Ground States and Dynamics of the Nonlinear Schrodinger / Gross-Pitaevskii Equations

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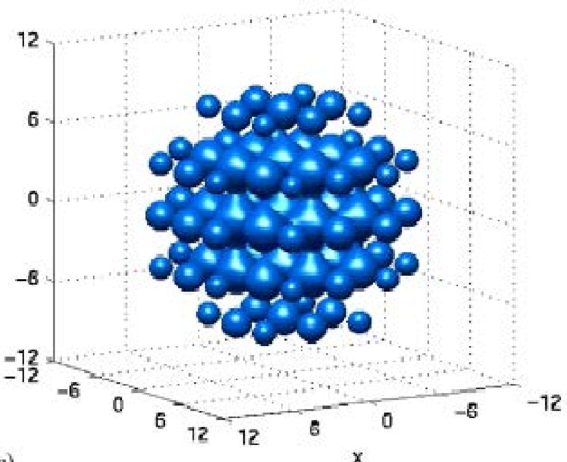
Outline

- Nonlinear Schrodinger / Gross-Pitaevskii equations
- Ground states
  - Existence, uniqueness & non-existence
  - Numerical methods & results
- Dynamics
  - Well-posedness & dynamical laws
  - Numerical methods & results
- Applications --- collapse & explosion of a BEC
- Extension to rotation, nonlocal interaction & system
- Conclusions



(c)

NLSE / GPE

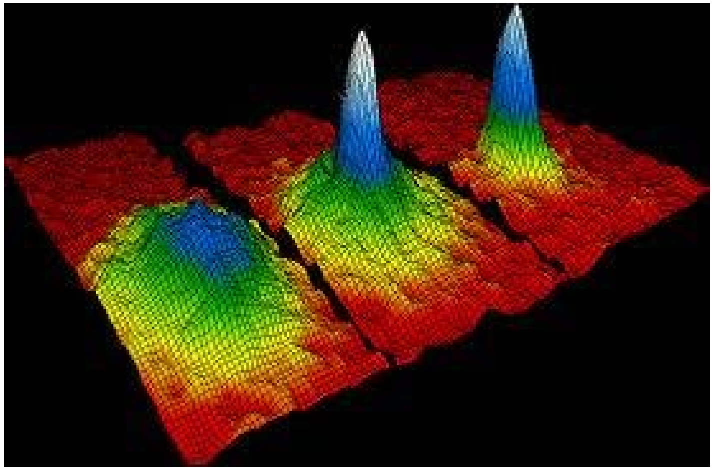
- The nonlinear Schrodinger equation (NLSE) ---1925

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

- t : time & $\vec{x}\ (\in \mathbb{R}^d)$: spatial coordinate (d=1,2,3)
- $\psi(\vec{x},t)$: complex-valued wave function
- $V(\vec{x})$: real-valued external potential
- β : dimensionless interaction constant
  - =0: linear; >0(<0): repulsive (attractive) interaction
- Gross-Pitaevskii equation (GPE) :
  - E. Schrodinger 1925';
  - E.P. Gross 1961'; L.P. Pitaevskii 1961'

Model for BEC

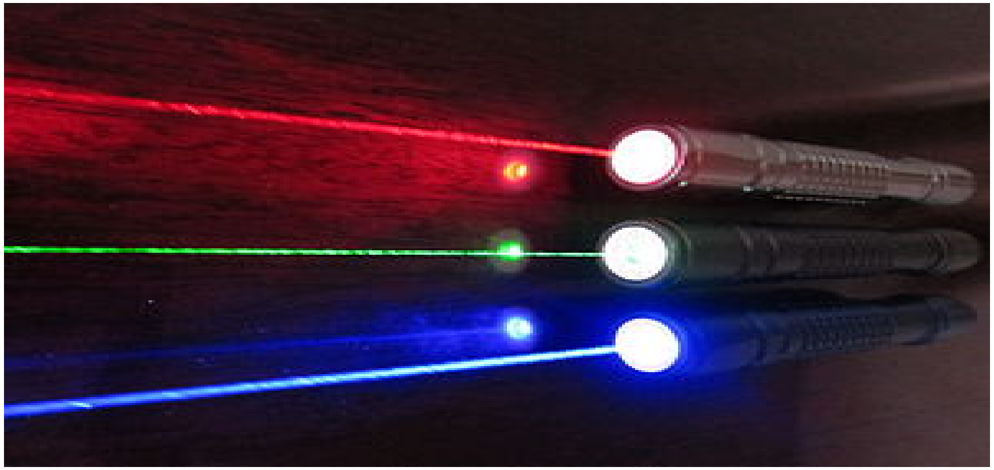
- Bose-Einstein condensation (BEC):
  - Bosons at nano-Kevin temperature
  - Many atoms occupy in one obit -- at quantum mechanical ground state
  - Form like a `super-atom', New matter of wave --- fifth state
- Theoretical prediction – S. Bose & E. Einstein 1924'
- Experimental realization – JILA 1995'
- 2001 Noble 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

