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

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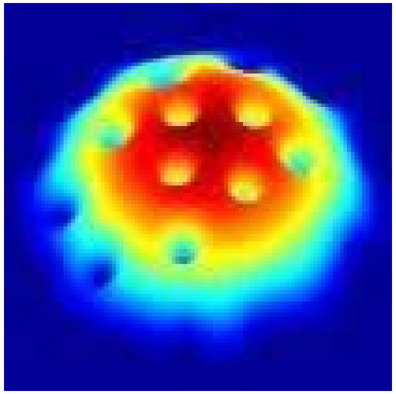
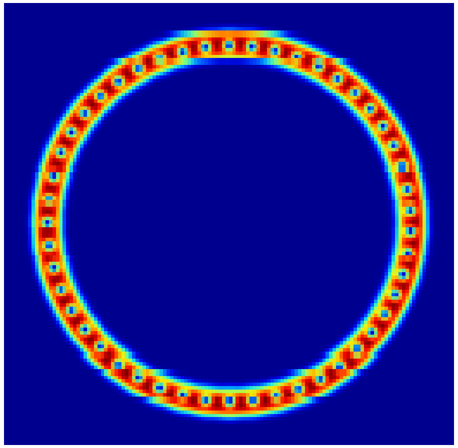


Vortex@ENS

Outline

- Nonlinear Schroedinger / 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 – collapse & explosion of a BEC, vortex lattice dynamics
- Extension to -- rotation, nonlocal interaction
- Conclusions



NLSE / GPE

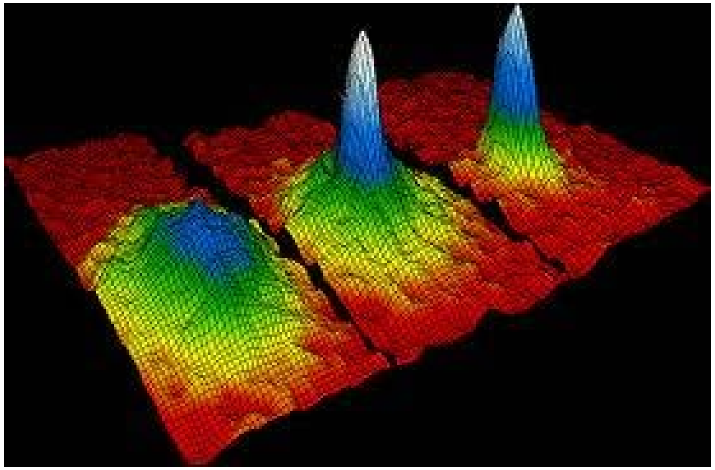
- The nonlinear Schroedinger equation (NLSE) --1925

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

- 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)

Model for BEC

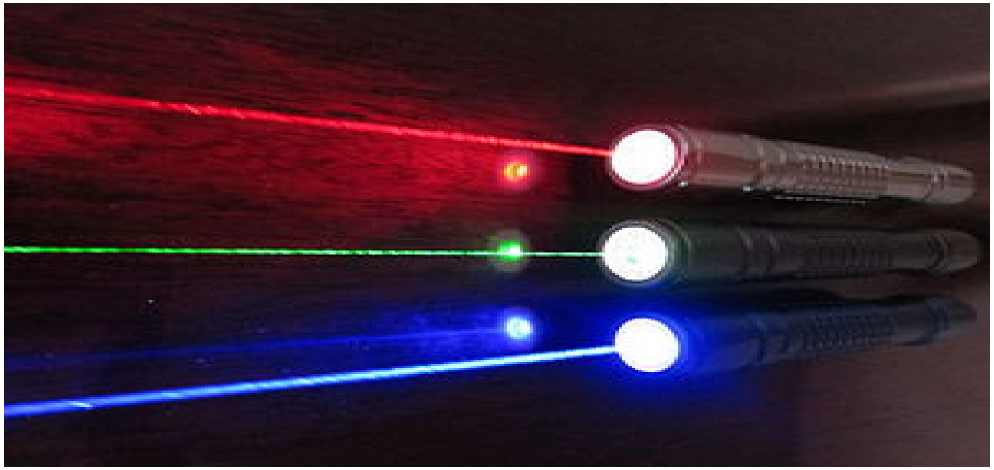
- Bose-Einstein condensation (BEC):
  - Bosons at nano-Kevin temperature
  - Many atoms occupy in one obit -- at quantum mechanical ground state
  - Form like a `super-atom', New matter of wave --- fifth state
- Theoretical prediction – S. Bose & E. Einstein 1924'
- Experimental realization – JILA 1995'
- 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

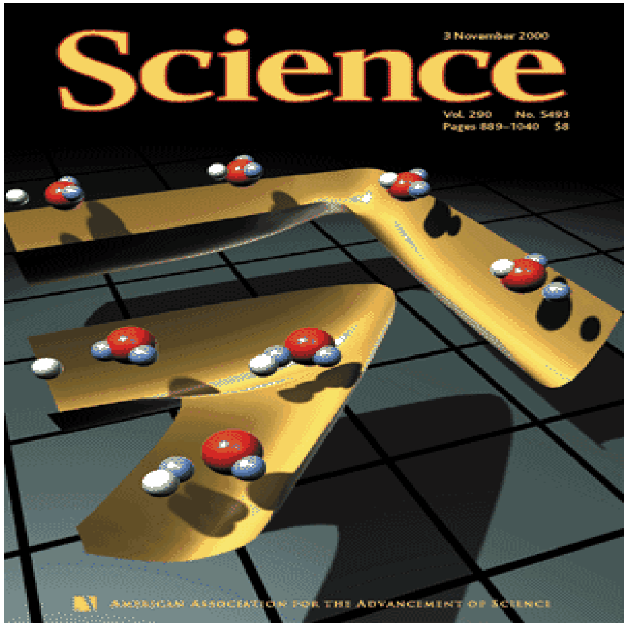
Laser beam propagation

- Nonlinear wave (or Maxwell) equations
- Helmholtz equation – time harmonic
- In a Kerr medium
- Paraxial (or parabolic) approximation -- NLSE



