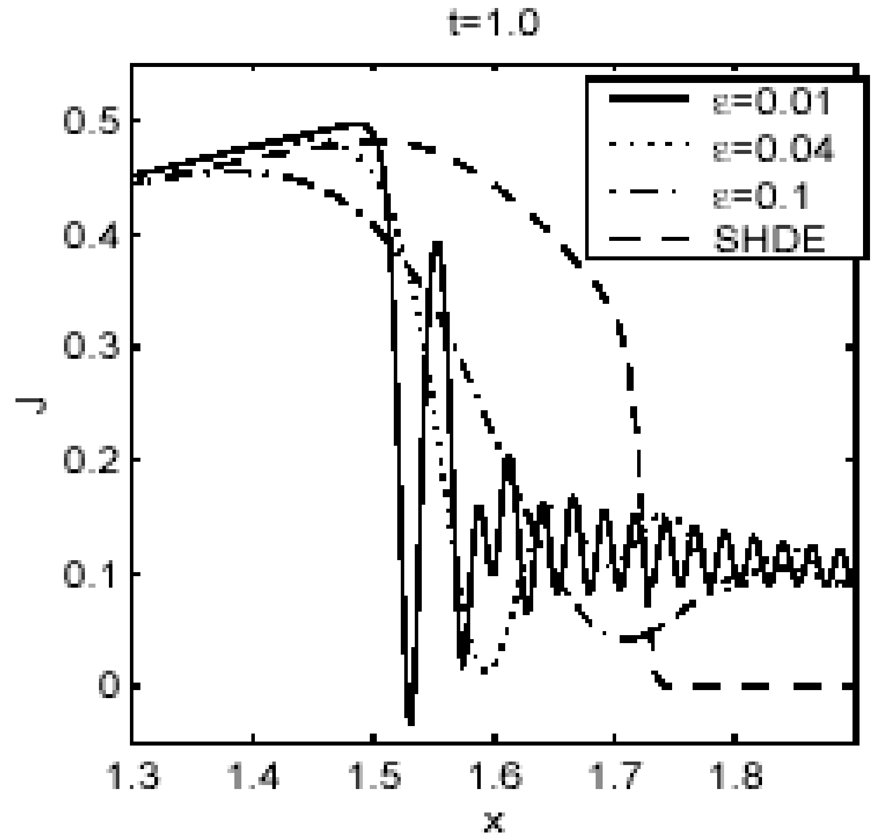




$$\int_0^t \rho^{\varepsilon}(x, s)\, ds$$




Before caustics



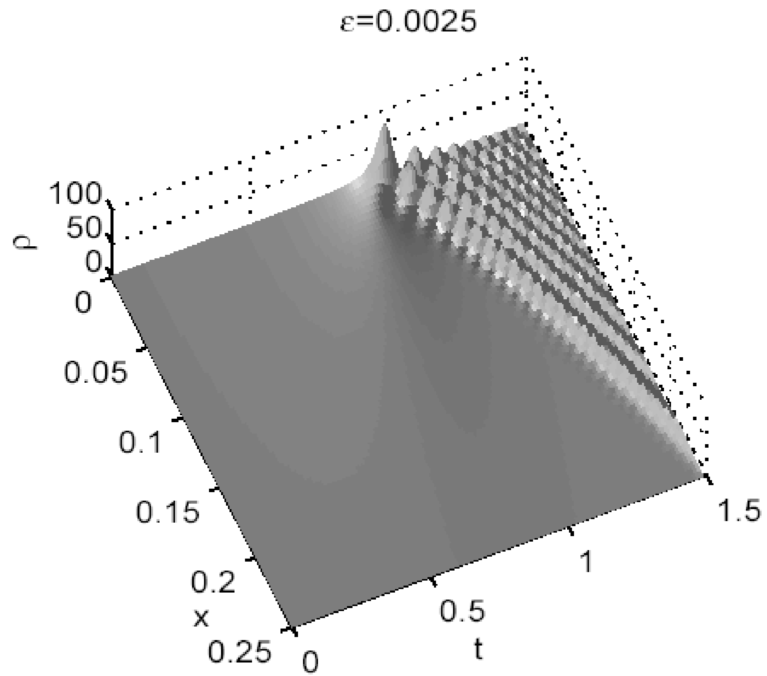

After caustics

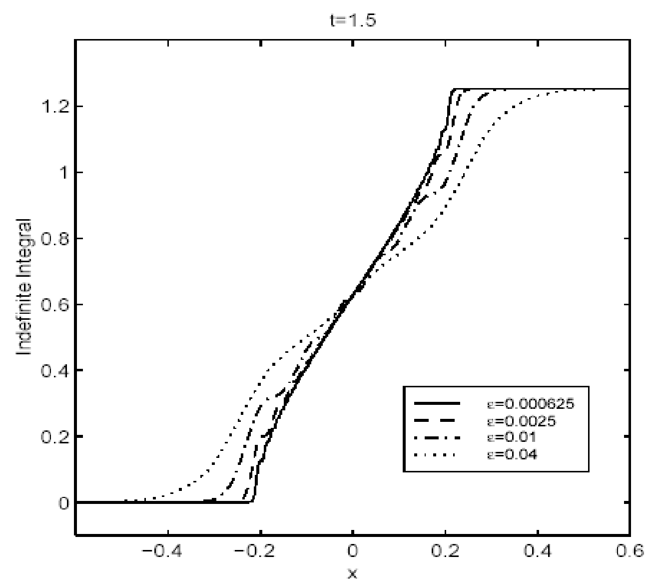
- Observations
  - Before caustics: converge strongly & converge to QHD