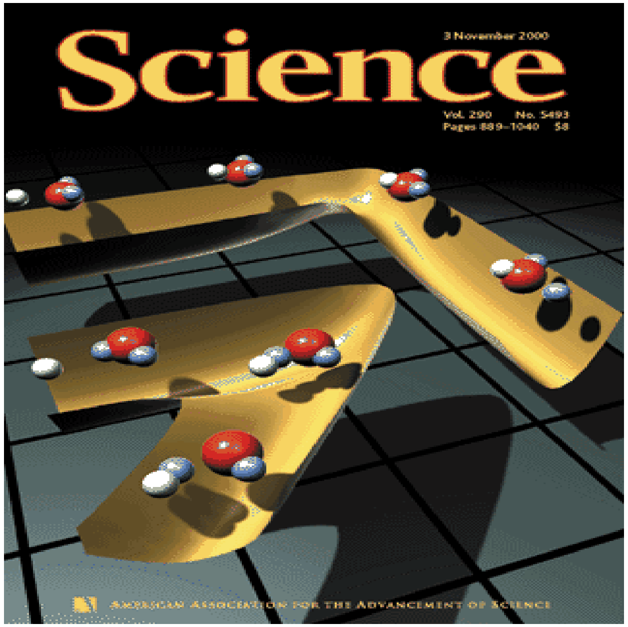
Laser beam propagation

- 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

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

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

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

- Mass 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 conservation

$$E(t) := E(\psi(\bullet,t)) = \int_{\mathbb{R}^d} \left[\frac{1}{2}|\nabla\psi|^2 + V(x)|\psi|^2 + \frac{\beta}{2}|\psi|^4\right] d\vec{x} \equiv E(0), \quad t \ge 0$$

Stationary states

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

- Stationary states (ground & excited states)

$$\psi(\vec{x},t) = \phi(\vec{x})\,e^{-i\,t\,\mu}$$

- Nonlinear eigenvalue problems: Find (μ,ϕ) s.t.

$$\mu\,\phi(\vec{x}) = -\frac{1}{2}\nabla^2\phi(\vec{x}) + V(\vec{x})\phi(\vec{x}) + \beta\,|\phi(\vec{x})|^2\,\phi(\vec{x}), \quad \vec{x}\in\mathbb{R}^d$$

$$\text{with} \qquad \|\phi\|^2 := \int_{\mathbb{R}^d} |\phi(\vec{x})|^2\, d\vec{x} = 1$$

- Time-independent NLSE or GPE:
- Eigenfunctions are
  - Orthogonal in linear case & Superposition is valid for dynamics!!
  - Not orthogonal in nonlinear case !!!! No superposition for dynamics!!!

Ground states

- The eigenvalue is also called as chemical potential

$$\mu := \mu(\phi) = E(\phi) + \frac{\beta}{2}\int_{\mathbb{R}^d} |\phi(\vec{x})|^4 \, d\vec{x}$$

  - With energy

$$E(\phi) = \int_{\mathbb{R}^d} [\frac{1}{2}|\nabla\phi(\vec{x})|^2 + V(\vec{x})|\phi(\vec{x})|^2 + \frac{\beta}{2}|\phi(\vec{x})|^4] \, d\vec{x}$$

- Ground states -- nonconvex minimization problem

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

  - Euler-Lagrange equation → nonlinear eigenvalue problem

Existence & uniqueness

$$C_b = \inf_{0\neq f\in H^1(\mathbb{R}^2)} \frac{\|\nabla f\|^2_{L^2(\mathbb{R}^2)}\|f\|^2_{L^2(\mathbb{R}^2)}}{\|f\|^4_{L^4(\mathbb{R}^2)}}$$