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

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

Dynamics with no potential

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

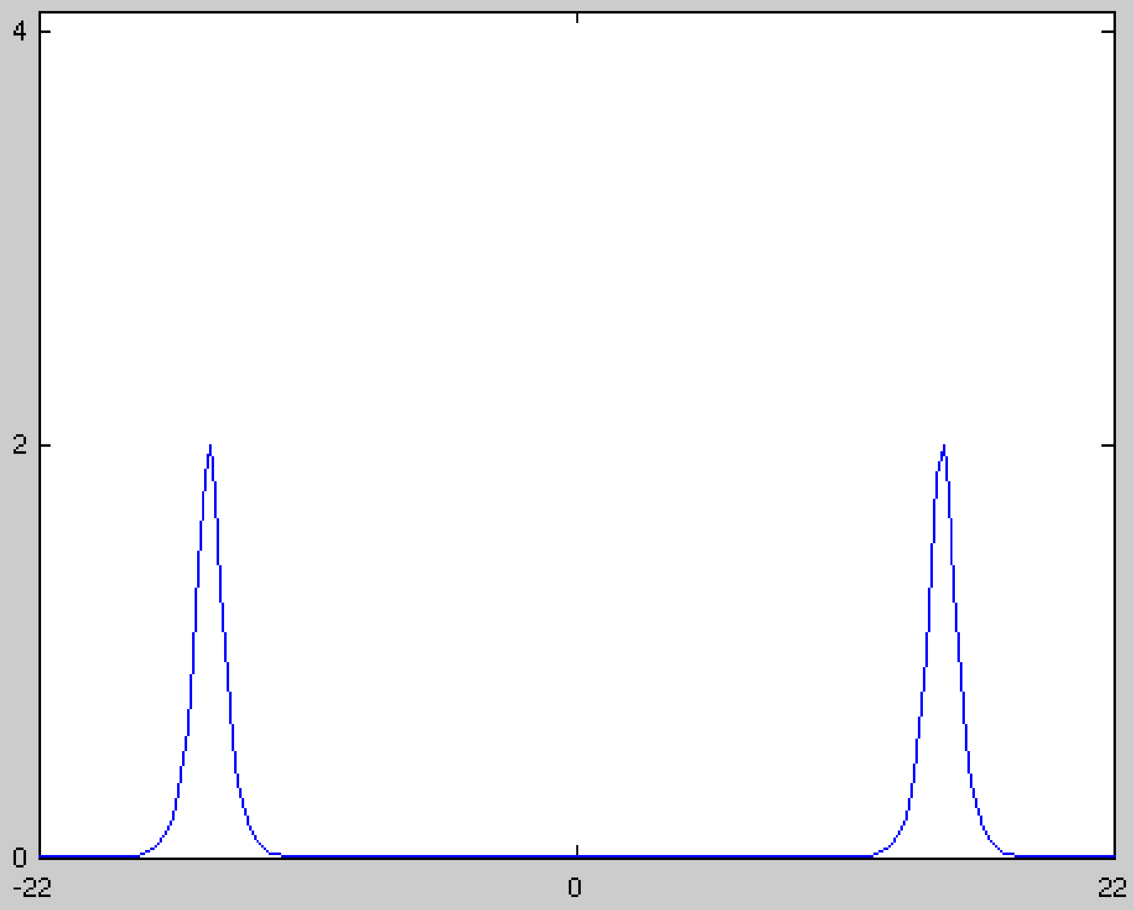
- Momentum conservation $\vec{J}(t) := \mathrm{Im} \int_{\mathbb{R}^d} \bar{\psi}\, \nabla \psi \, d\vec{x} \equiv \vec{J}(0) \quad t \geq 0$
- Dispersion relation $\psi(\vec{x},t) = Ae^{i(\vec{k}\bullet\vec{x}-\omega t)} \Rightarrow \omega = \frac{\varepsilon}{2}\left|\vec{k}\right|^2 + \frac{\beta}{\varepsilon}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

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

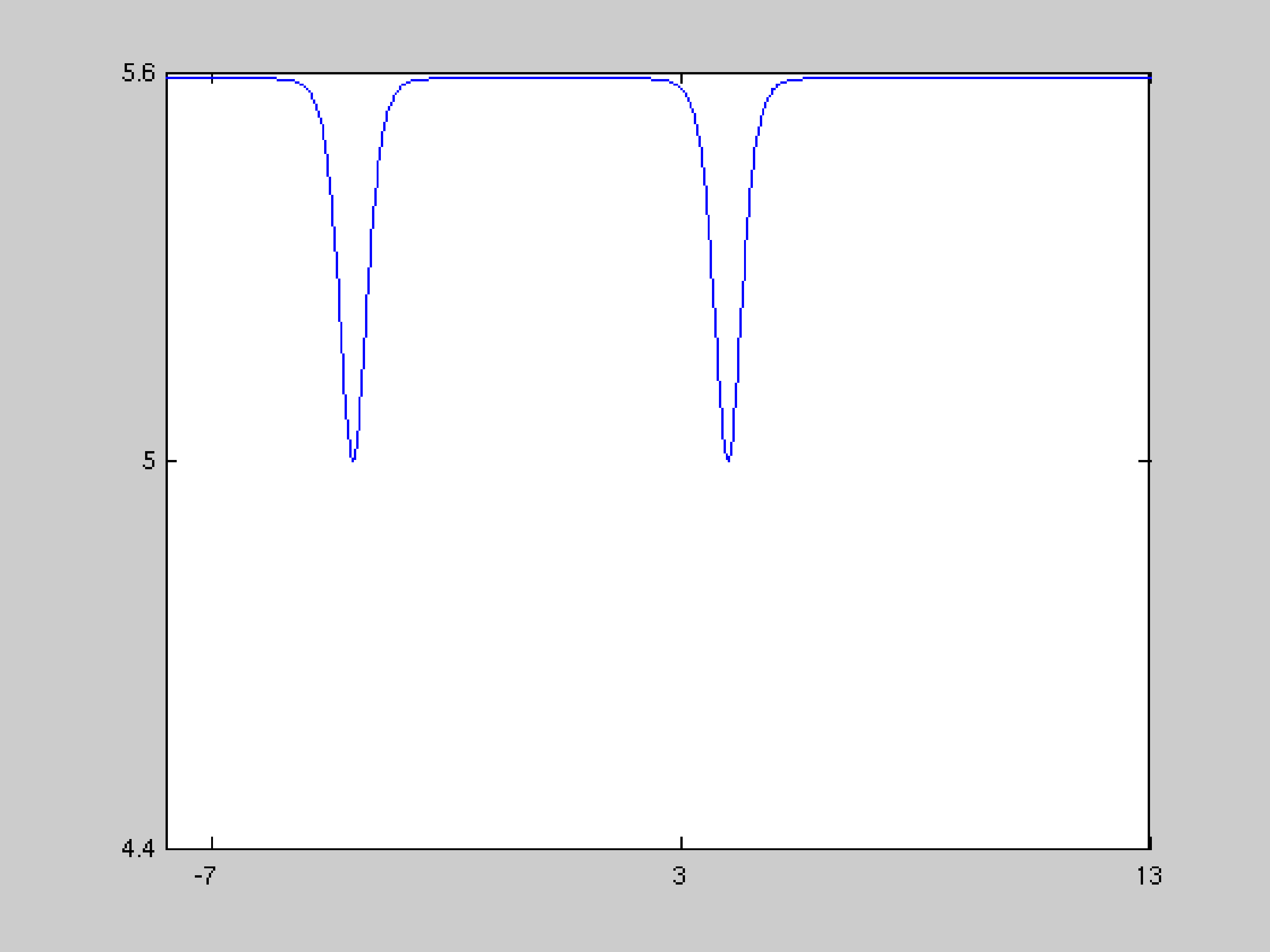
  - Dark (or gray) soliton $\beta > 0$ ---- nonzero &oscillatory at far-field

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

Interaction of two bright solitons



Interaction of two 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 $\psi_0(\vec{x}) = \phi_s(\vec{x} - \vec{x}_0)$

