Numerical Methods for the Dynamics of the Nonlinear Schrodinger / Gross-Pitaevskii Equations

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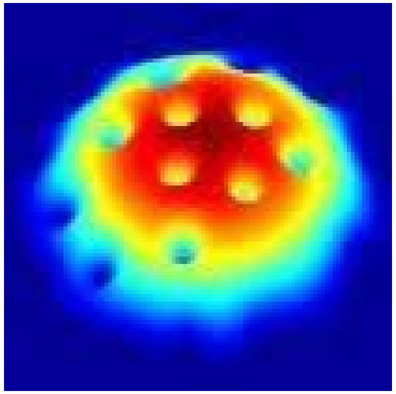
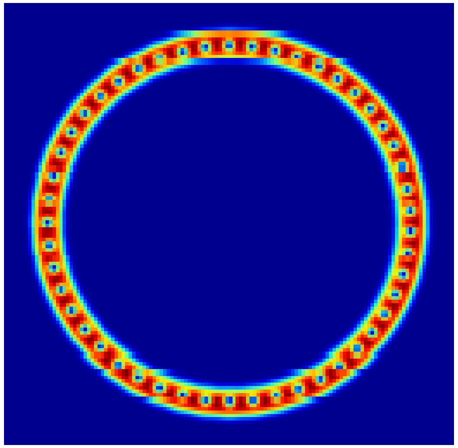


Vortex@ENS

Outline

- Nonlinear Schrodinger / Gross-Pitaevskii equations
- Dynamical properties
  - Conserved quantities
  - Center-of-mass & an analytical solution
  - Specific solutions – soliton in 1D



- Numerical methods
  - Finite difference time domain (FDTD) methods
  - Time-splitting spectral (TSSP) method
  - Applications – atomic transport, collapse & explosion of a BEC, vortex lattice dynamics
  - Semiclassical limit and its computation
- Extension to -- rotation, nonlocal interaction & system
- Conclusions

NLSE / GPE

- The nonlinear Schrodinger equation (NLSE) --- Schrodinger 1925; – Gross & Pitaevskii 1961

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

  - 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
  - β : given interaction constant
    - =0: linear; >0: repulsive & <0: attractive
  - $0 < \varepsilon \le 1$: scaled Planck constant
    - ($\varepsilon = 1$: standard; $0 < \varepsilon \ll 1$ & $\beta = \pm 1$: semiclassical)

The Schrodinger equation

$$i\hbar\,\partial_t\psi(\vec{x},t)=\left(-\frac{\hbar^2}{2m}\nabla^2+V(\vec{x})\right)\psi(\vec{x},t)\overset{\psi=e^{-iEt/\hbar}\phi}{\Rightarrow}H\phi=E\phi$$

- Derived by Ewin Schrodinger in 1925 —Nobel prize in 1933
- It describes the evolution over time of a physical system in which quantum effects, such as wave–particle duality, are significant in quantum mechanics.
- Informal history
  - Max Planck (1858-1947) proposed light is emitted in discrete quanta of energy in 1900 (Nobel Prize in 1918 for energy quanta). Planck-Einstein relation: $E = h\nu$
  - Albert Einstein (1879-1955) proposed light is propagated and absorbed in quanta in 1905 –photon- (Nobel Prize in 1921 for photoelectronic effect). Mementum: $p = E/c = h/\lambda$
  - Louis de Broglie (1892-1987) proposed matter behaves like a wave—wave-matter duality (Nobel Prize in 1927 for wave-like behaviour of matter). wavelength: $\lambda = h/p$
  - Peter Debye told Ewin Schrodinger: ``your research is not focus on a good direction, can you read Louis de Broglie's work on wave-matter and give a report in my seminar''. ``The idea is naïve and interesting, if it is wave, there should be a wave equation!!!''

The Schrodinger equation

- Formal derivation via first quantization

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

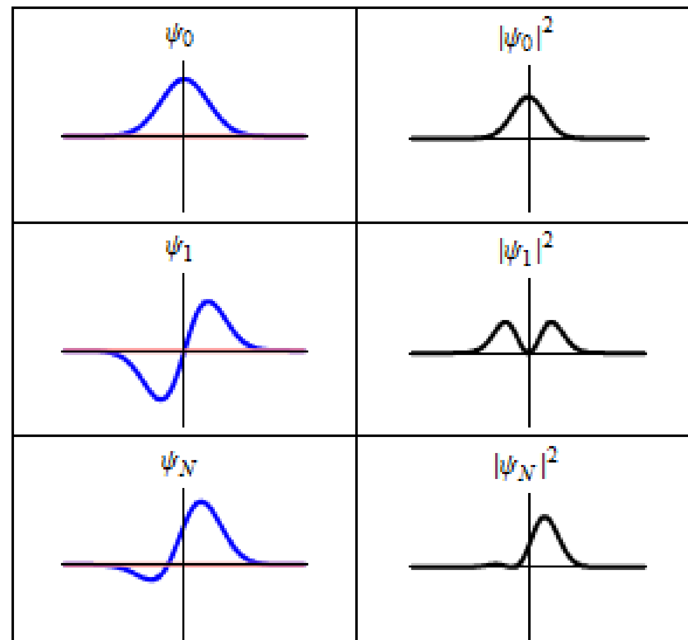
- Continuity equation

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

  – With probability density and current

$$\rho = |\psi|^2 = \psi^*\psi, \qquad j = \frac{-i\hbar}{2m}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right)$$

- Analytical solutions $-\frac{\hbar^2}{2m}\nabla^2\psi + V(\vec{x})\psi = E\psi$
  – free particle, step potential,
  – box potential & harmonic potentials,…



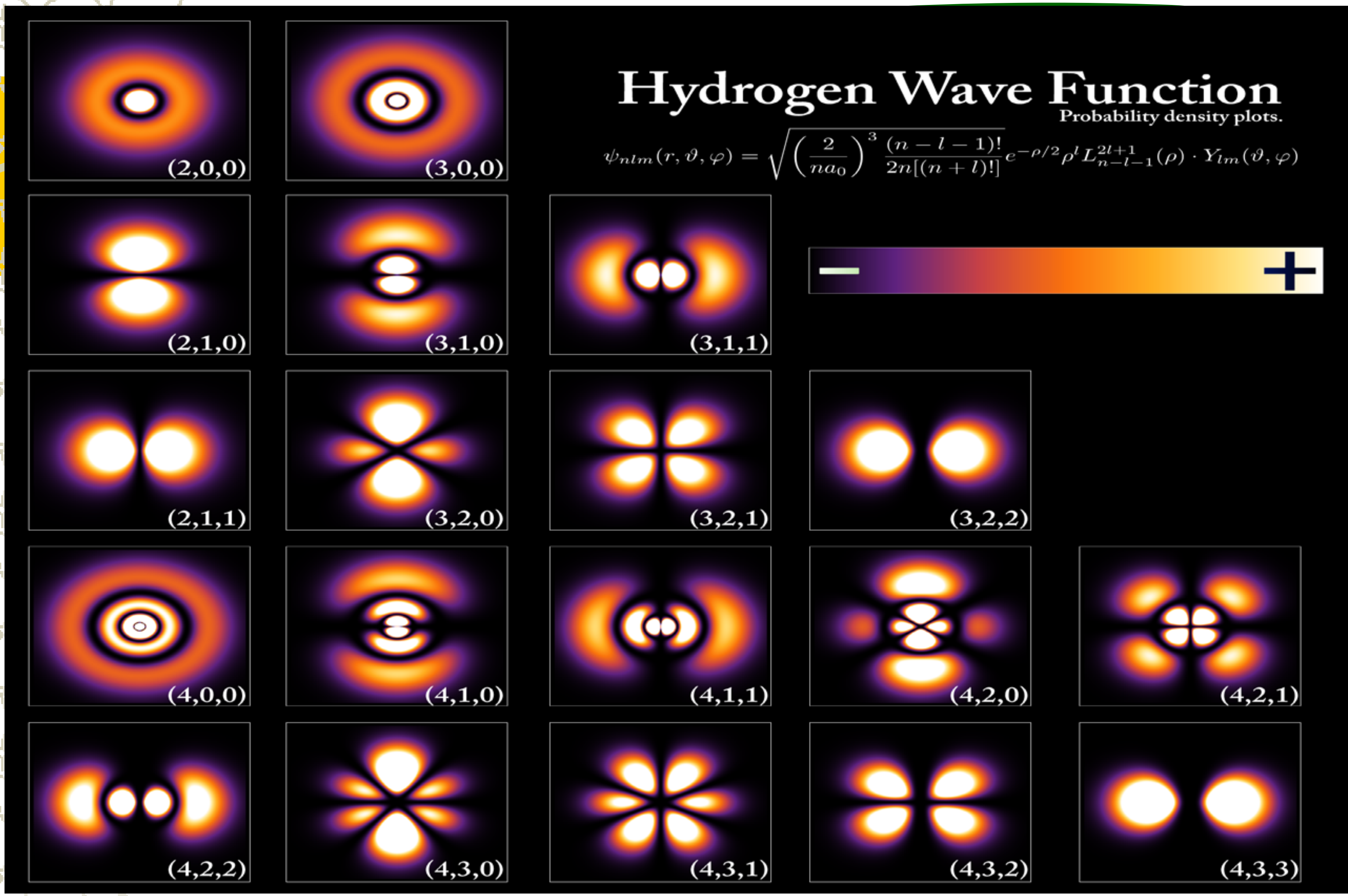
Quantum many-body problems

- Central role via many-body (N-body) problem
  - quantum physics & chemistry
  - materials science, electronic structure --- DFT
  - mathematical physics, …..

$$\Psi := \Psi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N, t)$$

$$i\hbar\,\partial_t \Psi = \left[\sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m}\Delta_j + V(\vec{x}_j)\right) - \sum_{j=1}^{N}\sum_{l=1}^{K}\frac{Z_l}{\left|\vec{x}_j - \vec{a}_l\right|} + \sum_{1\le j<l\le N}\frac{1}{\left|\vec{x}_j - \vec{x}_l\right|}\right]\Psi$$

- Relativistic quantum physics
  - Klein-Gordon equation for spinless particle -- pion
  - Dirac equation for spin particle -- electron and quarks



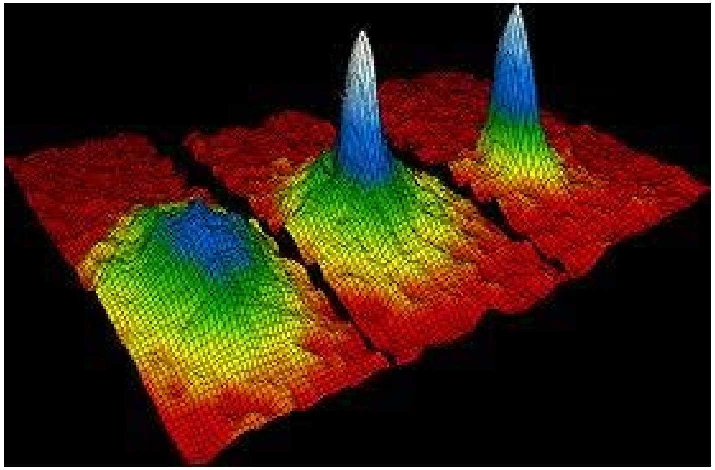
$$N=1\,\&\,K=1\Rightarrow -\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec{r})-\frac{e^2}{4\pi\varepsilon_0 r}\psi(\vec{r})=E\psi(\vec{r}),\qquad \mu=\frac{m_e m_p}{m_e+m_p},\Leftarrow \text{spectrum of Hydrogen atom}$$

$$\Rightarrow \psi_{nlm}(r,\theta,\phi)=\sqrt{\left(\frac{2}{na_0}\right)^3\frac{(n-l-1)!}{2n[(n+l)!]}}\,e^{-r/(na_0)}\left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right)Y_l^m(\theta,\phi),\ n\geq 1, l=0,\ldots,n-1, |m|\leq l$$

Schrödinger equation as part of a monument in front of Warsaw University's Centre of New Technologies

Model for BEC via GPE/NLSE

- Bose-Einstein condensation (BEC):
  - Bosons at nano-Kevin temperature
  - Many atoms occupy in one obit -- at quantum mechanical ground state
  - Form like a `super-atom', New matter of wave --- fifth state
- Theoretical prediction – S. Bose & E. Einstein 1924'
- Experimental realization – JILA 1995'
- 2001 Nobel prize in physics
  - E. A. Cornell, W. Ketterle, C. E. Wieman
- Mean-field approximation
  - Gross-Pitaevskii equation (GPE) :
    - E.P. Gross 1961'; L.P. Pitaevskii 1961'



BEC@ JILA

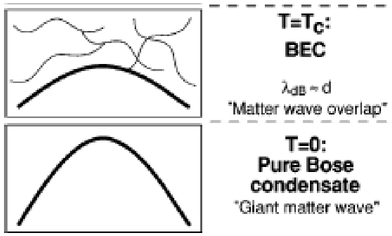
Model for a BEC at zero temperature

– with N identical bosons

- N-body problem –$3N+1$ dim. (linear) Schrodinger equation

$$i\hbar\partial_t \Psi_N(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t) = H_N \Psi_N(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t), \qquad \text{with}$$

$$H_N = \sum_{j=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla_j^2 + V(\vec{x}_j)\right) + \sum_{1\le j<k\le N} V_{\text{int}}(\vec{x}_j - \vec{x}_k)$$



- Hartree ansatz $\Psi_N(\vec{x}_1,\vec{x}_2,\ldots,\vec{x}_N,t) = \prod_{j=1}^{N}\psi(\vec{x}_j,t), \vec{x}_j \in \mathbb{R}^3$
- Fermi interaction $V_{\text{int}}(\vec{x}_j - \vec{x}_k) = g\delta(\vec{x}_j - \vec{x}_k)$ with $g = \frac{4\pi\hbar^2 a_s}{m}$
- Dilute quantum gas -- two-body elastic interaction

$$E_N(\Psi_N) := \int_{\mathbb{R}^{3N}} \bar{\Psi}_N H_N \Psi_N \, d\vec{x}_1 \cdots d\vec{x}_N \approx N E(\psi) \text{--energy per particle}$$

Model for a BEC – with N identical bosons

- Energy per particle – mean field approximation (Lieb et al, 00')

$$E(\psi)=\int_{\mathbb{R}^3}\left[\frac{\hbar^2}{2m}|\nabla\psi|^2+V(\vec{x})|\psi|^2+\frac{Ng}{2}|\psi|^4\right]d\vec{x}\quad \text{with}\quad \psi:=\psi(\vec{x},t)$$

- Dynamics (Gross, Pitaevskii 1961'; Erdos, Schlein & Yau, Ann. Math. 2010')

$$i\hbar\partial_t\psi(\vec{x},t)=\frac{\delta E(\psi)}{\delta\overline{\psi}}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{x})+Ng|\psi|^2\right]\psi,\quad \vec{x}\in\mathbb{R}^3$$

- Proper non-dimensionalization & dimension reduction– GPE/NLSE

$$i\,\partial_t\psi(\vec{x},t)=-\frac{1}{2}\nabla^2\psi+V(\vec{x})\psi+\beta\,|\psi|^2\,\psi,\quad \vec{x}\in\mathbb{R}^d\quad \text{with}\quad \beta=\frac{4\pi N a_s}{x_s}$$

Laser beam propagation

- Nonlinear wave (or Maxwell) equations

$$c(|u|)^{-2}\partial_{tt}u(\vec{x},t)-\Delta u(\vec{x},t)=0, \qquad \vec{x}\in\mathbb{R}^3, \quad t>0$$

- Helmholtz equation – time harmonic $\quad u(\vec{x},t)=e^{i\omega t}v(\vec{x})$

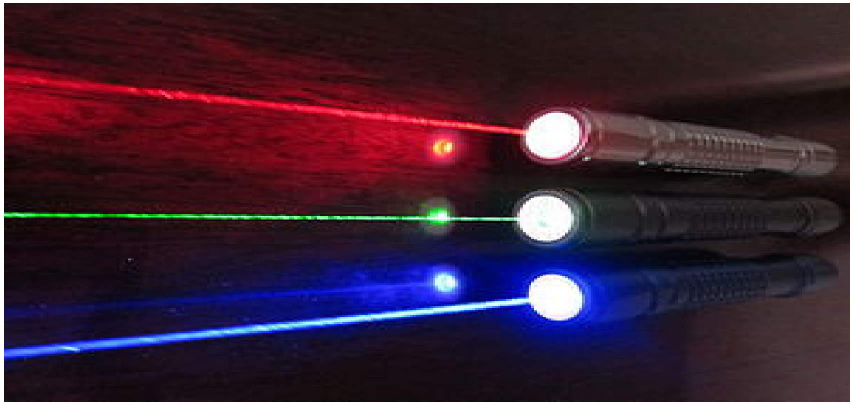
$$\Delta v(\vec{x})+k_0^2n^2(|v|)v(\vec{x})=0, \quad \vec{x}\in\mathbb{R}^3; \quad k_0=\frac{\omega}{c_0}\gg 1, \quad n(|v|)=\frac{c_0}{c(|v|)}$$

- In a Kerr medium

$$n(|v|)=\left(1+\frac{4n_2}{n_0}|v|^2\right)^{1/2}$$

n_2--Kerr coefficient

n_0--refraction index



Laser beam propagation

- Laser propagates in *z*-direction & take ansatz

$$v(x,y,z) = e^{ik_0 z}\psi(x,y,z)$$

- Reduced wave equation (C. Sulem & P.L. Sulem, 99')

$$2ik_0\partial_z\psi(\vec{x}_\perp,z) + \Delta_\perp\psi + \frac{4n_2k_0^2}{n_0}|\psi|^2\psi + \partial_{zz}\psi = 0, \quad \vec{x}_\perp = (x,y)\in\mathbb{R}^2$$

- Non-dimensionalization $z \to t$ & $\vec{x}_\perp \to \vec{x}$

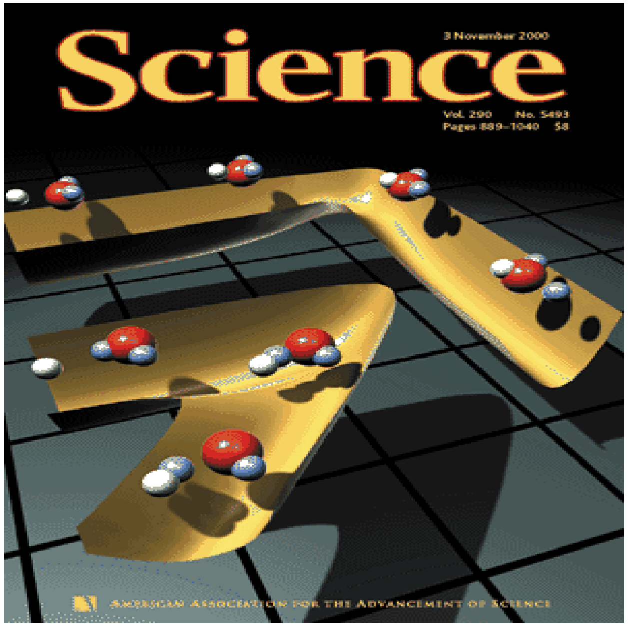
$$i\partial_t\psi(\vec{x},t) = -\frac{1}{2}\Delta\psi - |\psi|^2\psi - \delta\partial_{tt}\psi, \quad \vec{x}\in\mathbb{R}^2 \quad \text{with} \quad \delta \ll 1$$

- Paraxial (or parabolic) approximation -- NLSE

$$i\partial_t\psi(\vec{x},t) = -\frac{1}{2}\Delta\psi - |\psi|^2\psi, \quad \vec{x}\in\mathbb{R}^2, \quad t>0$$

Other applications

- In plasma physics: wave interaction between electrons and ions
  - Zakharov system, …..
- In quantum chemistry: chemical interaction based on the first principle
  - Schrodinger-Poisson system
- In materials science:
  - First principle computation
  - Semiconductor industry
- In nonlinear (quantum) optics
- In biology – protein folding
- In superfluids – flow without friction



Conservation laws

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

- Dispersive
- Time symmetric: $t \to -t$ & take conjugate $\Rightarrow$ unchanged!!
- Time transverse (gauge) invariant

$$V(\vec{x}) \to V(\vec{x}) + \alpha \Rightarrow \psi \to \psi e^{-i\alpha t/\varepsilon} \Rightarrow \rho = |\psi|^2 \text{ --unchanged!!}$$

- Mass (or wave energy) conservation

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

- Energy (or Hamiltonian) conservation

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

Dynamics with no potential

$$V(\vec{x}) \equiv 0, \quad \vec{x} \in \mathbb{R}^d$$

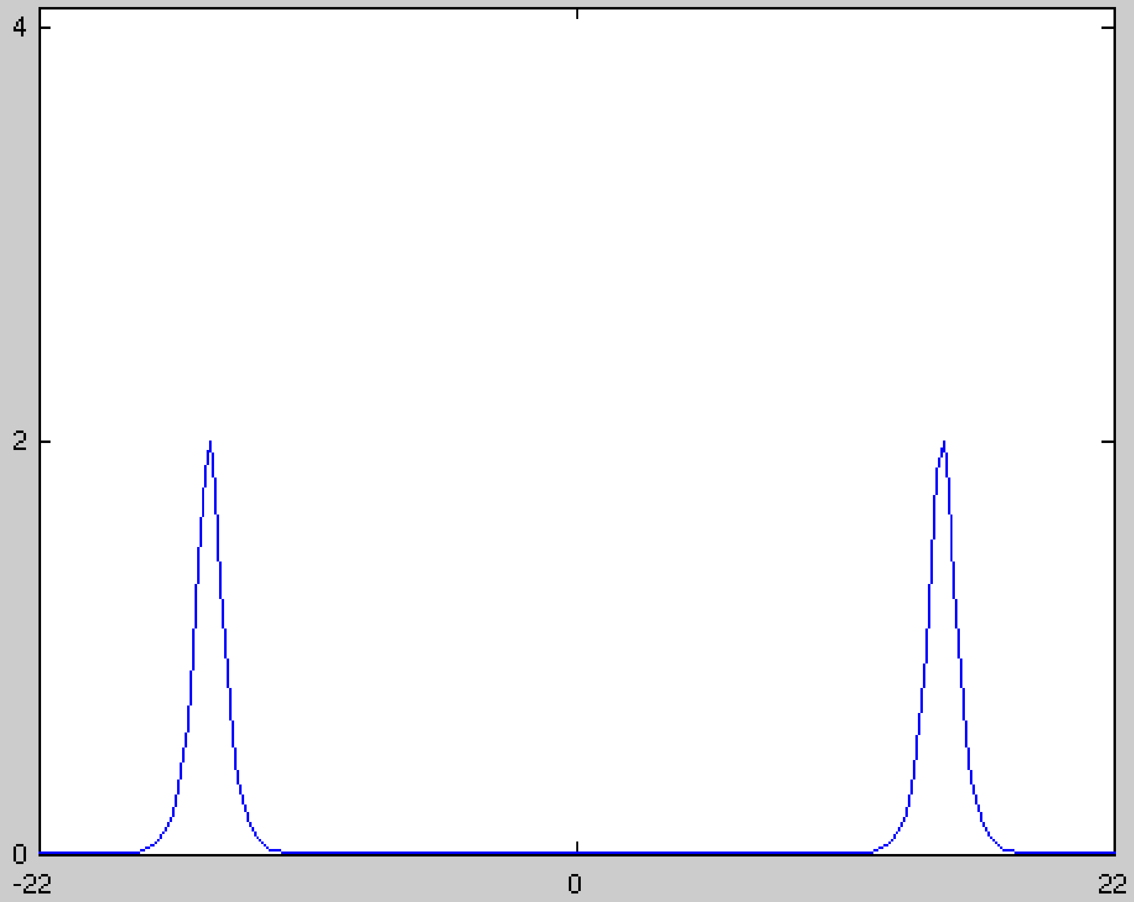
- Momentum conservation $\vec{J}(t) := \mathrm{Im} \int_{\mathbb{R}^d} \overline{\psi}\, \nabla \psi \, d\vec{x} \equiv \vec{J}(0) \quad t \geq 0$
- Dispersion relation $\psi(\vec{x},t) = Ae^{i(\vec{k}\bullet\vec{x}-\omega t)} \Rightarrow \omega = \frac{\varepsilon}{2}|\vec{k}|^2 + \frac{\beta}{\varepsilon}A^2$
- Soliton solutions in 1D: $\varepsilon = 1$
  - Bright soliton when $\beta < 0$ ---- decaying to zero at far-field

$$\psi(x,t) = \frac{a}{\sqrt{-\beta}} \mathrm{sech}(a(x - vt - x_0))\, e^{i(vx - \frac{1}{2}(v^2 - a^2)t + \theta_0)}, \quad x \in \mathbb{R}, \quad t \geq 0$$