- Theorem (Lieb, etc, PRA, 02'; Bao & Cai, KRM, 13') If potential is confining

$$V(\vec{x})\geq 0 \quad \text{for} \quad \vec{x}\in\mathbb{R}^d \quad \& \quad \lim_{|\vec{x}|\to\infty} V(\vec{x})=\infty$$

  - There exists a ground state if one of the following holds

$$(i)\ d=3\ \&\ \beta\geq 0;\quad (ii)\ d=2\ \&\ \beta>-C_b;\quad (iii)\ d=1\ \&\ \beta\in\mathbb{R}$$

  - The ground state can be chosen as nonnegative $|\phi_g|$, $i.e.\ \phi_g=|\phi_g|e^{i\theta_0}$
  - Nonnegative ground state is unique if $\beta\geq 0$
  - The nonnegative ground state is strictly positive if $V(\vec{x})\in L^2_{\text{loc}}$
  - There is no ground stats if one of the following holds

$$(i)'\quad d=3\ \&\ \beta<0;\quad (ii)'\quad d=2\ \&\ \beta\leq -C_b$$

Key Techniques in Proof

- Positivity & semi-lower continuous

$$E(\phi) \geq E(|\phi|) = E(\sqrt{\rho}), \quad \forall \phi \in S \qquad \text{with} \quad \rho = |\phi|^2$$

- The energy $\tilde{E}(\rho) := E(\sqrt{\rho})$ is bounded below if conditons (i) or (ii) or (iii) and strictly convex if $\beta \geq 0$
- Confinement potential implies decay at far field
- The set $S = \left\{ \rho \mid \int_{\mathbb{R}^d} \rho(\vec{x}) d\vec{x} = 1 \ \& \ \tilde{E}(\rho) < \infty \right\}$ is convex in ρ
- Using convex minimization theorem
- Non-existence result

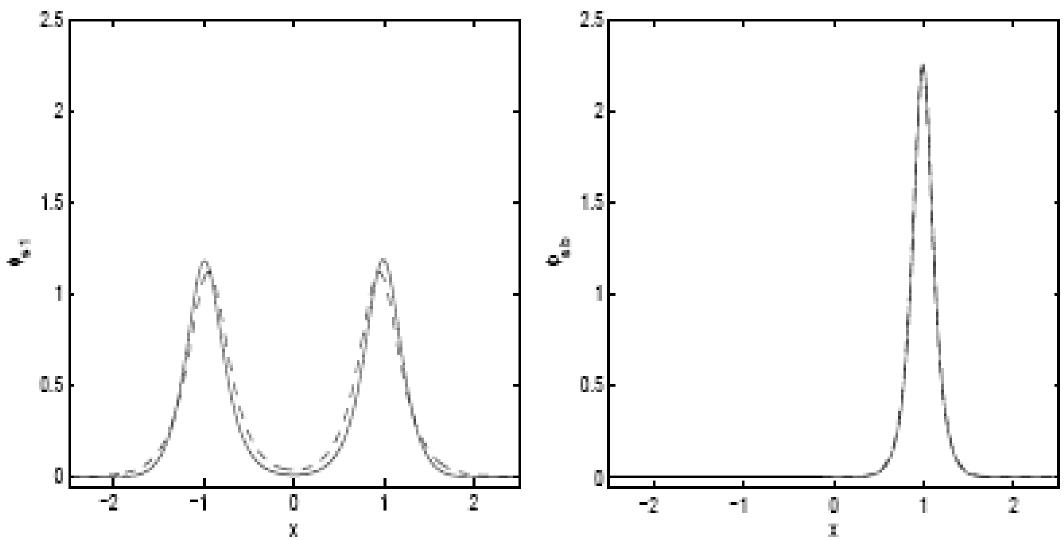
$$\phi_\varepsilon(\vec{x}) = \frac{1}{(2\pi\varepsilon)^{d/4}} \exp\left(-\frac{|\vec{x}|^2}{2\varepsilon} \right), \quad \vec{x} \in \mathbb{R}^d \quad \text{with} \quad \varepsilon \to 0$$