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

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

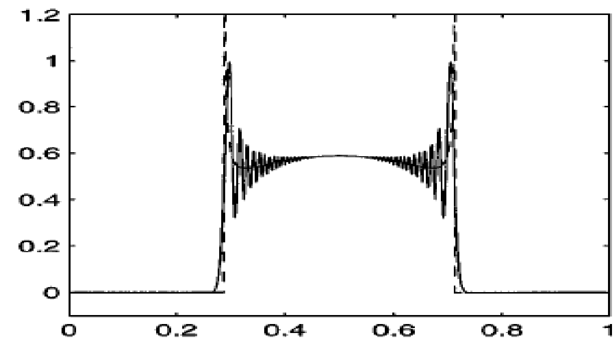
$$\mu_s \phi_s(\vec{x}) = -\frac{\varepsilon^2}{2}\nabla^2 \phi_s + V(\vec{x})\phi_s + \beta |\phi_s|^2 \phi_s$$

Numerical methods for dynamics

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

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

- 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: $\beta \gg 1 \;\&\; \varepsilon = 1 \;\text{ or }\; 0 < \varepsilon \ll 1 \;\&\; \beta = \pm 1$

Crank-Nicolson finite difference (CNFD)

$$i\varepsilon\,\partial_t \psi(x,t) = -\frac{\varepsilon^2}{2}\partial_{xx}\psi + V(x)\psi + \beta|\psi|^2\psi, \quad a < x < b, \quad t > 0$$

$$\psi(a,t) = \psi(b,t) = 0, \quad \text{with} \quad \psi(x,0) = \psi_0(x), \quad a \le x \le b$$

- Crank-Nicolson finite difference (CNFD) method (Chan&Shen, SINUM, 86'&87'; Guo, JCM, 86'; Glassey, JCP, 92'; Chan, Guo & Jiang, Math. Comp., 94'; Chang & Sun, JCP 03'; Bao&Cai, Math. Comp., 13'; ....)

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

$$+\frac{V(x_j)}{2}(\psi_j^{n+1}+\psi_j^n)+\frac{\beta}{4}(|\psi_j^{n+1}|^2+|\psi_j^n|^2)(\psi_j^{n+1}+\psi_j^n)$$

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

CNFD for NLSE

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

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

CNFD for NLSE

$$\left\|e^n\right\|_{l^2} + \left\|\nabla_h e^n\right\|_{l^2} \le C(h^2+\tau^2)$$

- Error estimate in H^1-norm when $\varepsilon = 1$:
  - In 1D for CNFD --- Glassey, Math. Comp. 92'; Chang,Guo&Jiang, Math. Comp., 95':
    - Energy method
    - Key inequality $\| f \|_{L^\infty}^2 \le \| f \|_{L^2} \bullet \|\nabla f \|_{L^2}, \qquad f \in H_0^1(\Omega)$
  - In 2D&3D & for non-energy conservative: -- Bao&Cai , Math. Comp. 13'
    - Energy method
    - Inverse inequality $\left\|\psi^n\right\|_{l^\infty} \le \left\|\psi\right\|_{L^\infty} + \left\|e^n\right\|_{l^\infty}$
    - For CNFD ---- cut-off function techniques
    - For SIFD --- the method of mathematical induction

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 2nd or 4th order splitting (Bao,Jin & Markowich, JCP, 02'; citations >300 !!)
  - $\varepsilon = 1$: (Hardin & Tarppent, SIAM 73'; Taha&Ablowitz, JCP, 84'; Weideman&Herbst, SINUM, 86'; Pathria&Moris, JCP, 90'; Bao,Jin&Markowich, JCP, 02', SISC, 03', …..)

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

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

- Stability: yes

Properties of the method

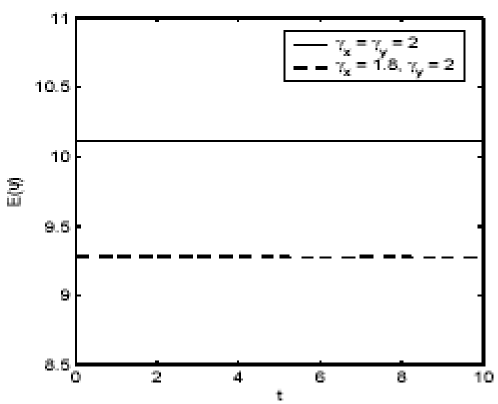
- Dispersion relation without potential: yes

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

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

  – 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: $0 < \beta = O(1)$

$$\|e^n\| \le C(h^m + \tau^2)$$

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

- Error estimate in L^2-norm and/or H^1 when $\varepsilon = 1$:
  - Besse,Bidegary&Descombes, 02'; Lubich, 08'; Koch&Thalhammer, M. Caliari, C. Neuhauser, Faou, 12'; A. Debussche, L. Gauckler, E. Hairer, Shen&Wang, 13'; Bao&Cai, 13'; etc.