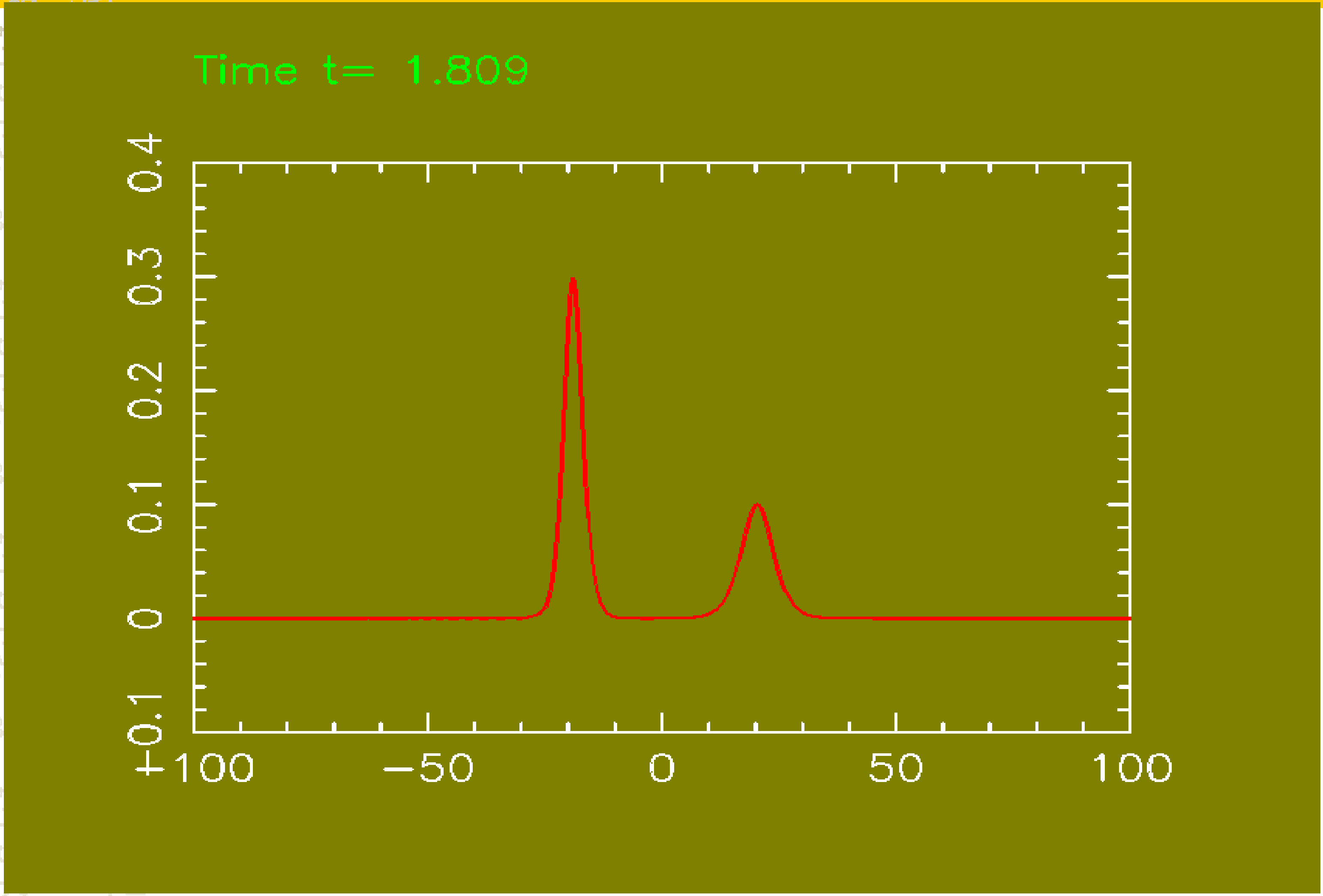
  - Dark (or gray) soliton $\beta > 0$ ---- nonzero &oscillatory at far-field

$$\psi(x,t) = \frac{1}{\sqrt{\beta}} [a \tanh(a(x - vt - x_0)) + i(v-k)]\, e^{i(kx - \frac{1}{2}(k^2 + 2a^2 + 2(v-k)^2)t + \theta_0)}, \quad x \in \mathbb{R}, \quad t \geq 0$$

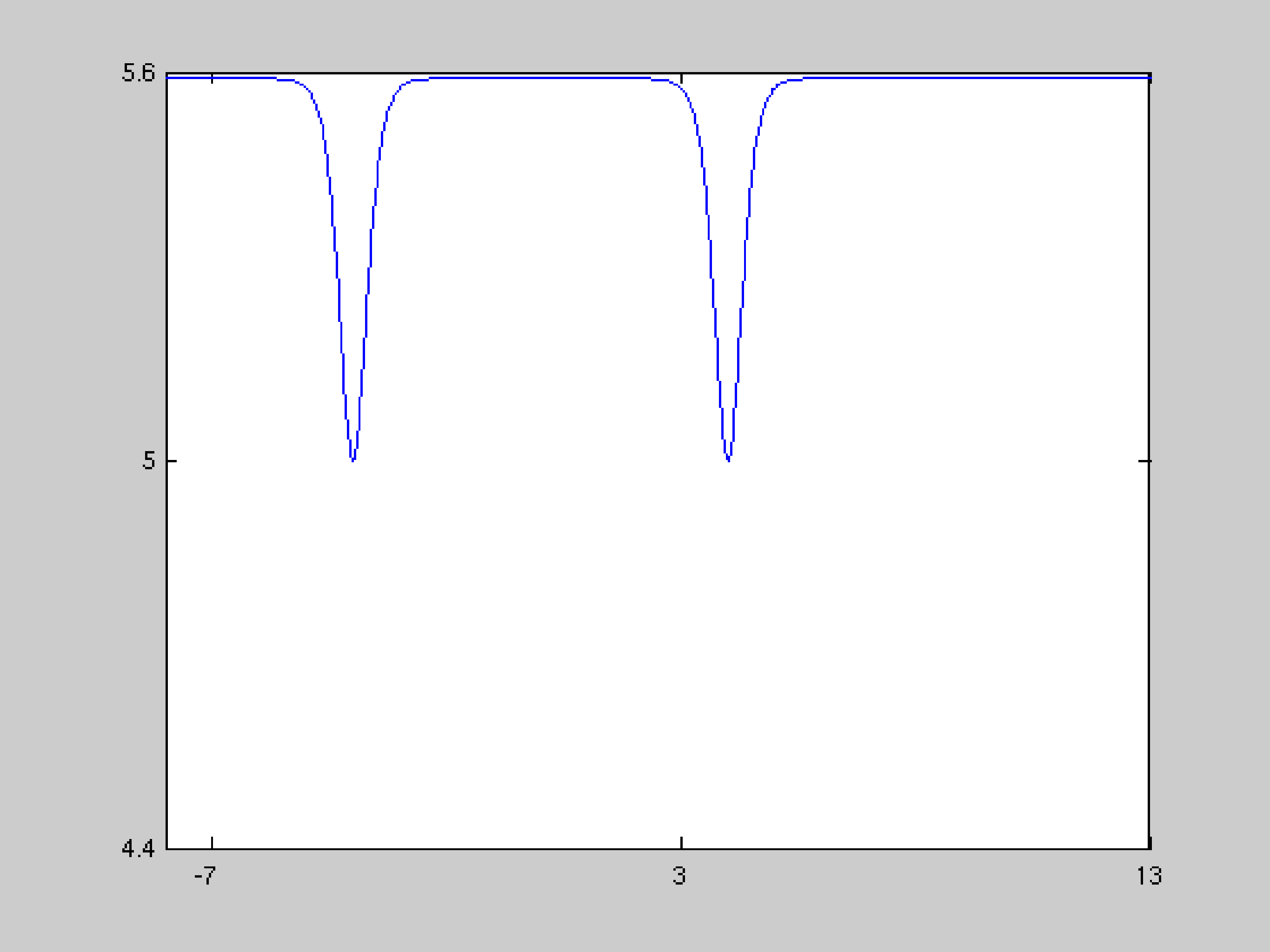
Interaction of two bright solitons



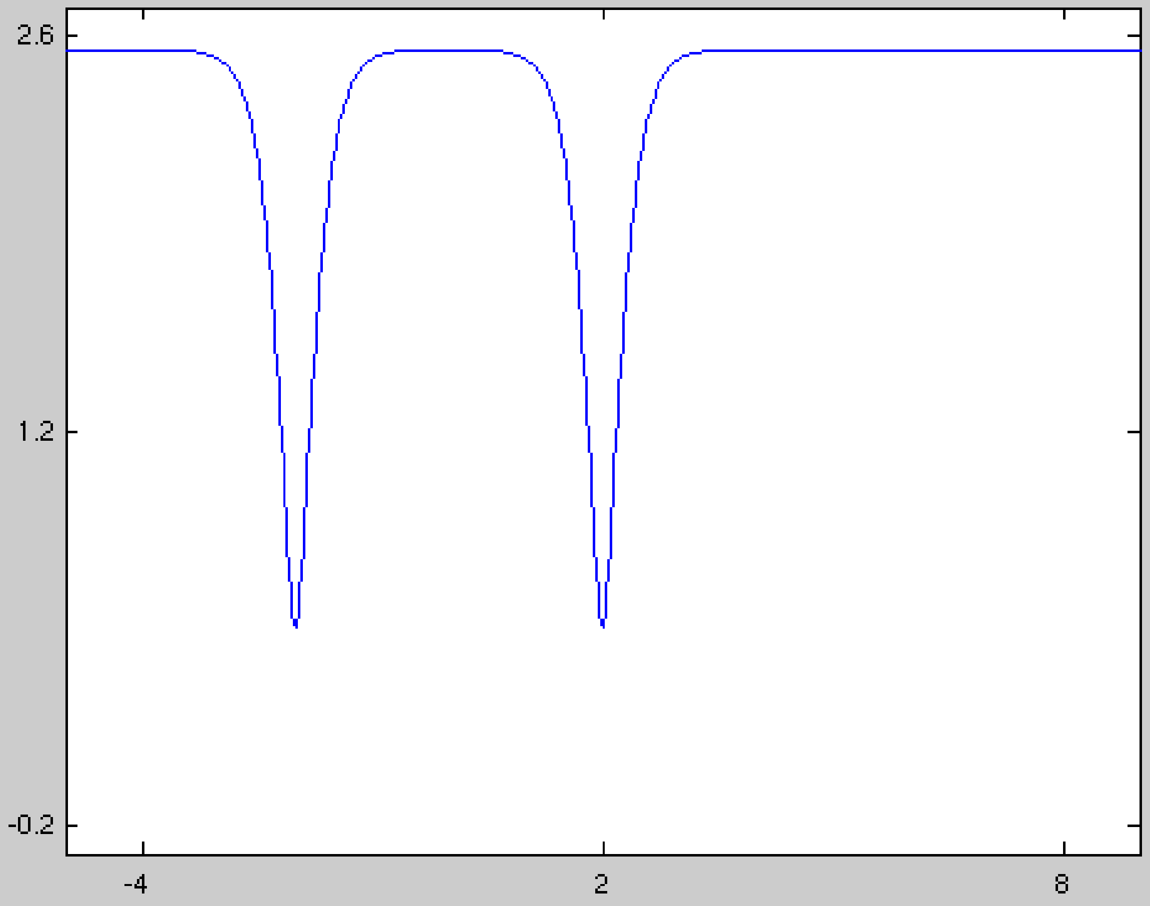
Interaction of Two Bright Solitons



Interaction of two dark solitons



Interactions of two dark solitons



Dynamics with harmonic potential

$\varepsilon = 1$

- Harmonic potential $V(\vec{x}) = \frac{1}{2}\begin{cases} \gamma_x^2 x^2 & d=1 \\ \gamma_x^2 x^2 + \gamma_y^2 y^2 & d=2 \\ \gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2 & d=3 \end{cases}$

- Center-of-mass: $\vec{x}_c(t) = \int_{\mathbb{R}^d} \vec{x}\,|\psi(\vec{x},t)|^2 d\vec{x}$

$$\ddot{\vec{x}}_c(t) + \mathrm{diag}(\gamma_x^2, \gamma_y^2, \gamma_z^2)\vec{x}_c(t) = 0, \quad t > 0 \Rightarrow \text{each component is periodic!!}$$

- An analytical solution if $\psi_0(\vec{x}) = \phi_s(\vec{x} - \vec{x}_0)$

$$\psi(\vec{x},t) = e^{-i\mu_s t}\,\phi_s(\vec{x} - \vec{x}_c(t))\,e^{iw(\vec{x},t)}, \qquad \vec{x}_c(0) = \vec{x}_0 \quad \& \,\Delta w(\vec{x},t) = 0$$

$$\Rightarrow \rho(\vec{x},t) := |\psi(\vec{x},t)|^2 = |\phi_s(\vec{x} - \vec{x}_c(t))|^2 \quad \text{-- moves like a particle!!}$$

$$\mu_s\,\phi_s(\vec{x}) = -\frac{\varepsilon^2}{2}\nabla^2\phi_s + V(\vec{x})\phi_s + \beta\,|\phi_s|^2\,\phi_s$$

Well-posedenss

- Theorem (T. Cazenave, 03'; C. Sulem & P.L. Sulem, 99'') Assumptions

(i) $V(\vec{x}) \in C^\infty(\mathbb{R}^d), \quad V(\vec{x}) \geq 0, \forall \vec{x} \in \mathbb{R}^d \quad \& \quad D^\alpha V(\vec{x}) \in L^\infty(\mathbb{R}^d) \quad |\alpha| \geq 2$

(ii) $\psi_0 \in X = \left\{ u \in H^1(\mathbb{R}^d) \mid \|u\|_X^2 = \|u\|_{L^2}^2 + \|\nabla u\|_{L^2}^2 + \int_{\mathbb{R}^d} V(\vec{x}) u(\vec{x}) d\vec{x} < \infty \right\}$

  – Local existence, i.e.

$\exists T_{\max} \in (0, \infty]$, s. t. the problem has a unique solution $\psi \in C([0, T_{\max}), X)$

  – Global existence, i.e. $T_{\max} = +\infty$ if

$d = 1$ or $d = 2$ with $\beta \geq -C_b / \|\psi_0\|_{L^2(\mathbb{R}^d)}^2$ or $d = 3 \, \& \, \beta \geq 0$

Finite time blowup

- Theorem (T. Cazenave, 03'; C. Sulem & P.L. Sulem, 99') Assumptions

$$\beta<0 \quad \& \quad V(\vec{x})d+\vec{x}\cdot\nabla V(\vec{x})\ge 0, \quad \forall \vec{x}\in\mathbb{R}^d \quad \text{with} \quad d=2,3$$

$$\psi_0\in X \qquad \text{with finite variance} \quad \delta_V(0):=\int_{\mathbb{R}^d} \left|\vec{x}\right|^2 \psi_0(\vec{x})d\vec{x}<\infty$$

– There exists finite time blowup, i.e. $T_{\max}<+\infty$ if one of the following holds

$$\text{(i)} \quad E(\psi_0)<0$$

$$\text{(ii)} \quad E(\psi_0)=0 \quad \& \quad \operatorname{Im}\int_{\mathbb{R}^d} \overline{\psi}_0(x)\,(\vec{x}\cdot\nabla\psi_0(\vec{x}))\,d\,\vec{x}<0$$

$$\text{(iii)} \quad E(\psi_0)>0 \quad \& \quad \operatorname{Im}\int_{\mathbb{R}^d} \overline{\psi}_0(x)\,(\vec{x}\cdot\nabla\psi_0(\vec{x}))\,d\,\vec{x}<-\sqrt{E(\psi_0)d}\,\left\|\vec{x}\,\psi_0\right\|_{L^2}$$

– Proof:

$$\delta_V(t):=\int_{\mathbb{R}^d}\left|\vec{x}\right|^2 |\psi(\vec{x},t)|^2\,d\vec{x}\Rightarrow \ddot{\delta}_V(t)\le 2d\;E(\psi_0), \quad t\ge 0, \quad d=2,3$$

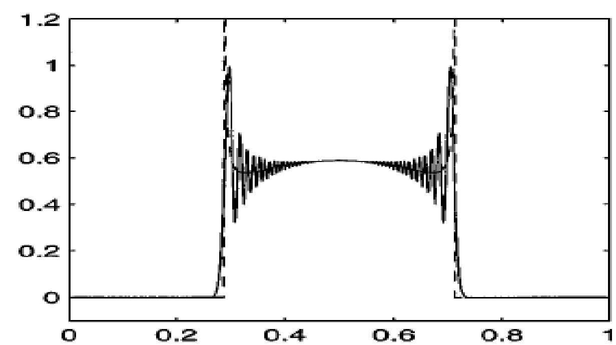
$$\Rightarrow \delta_V(t)\le d\;E(\psi_0)t^2+\delta_V^{'}(0)t+\delta_V(0)\Rightarrow \exists 0<t^*<\infty \;\&\; \delta_V(t^*)=0!!$$

Numerical methods for dynamics

$$i\varepsilon\,\partial_t\,\psi(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi + V(\vec{x})\psi + \beta\,|\psi|^2\psi, \quad \vec{x}\in\mathbb{R}^d, \quad t>0$$

with $\quad \psi(\vec{x},0)=\psi_0(\vec{x})$

- Dispersive & nonlinear
- Solution and/or potential are smooth but may oscillate wildly
- Keep the properties of NLSE on the discretized level
  - Time reversible & time transverse invariant
  - Mass & energy conservation
  - Dispersion relation



- In high dimensions: many-body problems
- Design efficient & accurate numerical algorithms
  - Explicit vs implicit (or computation cost)
  - Spatial/temporal accuracy, Stability
  - Resolution in strong interaction regime: $\beta \gg 1\,\&\,\varepsilon = 1$ or $0<\varepsilon\ll 1\,\&\,\beta=\pm 1$

Numerical difficulties

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

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

Different Numerical Methods

- Lattice Boltzmann Method (Succi, Phys. Rev. E, 96'; Int. J. Mod. Phys., 98')
- Explicit FDM (Edwards & Burnett et al., Phys. Rev. Lett., 96')
- Particle-inspired scheme (Succi et al., Comput. Phys. Comm., 00')
- Leap-frog FDM (Succi & Tosi et al., Phys. Rev. E, 00')
- Crank-Nicolson FDM (Adhikari, Phys. Rev. E 00')
- Time-splitting spectral (TSSP) method (Bao,Jaksch&Markowich,JCP, 03')
- Runge-Kutta spectral method (Adhikari et al., J. Phys. B, 03')
- Symplectic FDM (M. Qin et al., Comput. Phys. Comm., 04')

NLS in 1D

- Time-dependent NLS in 1D

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

$$x \in \Omega = (a,b), \quad t > 0,$$

$$\psi(x,0) = \psi_0(x), \qquad a \le x \le b.$$

- Boundary conditions (BC)
  - Periodic BC: $\psi(a,t) = \psi(b,t), \quad \partial_x\psi(a,t) = \partial_x\psi(b,t), \quad t \ge 0$
  - Or homogeneous Dirichlet BC: $\psi(a,t) = \psi(b,t) = 0, \quad t \ge 0$
  - Or homogeneous Neumann BC:
  - Or PML / TBC / ABC, …

Time-splitting (or split-step) Method

$$\partial_t u = (T+V)u, \quad u(0) = u_0$$

- Lie-Trotter splitting

$$u(\tau) = e^{\tau(T+V)}u_0 \approx u^{(1)} := e^{\tau T}e^{\tau V}u_0 \Rightarrow \left\| u(\tau) - u^{(1)} \right\| \le C\tau^2 \Rightarrow \text{1st order}$$

- Strang splitting – G. Strang, SINUM, 1968

$$u(\tau) = e^{\tau(T+V)}u_0 \approx u^{(2)} := e^{\frac{1}{2}\tau V}e^{\tau T}e^{\frac{1}{2}\tau V}u_0 \Rightarrow \left\| u(\tau) - u^{(2)} \right\| \le C\tau^3 \Rightarrow \text{2nd order}$$

- Higher order splitting –M. Suzuki, 90'; H. Yoshida, 90'; R.I. McLachlan, et. Acta 02';..

$$u(\tau) \approx u^{(r)} := e^{a_1\tau T}e^{b_1\tau V}e^{a_2\tau T}\cdots e^{b_r\tau V}e^{a_r\tau T}\cdots e^{b_1\tau V}e^{a_1\tau T}u_0$$

  - 4th order: $r = 2, a_1 = \theta, b_1 = 2\theta, a_2 = 0.5-\theta, b_2 = 1-4\theta; \quad \theta = \frac{1}{6}\left(2 + 2^{\frac{1}{3}} + 2^{-\frac{1}{3}}\right)$
  - Partition Runge-Kutta: $r = 4, b_4 = 0, a_1 = \ldots$

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

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

  - Step 2: solve the nonlinear ODE analytically

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

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

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

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

- Use 2^{nd} or 4^{th} order splitting (Bao,Jin & Markowich, JCP, 02'; citations about 300 !!)
  - $\varepsilon = 1:$ (Tarppent, SIAM 78'; Moris etc., JCP, 88'; Ablowitz etc. JCP, 84',.....)

An algorithm in 1D for NLSE

- Choose time step: $\tau = \Delta t$; set $t_n = n\,\tau, n = 0, 1, \cdots$
- 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')

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

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

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

  – 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

$$n+1 \leftrightarrow n \quad \& \quad \tau \leftrightarrow -\tau \Rightarrow \quad \text{scheme unchanged!!}$$

- Time transverse invariant: yes

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

- Mass conservation: yes

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

- Stability: yes

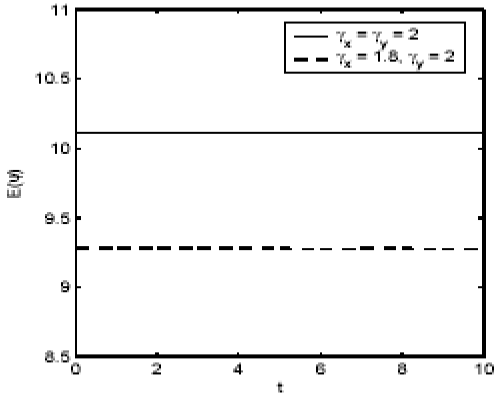
Properties of the method

- Dispersion relation without potential: yes

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

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

  - 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: 2^{nd} order
- Resolution in semiclassical regime (Bao, Jin & Markowich, JCP, 02')
  - Linear case: $\beta = 0$

    $$h = O(\varepsilon) \quad \& \quad \tau - \text{independent of } \varepsilon$$
  - Weakly nonlinear case: $\beta = O(\varepsilon)$

    $$h = O(\varepsilon) \quad \& \quad \tau - \text{independent of } \varepsilon$$
  - Strongly repulsive case: $0 < \beta = O(1)$

    $$h = O(\varepsilon) \quad \& \quad \tau = O(\varepsilon)$$
- Error estimate in L^2-norm and/or H^1: $\|e^n\| \le C(h^m + \tau^2)$
  - C. Besse, C. Lubich, O. Koch, M. Thalhammer, M. Caliari, C. Neuhauser, E. Faou, A. Debussche, L. Gauckler, E. Hairer, J. Shen&Z.Q. Wang, W. Bao&Y. Cai, etc.

Crank-Nicolson finite difference (CNFD) method

- Crank-Nicolson finite difference (CNFD)method

$$i\,\varepsilon\,\frac{\psi_j^{n+1}-\psi_j^n}{\tau}=-\frac{\varepsilon^2}{4}\left[\frac{\psi_{j+1}^{n+1}-2\psi_j^{n+1}+\psi_{j-1}^{n+1}}{h^2}+\frac{\psi_{j+1}^{n}-2\psi_j^{n}+\psi_{j-1}^{n}}{h^2}\right]$$

$$+\frac{V(x_j)}{2}(\psi_j^{n+1}+\psi_j^n)+\frac{\beta}{4}(|\psi_j^{n+1}|^2+|\psi_j^n|^2)\,(\psi_j^{n+1}+\psi_j^n),\quad 1\le j\le M-1,\quad n\ge 0$$

$$\psi_0^{n+1}=\psi_M^{n+1}=0,\quad n\ge 0 \qquad\qquad \psi_j^0=\psi_0(x_j),\quad 0\le j\le M$$

- Implicit: need solve a fully nonlinear system per time step via iterations!!!
- Time reversible: Yes
- Time transverse invariant: No
- Mass conservation: Yes

CNFD

- Stability: Yes
- Energy conservation: Yes
- Dispersion relation without potential: No
- Accuracy
  - Spatial: 2nd order
  - Temporal: 2^{nd} order
- Resolution in semiclassical regime (Markowich, Poala & Mauser, SINUM, 02')

$$h = o(\varepsilon) \quad \& \quad \tau = o(\varepsilon) \Leftarrow \quad h = O(\varepsilon^2) \quad \& \quad \tau = O(\varepsilon^2)$$

- Error estimate: Yes

Error estimates for CNFD

- Assume $e_j^n = \psi(x_j, t_n) - \psi_j^n$

$$\psi \in C^3([0,T];W^{1,\infty}) \cap C^2([0,T];W^{3,\infty}) \cap C^0([0,T];W^{5,\infty} \cap H_0^1) \quad \& \quad V \in C^1$$

- Theorem: Assume $\tau \le C_0 h$, there exist $h_0 > 0 \,\&\, \tau_0 > 0$ sufficiently small, when $0 < h \le h_0 \,\&\, 0 < \tau < \tau_0$, we have the following error estimate

$$\|e^n\| \le C[h^2 + \tau^2] \quad \& \quad \|\delta^+ e^n\| \le C[h^{3/2} + \tau^{3/2}], \qquad 0 \le n \le T/\tau$$

In addition, if either $\partial_n V(\vec{x})|_{\partial\Omega} = 0$ or $\psi \in C^0([0,T]; H_0^2)$, we have

$$\|e^n\| + \|\delta^+ e^n\| \le C[h^2 + \tau^2], \qquad 0 \le n \le T/\tau$$

Semi-Implicit finite difference (SIFD)method

- Semi-Implicit finite difference (SIFD)method

$$i\varepsilon \frac{\psi_j^{n+1}-\psi_j^{n-1}}{\tau} = -\frac{\varepsilon^2}{4}\left[\frac{\psi_{j+1}^{n+1}-2\psi_j^{n+1}+\psi_{j-1}^{n+1}}{h^2}+\frac{\psi_{j+1}^{n-1}-2\psi_j^{n-1}+\psi_{j-1}^{n-1}}{h^2}\right] \qquad 1\le j\le M-1, \quad n\ge 1$$

$$+\frac{V(x_j)}{2}(\psi_j^{n+1}+\psi_j^{n-1})+\beta|\psi_j^n|^2\psi_j^n \quad \text{or} \quad +\frac{V(x_j)}{2}\psi_j^n+\beta|\psi_j^n|^2\psi_j^n$$

$$\psi_0^{n+1}=\psi_M^{n+1}=0, \quad n\ge 0 \qquad \psi_j^0=\psi_0(x_j), \quad 0\le j\le M$$

$\psi_j^1 \quad (j=1,2,\ldots,M-1)$ by 2nd explicit time integrator, e.g. modified Euler method

- Implicit: need solve linear system per time step via fast Poisson solver!!
- Time reversible: Yes
- Time transverse invariant: No
- Mass conservation: no

SIFD

- Stability: conditional stable
- Energy conservation: no
- Dispersion relation without potential: No
- Accuracy
  - Spatial: 2nd order
  - Temporal: 2^{nd} order
- Resolution in semiclassical regime (Markowich, Poala & Mauser, SINUM, 02')

$$h = o(\varepsilon) \quad \& \quad \tau = o(\varepsilon) \Leftarrow \quad h = O(\varepsilon^2) \quad \& \quad \tau = O(\varepsilon^2)$$

- Error estimate: Yes

Error estimates for SIFD

- Assume $$e_j^n = \psi(x_j, t_n) - \psi_j^n$$

$$\psi \in C^3([0,T];W^{1,\infty}) \cap C^2([0,T];W^{3,\infty}) \cap C^0([0,T];W^{5,\infty} \cap H_0^1) \quad \& \quad V \in C^1$$

- Theorem: Assume $\tau \le C_0 h$, there exist $h_0 > 0 \,\&\, \tau_0 > 0$ sufficiently small, when $0 < h \le h_0 \,\&\, 0 < \tau < \tau_0$, we have the following error estimate

$$\|e^n\| \le C[h^2 + \tau^2] \quad \& \quad \|\delta^+ e^n\| \le C[h^{3/2} + \tau^{3/2}], \qquad 0 \le n \le T/\tau$$

In addition, if either $\partial_n V(\vec{x})|_{\partial\Omega} = 0$ or $\psi \in C^0([0,T]; H_0^2)$ we have

$$\|e^n\| + \|\delta^+ e^n\| \le C[h^2 + \tau^2], \qquad 0 \le n \le T/\tau$$

Other approaches for NLS

- Leap-frog finite difference (LPFD) method

$$i\varepsilon \frac{\psi_j^{n+1}-\psi_j^{n-1}}{2\tau} = -\frac{\varepsilon^2}{2h^2}(\psi_{j+1}^n - 2\psi_j^n + \psi_{j-1}^n) + V(x_j)\psi_j^n + \frac{\beta}{2}|\psi_j^n|^2\psi_j^n$$

$$\psi_0^{n+1} = \psi_M^{n+1} = 0, \quad n \geq 0 \qquad \psi_j^0 = \psi_0(x_j), \quad 0 \leq j \leq M$$

$\psi_j^1 \quad (j = 1, 2, \ldots, M-1)$ by 2nd explicit method, e.g. modified Euler

- Time-splitting finite difference (TSFD) method
  - Step 1. Solve by CNFD
  - Step 2. Solve the ODE analytically

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

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

Other approaches for NLS

- Crank-Nicolson spectral (CNSP) method

$$i\,\varepsilon\,\frac{\psi_j^{n+1}-\psi_j^n}{\tau}=-\frac{\varepsilon^2}{4}\left[D_{xx}^h\,\psi^{n+1}\Big|_{x=x_j}+D_{xx}^h\,\psi^n\Big|_{x=x_j}\right]$$
$$+\frac{V(x_j)}{2}(\psi_j^{n+1}+\psi_j^n)+\frac{\beta}{4}(|\psi_j^{n+1}|^2+|\psi_j^n|^2)(\psi_j^{n+1}+\psi_j^n)$$

D_{xx}^h : pseudo-spectral differential approximation to ∂_{xx}

- 4^{th} order Runge-Kutta spectral (RKSP4) method
- Compact scheme in space, ……
- Multi-symplectic scheme in time, …….