Phase transition –symmetry breaking

- Attractive interaction with double-well potential in 1D

$$\mu\,\phi(x) = -\frac{1}{2}\phi''(x) + V(x)\phi(x) + \beta\,|\phi(x)|^2\,\phi(x), \quad \text{with} \quad \int_{-\infty}^{\infty} |\phi(x)|^2 dx = 1$$

$$V(x) = (x^2-1)^2 \qquad \& \qquad \beta: \text{ positive } \rightarrow 0 \rightarrow \text{ negative}$$



Excited states

- Excited states: $\phi_1, \quad \phi_2, \quad \phi_3, \quad \cdots$
- Open question: (Bao & W. Tang, JCP, 03'; Bao, F. Lim & Y. Zhang, Bull Int. Math, 06')

$$\varphi_g, \qquad \varphi_1, \qquad \varphi_2, \qquad \cdots$$

$$E(\varphi_g) < E(\varphi_1) \le E(\varphi_2) \le \cdots$$

$$\mu(\varphi_g) < \mu(\varphi_1) \le \mu(\varphi_2) \le \cdots \quad ???????$$

- Gaps between ground and first excited states

$$\delta_\mu(\beta) := \mu(\phi_1^\beta) - \mu(\phi_g^\beta) > 0, \qquad \delta_E(\beta) := E(\phi_1^\beta) - E(\phi_g^\beta) > 0$$

  - Linear case – fundamental gap conjecture (B. Andrews & J. Clutterbuck, JAMS 11')

$$\delta := \delta_\mu(0) = \delta_E(0) \ge \frac{3\pi^2}{|D|} \qquad \text{on bounded domain } D \subset \mathbb{R}^d$$

  - Nonlinear case ?????

$$\delta_\mu(\beta) \ge C_1 > 0, \qquad \delta_E(\beta) \ge C_2 > 0, \quad \beta \ge 0\,????$$

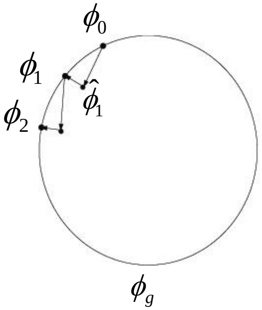
Computing ground states

- Idea: Steepest decent method + Projection

$$\partial_t \varphi(\vec{x},t) = -\frac{1}{2}\frac{\delta E(\varphi)}{\delta \varphi} = \frac{1}{2}\nabla^2\varphi - V(\vec{x})\varphi - \beta|\varphi|^2\varphi, \quad t_n \le t < t_{n+1}$$

$$\varphi(\vec{x},t_{n+1}) = \frac{\varphi(\vec{x},t_{n+1}^-)}{\|\varphi(\vec{x},t_{n+1}^-)\|}, \qquad n = 0,1,2,\cdots$$

$$\varphi(\vec{x},0) = \varphi_0(\vec{x}) \quad \text{with} \quad \|\varphi_0(\vec{x})\| = 1.$$



$E(\hat{\phi}_1) < E(\phi_0)$

$E(\hat{\phi}_1) < E(\phi_1)$

$E(\phi_1) < E(\phi_0)$??

  - The first equation can be viewed as choosing $t = i\tau$ in NLS
  - For linear case: (Bao & Q. Du, SIAM Sci. Comput., 03')

$$E_0(\phi(.,t_{n+1})) \le E_0(\phi(.,t_n)) \le \cdots \le E_0(\phi(.,0))$$

  - For nonlinear case with small time step, CNGF

Normalized gradient glow

- Idea: letting time step go to 0 (Bao & Q. Du, SIAM Sci. Comput., 03')

$$\partial_t \phi(\vec{x},t) = \frac{1}{2}\nabla^2\phi - V(\vec{x})\,\phi - \beta\,|\phi|^2\,\phi + \frac{\mu(\phi(.,t))}{\|\phi(.,t)\|^2}\,\phi, \quad t \ge 0,$$