  - After caustics: converge weakly but the location of discontinuity is different to QHD!!

# Numerical Results

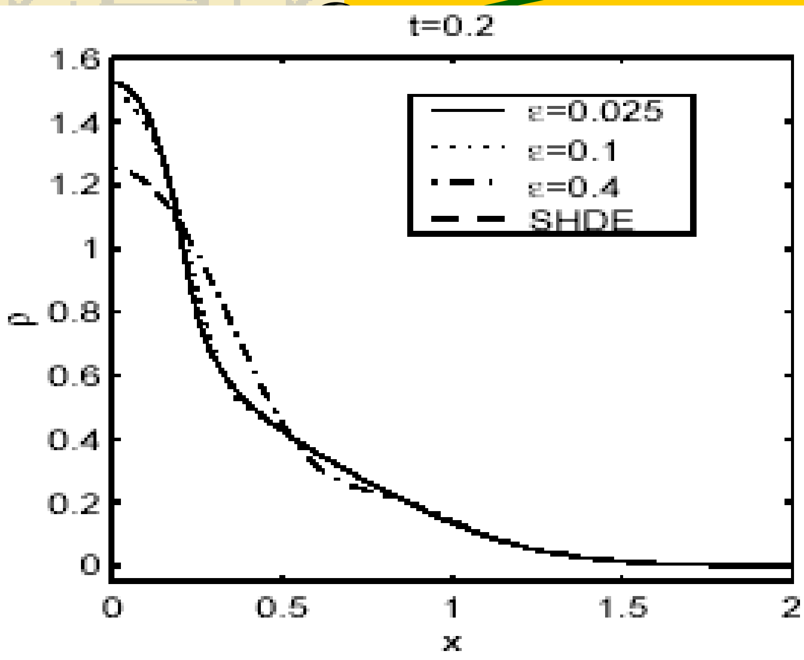
- Example 2. NLS with focusing nonlinearity (Bao,Jin,Markowich, SISC,03')

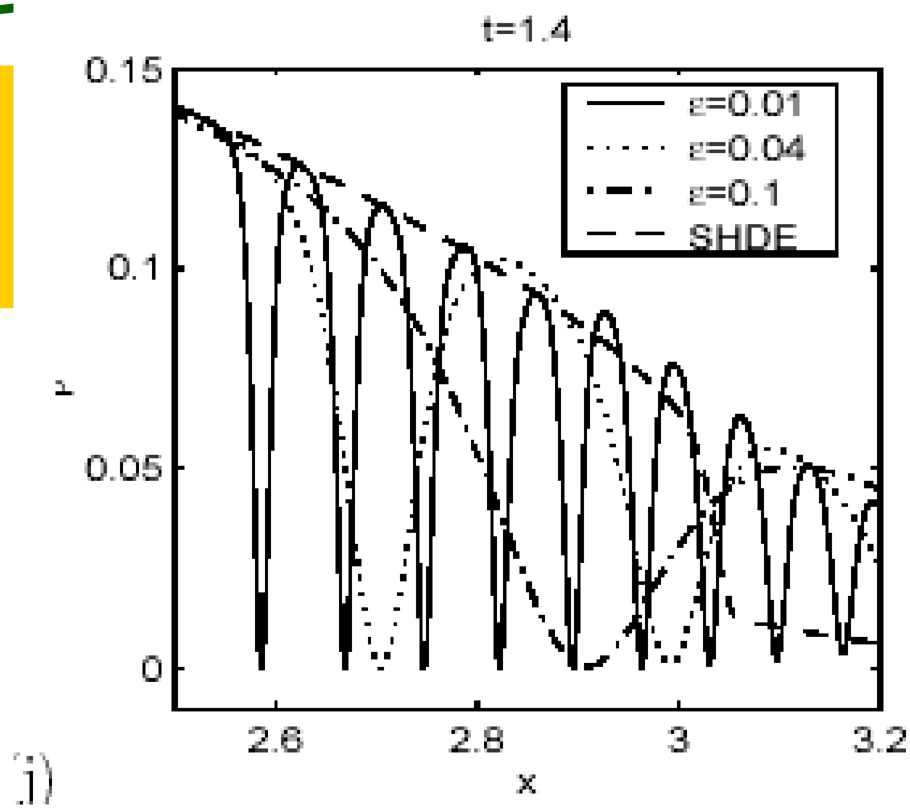
$$\beta = -\varepsilon, V(x) = 0, A_0(x) = e^{-x^2}, S_0(x) = 0$$