Other approaches

- Time discretization
  - Leap-frog scheme
  - 4th-order Runge-Kutta (RK4) --- not time symmetric
  - …….
- Spatial discretization
  - Finite element method
  - Finite volume method
  - Compact finite difference method
  - ……..
- Time + spatial discretization → different methods for NLSE

Numerical error comparison

h	$h_0 = 0.5$	$h_0/2$	$h_0/4$	$h_0/8$	$h_0/16$
CNFD	2.48	8.50E-1	1.79E-1	4.33E-2	1.07E-2
SIFD	2.48	8.50E-1	1.79E-1	4.33E-2	1.07E-2
TSFD	2.48	8.50E-1	1.79E-1	4.33E-2	1.07E-2
TSSP	3.95E-1	2.22E-4	3.93E-9	$<$1E-9	$<$1E-9

τ	$\tau_0 = 0.1$	$\tau_0/2$	$\tau_0/4$	$\tau_0/8$	$\tau_0/16$
CNFD	1.07E-1	2.71E-2	6.72E-3	1.58E-3	2.95E-4
SIFD	7.61E-1	1.23E-1	2.88E-2	7.19E-3	1.81E-3
TSFD	3.74E-1	8.52E-2	2.10E-2	5.31E-3	1.35E-3
TSSP	2.18E-1	5.90E-2	1.51E-2	3.79E-3	9.49E-4

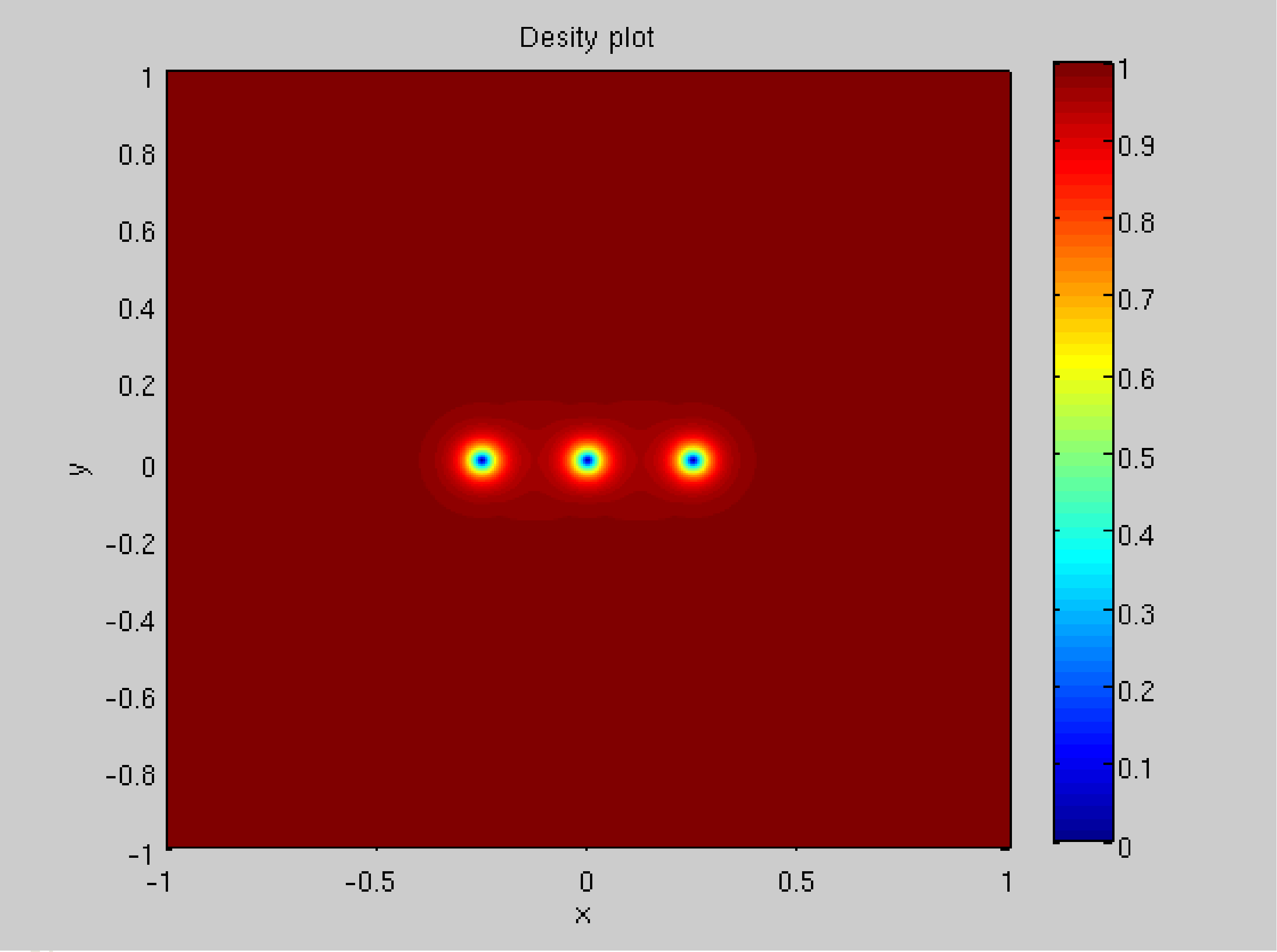
Comparison

Method	TSSP	CNFD	SIFD	ReFD	TSFD
Time Reversible	Yes	Yes	Yes	Yes	Yes
Time Transverse Invariant	Yes	No	No	No	Yes
Mass Conservation	Yes	Yes	No	Yes	Yes
Energy Conservation	No	Yes	No	Yes[4]	No
Dispersion Relation	Yes	No	No	No	Yes
Unconditional Stability	Yes	Yes	No	Yes	Yes
Explicit Scheme	Yes	No	No	No	No
Time Accuracy	2th or 4th	2th	2th	2th	2th
Spatial Accuracy	spectral	2th	2th	2th	2th
Memory Cost	$O(J^d)$	$O(J^d)$	$O(J^d)$	$O(J^d)$	$O(J^d)$
Computational Cost	$O(J^d \log J)$	$\gg O(J^d)$ [5]	$O(J^d \log J)$ [6]	$O(J^d \log J)$ [7]	$O(J^d \log J)$ [8]
Resolution when $0 < \varepsilon \ll 1$ [9]	$h = O(\varepsilon)$ $\tau = O(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$

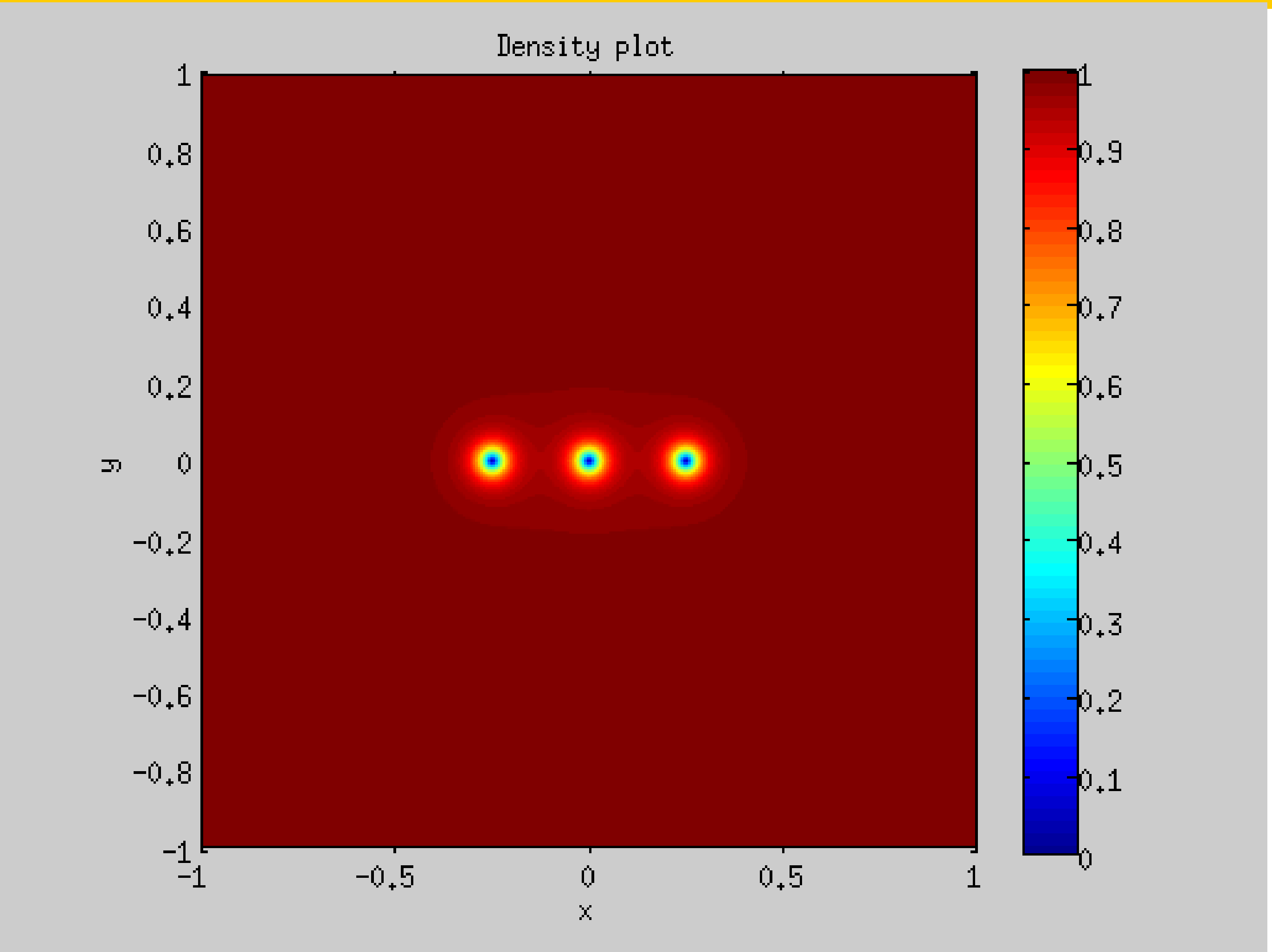
Comparison summary

- TSSP method
  - It is the best in computation in terms of stability, accuracy, easy to implement, resolution, …. !!
  - Its error estimate is well-understood in math now!
  - Keep most properties except the energy!!
  - TSFD is used for rough solution, e.g. random potential!!
- CNFD & SIFD methods
  - Error estimates are established in mathematics !!
  - CNFD conserves energy, but it is expensive to solve in 2D &3D!!
  - SIFD can be used in 2D &3D instead of CNFD.
- Other methods --- RK4FD, LPFD, RK4SP, ……
  - In general, not as good as either TSSP or CNFD or SIFD !!

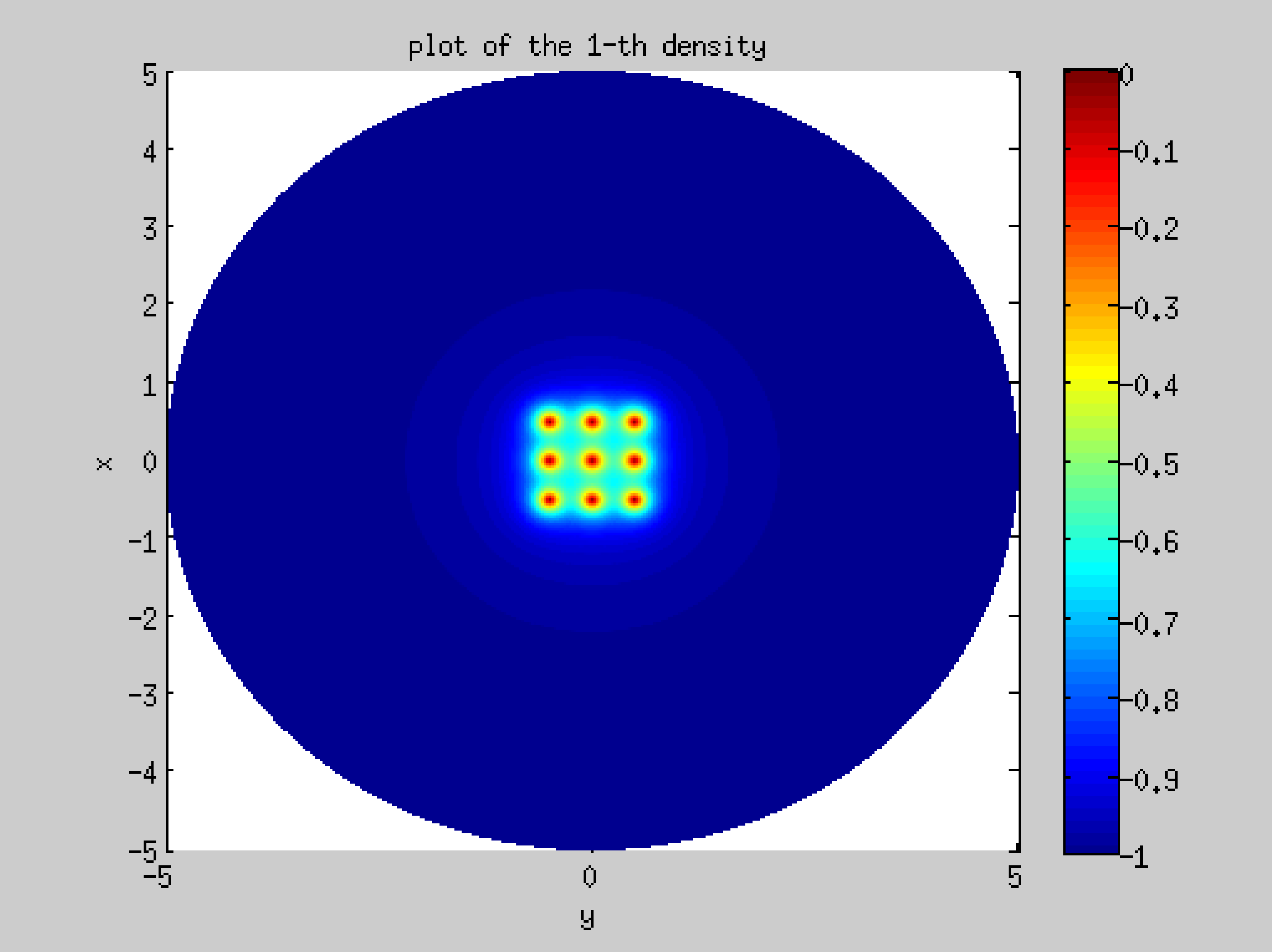
Interaction of 3 like vortices



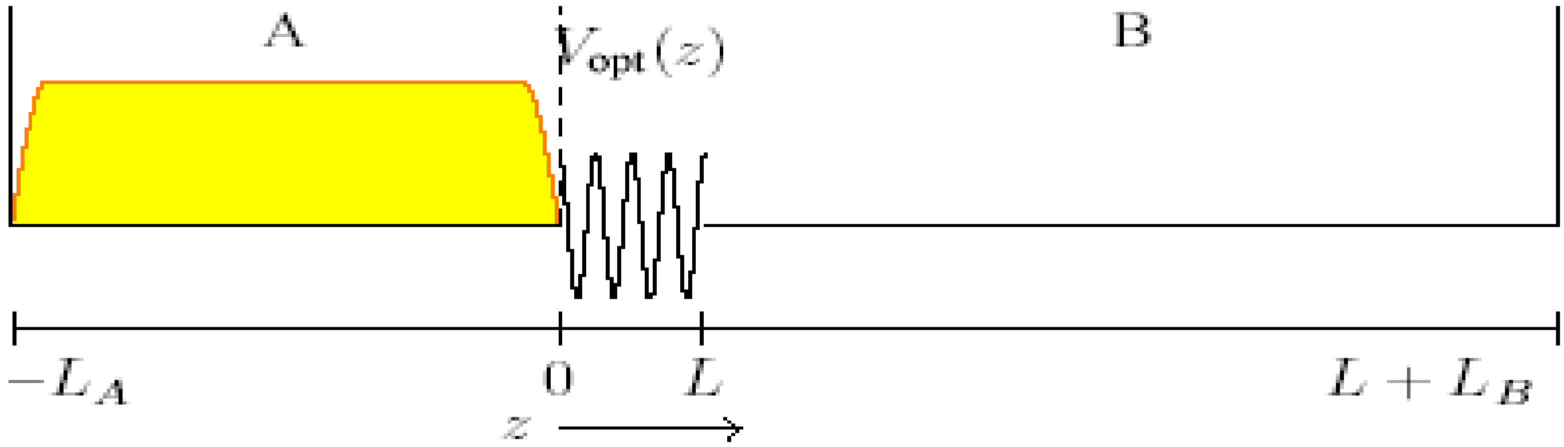
Interaction of 3 opposite vortices



Interaction of a lattice



Quantum transport --- setup



- Study
  - Finite size effects of the optical lattice: depth, width, recoil energy
  - Strong interaction in BEC
  - Density, current, Resonance, …..
- Reference: Dynamical self-trapping of Bose-Einstein condensates in shallow optical lattices, M. Rosenkranz, D. Jaksch, F. Y. Lim & W. Bao, PRA, 08'

GPE with lattice potential

- Quasi-1D GPE described by $\psi = \psi(z,t)$ (re-scaled)

$$i\frac{\partial}{\partial t}\psi(z,t) = \left[-\frac{1}{2}\frac{\partial^2}{\partial z^2} + V_{\text{ax}}(z) + \beta|\psi|^2\right]\psi(z,t)$$

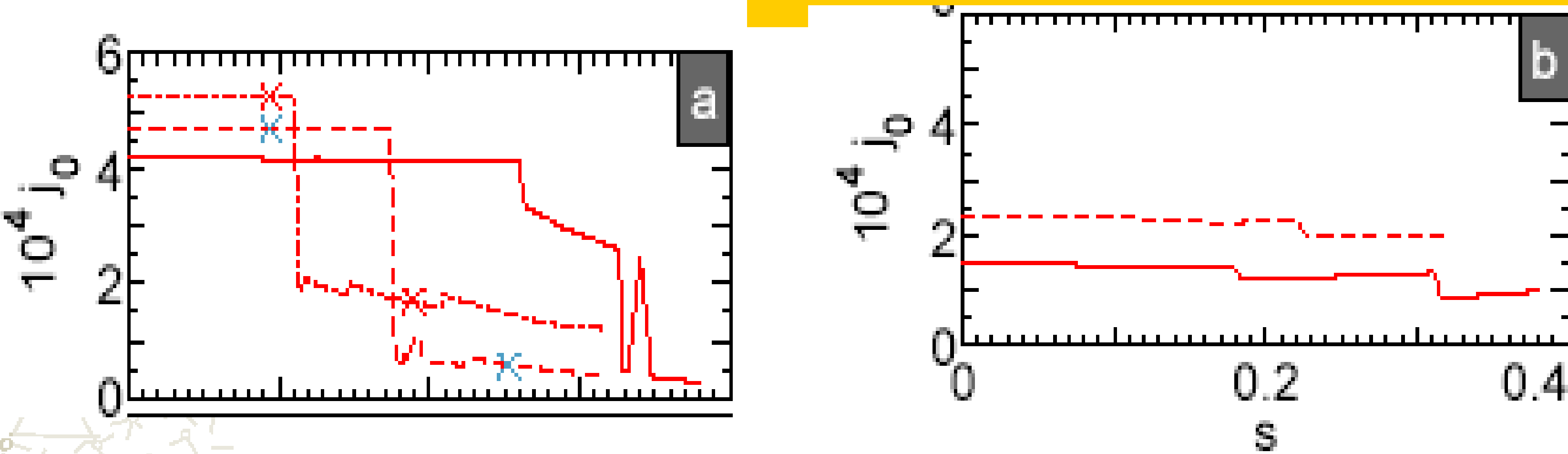
$$\psi(z,t=0) = \psi_0(z), \qquad \psi(-L_A,t) = \psi(L+L_B,t) = 0$$

$$V_{\text{ax}}(z) = \begin{cases} 0 & -L_A \le z \le 0 \\ V_{\text{opt}}(z) & 0 \le z \le L \\ 0 & L \le z \le L+L_B \end{cases} \qquad V_{\text{opt}}(z) = v + s\sin(2z)$$

$$\beta = \frac{N a_s k \hbar \omega_\perp}{E_R} \text{ (interaction constant)}, \quad E_R = \frac{\hbar^2 k^2}{2m} \text{ (photon recoil energy)}$$

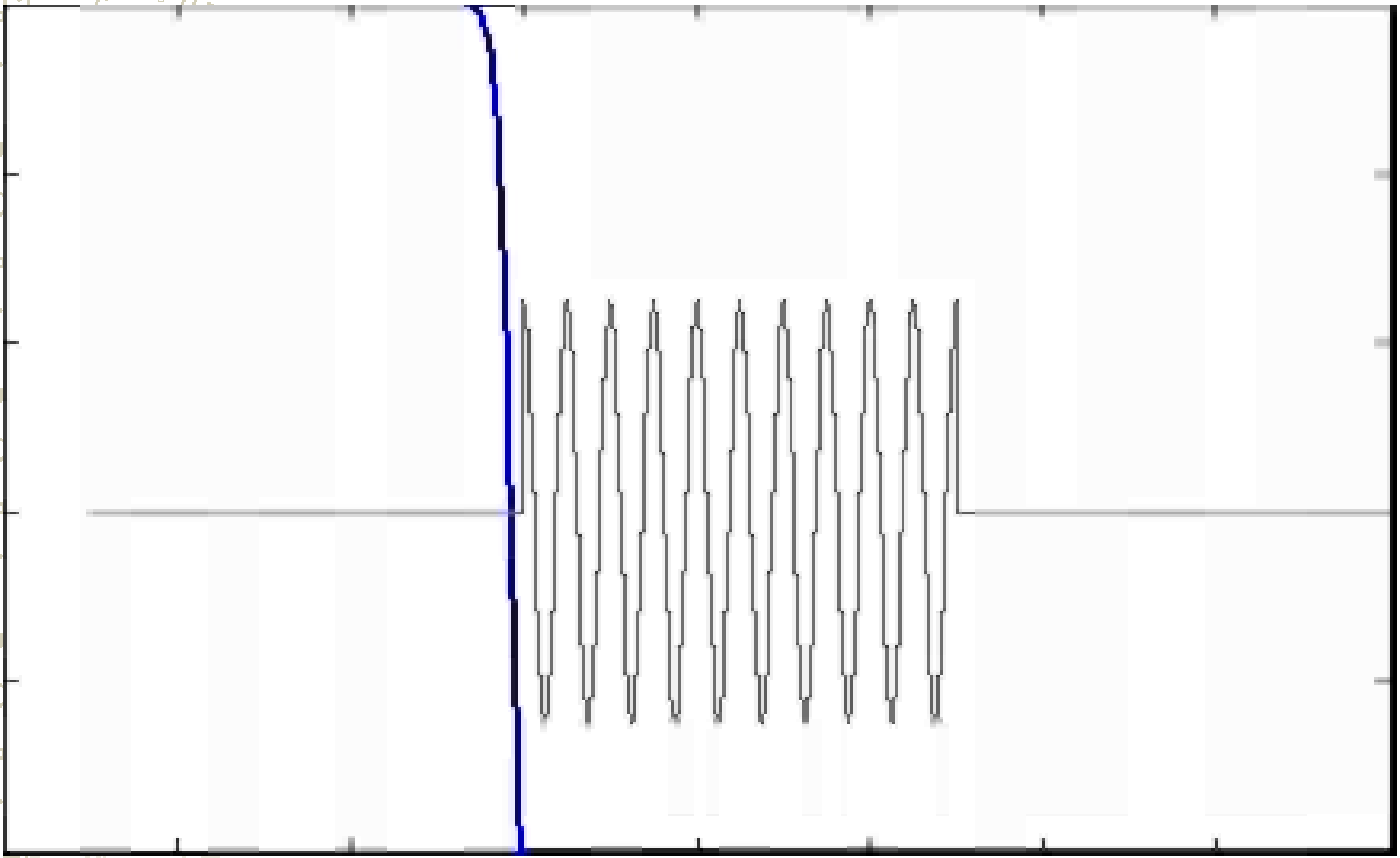
Normalization condition $$\int_{-L_A}^{L+L_B} |\psi(z,t)|^2\, dz = 1$$