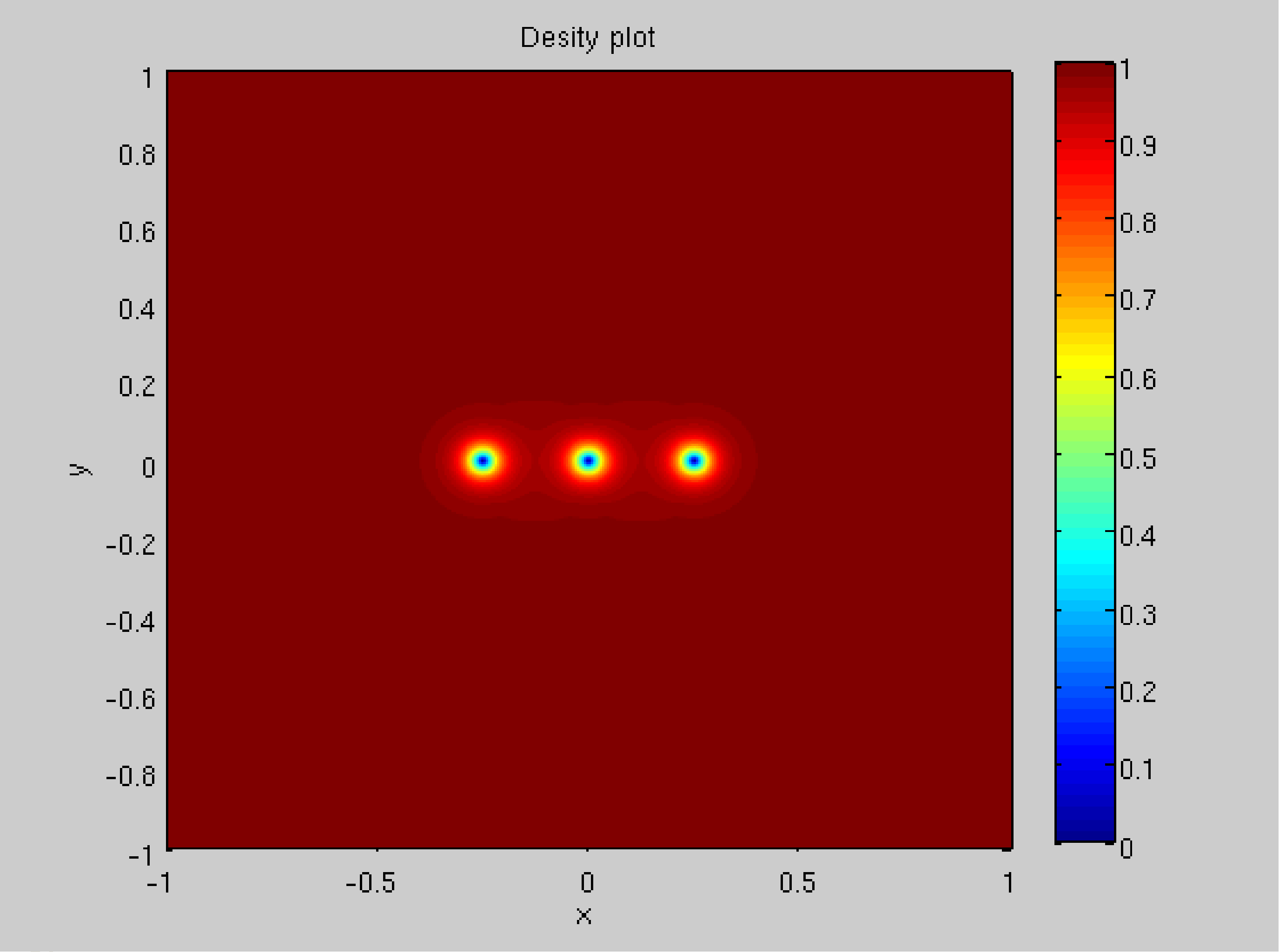
Other approaches

- Time discretization
  - Leap-frog or explicit scheme --- severe stability constraint!!
  - Multi-sympletic scheme --- Hong et al., 06—10, ….
  - 4th-order Runge-Kutta (RK4) --- not time symmetric , …….
- Spatial discretization
  - Finite element method –Akrivis, 91'; Akrivis, Dugalis & Karakashan, 91'
  - Finite volume method
  - Compact finite difference method, ……….
- Time + spatial discretization → different methods for NLSE
  - Bao & Cai, Kinet. Relat. Mod, 6 (2013), pp. 1--135 --- Review paper.
  - Antonie, Bao & Besse, Comput. Phys. Commun., 2013(arXiv: math.NA 1305.1093)– Feature article.

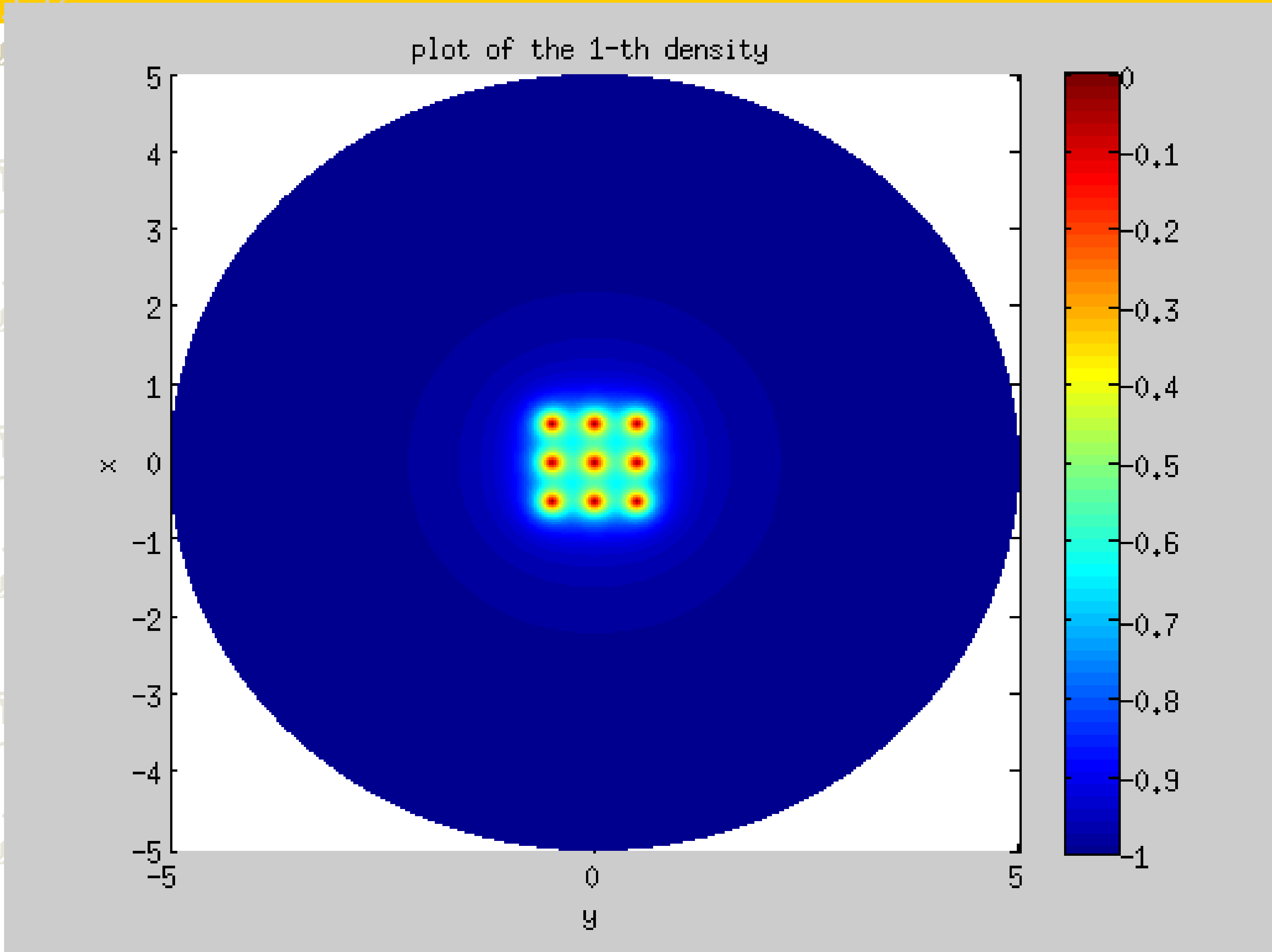
Comparison

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	2^{th} or 4^{th}	2^{th}	2^{th}	2^{th}	2^{th}
Spatial Accuracy	spectral	2^{th}	2^{th}	2^{th}	2^{th}
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]	$h = O(\varepsilon)$ $\tau = O(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$	$h = o(\varepsilon)$ $\tau = o(\varepsilon)$