$$\int_0^t \rho^{\varepsilon}(x,s)\,ds$$



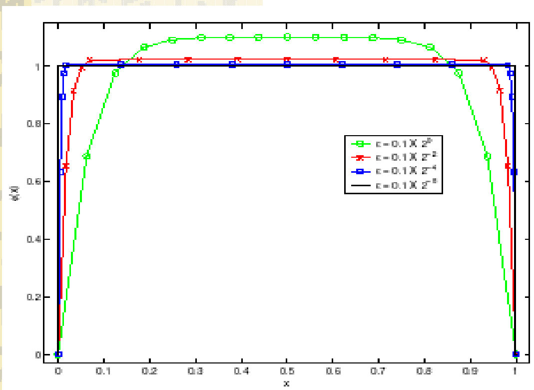

Before caustics

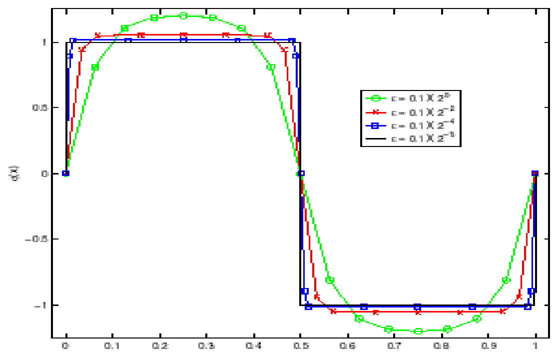
After caustics

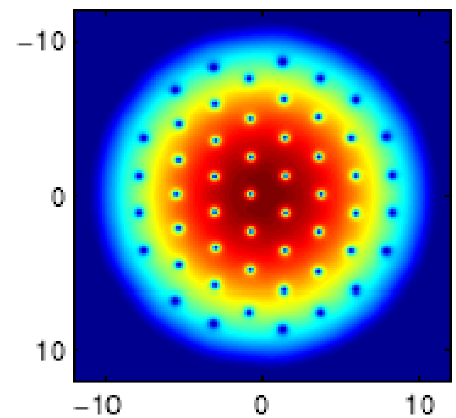
- Observations
  - Before caustics: converge strongly & converge to QHD
  - After caustics: converge weakly but the location of discontinuity is different to QHD!!