Stationary current – varying lattice depths

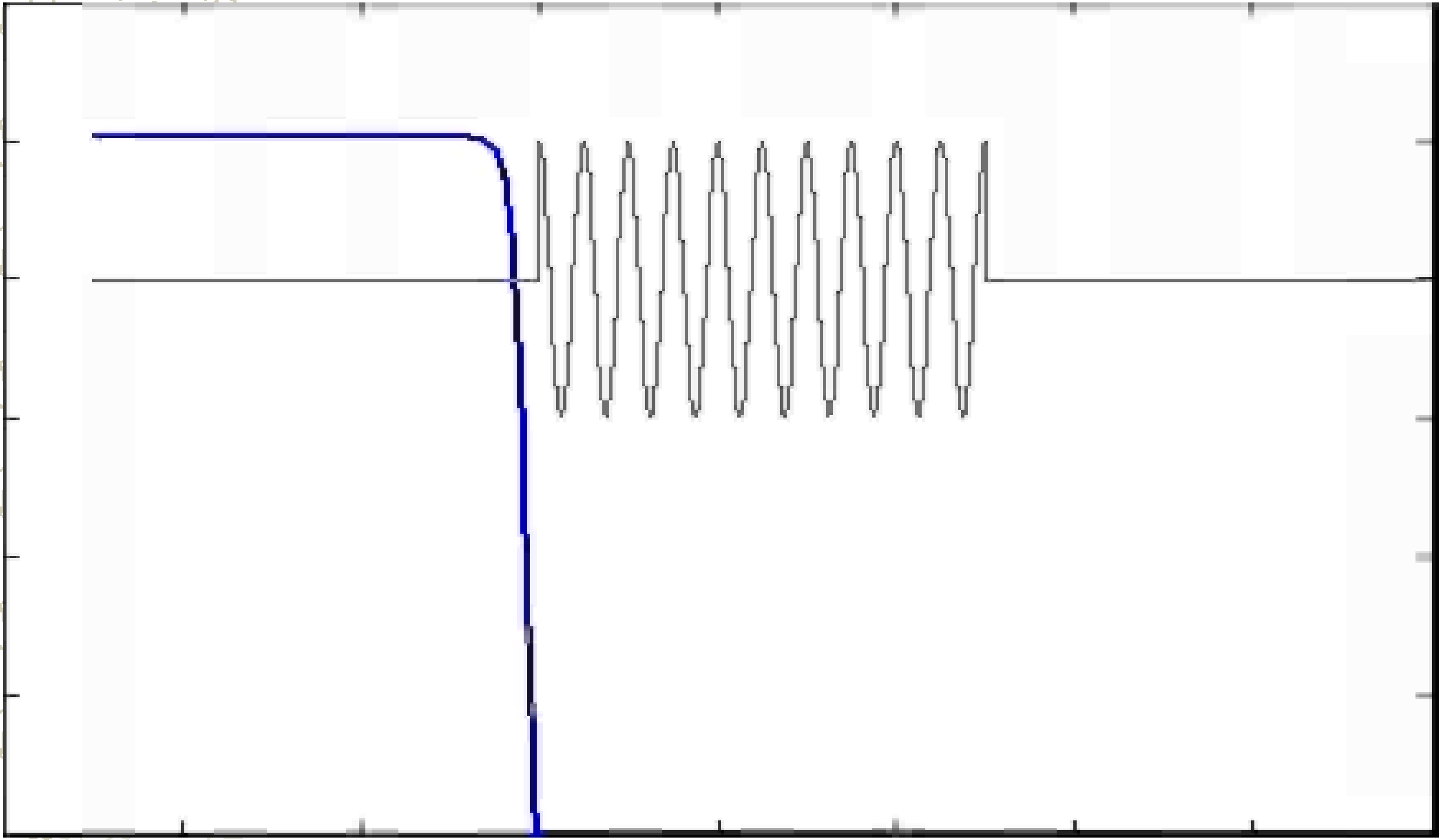


- Results
  - Left: $v = 0, \beta = 251.46(\text{solid}), 318.31(\text{dashed}), 397.89(\text{dotted})$
  - Right: $v = 0, \beta = 31.83(\text{solid}), 79.58(\text{dashed})$
- Observations
  - Characteristic drop in strong interaction & no drop in weak interaction
  - Drop position depends on lattice depth — self-trapping
  - After drop, transport of atoms through lattice almost blocked

Low lattice height

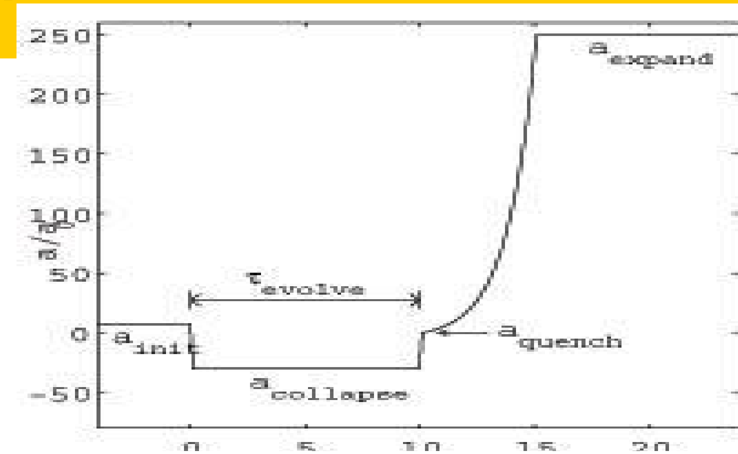


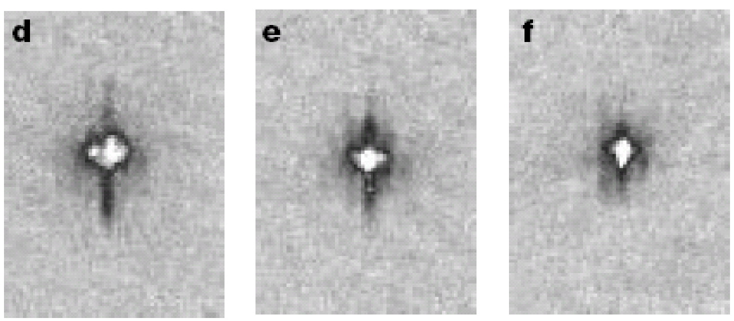
High lattice height

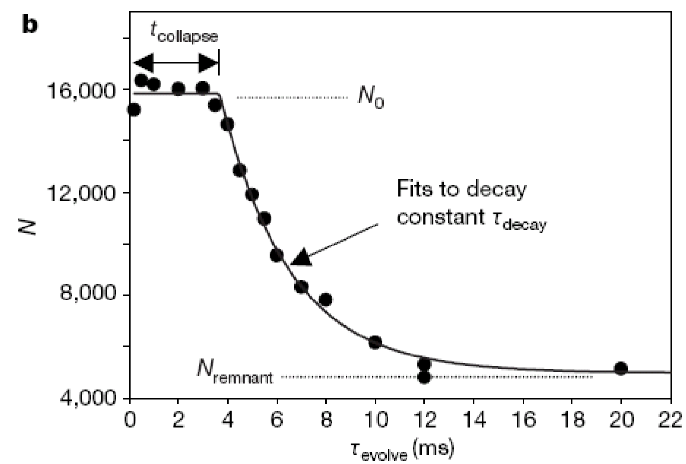


3D collapse & explosion of BEC

- Experiment (Donley et., Nature, 01')
  - Start with a stable condensate ($a_s>0$)
  - At t=0, change a_s from (+) to (-)
  - Three body recombination loss



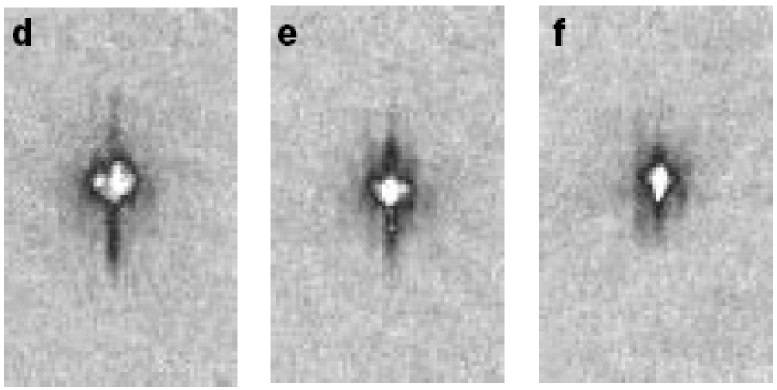


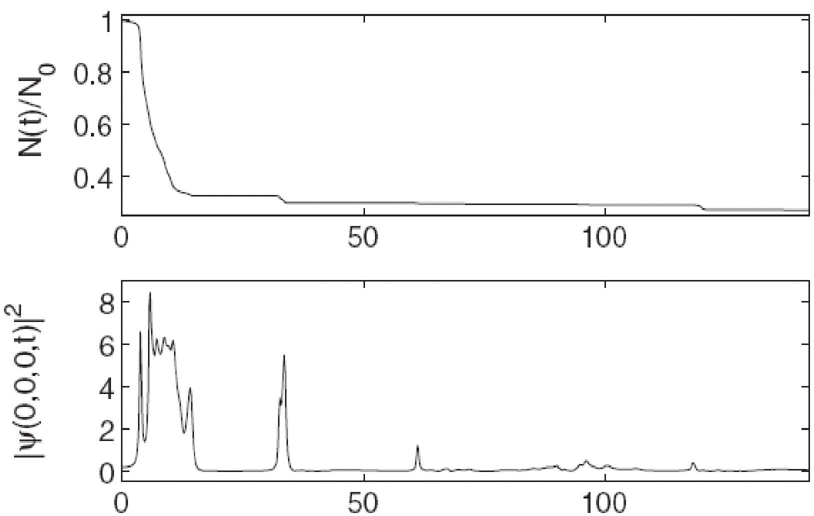


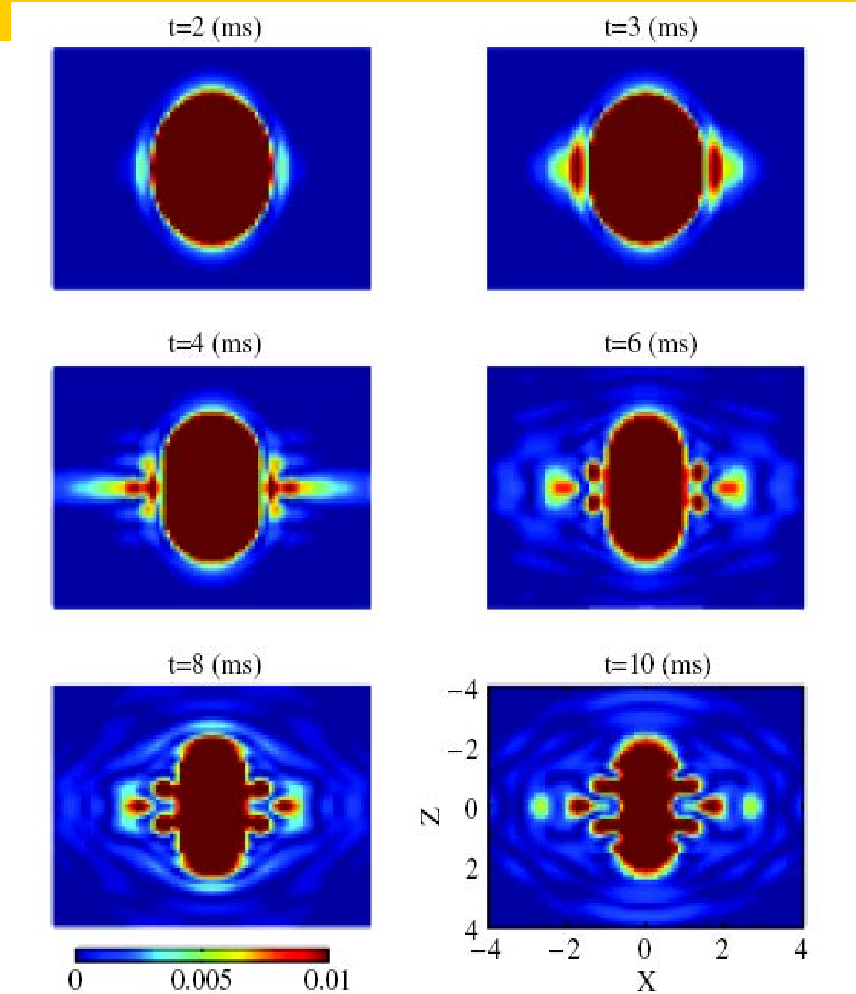
- Mathematical model (Duine & Stoof, PRL, 01')

$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x})\psi + \beta\,|\psi|^2\psi - i\delta_0\beta^2|\psi|^4\psi \qquad \beta = \frac{4\pi\, N\, a_s}{x_s}$$

Numerical results (Bao et., J Phys. B, 04)

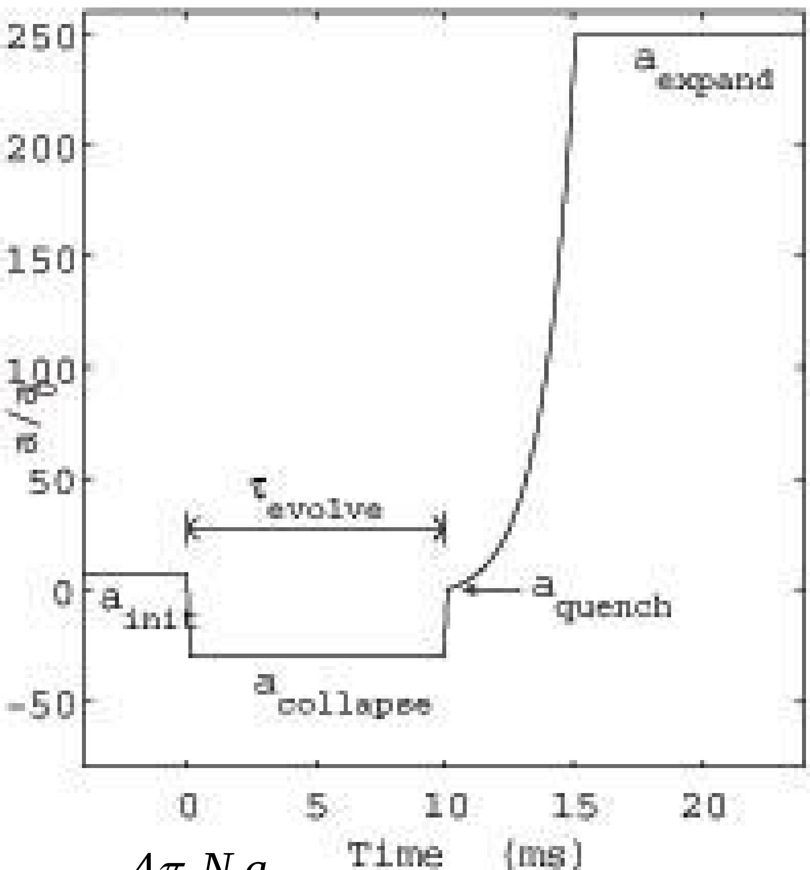


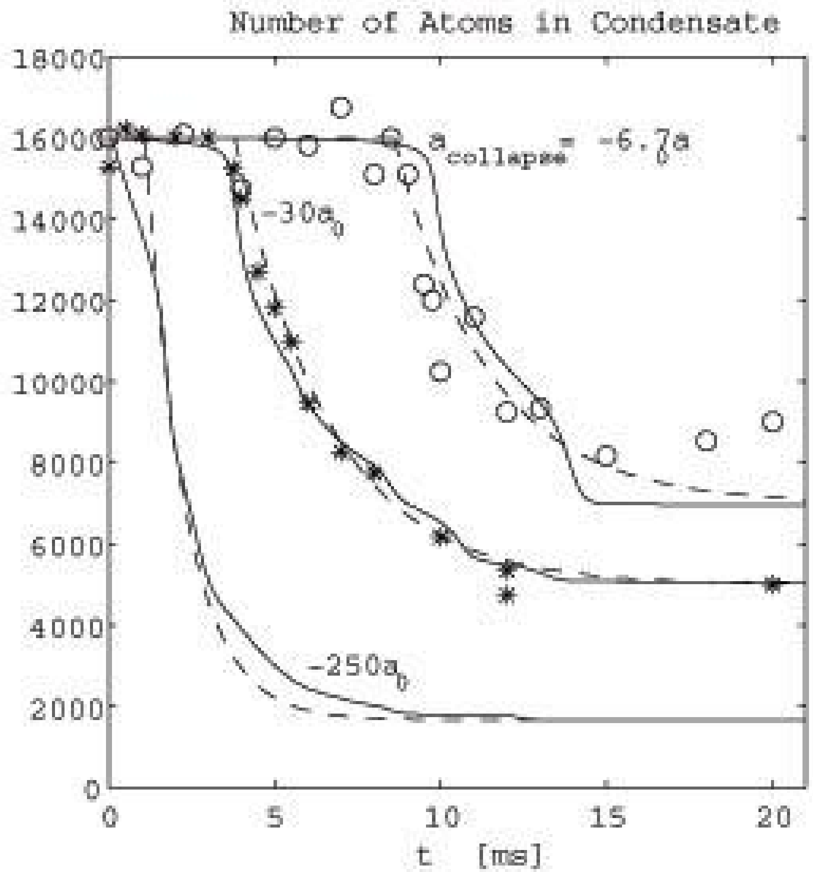




Jet formation

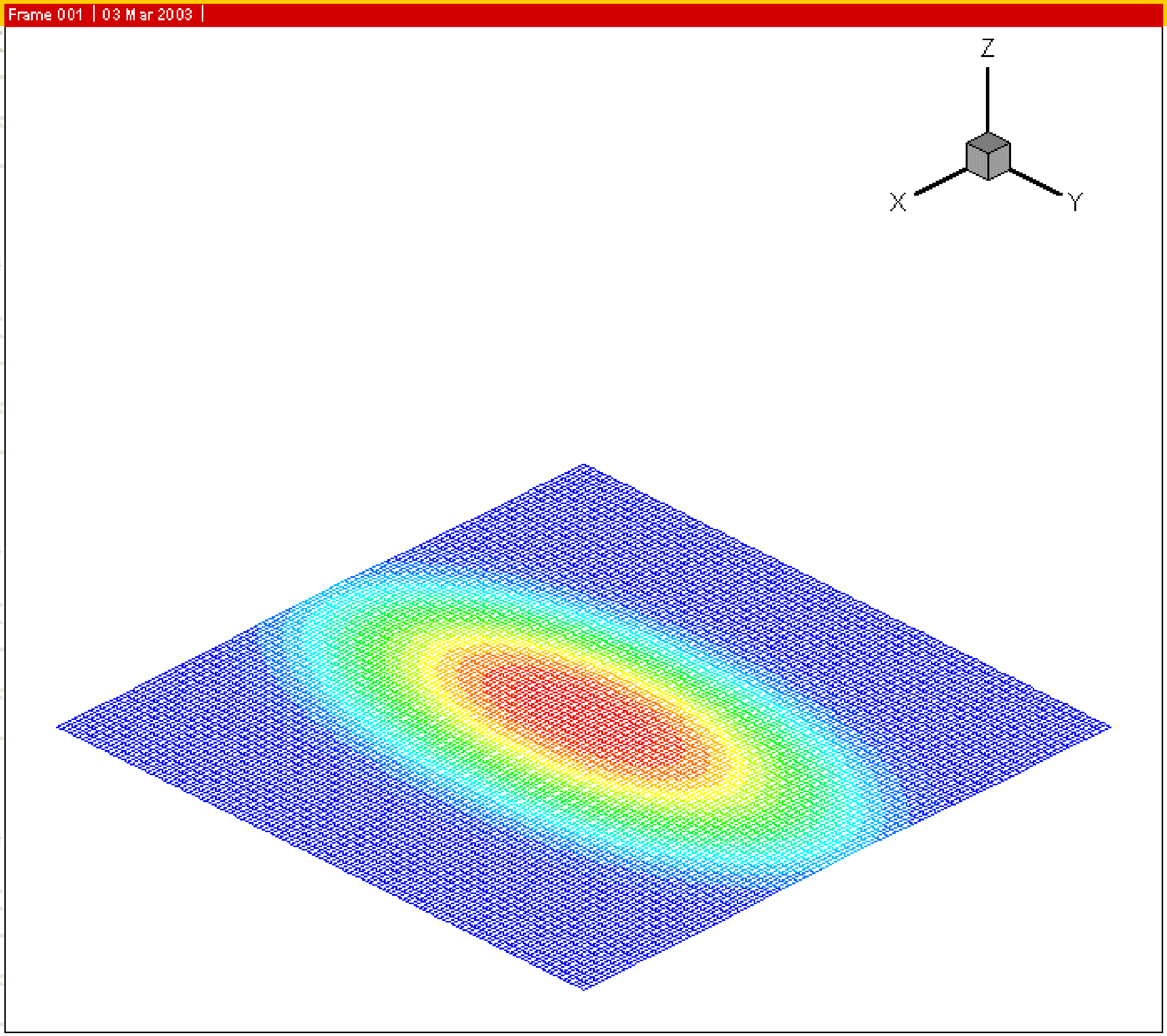
3D Collapse and explosion in BEC





$$\beta = \frac{4\pi\ N\, a_s}{x_s}$$

3D Collapse and explosion in BEC



Semiclassical limits

$$0 < \varepsilon \ll 1 \qquad i\varepsilon\, \partial_t \psi^\varepsilon(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi^\varepsilon + V(\vec{x})\psi^\varepsilon + \beta\,|\psi^\varepsilon|^2\,\psi^\varepsilon$$

$$\psi := \psi^\varepsilon \qquad \psi^\varepsilon(\vec{x},0) := \psi_0^\varepsilon(\vec{x}) = \sqrt{\rho_0^\varepsilon(\vec{x})}\; e^{i S_0^\varepsilon(\vec{x})/\varepsilon}$$

- WKB analysis -- Gregor Wentzel, Hans Kramers & Leon Brillouin, 1926
  - 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

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

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

From QM to fluid dynamics

– 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 --- Euler equations for fluids

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

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

- 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
  – NLSE before caustics

Efficient Computation

- 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, …….
  - ε 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
- Solve the limiting QHD system with multi-values
  - Level set method: S. Osher, H.L. Liu, S. Jin, L.T. Cheng, ….
  - K-branch method: L. Goss, P.A. Markowich, …..
- Solve the Liouville equation (obtained by Wigner transform): S. Jin, X. Wen, ……..

Properties of TSSP

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

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

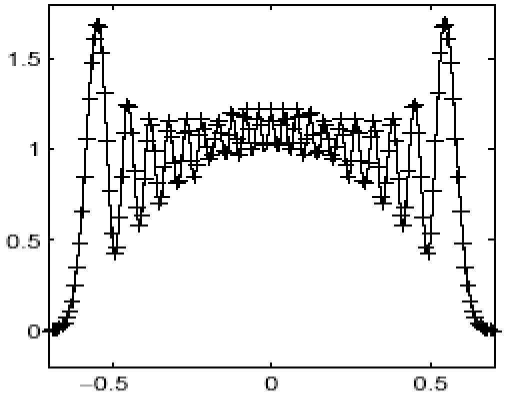
  - Weakly nonlinear case: $\beta = O(\varepsilon)$

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

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

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

- Error estimate: not available yet!!