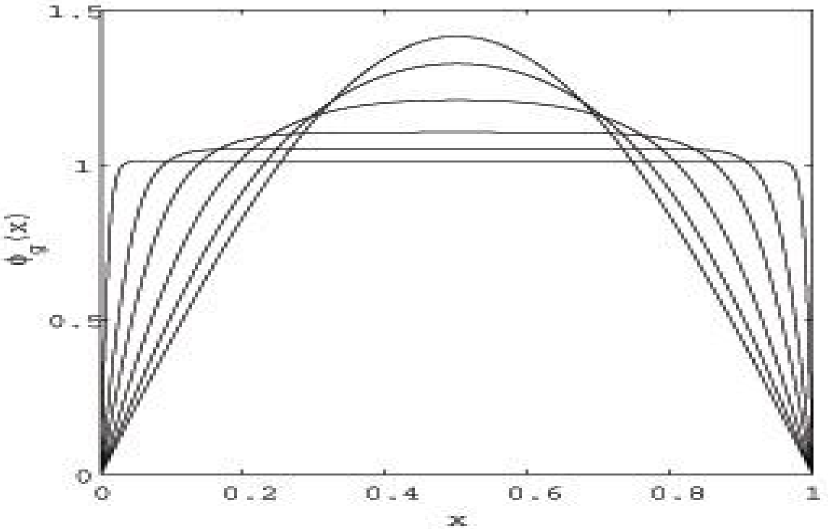
$$\phi(\vec{x},0) = \phi_0(\vec{x}) \qquad \text{with} \qquad \|\phi_0(\vec{x})\| = 1.$$

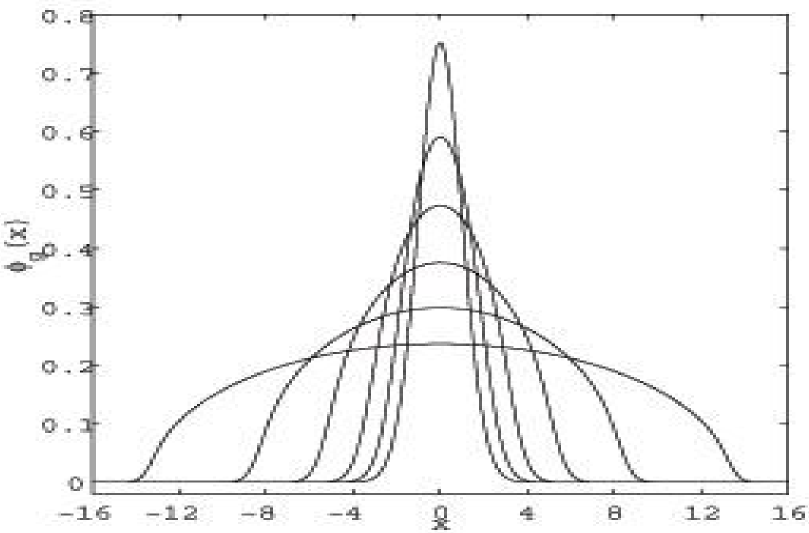
  - Mass conservation & energy diminishing

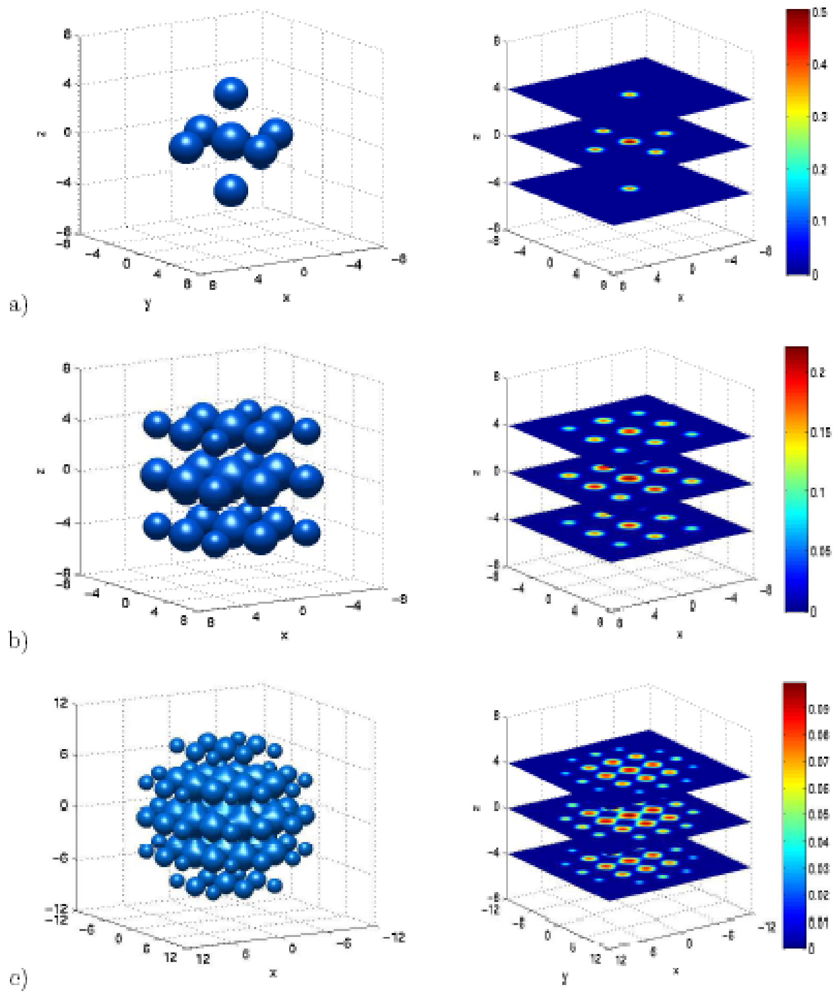
$$\|\varphi(.,t)\| = \|\varphi_0\| = 1, \qquad \frac{d}{d\,t}E(\varphi(.,t)) \le 0, \qquad t \ge 0$$