# Initial data with vacuum

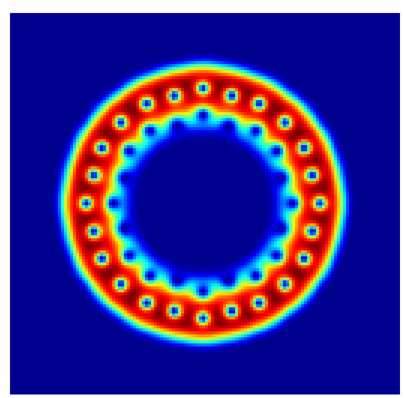
- Vacuum at a point

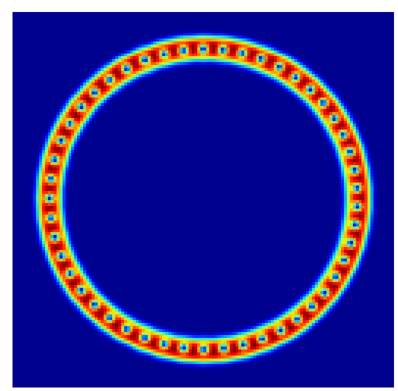




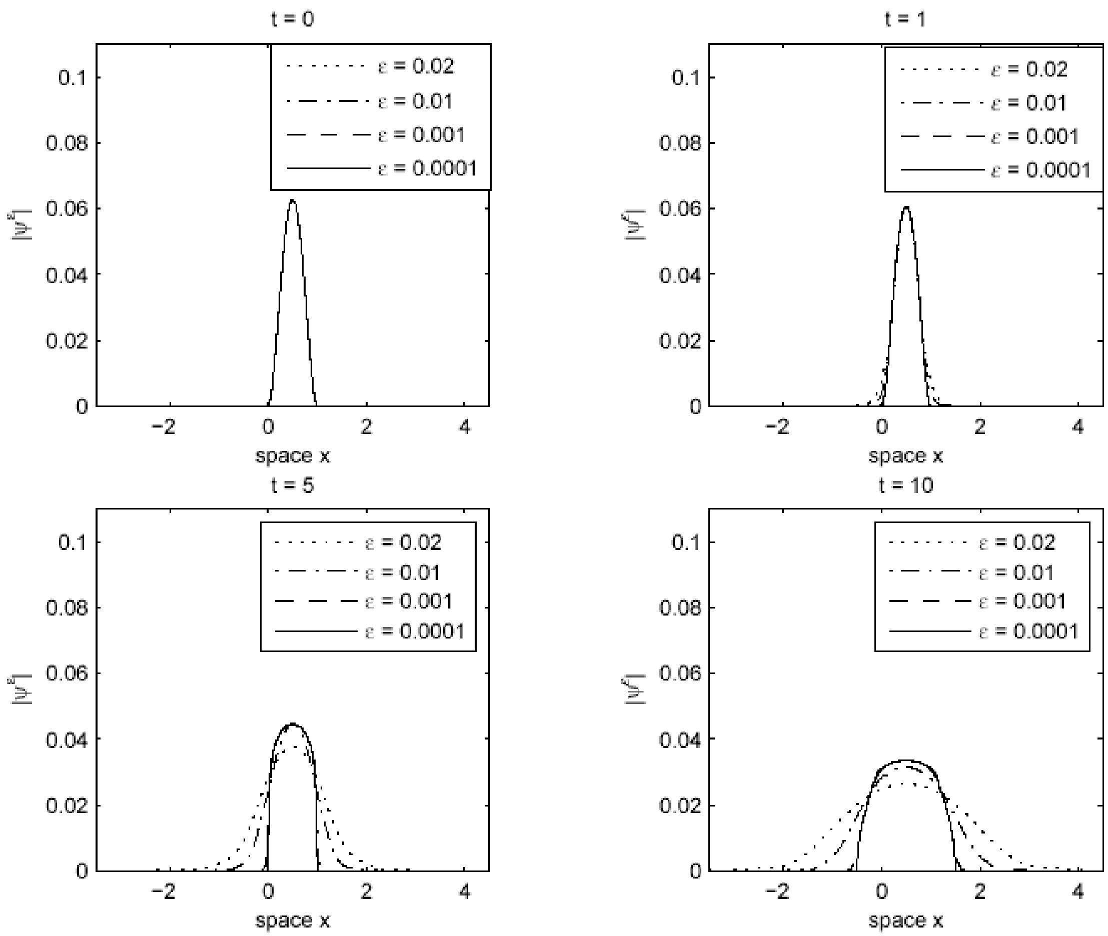


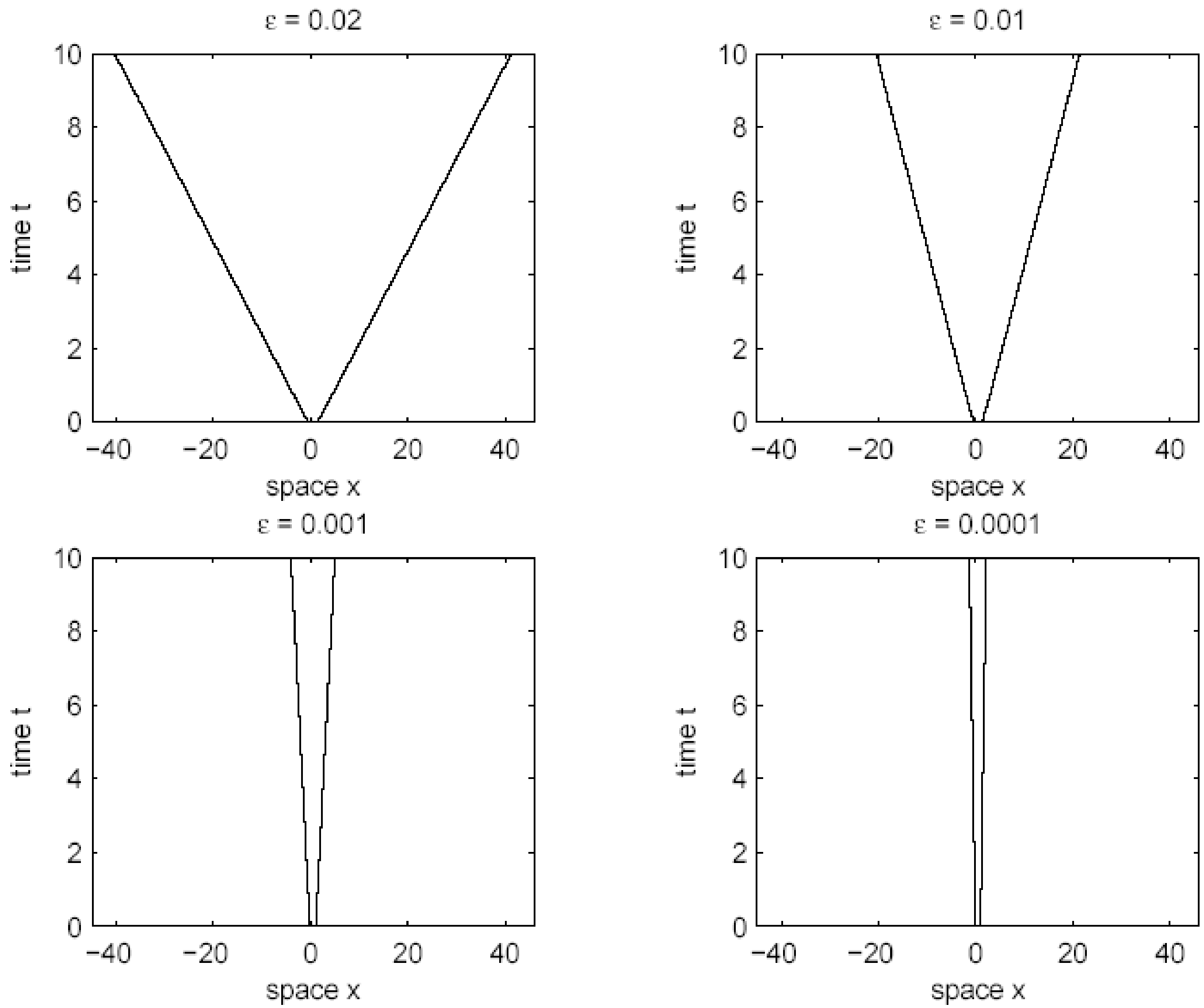

- Vacuum at a region