For Schrodinger Equation

- 4^{th} order compact time-splitting ---– S.A. Chin, Phys. Lett. A, 97'

- Zassenhaus splitting --- P. Bader, A. Iserles, K. Kropielnicka & P. Singh, 15'; 17'; …. (see talk by Prof K. Kropielnicka in the workshop)

4th-order Compact time-splitting

$$e^T e^V = e^Z$$

- Baker-Campbell-Hausdorff (BCH) formula

$$Z = \sum_{n=1}^{\infty} Z_n = T + V + \frac{1}{2}[T,V] + \frac{1}{12}\left([T,[T,V]] + [V,[V,T]]\right) - \frac{1}{24}[V,[T,[T,V]]] + \ldots$$

$$[T,V] := TV - VT$$

- 4th compact method – S.A. Chin, Phys. Lett. A, 97'

$$u(\tau) = e^{\tau(T+V)} u_0 \approx u^{(4)} := e^{\frac{1}{6}\tau V} e^{\frac{1}{2}\tau T} e^{\frac{2}{3}\tau F(V)} e^{\frac{1}{2}\tau T} e^{\frac{1}{6}\tau V} u_0$$

$$F(V) := V + \frac{\tau^2}{48}[V,[T,V]]$$

$$\left\| u(\tau) - u^{(4)} \right\| \le C\tau^5$$

Application to (linear) Schrodinger equation

- The Schrodinger equation

$$i\,\partial_t \psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x})\psi \Leftrightarrow \partial_t \psi = (T+V)\psi$$

  - With

$$V := -iV(\vec{x}), \quad T := \frac{i}{2}\nabla^2, \quad F(V) := -iV(x) + \frac{i\tau^2}{48}\left|\nabla V(\vec{x})\right|^2$$

- 4th compact time-splitting $\left\|\psi(\tau) - \psi^{(4)}\right\| \le C\tau^5$

$$\psi(\tau) \approx \psi^{(4)} := e^{\frac{1}{6}\tau V} e^{\frac{1}{2}\tau T} e^{\frac{2}{3}\tau F(V)} e^{\frac{1}{2}\tau T} e^{\frac{1}{6}\tau V} \psi(0)$$

Application to Damped NLS

- NLS with damping term (Bao & Jaksch, SINUM, 03')

$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x})\psi + \beta|\psi|^2\psi - \underline{i\delta_0\beta^2|\psi|^4\psi}$$

- Time-splitting spectral method (TSSP)
  - Step 1:

$$i\ \partial_t\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi$$

  - Step 2:

$$i\ \partial_t\psi(\vec{x},t) = V(\vec{x})\psi(\vec{x},t) + \beta|\psi(\vec{x},t)|^2\psi(\vec{x},t) - \underline{i\delta_0\beta^2|\psi(\vec{x},t)|^4\psi(\vec{x},t)}$$

$$\Downarrow \rho=|\psi|^2$$

$$\partial_t\rho = -2\delta_0\beta^2\rho^3 \Rightarrow \rho(x,t) = \frac{\rho(x,t_n)}{\sqrt{1+4\delta_0\beta^2(t-t_n)\rho^2(x,t_n)}}, \quad t_n \le t \le t_{n+1}$$

To NLS with time-dependent potential

- NLS with time-dependent potential (Bao & Jaksch, SINUM, 03')

$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x},t)\psi + \beta(t)\,|\psi|^2\,\psi$$

- Time-splitting spectral method (TSSP)
  - Step 1:

$$i\ \partial_t\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi$$

  - Step 2:

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

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

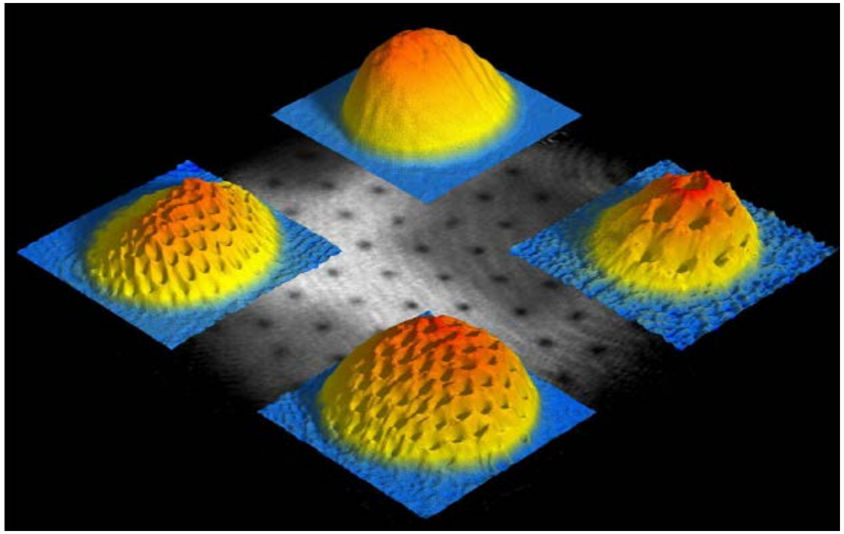
$$\Rightarrow \psi(\vec{x},t) = e^{-i\left[\int_{t_n}^{t} V(\vec{x},s)ds + |\psi(\vec{x},t_n)|^2\int_{t_n}^{t}\beta(s)ds\right]}\ \psi(\vec{x},t_n)$$

GPE with angular rotation

- GPE / NLSE with an angular momentum rotation

$$i\,\partial_t\,\psi(\vec{x},t)=[-\frac{1}{2}\nabla^2+V(\vec{x})-\Omega\,L_z+\beta\,|\psi|^2]\,\psi,\quad \vec{x}\in\mathbb{R}^d,\quad t>0$$

$$L_z := xp_y - yp_x = -i(x\partial_y - y\partial_x) \equiv -i\partial_\theta\,,\quad L=\vec{x}\times\vec{P},\quad \vec{P}=-i\nabla$$



Vortex @MIT

Numerical methods

- Time-splitting + polar (cylindrical) coordinates –Bao, Du & Zhang, SIAP, 05'

$$\text{Step 1:}\quad i\,\partial_t\,\psi(\vec{x},t)=[-\frac{1}{2}\nabla^2-\Omega\,L_z]\,\psi$$

$$\text{Step 2:}\quad i\,\partial_t\,\psi(\vec{x},t)=[V(\vec{x})+\beta\,|\,\psi\,|^2]\,\psi$$

- Time-splitting + ADI -- Bao & Wang, JCP, 06'

$$\text{Step 1:}\quad i\,\partial_t\,\psi(\vec{x},t)=[-\frac{1}{2}\partial_{xx}-i\Omega y\partial_x]\,\psi$$

$$\text{Step 2:}\quad i\,\partial_t\,\psi(\vec{x},t)=[-\frac{1}{2}\partial_{yy}+i\Omega x\partial_y]\,\psi$$

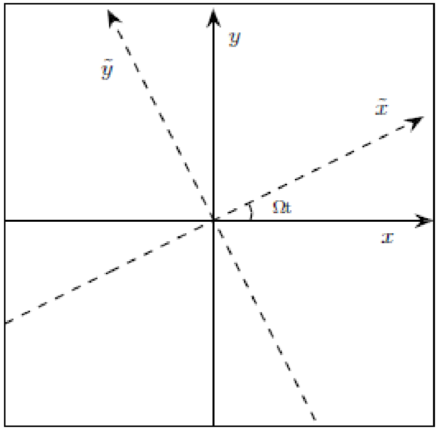
$$\text{Step 3:}\quad i\,\partial_t\,\psi(\vec{x},t)=[V(\vec{x})+\beta\,|\,\psi\,|^2]\,\psi$$

- Time-splitting + Laguerre-Hermite functions –Bao, Li &Shen, SISC, 09'

$$\text{Step 1:}\quad i\,\partial_t\,\psi(\vec{x},t)=[-\frac{1}{2}\nabla^2-\Omega\,L_z+\left|\vec{x}\right|^2/2]\,\psi:=L\psi$$

$$\text{Step 2:}\quad i\,\partial_t\,\psi(\vec{x},t)=[W(\vec{x})+\beta\,|\,\psi\,|^2]\,\psi$$

A simple & efficient method



- **Ideas** – Bao, Marahrens,Tang & Zhang, 13'; Bao & Cai, KRM, 13'; ……
  - A rotating Lagrange coordinate:

$$\tilde{\vec{x}} = A(t)^{-1}\vec{x} \quad \& \quad \phi(\tilde{\vec{x}},t) := \psi(\vec{x},t) = \psi(A(t)\vec{x},t)$$

$$A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) \\ -\sin(\Omega t) & \cos(\Omega t) \end{bmatrix} \text{ for } d=2; \quad A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \text{ for } d=3$$

  - GPE in rotating Lagrange coordinates

$$i\,\partial_t\,\phi(\tilde{\vec{x}},t) = [-\frac{1}{2}\nabla^2 + V(A(t)\tilde{\vec{x}}) + \beta\,|\phi|^2]\,\phi, \quad \tilde{\vec{x}} \in \mathbb{R}^d, \quad t>0$$

  - TSSP method

$$\text{Step 1:} \quad i\,\partial_t\,\phi(\tilde{\vec{x}},t) = -\frac{1}{2}\nabla^2\phi,$$

$$\text{Step 2:} \quad i\,\partial_t\,\phi(\tilde{\vec{x}},t) = [V(A(t)\tilde{\vec{x}}) + \beta\,|\phi|^2]\,\phi,$$

Dynamics of ground state

- Choose initial data as: $\beta = 100, \quad \Omega = 0.8, \quad \gamma_y = \gamma_z = 1$

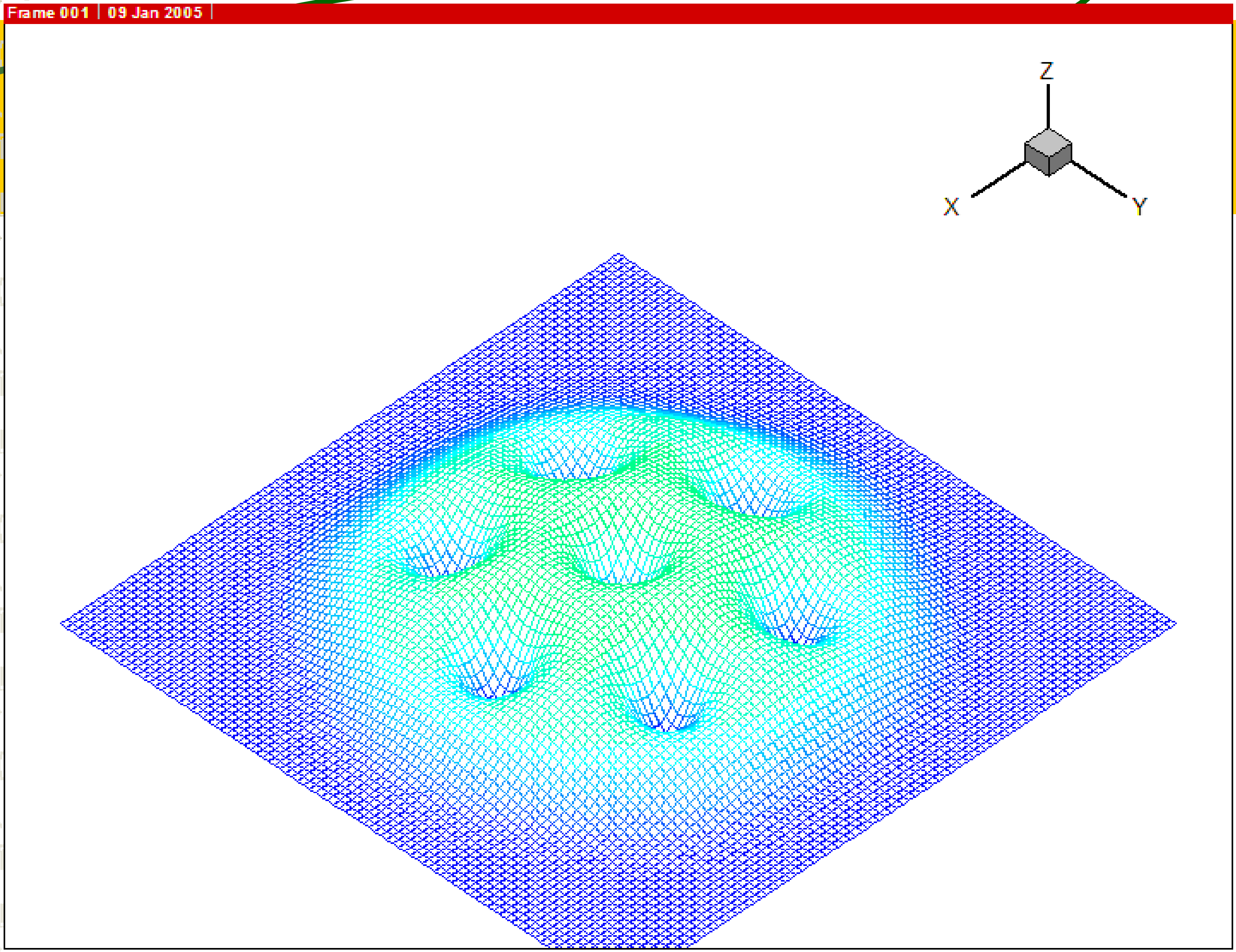
  $\psi_0(\vec{x}) = \phi_g(\vec{x})$: ground state

- Change the frequency in the external potential:
  - Case 1: symmetric: $\gamma_x : 1 \to 2 \quad \& \quad \gamma_y : 1 \to 2$

    surface contour
  - Case 2: non-symmetric: $\gamma_x : 1 \to 1.8 \quad \& \quad \gamma_y : 1 \to 2.2$

    surface contour
  - Case 3: dynamics of a vortex lattice with 45 vortices:

    image contour $\beta = 1000, \Omega = 0.9, V(\vec{x}, t)$: anisotropic next



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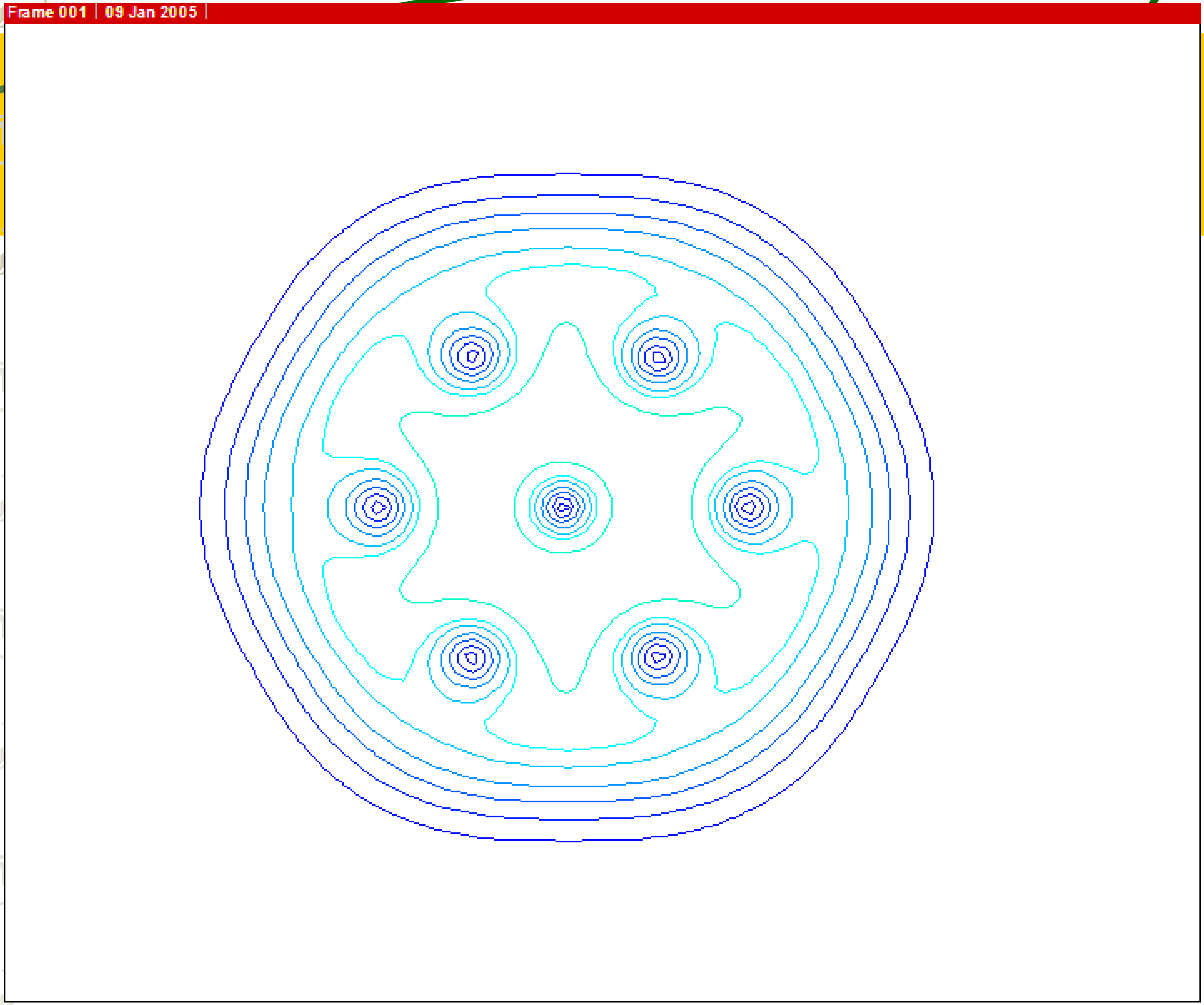

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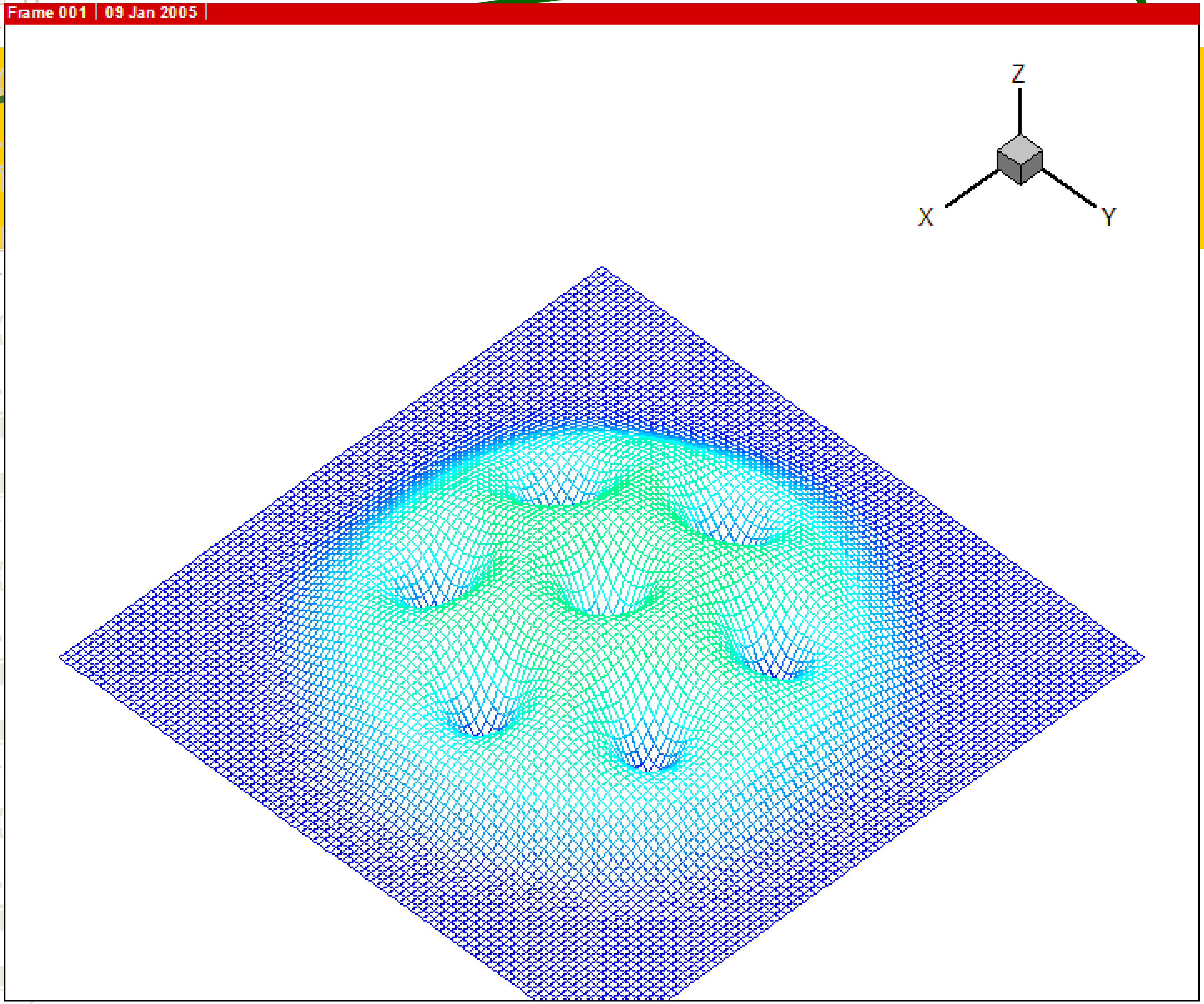

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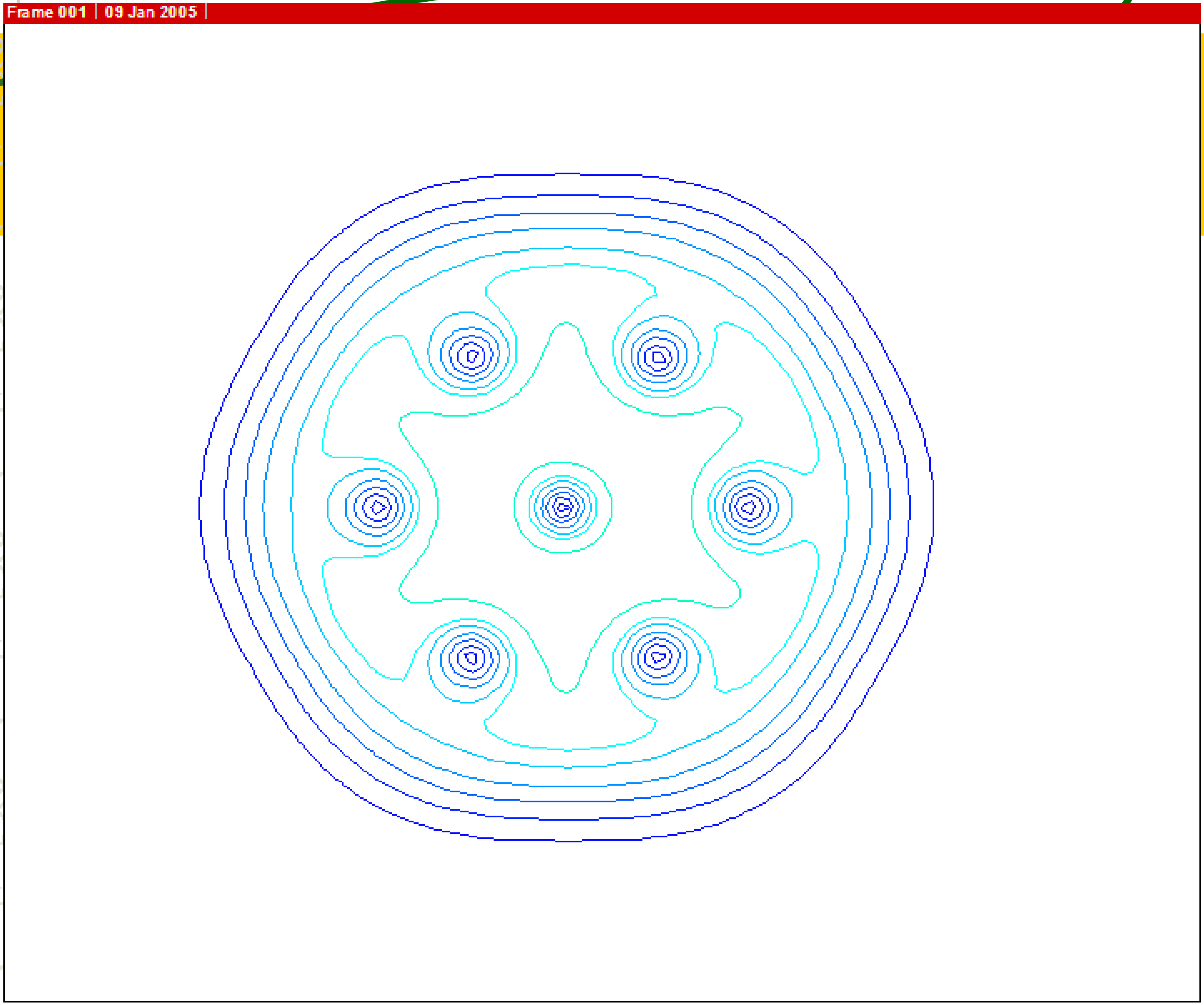

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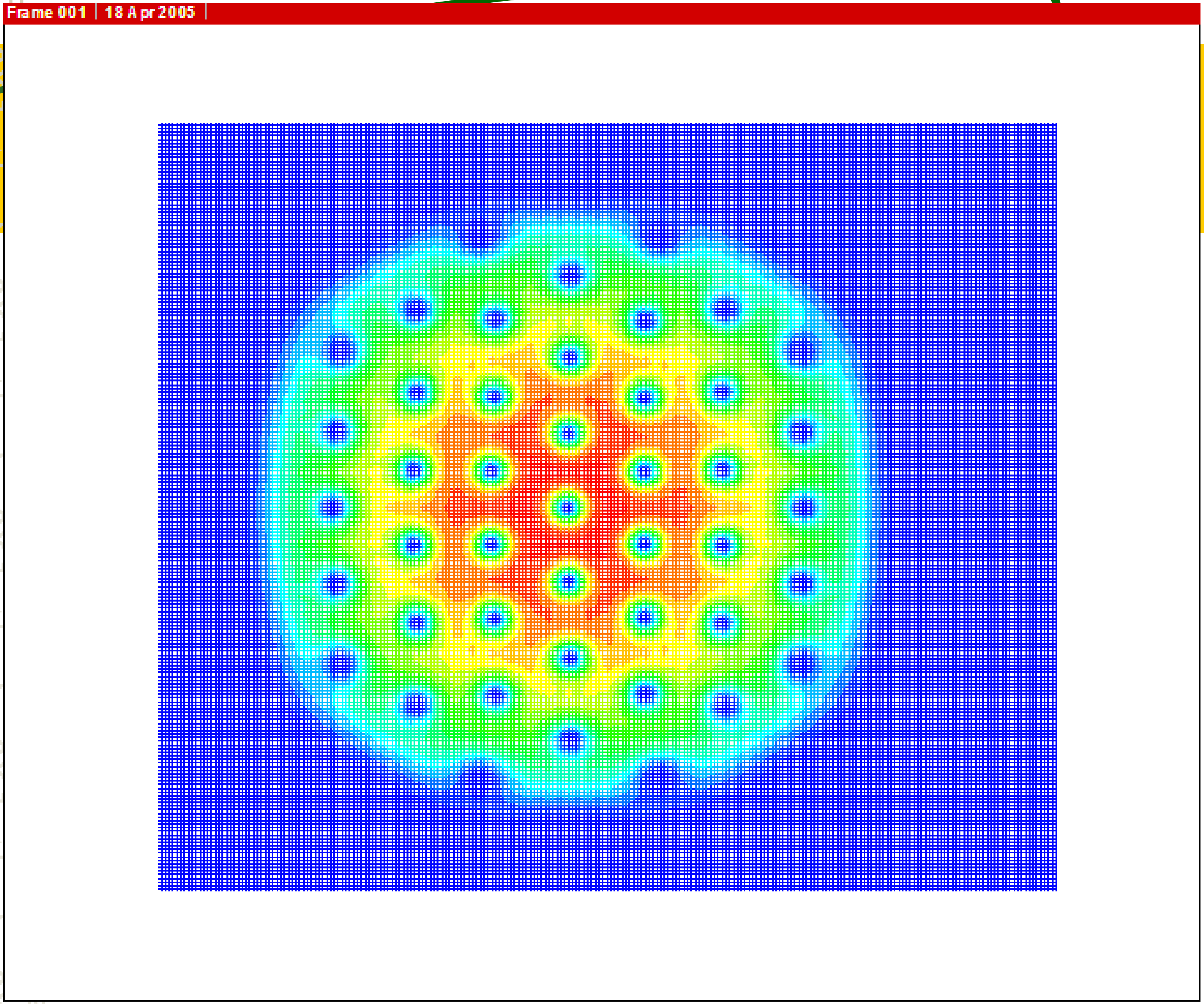