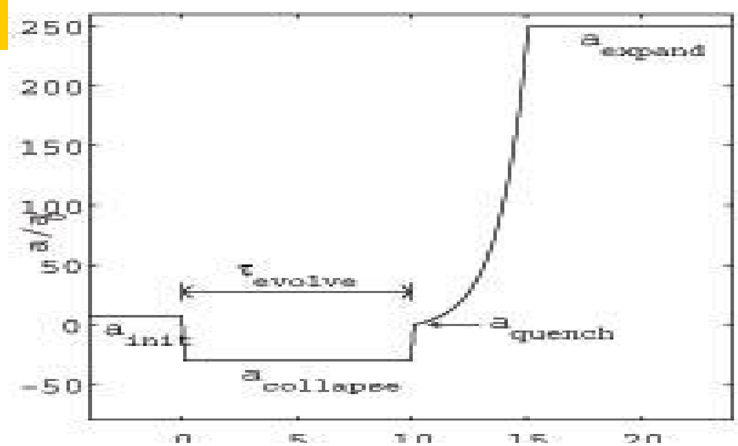
Interaction of 3 like vortices



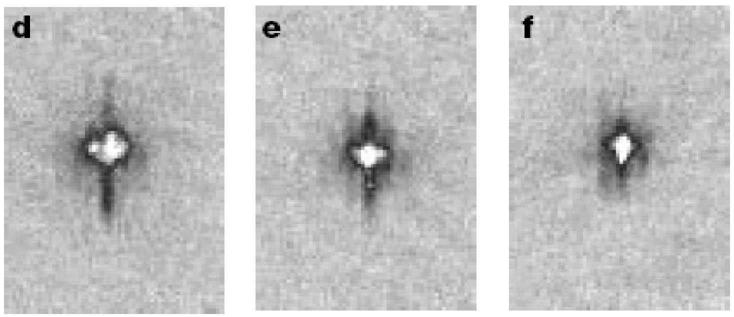
Interaction of a lattice

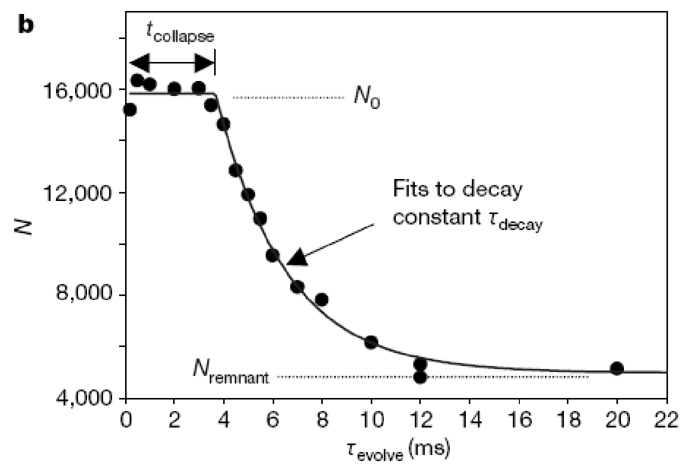


3D collapse & explosion of BEC



- 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

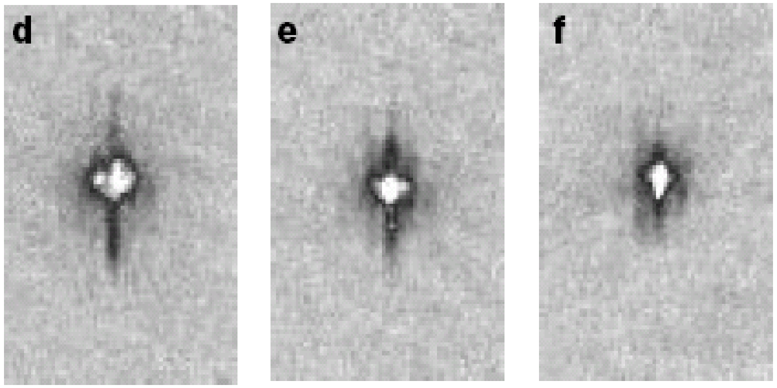


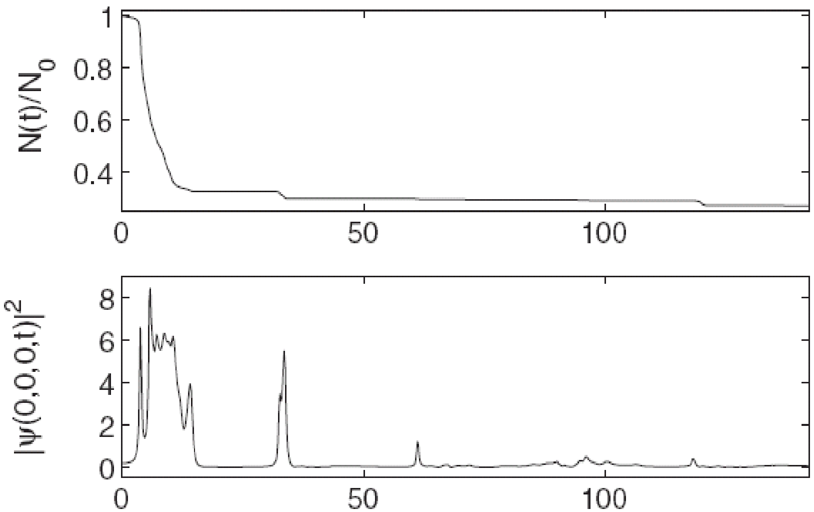


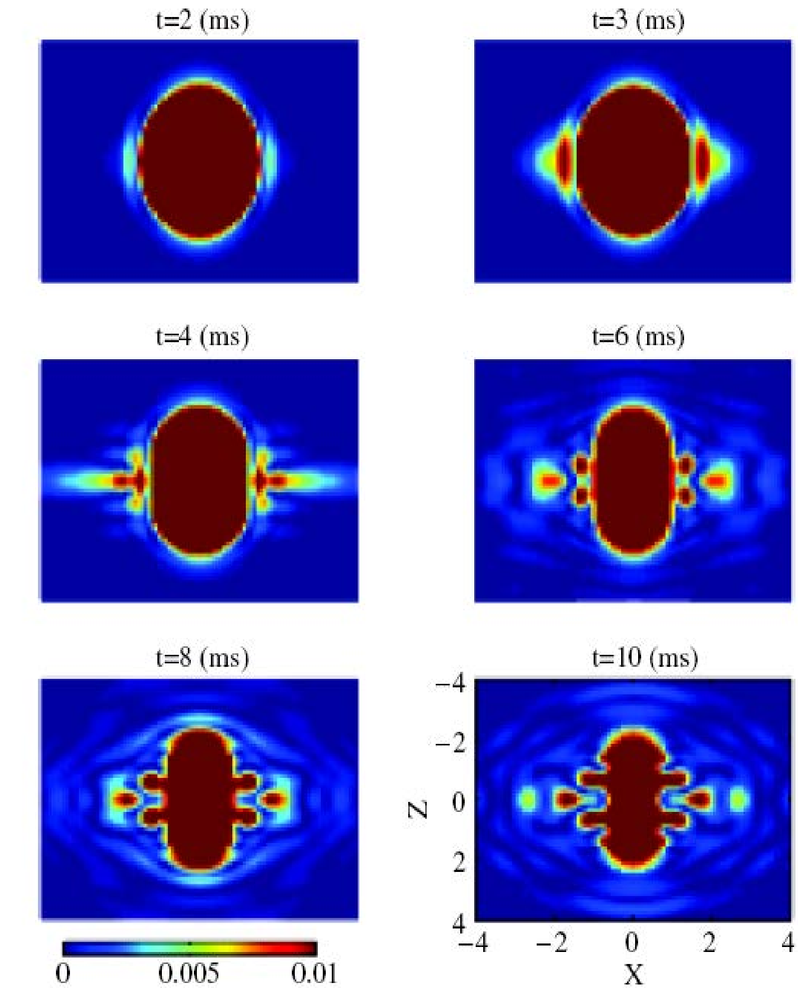
- Mathematical model (Duine & Stoof, PRL, 01')