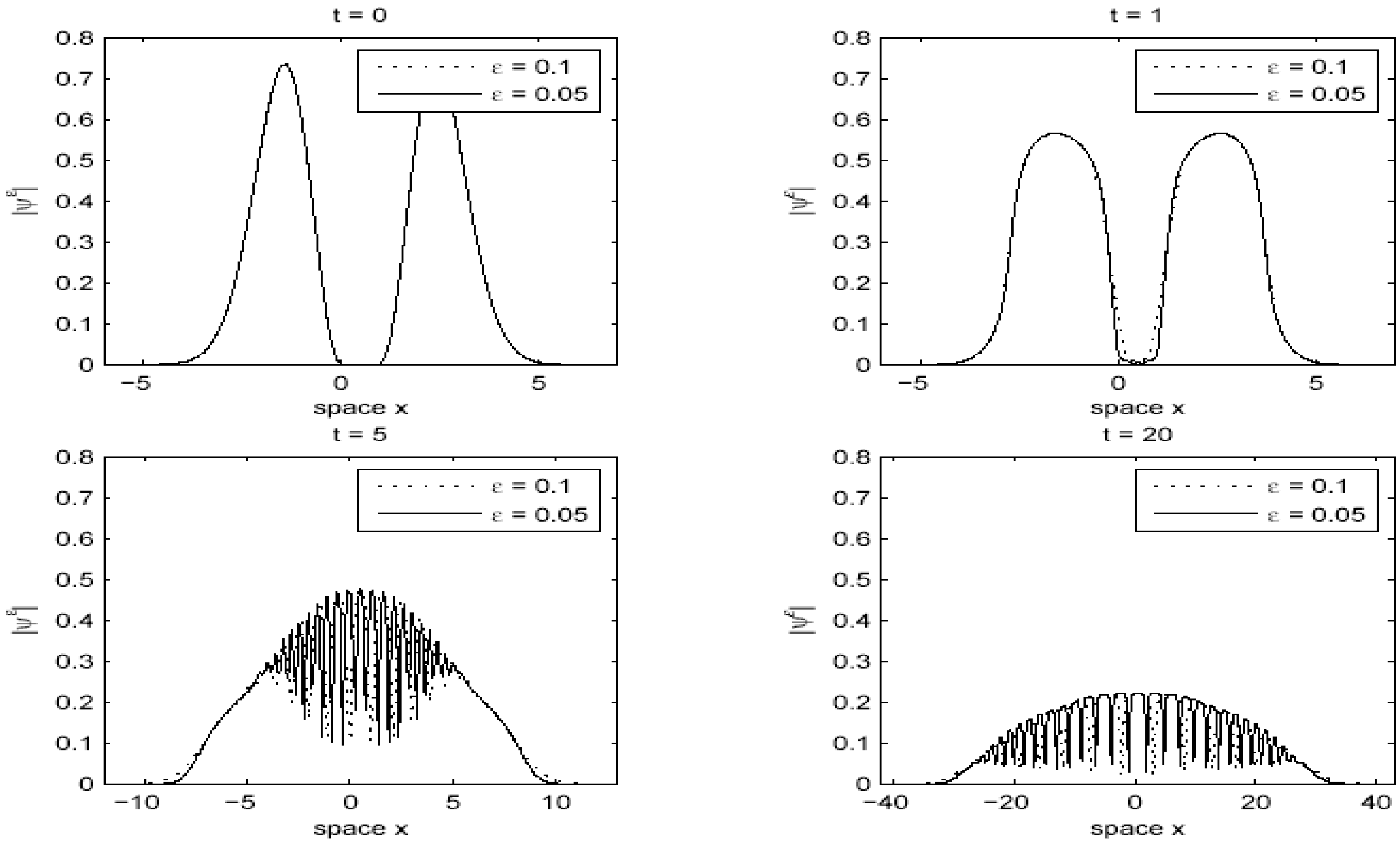
$$\beta=1, V(x)=0, A_0(x)=\begin{cases} x^2(1-x)^2 & 0<x<1 \\ 0 & \text{otherwise} \end{cases}, S_0(x)=0$$