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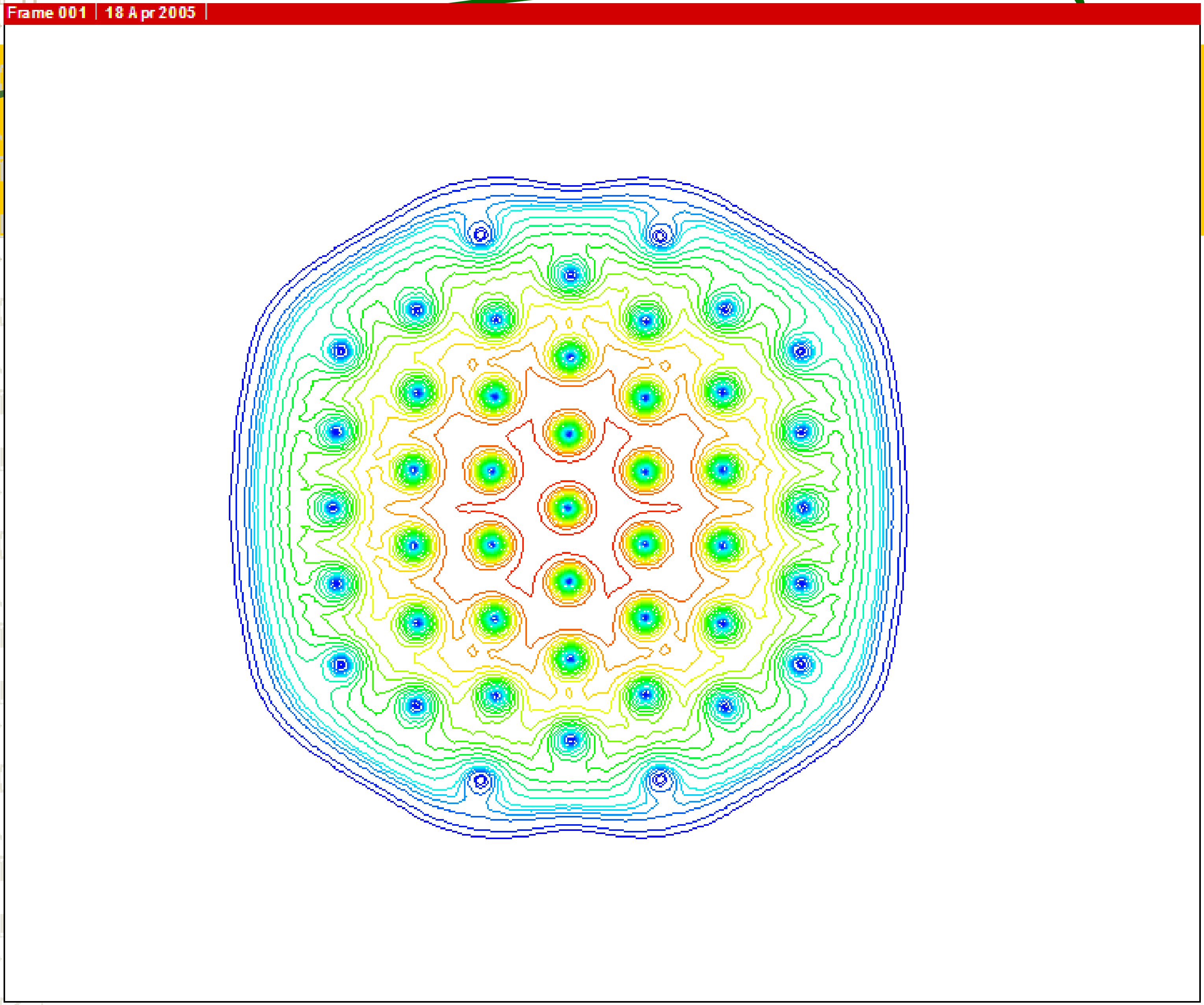

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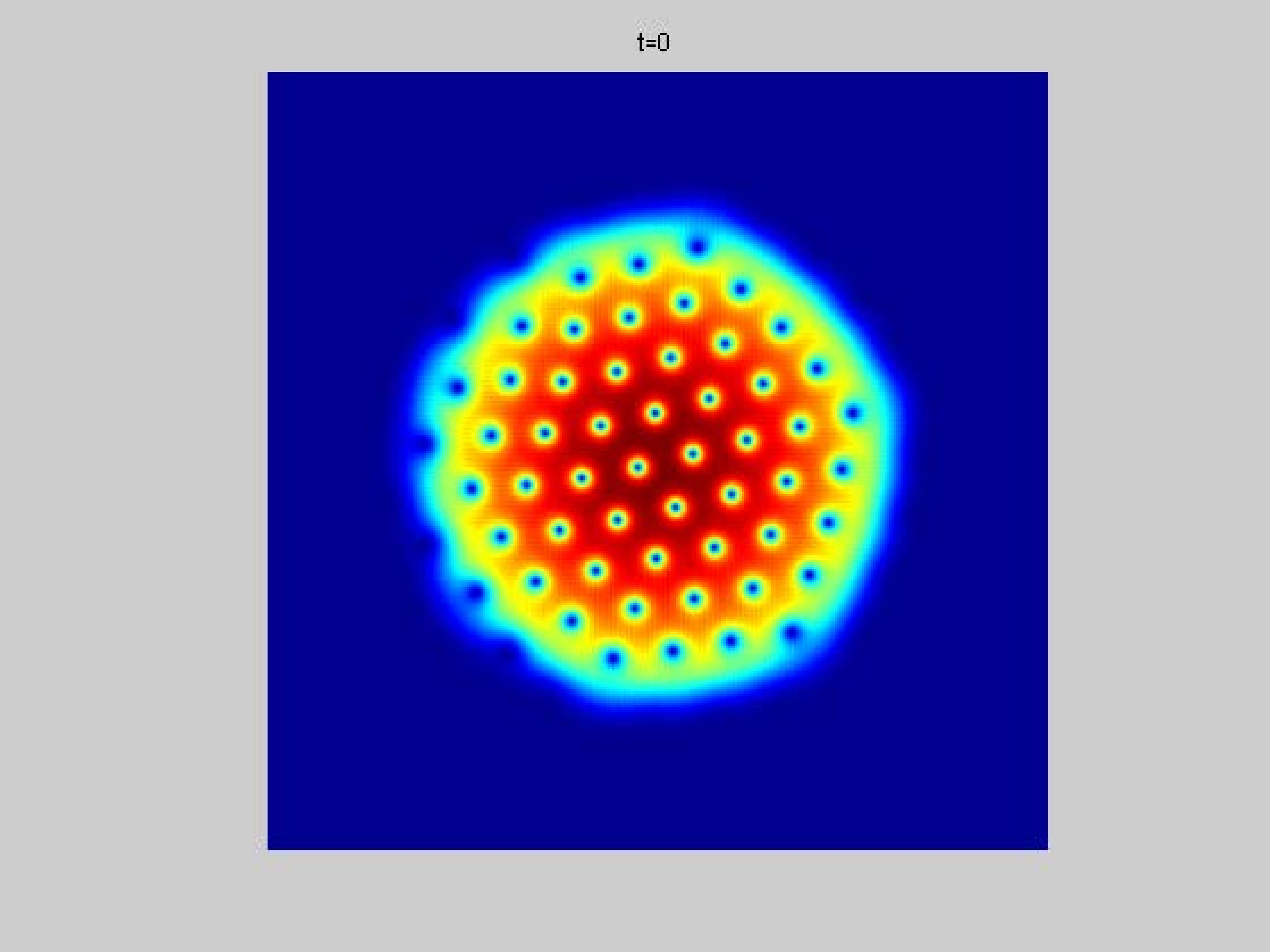
Dynamics of a vortex lattice



Application to NLSE with Coulomb interaction

- NLSE with Coulomb interaction (Bao, Mauser & Stimming, CMS, 04'; Bao, Jian, Mauser & Zhang, SIAP, 13'; Greengard, Jiang& Bao, SISC, 14'; Bao, Jiang, Tang & Zhang, JCP, 15')

$$i\varepsilon\,\partial_t\psi(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi + V(\vec{x})\psi + \frac{\sigma_0}{|\vec{x}|} * |\psi|^2\,\psi,$$

- Schrodinger-Poisson-type equation
  - In 3D

$$i\varepsilon\,\partial_t\psi(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi + V(\vec{x})\psi + \tilde{\sigma}_0 W\psi, \quad -\Delta W = |\psi|^2, \quad \lim_{|\vec{x}|\to\infty} W(\vec{x},t) = 0$$

  - In 2D

$$i\varepsilon\,\partial_t\psi(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi + V(\vec{x})\psi + \tilde{\sigma}_0 W\psi, \quad (-\Delta)^{1/2} W = |\psi|^2, \quad \lim_{|\vec{x}|\to\infty} W(\vec{x},t) = 0$$

Application to NLSE with Coulomb interaction

- Time-splitting spectral (TSSP) method
  - Step 1: $$i\,\varepsilon\,\partial_t \psi(\vec{x},t) = -\frac{\varepsilon^2}{2}\nabla^2\psi$$
  - Step 2:

$$i\,\varepsilon\,\partial_t \psi(\vec{x},t) = V(\vec{x})\psi + \tilde{\sigma}_0 W\psi, \quad -\Delta W = |\psi|^2, \quad \lim_{|\vec{x}|\to\infty} W(\vec{x},t) = 0$$

  - Boundary condition when truncation
  - Dirichlet BC is OK, periodic BC is wrong!!

  - NUFFT for Coulomb interaction (Greengard, Jiang& Bao, SISC, 14'; Bao, Jiang, Tang & Zhang, JCP, 15')

$$W(\vec{x},t) = \int_{\mathbb{R}^d} \frac{1}{|\xi|^{d-1}}\widehat{\rho}(\xi,t)e^{-i\vec{x}\cdot\xi}d\xi \overset{\text{sphere coordinate}}{=} \int_{S^{d-1}\times\mathbb{R}^+} |\xi|^{d-1}\frac{1}{|\xi|^{d-1}}\widehat{\rho}(\xi,t)e^{-i\vec{x}\cdot\xi}\cdots$$

$$= \int_{S^{d-1}\times\mathbb{R}^+} \widehat{\rho}(\zeta,t)e^{-i\vec{x}\cdot\xi}\cdots, \quad \rho = |\psi|^2, \quad d = 3,2$$

Extension to dipolar quantum gas

- Gross-Pitaevskii equation (re-scaled) $\psi=\psi(\vec{x},t) \quad \vec{x}\in\mathbb{R}^3$

$$i\,\partial_t\,\psi(\vec{x},t)=\left[-\frac{1}{2}\nabla^2+V(\vec{x})+\beta\,|\psi|^2+\lambda\left(U_{\rm dip}*|\psi|^2\right)\right]\psi$$

  – Trap potential $V(\vec{x})=\frac{1}{2}\left(\gamma_x^2\,x^2+\gamma_y^2\,y^2+\gamma_z^2\,z^2\right)$

  – Interaction constants $\beta=\frac{4\pi N\,a_s}{x_s}$ (short-range), $\lambda=\frac{mN\,\mu_0\mu_{\rm dip}^2}{3\hbar^2 x_s}$ (long-range)

  – Long-range dipole-dipole interaction kernel

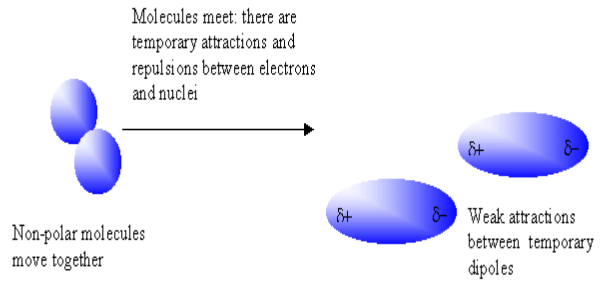
$$U_{\rm dip}(\vec{x})=\frac{3}{4\pi}\frac{1-3(\vec{n}\cdot\vec{x})^2/|\vec{x}|^2}{|\vec{x}|^3}=\frac{3}{4\pi}\frac{1-3\cos^2(\theta)}{|\vec{x}|^3}$$

- References:

  – L. Santos, et al. PRL 85 (2000), 1791-1797

  – S. Yi & L. You, PRA 61 (2001), 041604(R);

  – D. H. J. O'Dell, PRL 92 (2004), 250401



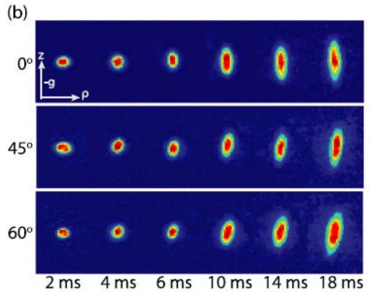
A New Formulation

$$r = |\vec{x}| \quad \& \quad \partial_{\vec{n}} = \vec{n} \cdot \nabla \quad \& \quad \partial_{\vec{n}\vec{n}} = \partial_{\vec{n}}(\partial_{\vec{n}})$$

- Using the identity (O'Dell et al., PRL 92 (2004), 250401, Parker et al., PRA 79 (2009), 013617)

$$U_{\rm dip}(\vec{x}) = \frac{3}{4\pi r^3}\left(1 - \frac{3(\vec{n}\cdot\vec{x})^2}{r^2}\right) = -\delta(\vec{x}) - 3\partial_{\vec{n}\vec{n}}\left(\frac{1}{4\pi r}\right)$$

$$\Rightarrow \qquad \widehat{U}_{\rm dip}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2}$$



BEC@Stanford

- Dipole-dipole interaction becomes

$$U_{\rm dip} * |\psi|^2 = -|\psi|^2 - 3\partial_{\vec{n}\vec{n}}\varphi$$

$$\varphi = \frac{1}{4\pi r} * |\psi|^2 \Leftrightarrow -\nabla^2\varphi = |\psi|^2$$

Figure 1. The Rosensweig instability [32] of a ferrofluid (a colloidal dispersion in a carrier liquid of subdomain ferromagnetic particles, with typical dimensions of 10 nm) in a magnetic field perpendicular to its surface is a fascinating example of the novel physical phenomena appearing in classical physics due to long range, anisotropic interactions. Figure reprinted with permission from [34]. Copyright 2007 by the American Physical Society.

A New Formulation

- Gross-Pitaevskii-Poisson type equations (Bao,Cai & Wang, JCP, 10')

$$i\,\partial_t\,\psi(\vec{x},t)=\left[-\frac{1}{2}\nabla^2+V(\vec{x})+(\beta-\lambda)\,|\,\psi\,|^2\,-3\lambda\partial_{\vec{n}\vec{n}}\varphi\,\right]\psi$$

$$-\nabla^2\varphi(\vec{x},t)=|\,\psi(\vec{x},t)\,|^2,\quad \vec{x}\in\mathbb{R}^3,\quad \lim_{|\vec{x}|\to\infty}\varphi(\vec{x},t)=0$$

  – Energy

$$E(\psi(\cdot,t)):=\int_{\mathbb{R}^3}\left[\frac{1}{2}\,|\,\nabla\psi\,|^2+V(\vec{x})\,|\,\psi\,|^2+\frac{\beta-\lambda}{2}\,|\,\psi\,|^4+\frac{3\lambda}{2}\,|\,\partial_{\vec{n}}\nabla\varphi\,|^2\right]d\,\vec{x}$$

  – Model in 2D $\overset{2D}{\rightarrow}$ $(-\Delta_\perp)^{1/2}\varphi(\vec{x},t)=|\,\psi(\vec{x},t)\,|^2,\quad \vec{x}\in\mathbb{R}^2,\quad \lim_{|\vec{x}|\to\infty}\varphi(\vec{x},t)=0$

- Numerical methods --- TSSP with sine basis instead of Fourier basis
  – Bao, Cai & Wang, JCP, 10'; Bao & Cai, KRM, 13'
  – Bao, Marahrens,Tang & Zhang, 13''; Bao & Cai, KRM, 13'; ……

Numerical Method for dynamics

- Time-splitting sine pseudospectral (TSSP) method, $[t_n, t_{n+1}]$
  - Step 1: Discretize by spectral method & integrate in phase space exactly

$$i\,\partial_t \psi(\vec{x},t) = -\frac{1}{2}\nabla^2 \psi$$

  - Step 2: solve the nonlinear ODE analytically

$$i\,\partial_t \psi(\vec{x},t) = \left[V_{\text{ext}}(\vec{x}) + (\beta-\lambda)\,|\psi(\vec{x},t)|^2 - 3\lambda\,\partial_{\vec{n}\vec{n}}\varphi(\vec{x},t)\right]\psi(\vec{x},t)$$

$$-\Delta\varphi(\vec{x},t) = |\psi(\vec{x},t)|^2,$$

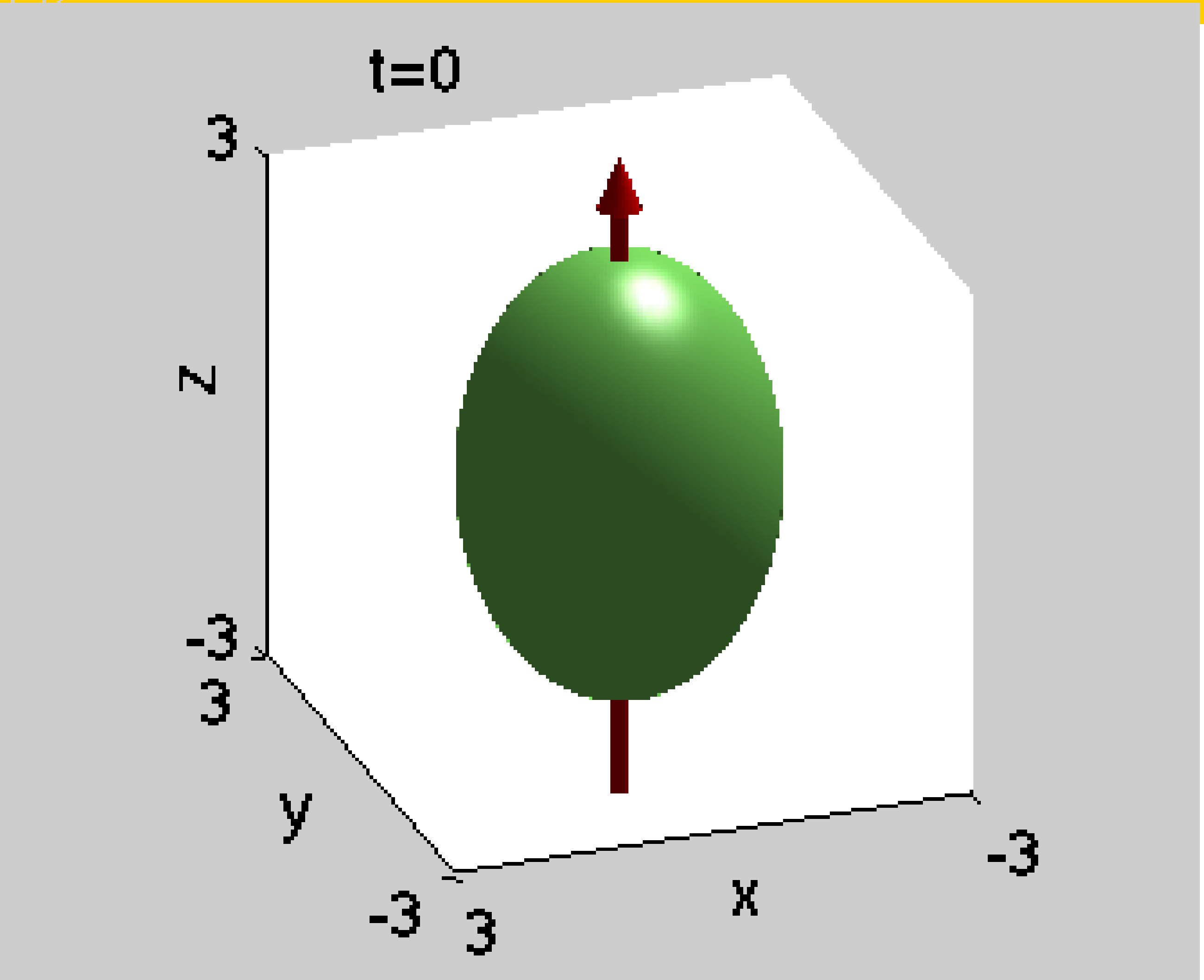
$$\Downarrow\ \partial_t(|\psi(\vec{x},t)|^2) = 0 \Rightarrow |\psi(\vec{x},t)| = |\psi(\vec{x},t_n)| \quad \& \quad \varphi(\vec{x},t) = \varphi(\vec{x},t_n)$$

$$i\,\partial_t \psi(\vec{x},t) = \left[V_{\text{ext}}(\vec{x}) + (\beta-\lambda)\,|\psi(\vec{x},t_n)|^2 - 3\lambda\,\partial_{\vec{n}\vec{n}}\varphi(\vec{x},t_n)\right]\psi(\vec{x},t)$$

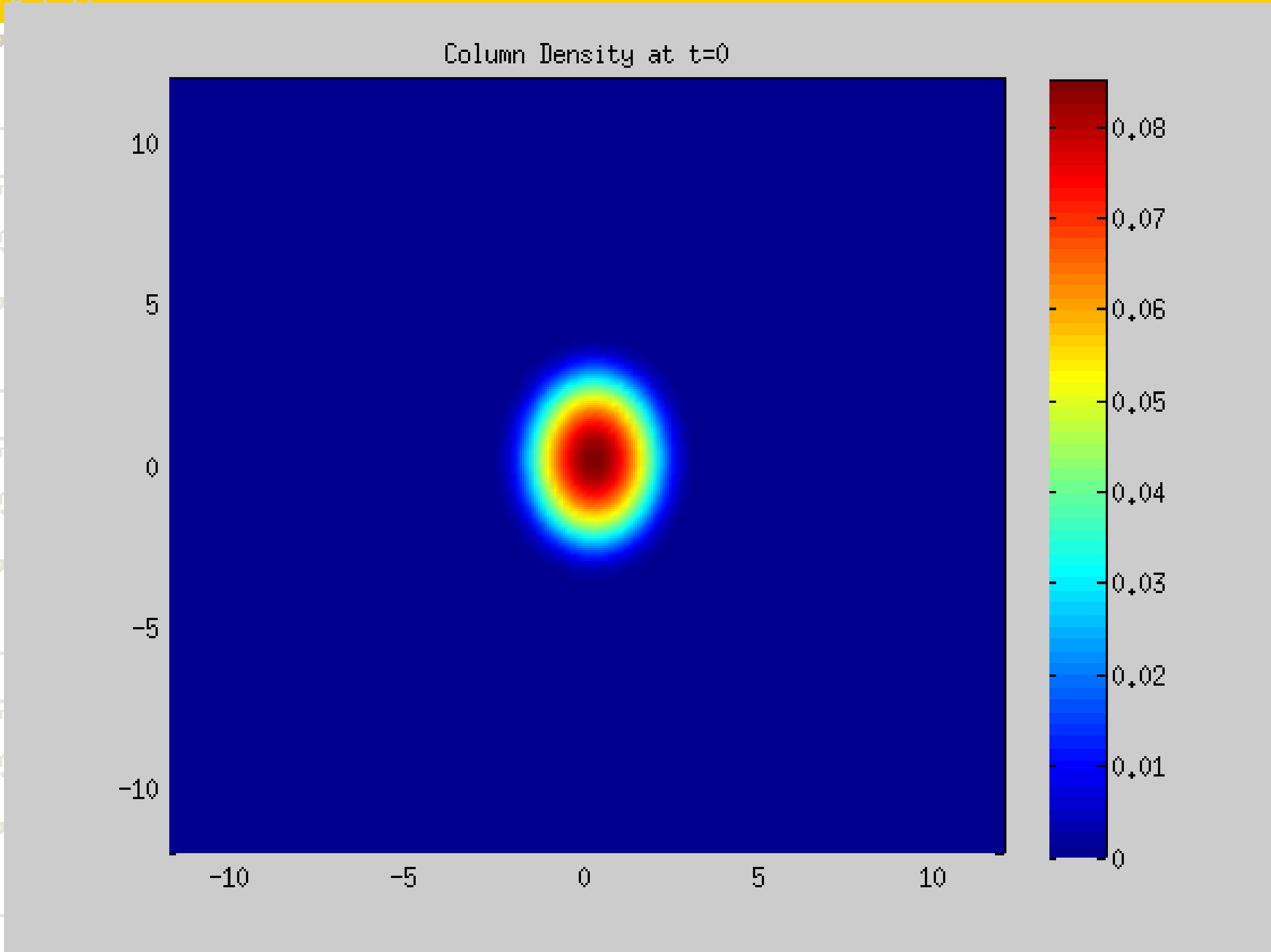
$$-\Delta\varphi(\vec{x},t_n) = |\psi(\vec{x},t_n)|^2,$$

$$\Rightarrow \psi(\vec{x},t) = e^{-i\,(t-t_n)[V_{\text{ext}}(\vec{x})+(\beta-\lambda)|\psi(\vec{x},t_n)|^2-3\lambda\,\partial_{\vec{n}\vec{n}}\varphi(\vec{x},t_n)]}\,\psi(\vec{x},t_n)$$