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

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

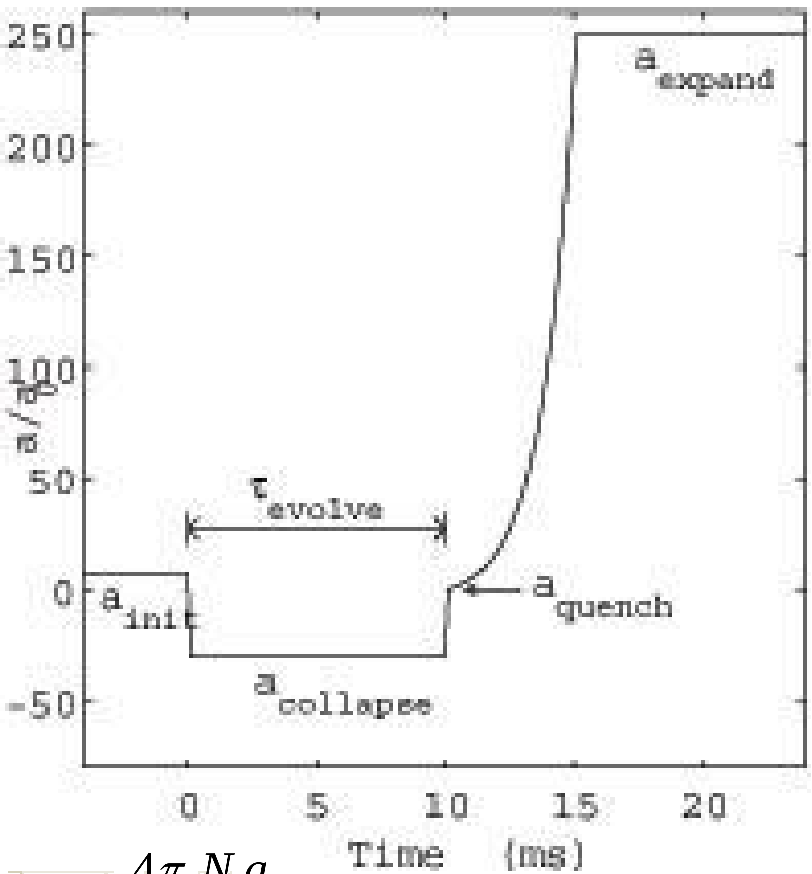


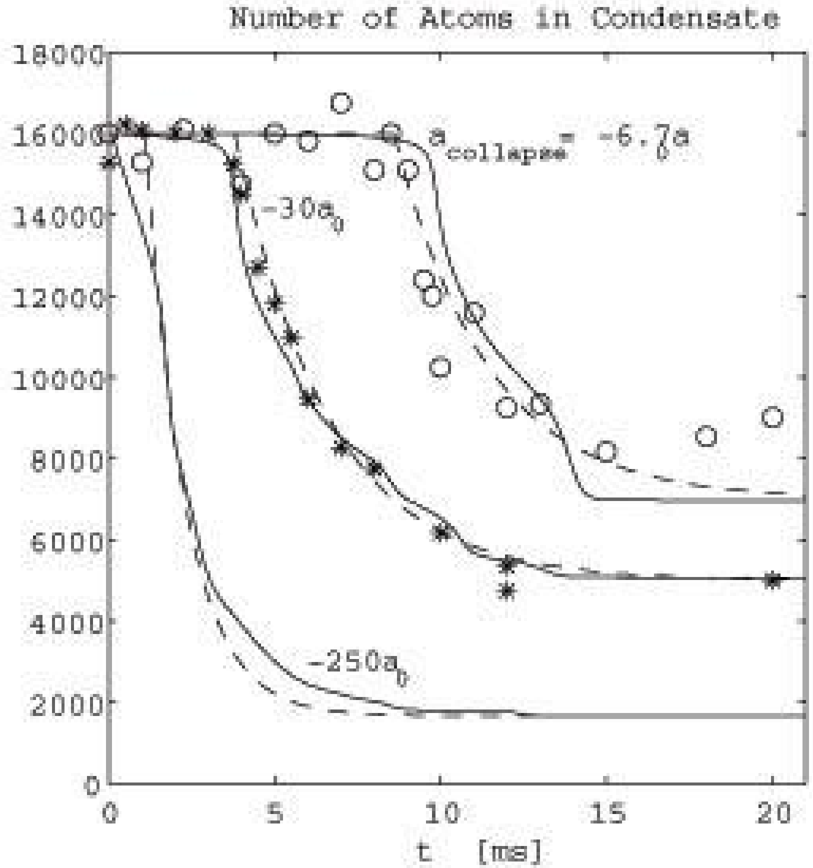




Jet formation

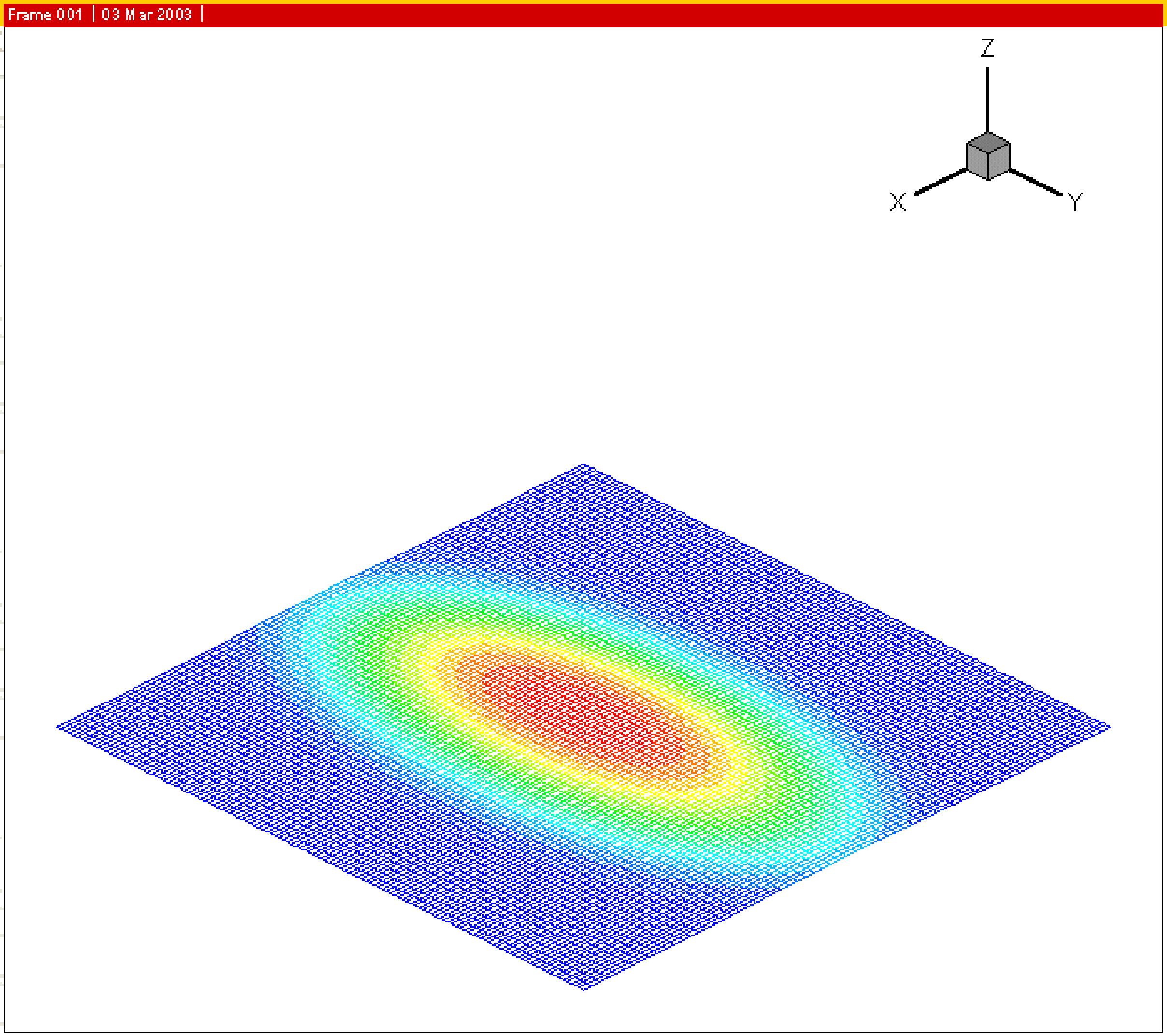
3D Collapse and explosion in BEC





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

3D Collapse and explosion in BEC

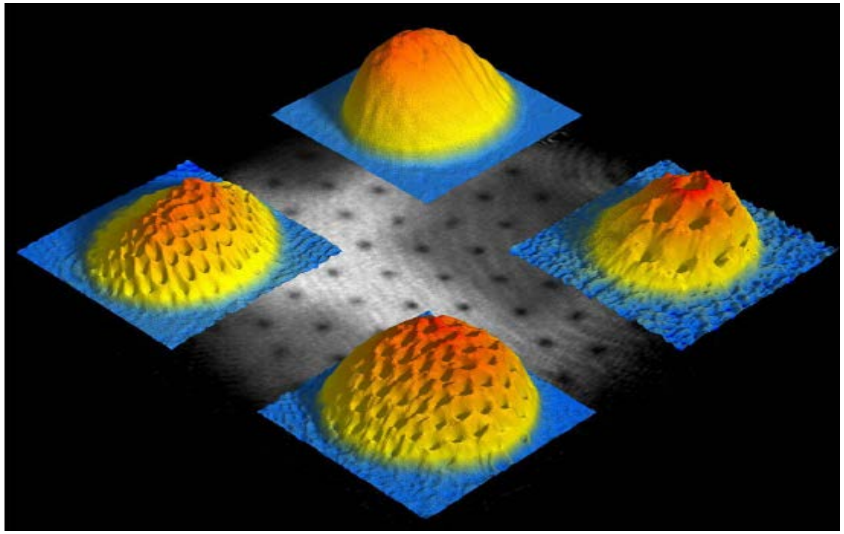


GPE with angular rotation

- GPE / NLSE with an angular momentum rotation

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

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