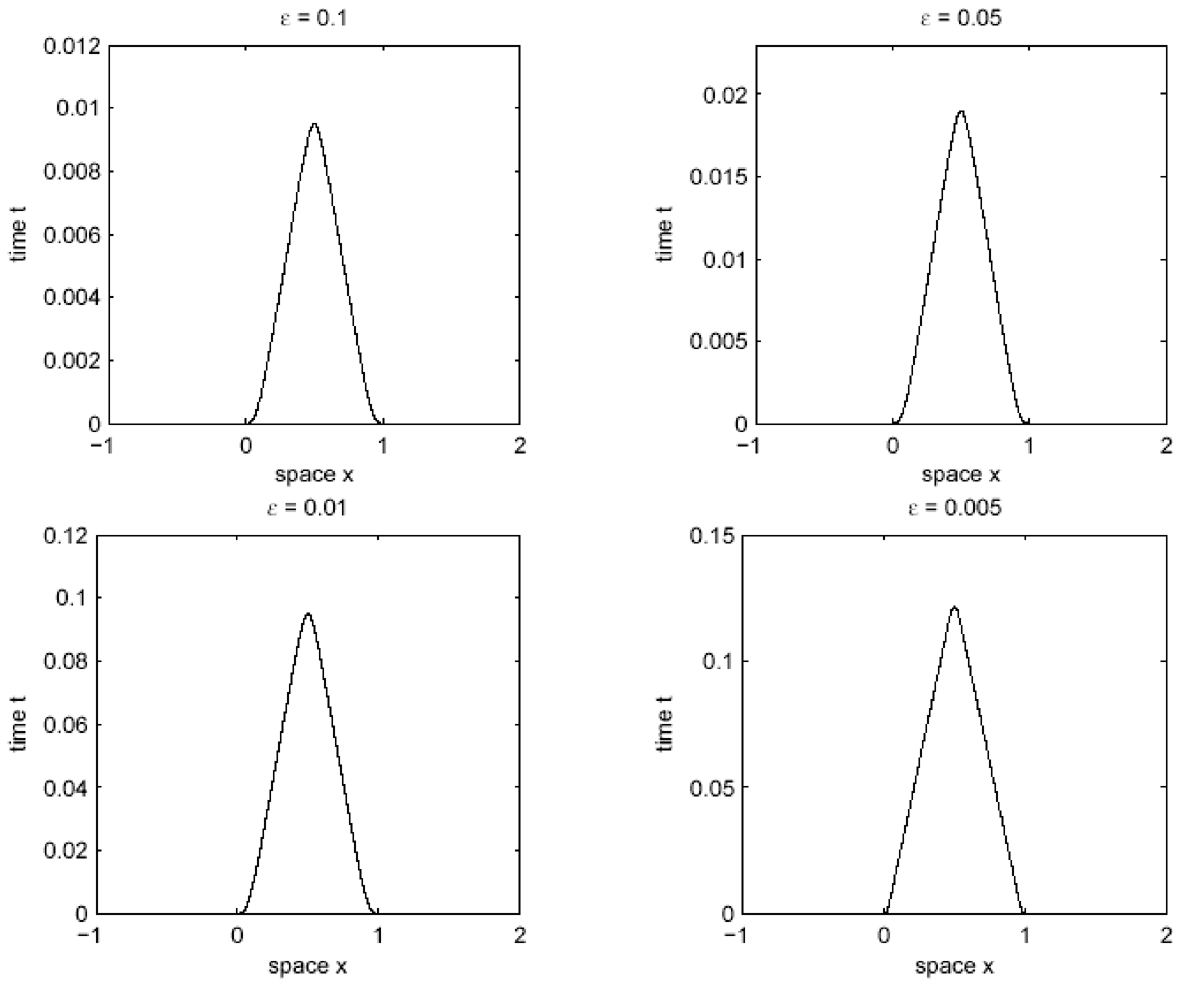




ε = 0.02
ε = 0.01
ε = 0.001
ε = 0.0001
time t
space x
10
8
6
4
2
0
−40
−20
0
20
40

$$\beta = 1, V(x) = 0, A_0(x) = \begin{cases} x^2 e^{-x^2} & x < 0 \\ 0 & 0 \le x \le 1, S_0(x) = 0 \\ (x-1)^2 e^{-(x-1)^2} & x > 1 \end{cases}$$






## Observations

- For fixed $\mathcal{E}$ : the location of vacuum moves and interact
- When $\varepsilon \to 0$ : compare the motion of vacuum with Euler system, compressible Navier-Stokes equations (with Z.P. Xin & H.L. Li,ongoing)

# Difficulties in rotating frame

- GPE in a rotational frame

$$i\,\varepsilon\frac{\partial}{\partial t}\psi^{\varepsilon}(\vec{x},t)=[-\frac{\varepsilon^{2}}{2}\nabla^{2}+V(\vec{x})-\varepsilon\,\Omega\,L_{z}+|\psi^{\varepsilon}|^{2}]\psi^{\varepsilon}$$

  – Angular momentum rotation

$$L_{z}:=xp_{y}-yp_{x}=-i(x\partial_{y}-y\partial_{x})\equiv-i\partial_{\theta}\,,\quad \vec{L}=\vec{x}\times\vec{P},\quad \vec{P}=-i\nabla$$

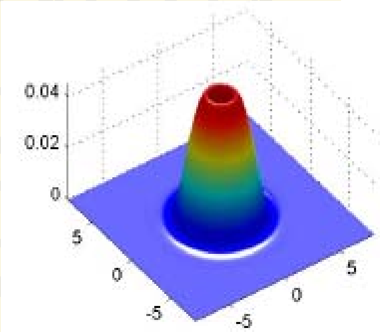
  – Formal WKB analysis

$$\partial_{t}\rho^{\varepsilon}+\nabla\bullet(\rho^{\varepsilon}\vec{v}^{\varepsilon})+\Omega\hat{L}_{z}\rho^{\varepsilon}=0,\qquad \hat{L}_{z}:=(x\partial_{y}-y\partial_{x})\equiv\partial_{\theta}$$