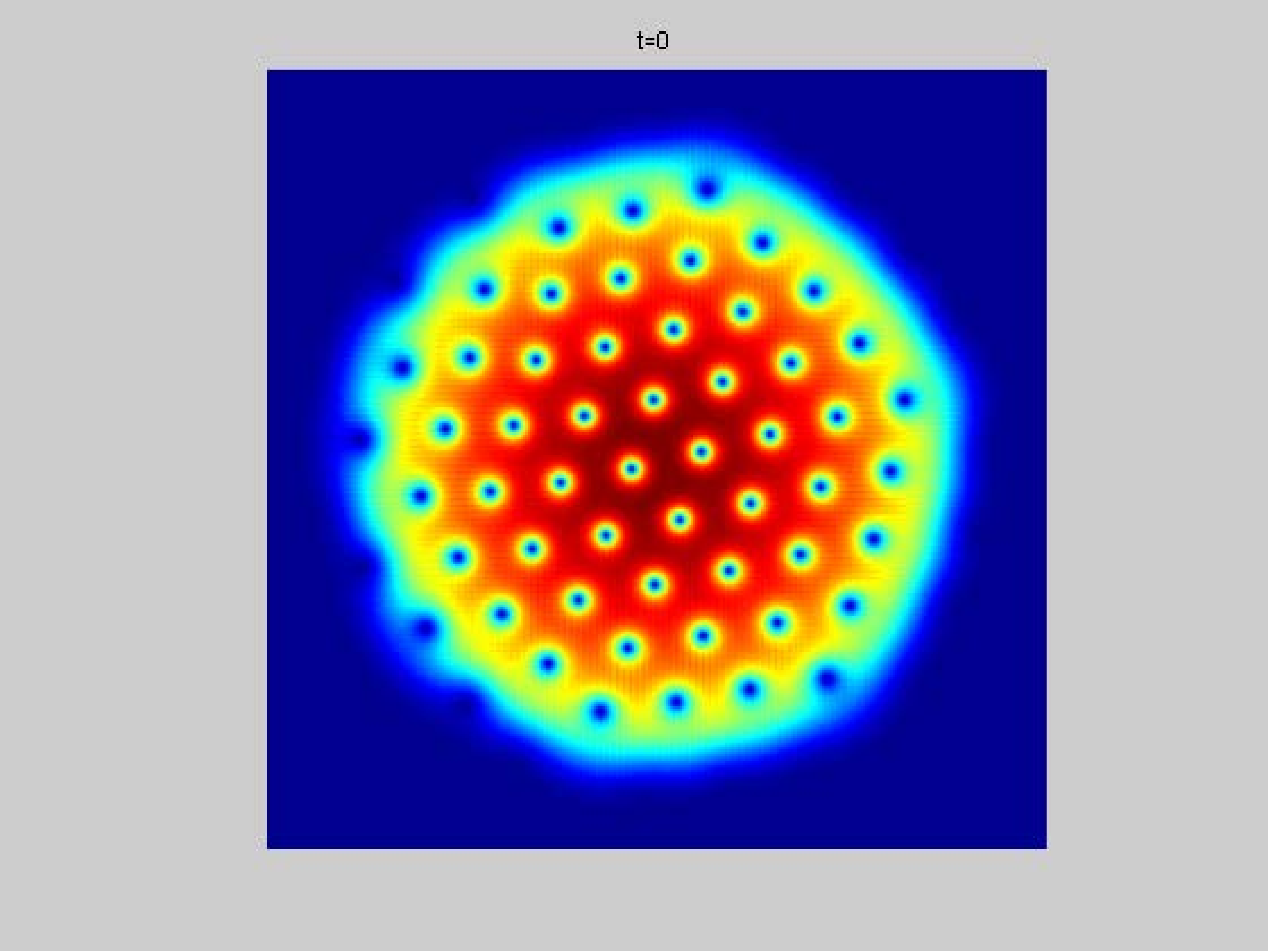
Dynamics of a BEC with DDI



Collapse of a BEC with DDI



Dynamics of a vortex lattice with DDI



New numerical methods for DDI

- How to compute nonlocal DDI $\phi := U_{\text{dip}} * |\psi|^2$
  - FFT (fast Fourier transform)
  - DST (discrete sine transform)

$$\widehat{U}_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2}$$

$$\phi = -|\psi|^2 - 3\partial_{nn}\varphi \quad \& \quad -\Delta\varphi(\vec{x},t) = |\psi(\vec{x},t)|^2$$

  - Nonuniform FFT (Bao, Jiang, Greengard, SISC,14'; Bao, Tang & Zhang, CiCP, 16')

$$\phi(\vec{x},t) = \int_{\mathbb{R}^3} \widehat{U}_{\text{dip}}(\xi)\widehat{\rho}(\zeta,t)e^{-i\vec{x}\cdot\xi}d\xi \qquad \rho = |\psi|^2$$

sphere coordinate

$$= \int_{S^2\times\mathbb{R}^+} \widehat{U}_{\text{dip}}(\xi)\,|\xi|^2\,\widehat{\rho}(\zeta,t)e^{-i\vec{x}\cdot\xi}\cdots$$

Numerical results (Bao, Tang & Zhang, CiCP, 16')

$$\Phi(\mathbf{x},t)=\int_{\mathbb{R}^d}U_{\text{dip}}(\mathbf{x}-\mathbf{y})\rho(\mathbf{y},t)d\mathbf{y}:\quad e_h:=\|\Phi-\Phi_h\|_{l^2}/\|\Phi\|_{l^2},$$

NUFFT	$h=2$	$h=1$	$h=1/2$	$h=1/4$
$L=4$	1.118E-01	3.454E-04	1.335E-04	1.029E-04
$L=8$	5.281E-02	3.428E-04	9.834E-12	1.601E-14
$L=16$	5.202E-02	3.551E-04	1.143E-11	8.089E-15
DST	$h=1$	$h=1/2$	$h=1/4$	$h=1/8$
$L=8$	6.919E-02	7.720E-02	8.124E-02	8.327E-02
$L=16$	2.709E-02	2.853E-02	2.925E-02	2.961E-02
$L=32$	1.008E-02	1.033E-02	1.046E-02	1.052E-02

Application to fractional Schrodinger equation

- Fractional Schrodinger equation (A. Elgart & B. Schlein, CPAM, 07'; Bao & Dong, JCP, 11'; I. Carusotto & C. Ciutti, Rev. Mod. Phys, 85 (299), 13'; F. Pinsker et al., PRB, 15', ….)

$$i\partial_t \psi(\vec{x},t) = \left(\delta - \Delta\right)^{\alpha/2} \psi + V(\vec{x})\psi + f(|\psi|^2)\psi,$$

  – Relativistic Hartree equation for Boson star $\delta \geq 0 \,\&\, 0 < \alpha \leq 2$
  – Polariton condensates
  – ….. $i\partial_t \psi(\vec{x},t) = q * \psi + V(\vec{x})\psi + f(|\psi|^2)\psi + ig(\vec{x},|\psi|^2)\psi, \quad \hat{q}(\vec{k}) = ...$

- Time-splitting spectral method
  – Step 1 $$i\partial_t \psi(\vec{x},t) = \left(\delta - \Delta\right)^{\alpha/2} \psi$$
  – Step 2. $$i\partial_t \psi(\vec{x},t) = V(\vec{x})\psi + f(|\psi|^2)\psi,$$

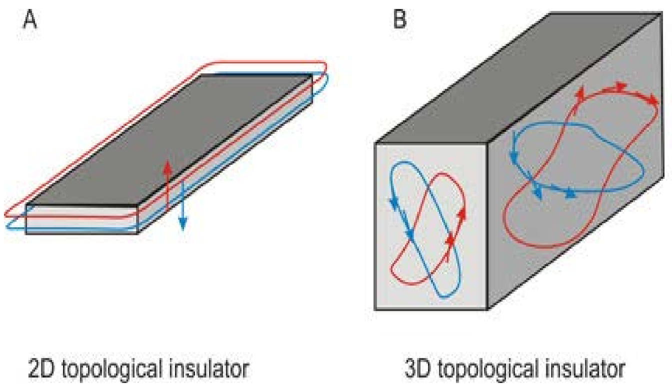
Spin-orbit coupled BEC

- Coupled GPE with a spin-orbit coupling & internal Josephson junction

$$i\frac{\partial}{\partial t}\psi_1 = [-\frac{1}{2}\nabla^2 + V(\vec{x}) + ik_0\partial_x + \delta + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2)]\psi_1 + \Omega\psi_{-1}$$

$$i\frac{\partial}{\partial t}\psi_{-1} = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - ik_0\partial_x - \delta + (\beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2)]\psi_{-1} + \Omega\psi_1$$

- Experiments: Lin, et al, Nature, 471(2011), 83.
- Applications ----Topological insulator
- Analysis & numerical methods:
  - For ground state & dynamics (Bao & Cai, 14')



Spin-orbit coupled BEC

- Time-splitting spectral (TSSP) method (Bao & Cai, SIAP, 14')
  - Step 1. Solve

$$i\frac{\partial}{\partial t}\psi_1=[-\frac{1}{2}\nabla^2+ik_0\partial_x+\delta]\psi_1+\Omega\psi_{-1}$$

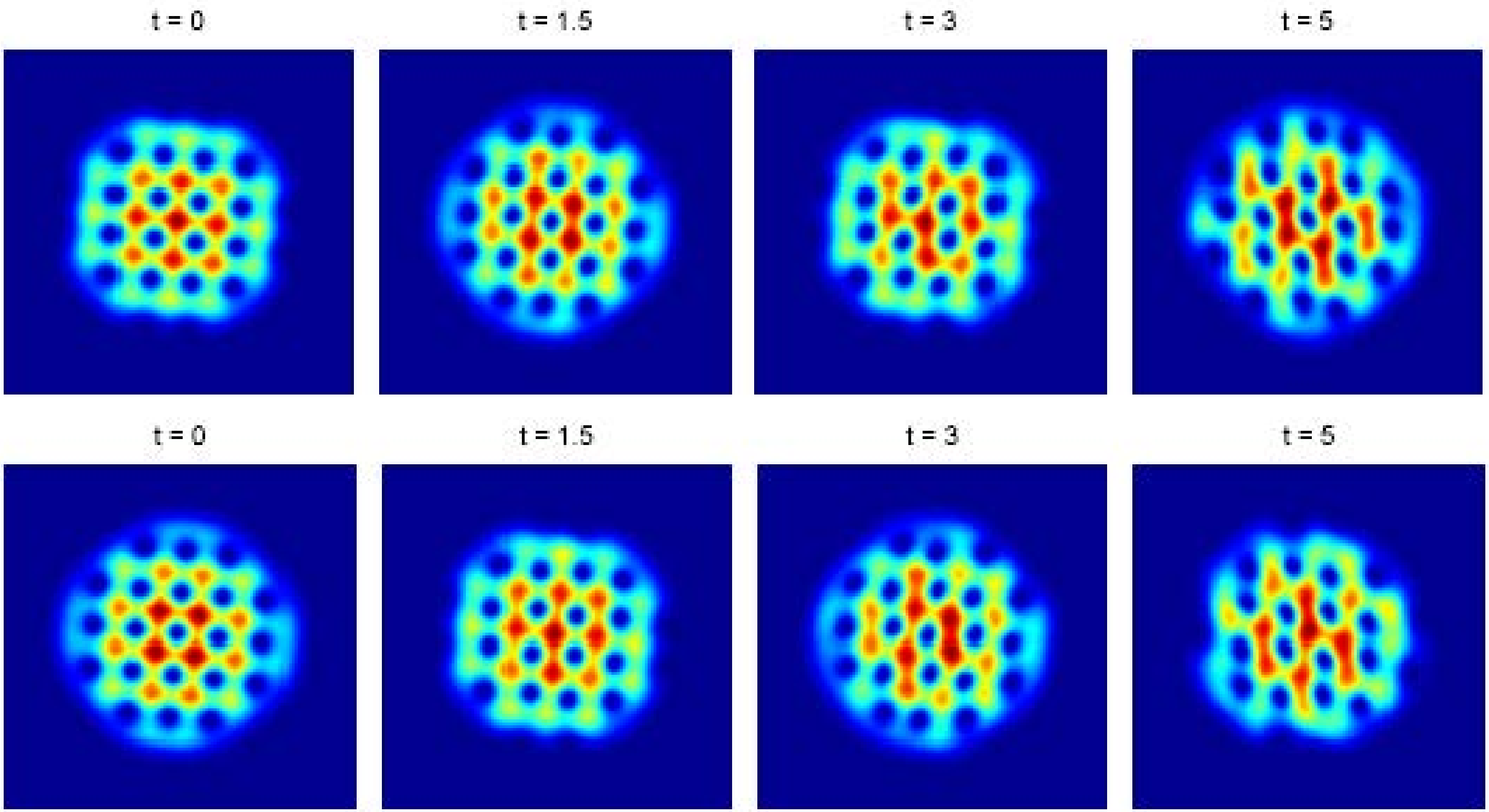
$$i\frac{\partial}{\partial t}\psi_{-1}=[-\frac{1}{2}\nabla^2-ik_0\partial_x-\delta]\psi_{-1}+\Omega\psi_1$$

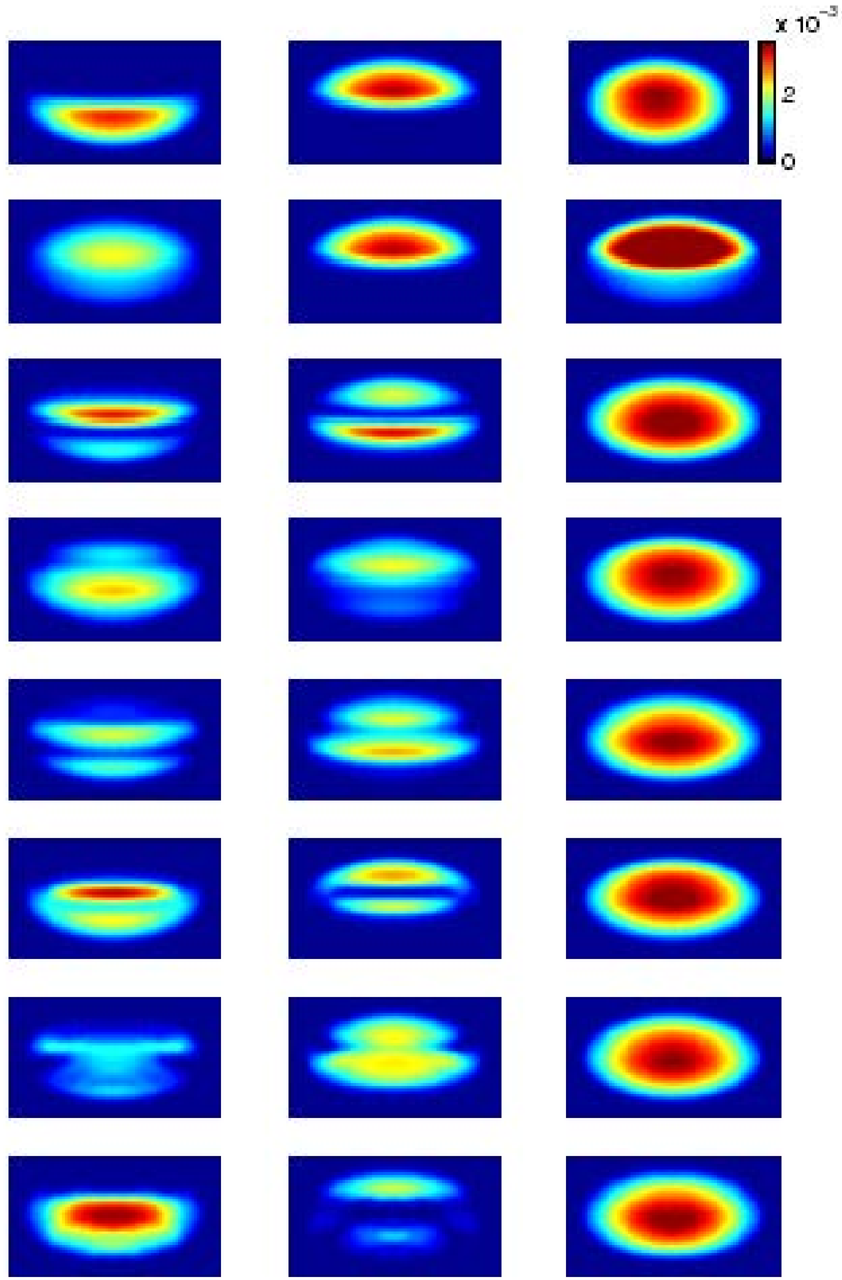
  - Step 2. Solve

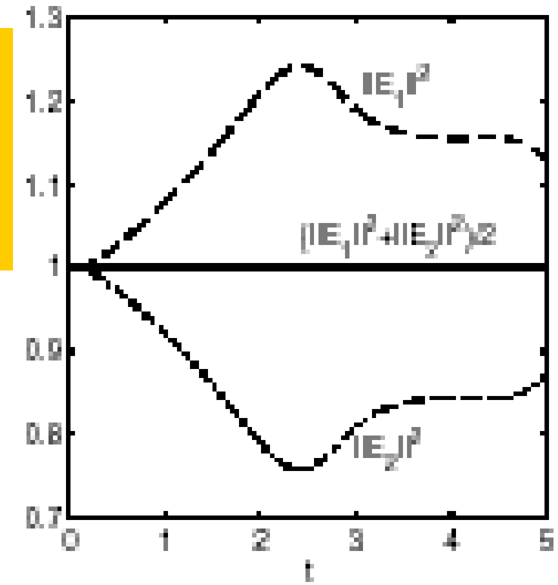
$$i\frac{\partial}{\partial t}\psi_1=[V(\vec{x})+(\beta_{11}|\psi_1|^2+\beta_{12}|\psi_2|^2)]\psi_1$$

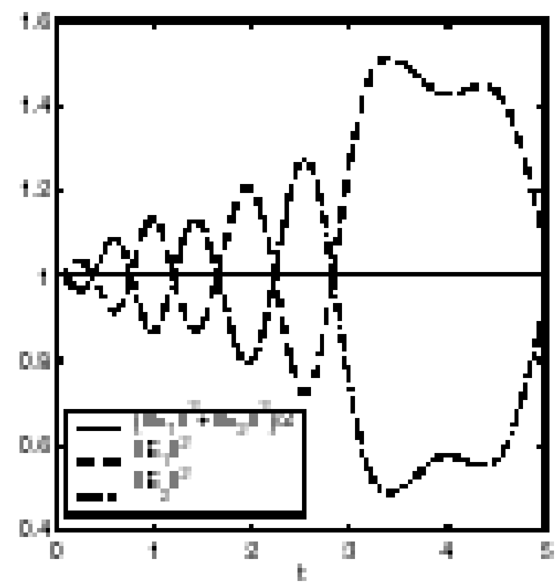
$$i\frac{\partial}{\partial t}\psi_{-1}=[V(\vec{x})+(\beta_{21}|\psi_1|^2+\beta_{22}|\psi_2|^2)]\psi_{-1}$$

Dynamical results

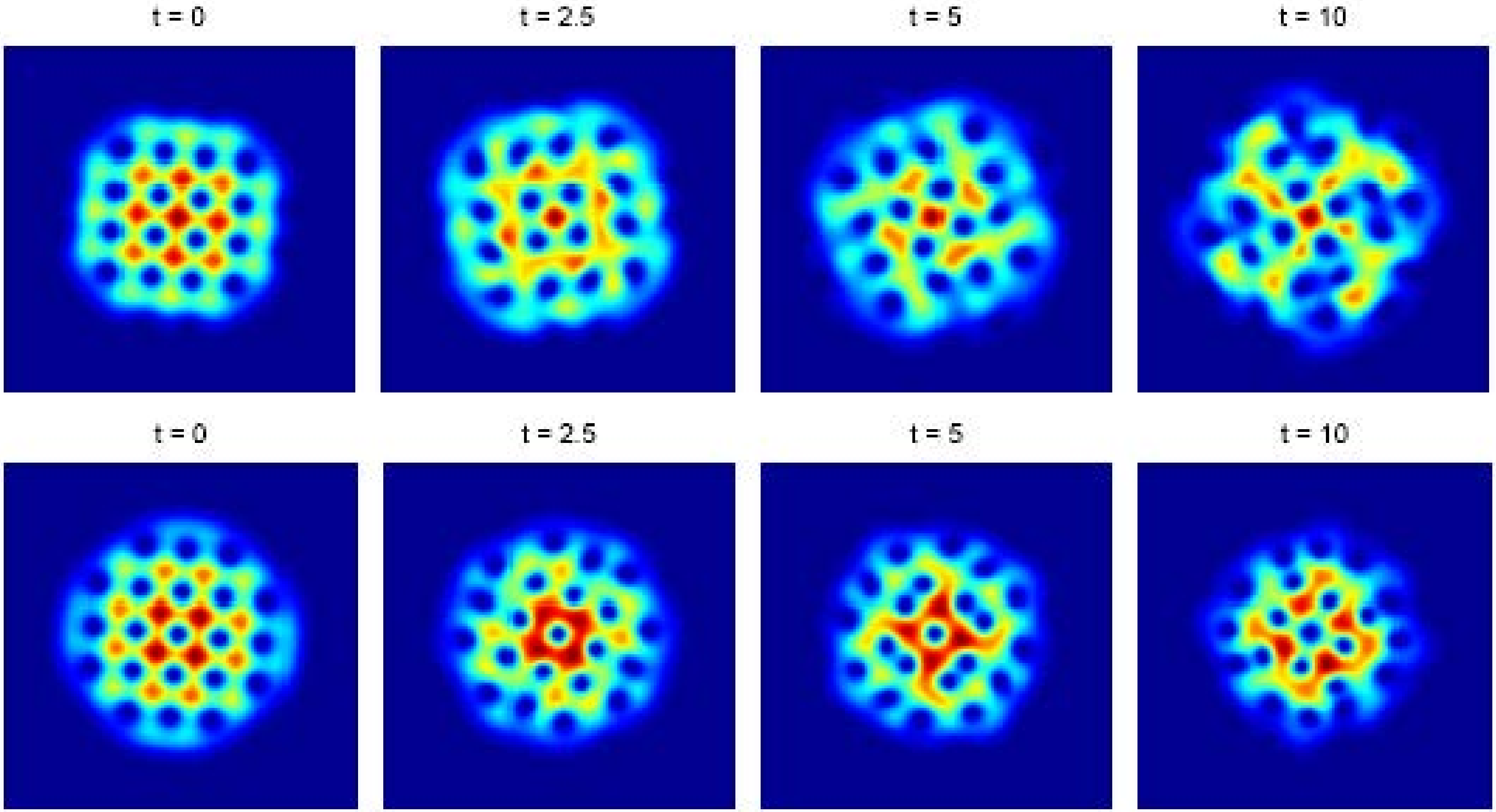



x 10^-3
2
0


|E1|²
(|E1|²+|E2|²)/2
|E2|²
t
1.3
1.2
1.1
1
0.9
0.8
0.7
0
1
2
3
4
5


t
1.6
1.4
1.2
1
0.8
0.6
0.4
0
1
2
3
4
5

Dynamical results



Coupled GPEs

- Spinor F=1 BEC

$$i\frac{\partial}{\partial t}\psi_1 = [-\frac{1}{2}\nabla^2 + V(\vec{x}) + \beta_n\rho]\psi_1 + \beta_s(\rho_1+\rho_0-\rho_{-1})\psi_1 + \beta_s\psi_{-1}^*\psi_0^2$$

$$i\frac{\partial}{\partial t}\psi_0 = [-\frac{1}{2}\nabla^2 + V(\vec{x}) + \beta_n\rho]\psi_0 + \beta_s(\rho_1+\rho_{-1})\psi_0 + 2\beta_s\psi_1\psi_{-1}\psi_0^*$$

$$i\frac{\partial}{\partial t}\psi_{-1} = [-\frac{1}{2}\nabla^2 + V(\vec{x}) + \beta_n\rho]\psi_{-1} + \beta_s(\rho_{-1}+\rho_0-\rho_1)\psi_{-1} + \beta_s\psi_1^*\psi_0^2$$

- With

$$\rho = \rho_{-1}+\rho_0+\rho_1, \quad \rho_j = |\psi_j|^2, \quad \beta_n = \frac{4\pi N(a_0+2a_2)}{3x_s}, \quad g_s = \frac{4\pi N(a_2-a_0)}{3x_s}$$

a_0, a_2: s-wave scattering length with the total spin 0 and 2 channels

- Numerical methods ---- TSSP with 3 steps
  - Bao, Markowich, Schmeiser & Weishaupl, M3AS, 05'
  - Bao & Cai, KRM, 13', ……

Spin-1 BEC

- Time-splitting spectral (TSSP) method –3 steps– (Bao, Markowich, Schmeiser & Weishaupl, M3AS, 05';Bao & Cai, KRM, 13', ……)
  - Step 1. Solve

$$i\frac{\partial}{\partial t}\psi_1=-\frac{1}{2}\nabla^2\psi_1,\quad i\frac{\partial}{\partial t}\psi_0=-\frac{1}{2}\nabla^2\psi_0,\quad i\frac{\partial}{\partial t}\psi_{-1}=-\frac{1}{2}\nabla^2\psi_{-1},$$