  - Numerical discretizations
    - BEFD: Energy diminishing & monotone (Bao & Q. Du, SIAM Sci. Comput., 03')
    - TSSP: Spectral accurate with splitting error (Bao & Q. Du, SIAM Sci. Comput., 03')
    - BESP: Spectral accuracy in space & stable (Bao, I. Chern & F. Lim, JCP, 06')

Ground states in 1D & 3D







Dynamics

- Time-dependent NLSE / GPE

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

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

- Well-posedness & dynamical laws
  - Well-posedness & finite time blow-up
  - Dynamical laws
    - Soliton solutions
    - Center-of-mass
    - An exact solution under special initial data
  - Numerical methods and applications

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 $\psi(\vec{x},t) = A e^{i(\vec{k}\cdot\vec{x}-\omega t)} \Rightarrow \omega = \frac{1}{2}\left|\vec{k}\right|^2 + \beta A^2$
- Soliton solutions in 1D:
  - Bright soliton $\beta < 0$ ----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

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

Dynamics with harmonic potential

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

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

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

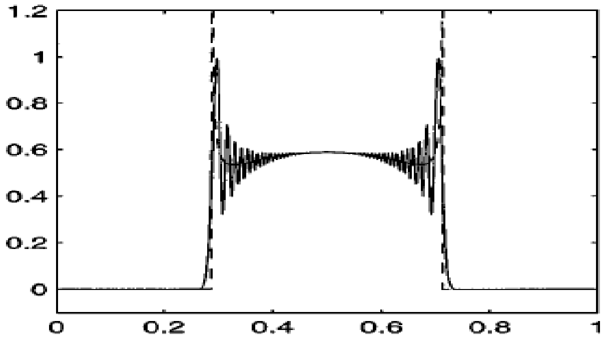
$$\mu_s\,\phi_s(\vec{x}) = -\frac{1}{2}\nabla^2\phi_s + V(\vec{x})\phi_s + \beta|\phi_s|^2\phi_s$$

Numerical difficulties

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

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

- Dispersive & nonlinear
- Solution and/or potential are smooth but may oscillate wildly
- Keep the properties of NLS 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: $\beta \gg 1$

Numerical methods

- Different methods
  - Crank-Nicolson finite difference method (CNFD)
  - Time-splitting spectral method (TSSP)
  - Leap-frog (or RK4) + FD (or spectral) methods
  - ……..
- Time-splitting spectral method (TSSP)

$$i\,\partial_t \psi(\vec{x},t) = (A+B)\psi \quad \text{with } A = -\frac{1}{2}\nabla^2, \quad B = V(\vec{x}) + \beta|\psi|^2$$

$$\psi(\vec{x},t_{n+1}) = e^{-i(A+B)\Delta t}\,\psi(\vec{x},t_n) \approx \begin{cases} e^{-iA\Delta t}e^{-iB\Delta t}\,\psi(\vec{x},t_n) + O((\Delta t)^2) \\ e^{-iA\Delta t/2}e^{-iB\Delta t}e^{-iA\Delta t/2}\,\psi(\vec{x},t_n) + O((\Delta t)^3) \\ \cdots + O((\Delta t)^5) \end{cases}$$