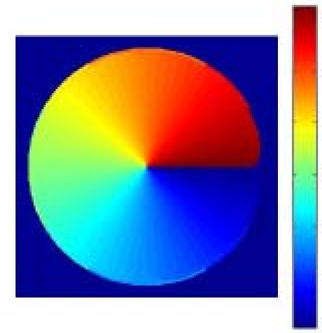
$$\partial_{t}(\vec{J}^{\varepsilon})+\nabla\bullet(\frac{\vec{J}^{\varepsilon}\otimes\vec{J}^{\varepsilon}}{\rho^{\varepsilon}})+\nabla P(\rho^{\varepsilon})+\rho^{\varepsilon}\nabla V_{d}+\Omega\hat{L}_{z}\vec{J}^{\varepsilon}+\Omega A\,\vec{J}^{\varepsilon}=\frac{\varepsilon^{2}}{4}\nabla(\rho^{\varepsilon}\Delta\ln\rho^{\varepsilon})$$

$$P(\rho)=\rho^{2}/2\,,\qquad \vec{J}^{\varepsilon}=\rho^{\varepsilon}\vec{v}^{\varepsilon},\qquad A=\begin{pmatrix}0&1\\-1&0\end{pmatrix}$$

  – Analysis & critical threshhold: E. Tadmor, H.L Liu, C. Sparber, ….




# Difficulties in rotational frame



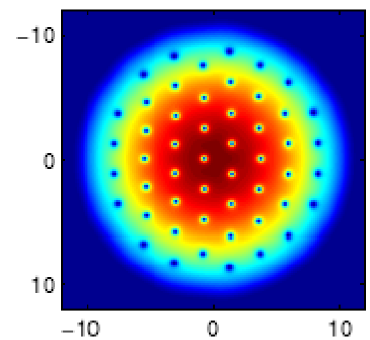

- Efficient computation for rotating GPE
  - Polar (2D) & cylindrical (3D) coordinates (Bao,Du,Zhang,S
  - ADI techniques (Bao, Wang, JCP, 06')
  - Generalized Laguerre-Fourier-Hermite function (Bao, Shen,08')
- Typical initial data: vacuum+two-scale in phase

$$\psi_0(x,y)=(x+i\,y)e^{-(x^2+y^2)/2}\,e^{-iS^0(x,y)/\varepsilon}\Rightarrow\psi^\varepsilon(\vec{x},t)=\vec{A}^\varepsilon(\vec{x},t)e^{iS^\varepsilon(\vec{x},t)/\varepsilon},\quad \vec{A}^\varepsilon=a^\varepsilon+i\,b^\varepsilon$$

- Grenier's approach (Grenier, 98'; Carles, CMP, 07')

$$\partial_t\vec{A}^\varepsilon+\nabla S^\varepsilon\cdot\nabla\vec{A}^\varepsilon+\frac{1}{2}\vec{A}^\varepsilon\Delta S^\varepsilon-\Omega\,\widehat{L}_z\vec{A}^\varepsilon=\frac{i\varepsilon}{2}\Delta\vec{A}^\varepsilon$$

$$\partial_t S^\varepsilon+\frac{1}{2}\left|\nabla S^\varepsilon\right|^2+V_d(\vec{x})+|\vec{A}^\varepsilon|^2-\Omega\,\widehat{L}_z S^\varepsilon=0$$



# Difficulties in system

- Couple GPE system

$$i\varepsilon\, \partial_t \psi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi^\varepsilon + V(\vec{x})\psi^\varepsilon + [\beta_1 |\psi^\varepsilon|^2 + \delta |\phi^\varepsilon|^2]\psi^\varepsilon + \lambda\, \phi^\varepsilon$$

$$i\varepsilon\, \partial_t \phi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\phi^\varepsilon + V(\vec{x})\phi^\varepsilon + [\delta |\psi^\varepsilon|^2 + \beta_2 |\phi^\varepsilon|^2]\phi^\varepsilon + \lambda\, \psi^\varepsilon$$

- Analysis
  - Formal WKB doesn't work!!!! No techniques are needed!
  - For linear case, Wigner transform can be applied; for nonlinear case???
  - V(x) is periodic and depends on $\varepsilon$
- Efficient computation for coupled GPE:
  - Numerical method (Bao, MMS, 04'; Bao, Li, Zhang, Physica D, 07')

# Conclusions

- For time-independent NLS
  - Matched asymptotic approximation
  - Boundary/interior layers
  - Semiclassical limits of ground and excited states
- For dynamics of NLS
  - Formal WKB analysis
  - Time-splitting spectral method (TSSP) for computation
  - Semiclassical limits: convergence, caustics, QHD, vacuum
  - Difficulties in rotational frame and system
  - Analysis and efficient computation are two important tools