  - Step 2. Solve

$$i\frac{\partial}{\partial t}\psi_1=[V(\vec{x})+\beta_n\rho]\psi_1+\beta_s(\rho_1+\rho_0-\rho_{-1})\psi_1$$

$$i\frac{\partial}{\partial t}\psi_0=[V(\vec{x})+\beta_n\rho]\psi_0+\beta_s(\rho_1+\rho_{-1})\psi_0$$

$$i\frac{\partial}{\partial t}\psi_{-1}=[V(\vec{x})+\beta_n\rho]\psi_{-1}+\beta_s(\rho_{-1}+\rho_0-\rho_1)\psi_{-1}$$

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_0\\ \psi_{-1}\end{pmatrix}=\beta_s\begin{pmatrix}0 & \psi_{-1}^*\psi_0 & 0\\ \psi_{-1}\psi_0^* & 0 & \psi_1\psi_0^*\\ 0 & \psi_1^*\psi_0 & 0\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_0\\ \psi_{-1}\end{pmatrix}$$

  - Step 3. Solve

$$i\frac{\partial}{\partial t}\psi_1=\beta_s\psi_{-1}^*\psi_0^2,\quad i\frac{\partial}{\partial t}\psi_0=2\beta_s\psi_1\psi_{-1}\psi_0^*,\quad i\frac{\partial}{\partial t}\psi_{-1}=\beta_s\psi_1^*\psi_0^2$$

Spin-1 BEC

- Time-splitting spectral (TSSP) method –2 steps– (L.M. Symes, R.I. McLachlan &B. Blake, PRE, 16')
  - Step 1. Solve

$$i\frac{\partial}{\partial t}\psi_1 = -\frac{1}{2}\nabla^2\psi_1, \quad i\frac{\partial}{\partial t}\psi_0 = -\frac{1}{2}\nabla^2\psi_0, \quad i\frac{\partial}{\partial t}\psi_{-1} = -\frac{1}{2}\nabla^2\psi_{-1},$$

  - Step 2. Solve

$$i\frac{\partial}{\partial t}\psi_1 = [V(\vec{x}) + \beta_n\rho]\psi_1 + \beta_s(\rho_1 + \rho_0 - \rho_{-1})\psi_1 + \beta_s\psi_{-1}^*\psi_0^2$$

$$i\frac{\partial}{\partial t}\psi_0 = [V(\vec{x}) + \beta_n\rho]\psi_0 + \beta_s(\rho_1 + \rho_{-1})\psi_0 + 2\beta_s\psi_1\psi_{-1}\psi_0^*$$

$$i\frac{\partial}{\partial t}\psi_{-1} = [V(\vec{x}) + \beta_n\rho]\psi_{-1} + \beta_s(\rho_{-1} + \rho_0 - \rho_1)\psi_{-1} + \beta_s\psi_1^*\psi_0^2$$

Spin-1 BEC

- Define

$$\rho(\vec{x},t) := |\psi_1|^2 + |\psi_0|^2 + |\psi_{-1}|^2, \quad F_z(\vec{x},t) := |\psi_1|^2 - |\psi_{-1}|^2$$

$$F_\perp(\vec{x},t) := \sqrt{2}\left(\psi_1^*\psi_0 + \psi_0^*\psi_{-1}\right), \quad |F|^2 = |F_z|^2 + |F_\perp|^2$$

$$\Rightarrow \rho(\vec{x},t) \equiv \rho(\vec{x},t_n), \quad F_z(\vec{x},t) \equiv F_z(\vec{x},t_n)$$

- Change of variable

$$\psi_j = \tilde{\psi}_j e^{-it\tilde{V}}, \quad \tilde{V} = V(\vec{x}) + \beta_n \rho(\vec{x},t_n), \quad j = -1, 0, 1;$$

$$i\frac{\partial}{\partial t}\begin{pmatrix}\tilde{\psi}_1\\ \tilde{\psi}_0\\ \tilde{\psi}_{-1}\end{pmatrix} = \beta_s \begin{pmatrix} \tilde{F}_z & \frac{1}{\sqrt{2}}\tilde{F}_\perp^* & 0 \\ \frac{1}{\sqrt{2}}\tilde{F}_\perp & 0 & \frac{1}{\sqrt{2}}\tilde{F}_\perp^* \\ 0 & \frac{1}{\sqrt{2}}\tilde{F}_\perp & -\tilde{F}_z \end{pmatrix} \begin{pmatrix}\tilde{\psi}_1\\ \tilde{\psi}_0\\ \tilde{\psi}_{-1}\end{pmatrix} \Leftrightarrow i\partial_t \tilde{\Psi} = \beta_s R \tilde{\Psi}$$

$$\Rightarrow \tilde{F}_z(\vec{x},t) \equiv \tilde{F}_z(\vec{x},t_n), \; \tilde{F}_\perp(\vec{x},t) \equiv \tilde{F}_\perp(\vec{x},t_n), \; R(\vec{x},t) = R(\vec{x},t_n)$$

$$\Rightarrow \tilde{\Psi}(t) = \cos(\beta_s |F| t)\Psi(0) - \frac{i}{|F|}\sin(\beta_s |F| t) R \Psi(0)$$

Extension to Zakharov System

- The Zakharov system (Bao, Sun & Wei, JCP, 04; Bao & Sun, SISC, 05')

$$i\,E_t + \Delta E - \alpha\, N\, E + \underline{\lambda |E|^2 E} + \underline{\underline{i\,\gamma\, E}} = 0$$

$$\varepsilon^2\, N_{tt} - \Delta(N + \underline{\nu}\,|E|^2) = 0, \qquad \vec{x} \in \mathbb{R}^d, \quad t > 0$$

  - E: envelope of the high-frequency electric field
  - N: deviation of the ion density from its equilibrium
  - $\varepsilon > 0$: inversely proportional to acoustic speed
  - $\gamma \geq 0$: a damping parameter
  - α, λ, ν : real parameters

Properties of Zakharov System

- Compatibility condition

$$\int N_1(\vec{x})\, d\vec{x} = 0$$

- Conservation laws when $\gamma = 0$
  - The wave energy

$$D(t) = \int |E(\vec{x},t)|^2\, d\vec{x}$$

  - The momentum

$$\vec{P} = \int \left[\frac{i}{2}(E\,\nabla\bar{E} - \bar{E}\,\nabla E) + \frac{\varepsilon^2 \alpha}{\nu} N\,\vec{V} \right] d\vec{x} \qquad N_t + \nabla \bullet \vec{V} = 0$$

Properties of Zakharov System

– The Hamiltonian

$$H = \int [\, |\nabla E|^2 + \alpha\, N\, |E|^2 - \frac{\lambda}{2} |E|^4 + \frac{\alpha}{2\nu} N^2 + \frac{\alpha\,\varepsilon^2}{2\nu} |\vec{V}|^2]\, d\vec{x}$$

- Time reversible when $\gamma = 0$
- Time transverse invariant when $\gamma = 0$

$$N_0 \to N_0 + \beta \quad \Rightarrow \quad N(.,t) \to N(.,t) + \beta \quad \& \quad |E(.,t)| \text{ unchanged}$$

- Decay rate of the wave energy D(t) when $\gamma > 0$

$$D'(t) = -2\gamma\, D(t) \qquad \Rightarrow \qquad D(t) = e^{-2\gamma t}\, D(0)$$

Plane & solitary waves

- Plane wave in 1D when: $\gamma = 0$

$$N(x,t) = d, \quad E(x,t) = c\, e^{i\left(\frac{2\pi r x}{b-a} - \omega t\right)}, \quad \omega = \alpha\, d + \frac{4\pi^2 r^2}{(b-a)^2} - \lambda\, c^2$$

- Solitary wave in 1D: $\gamma = 0, \lambda = 0, \alpha = 1, \nu = 1$

$$E(x,t) = \sqrt{2B^2 (1 - \varepsilon^2 C^2)}\ \mathrm{sech}(B(x - C\,t))\, e^{i(C\,x/2 - (C^2/4 - B^2)t)}$$

$$N(x,t) = -2B^2\ \mathrm{sech}^2(B(x - C\,t)), \quad -\infty < x < \infty, \quad t \ge 0$$

- Periodic soliton solution in 1D

Convergence of GZS to NLS

$$(\text{''subsonic limit''}) \Downarrow \varepsilon \to 0 \Rightarrow N = -\nu |E|^2 + O(\varepsilon^2)$$

$$i E_t + \Delta E + (\lambda + \alpha \nu) |E|^2 E + i \gamma E = 0$$

- Hamiltonian

$$\text{GZS}: \; H^{\text{GZS}} = \int [\, |\nabla E|^2 + \alpha N |E|^2 - \frac{\lambda}{2} |E|^4 + \frac{\alpha}{2\nu} N^2 + \frac{\alpha \varepsilon^2}{2\nu} |\vec{V}|^2]\, d\vec{x}$$

$$\varepsilon \to 0 \quad \Downarrow \quad N = -\nu |E|^2 + O(\varepsilon^2)$$

$$\text{NLS}: \; H^{\text{NLS}} = \underline{\int [\, |\nabla E|^2 - \frac{(\lambda - \alpha \nu)}{2} |E|^4]\, d\vec{x}} \; + \; \frac{\alpha \varepsilon^2}{2\nu} \int |\vec{V}|^2 \, d\vec{x}$$

  – Convergence rate: $H^{\text{GZS}} = H^{\text{NLS}} + O(\varepsilon^2) \quad \text{when} \quad \varepsilon \to 0$

- Momentum: $P^{\text{GZS}} = P^{\text{NLS}} + O(\varepsilon^2) \quad \text{when} \quad \varepsilon \to 0$

Well-posedness

- Solitary wave solution of ZS
  - Gibbons et al., 77'
- Global weak solution of ZS
  - Sulem et al., 79'
- Smooth solution provided smooth initial data
  - Bourgain et al., 96'
- Wellposedness of GZS
  - Colliander, 98'
- Blowup of ZS in 2D &3D when initial Hamiltonian < 0
  - Papanicolaou et al. 91', Wang 94', & Masselin 01'

Existing Numerical Methods

- Existing Numerical methods
  - RK2+spectral method: Payne, JCP, 83'
  - Implicit finite difference (FD): Glassey, JCP, 92'; Bao & Su, MMS, 17'
  - Semi-implicit finite difference (SI-FD): Chang, Guo & Jiang, JCP, 94'
  - Spectral method: Bao, Sun & Wei, JCP, 03'; Bao & Sun, SISC, 04'; Jin, Markowich & Zheng 04'; Bao & Su, 17',
- Numerical difficulties
  - Stiffness in time
  - Keep properties of GZS as much as possible in discretization
  - 3D & possible long time dynamics, …….
- Our goal: To develop an
  - explicit & unconditionally stable spectral method for GZS

New numerical Methods

- 1D GZS with periodic conditions:

$$i\,E_t + E_{xx} - \alpha\, N\, E + \lambda\, |E|^2\, E + i\,\gamma\, E = 0$$

$$\varepsilon^2\, N_{tt} - (N + \nu\, |E|^2)_{xx} = 0 \qquad\qquad a < x < b$$

$$E(x,0) = E_0(x), \quad N(x,0) = N_0(x), \quad N_t(x,0) = N_1(x)$$

$$E(a,t) = E(b,t), \quad N(b,t) = N(b,t),$$

$$\partial_x E(a,t) = \partial_x E(b,t), \quad \partial_x N(a,t) = \partial_x N(b,t)$$

- Compatibility conditions

$$E_0(a) = E_0(b), \quad N_0(a) = N_0(b), \quad N_1(a) = N_1(b), \quad \int_a^b N_1(x)\, dx = 0$$

New numerical Methods

- Our ideas (Bao, Sun & Wei, JCP, 03'; Bao & Sun SISC, 04'):
  - For the first (NLS-type) equation
    - time-splitting spectral method (TSSP)

$$\text{Step 1:} \quad i\,E_t + E_{xx} = 0, \qquad\qquad t_n \le t \le t_{n+1}$$

$$\text{Step 2:} \quad i\,E_t - \alpha\, N\, E + \lambda\, |E|^2\, E + i\,\gamma\, E = 0$$

$$\Downarrow |E(x,t)|^2 = e^{-2\gamma(t-t_n)}\,|E(x,t_n)|^2$$

$$i\,E_t(x,t) - \alpha\, N(x,t)\, E(x,t) + \lambda\, e^{-2\gamma(t-t_n)}\,|E(x,t_n)|^2\, E(x,t) + i\,\gamma\, E(x,t) = 0$$

    - 2nd time splitting

NLW in 1D

- Time-dependent NLW in 1D

$$\partial_{tt}u(x,t)-\partial_{xx}u(x,t)+f(u(x,t))=0,\quad x\in\Omega=(a,b),\quad t>0,$$
$$u(x,0)=u_0(x),\quad \partial_t u(x,0)=u_1(x),\quad a\le x\le b.$$

- Boundary conditions
  - Periodic BC: $u(a,t)=u(b,t),\quad \partial_x u(a,t)=\partial_x u(b,t),\quad t\ge 0$
  - Homogeneous Dirichlet BC $u(a,t)=u(b,t)=0,\quad t\ge 0$
- Time step $\tau=\Delta t$ and set $t_n=n\tau,\quad n=0,1,2,\ldots$
- Mesh size $h=(b-a)/M$ & set $x_j=a+jh,\quad j=0,1,\ldots,M$

$$u_j^n\approx u(x_j,t_n)$$

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 $s=\tau \quad \text{or} \quad s=-\tau$

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

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

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

- 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

- Gautschi-type exponential integrator (Gautschi, 68'):

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

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

- Via trapezoidal rule

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

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

Approximate first-order derivative

- Subtract

$$y'(t_n) = \frac{\omega}{2\sin(\omega\tau)}[y(t_n+\tau) - y(t_n-\tau)]$$

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

- Approximate by Gautschi-type or trapezoidal rule

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

Properties of Gautschi-type integrators

- Explicit
- Unconditionally stable for linear & Conditionally stable for nonlinear $\lambda\tau \le C$
- Give exact results when $f(y) = \alpha y$ is linear!!!
- Error estimate

$$\max_{0\le n\le T/\tau} |y(t_n) - y^n| \le C\tau^2$$

- Essentially conserves the energy when

$$\lambda \gg 1 \quad \& \quad \tau\lambda \approx 1$$

Exponential wave integrator spectral method for NLW

- Notations $\mu_l = \dfrac{l\pi}{b-a}, \quad l = 1, 2, \ldots, M-1$

$$Y_M = \mathrm{span}\left\{\phi_l(x) = \sin(\mu_l(x-a)), \quad l = 1, 2, \ldots, M-1\right\}$$

$$P_M : L^2(a,b) \to Y_M; \quad (P_M v)(x) = \sum_{l=1}^{M-1} \widehat{v}_l \sin(\mu_l(x-a))$$

- Sine spectral method
  - Find

$$u_M(x,t) \in Y_M \Rightarrow u_M(x,t) = \sum_{l=1}^{M-1} \widehat{u}_l(t) \sin(\mu_l(x-a)), \quad a \le x \le b, t \ge 0$$

  - Such that

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

EWI spectral method for NLW

– Take sine transform, for $l = 1, 2, \ldots, M-1$

$$\frac{d^2}{ds^2}\widehat{u}_l(t_n+s) + (\mu_l^2+\alpha)\widehat{u}_l(t_n+s) + \widehat{g}(u_M)_l(t_n+s) = 0, \quad s \in \mathbb{R}$$

$$\alpha = f'(0) \quad \& \quad g(u) = f(u) - \alpha u$$

– Solve this second-order ODE via Gautschi method

Properties of EWI-SP for NLW

- Explicit via DST
- Time reversible, i.e. unchanged if $\tau \to -\tau$
- Easy to extend to 2D & 3D
- Memory cost $O(M^d)$
- Computational cost $O(M^d \ln M)$
- Error estimate $\|u - u_M\|_{L^2} + \|\nabla(u - u_M)\|_{L^2} \le C[h^m + \tau^2]$
- Essentially conserves the energy well!!

For Klein-Gordon-Schrodinger

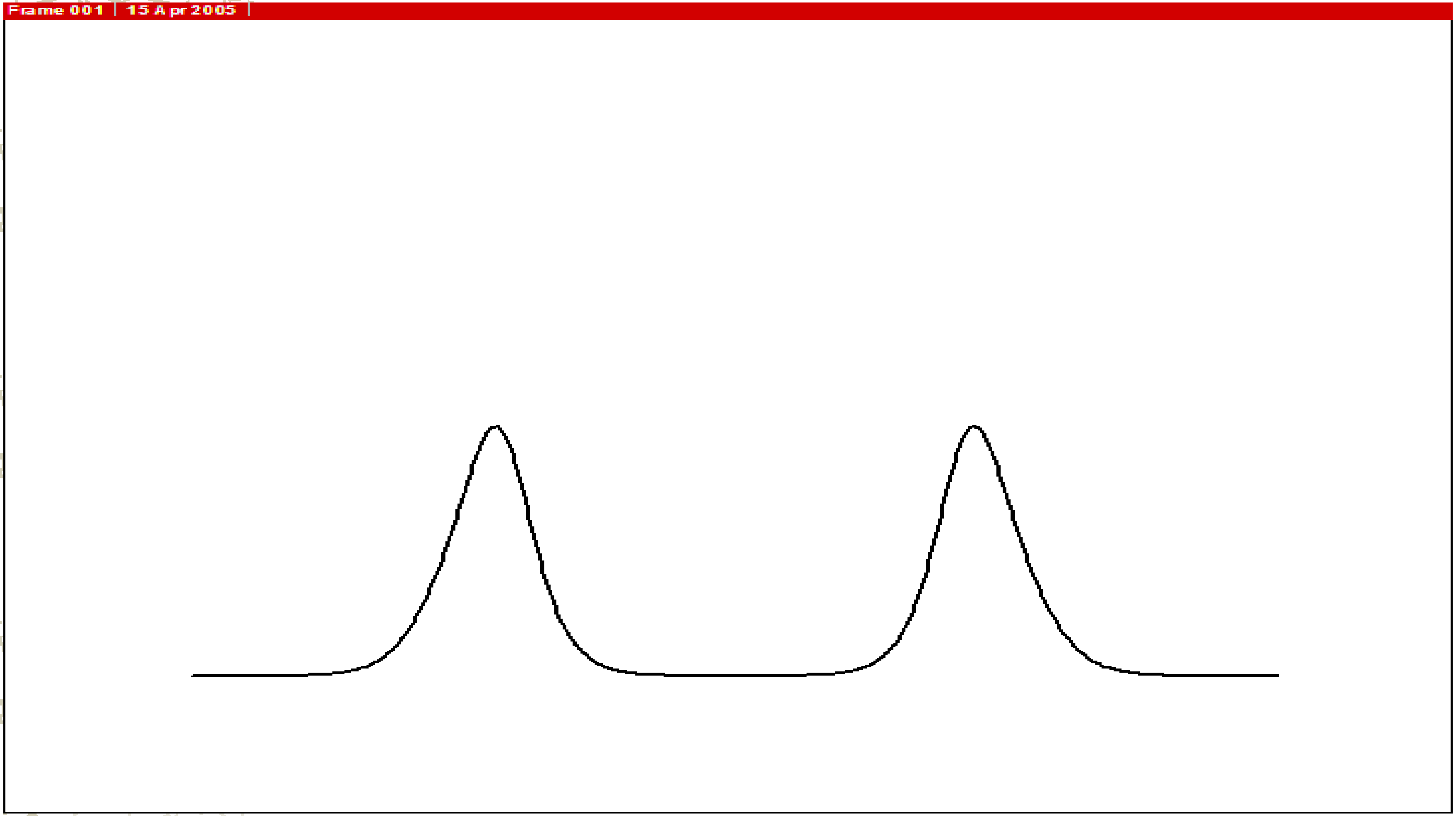
- KGS equations (Bao & L. Yang, JCP, 07'; Bao & Zhao, Numer. Math., 16')

$$i\partial_t \psi + \Delta \psi + \phi \psi + i\alpha\psi = 0$$

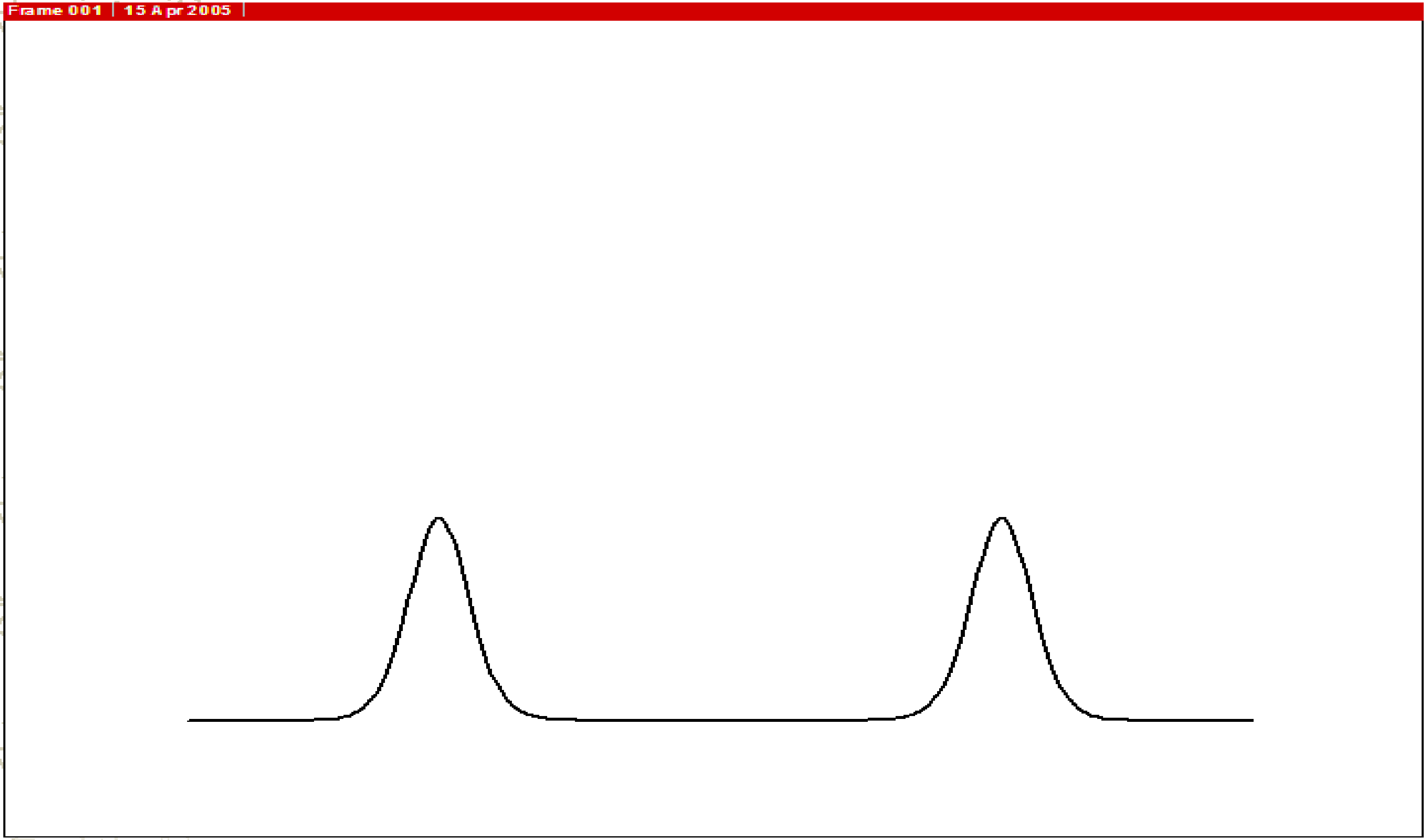
$$\partial_{tt}\phi - \Delta\phi + \mu^2\phi + \beta\phi_t - |\psi|^2 = 0$$

  – ψ : complex scalar nucleon field
  – ϕ : real meson field, $\alpha, \beta \,\&\, \mu$: constants
- Describes interaction of scalar nucleons interacting with neutral scalar mesons through Yukawa coupling
- Results: $\alpha = 0,\ \mu = 1,\ \beta = 1$

Meson Field



Nucleon Field



Conclusions & Future Challenges

- Conclusions:
  - NLSE / GPE – brief motivation
  - Dynamical properties
  - Numerical methods
    - Time-splitting spectral (TSSP) method & Applications
  - Extensions – rotations, nonlocal interaction, system
- Future Challenges
  - With random potential or high dimensions
  - Coupling GPE & Quantum Boltzmann equation (QBE) or other equations
  - NLSE / GPE in high dimension for quantum chemistry & materials science
  - BEC at finite temperature & quantum turbulence
  - Multiscale methods and analysis for highly oscillatory dispersive PDEs

Collaborators

- In Mathematics
  - External: P. Markowich (KAUST, Vienna, Cambridge); Q. Du (PSU); J. Shen (Purdue); L. Pareshi (Italy); P. Degond (France); N. Ben Abdallah (Toulouse), W. Tang (Beijing), I.-L. Chern (Taiwan), Y. Zhang (MUST), H. Wang (China), F. Mehats (France), C. Besse (France), X. Antonie (France), L. Greenguard (NYU), S. Jiang (NJIT), Y. Cai (Purdue), H. Li (Beijing), Z. Lei (Fudan), T. Li (Peking), F. Mehats (France); Z. Wen (Peking); X. Wu (Fudan), Y. Zhang (Vienna); Y. Yuan (Beijing); …;
  - Local: X. Dong, Q. Tang, X. Ruan, …….
- In Physics
  - External: D. Jaksch (Oxford); A. Klein (Oxfrod); M. Rosenkranz (Oxford); H. Pu (Rice), D. Zhang (Dalian), W. M. Liu (IOP, Beijing), X. J. Zhou (Peking U), …..
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