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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'

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

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

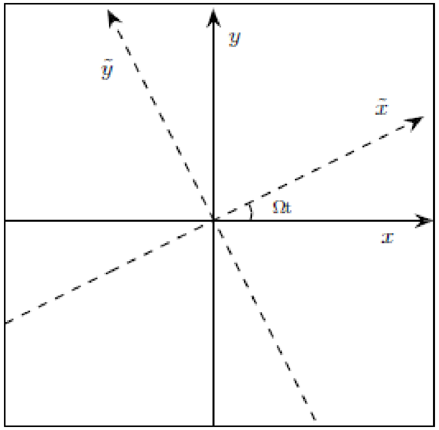
$$\text{Step 3:}\quad i\,\partial_t\,\psi(\vec{x},t) = [V(\vec{x}) + \beta\,|\psi|^2]\psi$$

- 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, SISC, 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

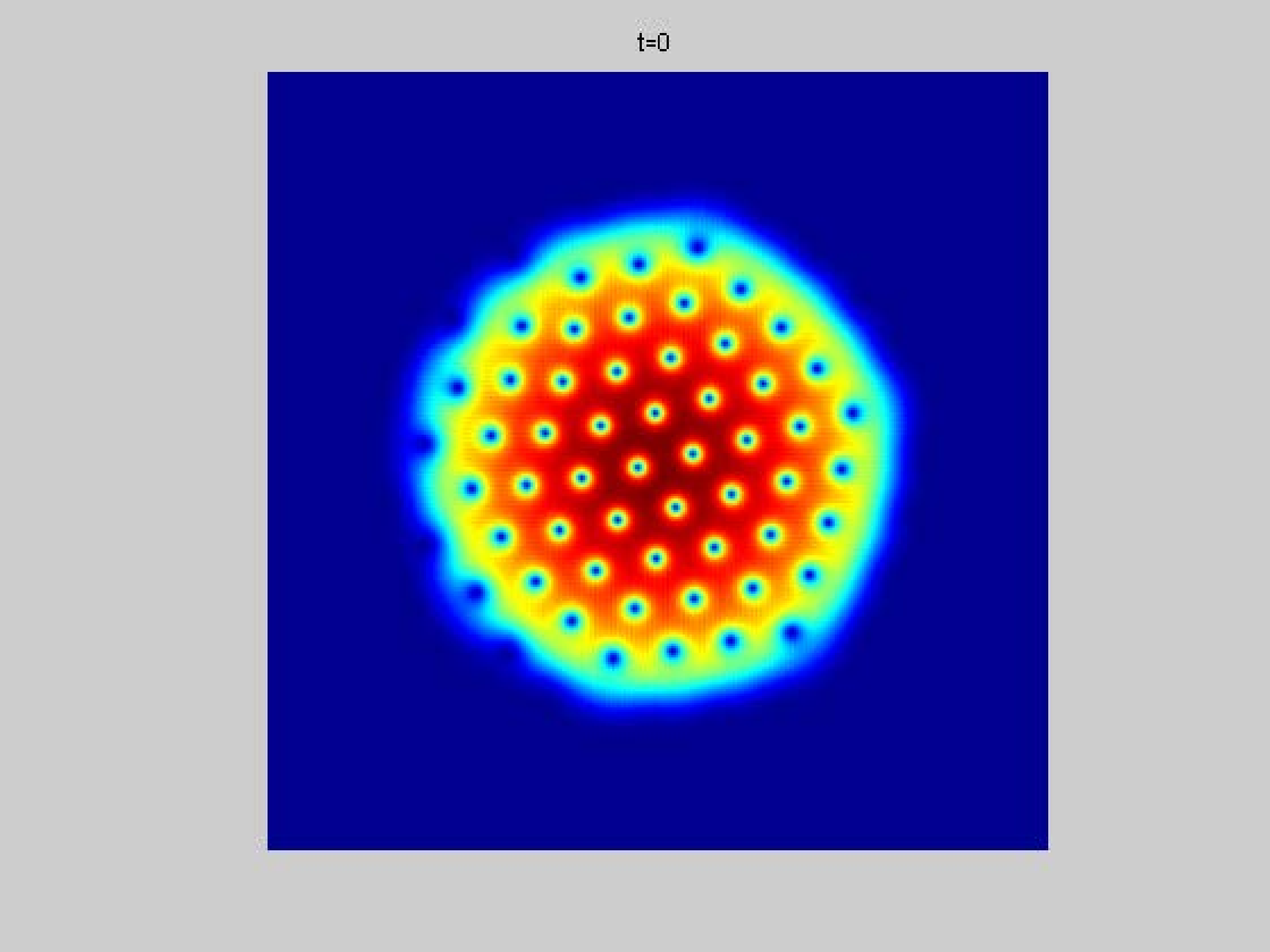
$$i\,\partial_t\,\phi(\tilde{\vec{x}},t) = [-\frac{1}{2}\nabla^2 + V(A(t)\tilde{\vec{x}}) + \beta\,|\phi|^2]\,\phi, \quad \tilde{\vec{x}} \in \mathbb{R}^d, \quad t>0$$

  - 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 a vortex lattice



Extension to dipolar quantum gas

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

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

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

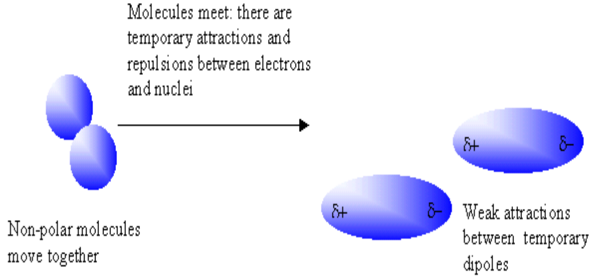
  – Interaction constants $\beta = \frac{4\pi N\,a_s}{x_s}$ (short-range), $\lambda = \frac{mN\,\mu_0\mu_{\text{dip}}^2}{3\hbar^2 x_s}$ (long-range)

  – Long-range dipole-dipole interaction kernel

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

- 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)

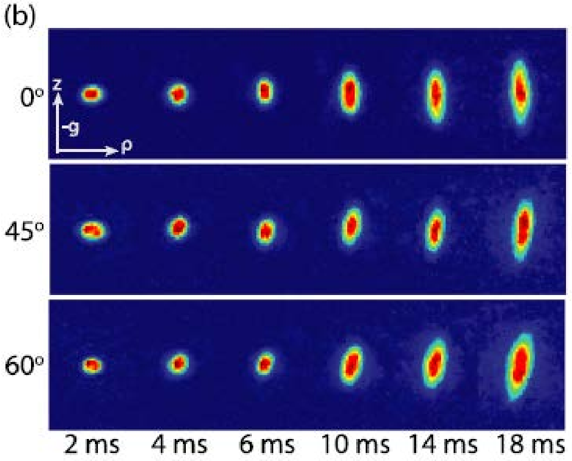
$$U_{\text{dip}}(\vec{x}) = \frac{3}{4\pi r^3}\left(1 - \frac{3(\vec{n}\cdot\vec{x})^2}{r^2}\right) = -\delta(\vec{x}) - 3\partial_{\vec{n}\vec{n}}\left(\frac{1}{4\pi r}\right)$$

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

- Dipole-dipole interaction becomes

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

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



BEC@Stanford

A New Formulation

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

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

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

  – Energy

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

  – 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, SISC, 13''; Bao & Cai, KRM, 13'; ……
  – Bao, Greengard &Jiang, 13' ---- nonuniform FFT

New numerical methods for DDI

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

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

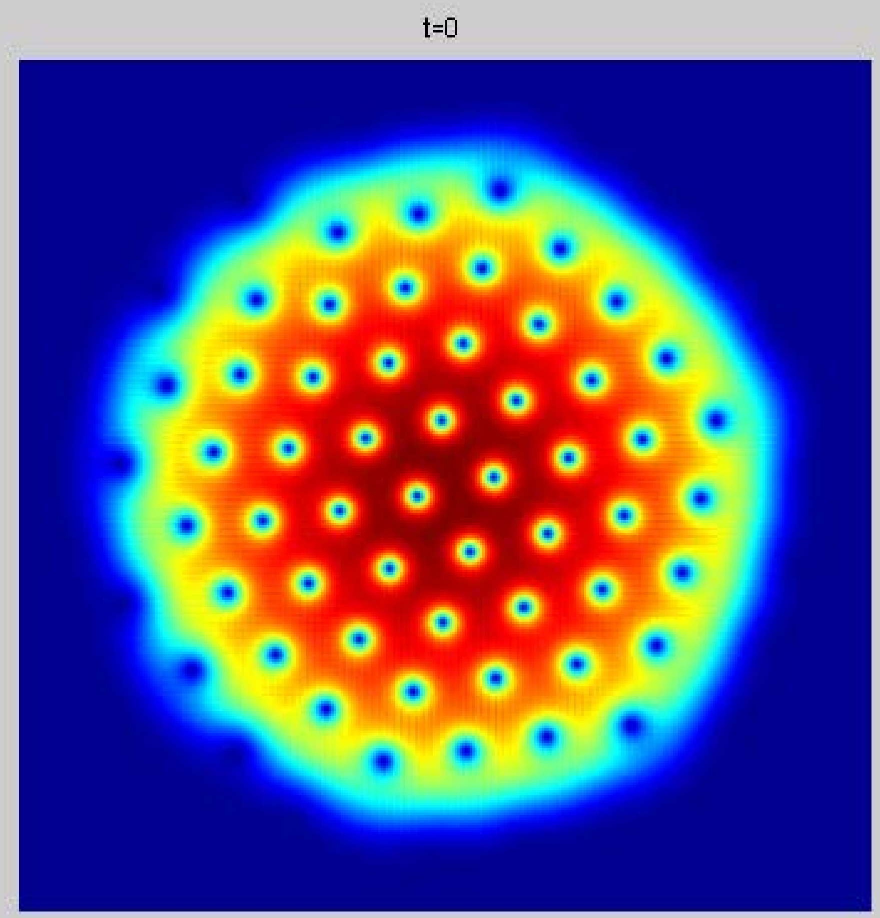
$$\phi = -|\psi|^2 - 3\partial_{nn}\varphi \quad \& \quad -\Delta\varphi(\vec{x},t) = |\psi(\vec{x},t)|^2$$

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

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

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

Dynamics of a vortex lattice



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', ……

Conclusions & Future Challenges

- Conclusions:
  - NLSE / GPE – brief motivation
  - Dynamical properties
  - Numerical methods
    - Time-splitting spectral (TSSP) method & Applications
  - Extensions – rotations, nonlocal, system
- Future Challenges
  - With random potential or high dimensions
  - Coupling GPE & Quantum Boltzmann equation (QBE)
  - NLSE / GPE coupled with other equations
  - BEC at finite temperature & quantum turbulence

Collaborators

- In Mathematics
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  - Local: X. Dong, Q. Tang, X. Zhao, …….
- In Physics
  - External: D. Jaksch (Oxford); A. Klein (Oxfrod); M. Rosenkranz (Oxford); H. Pu (Rice), Donghui Zhang (Dalian), W. M. Liu (IOP, Beijing), X. J. Zhou (Peking U), …..
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- Fund support: ARF Tier 1 & Tier 2