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

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

  - Step 2: solve the nonlinear ODE analytically

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

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

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

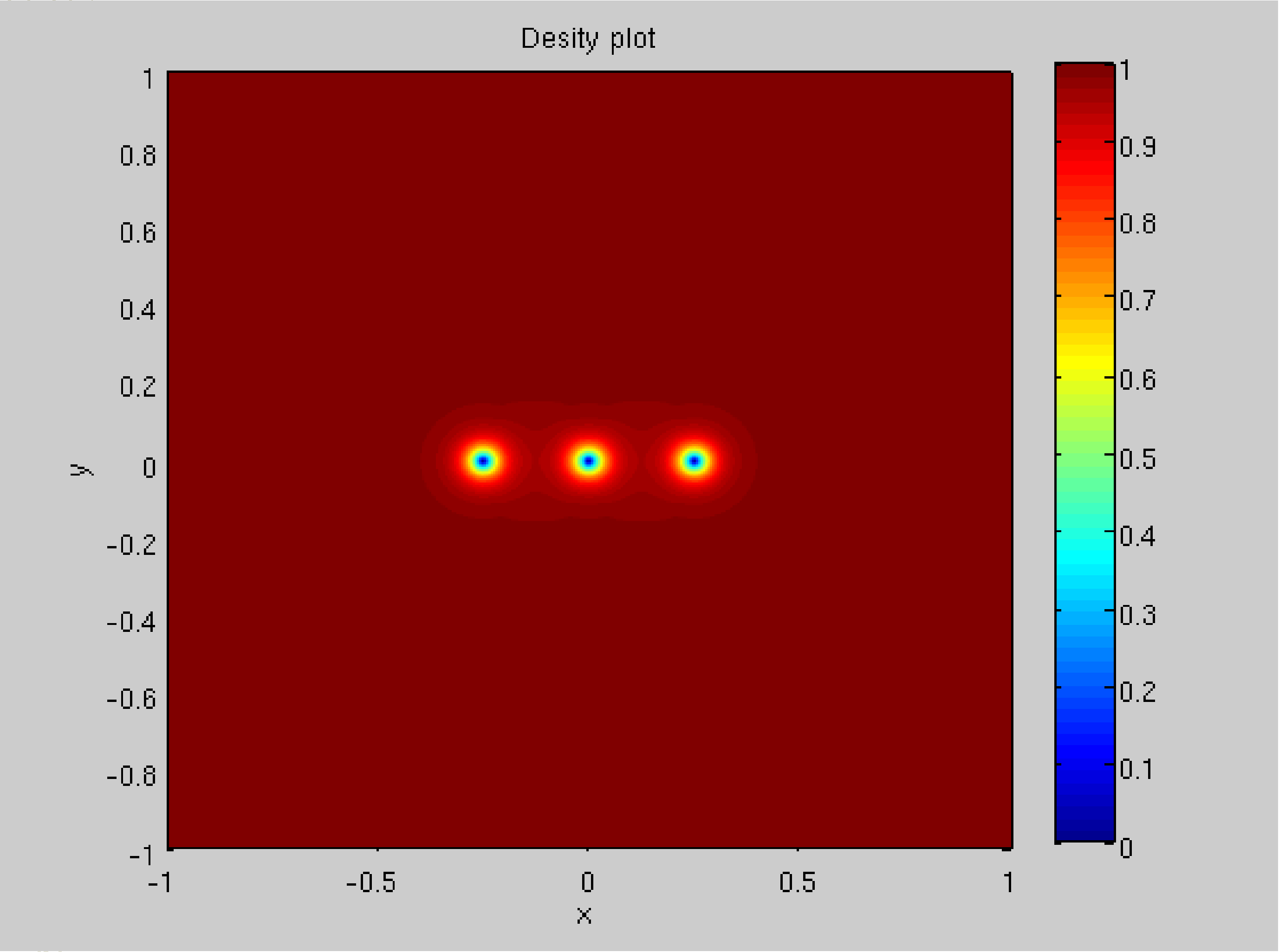
$$\Rightarrow \psi(\vec{x},t) = e^{-i\,(t-t_n)[V(x)+\beta|\psi(\vec{x},t_n)|^2]}\,\psi(\vec{x},t_n)$$

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

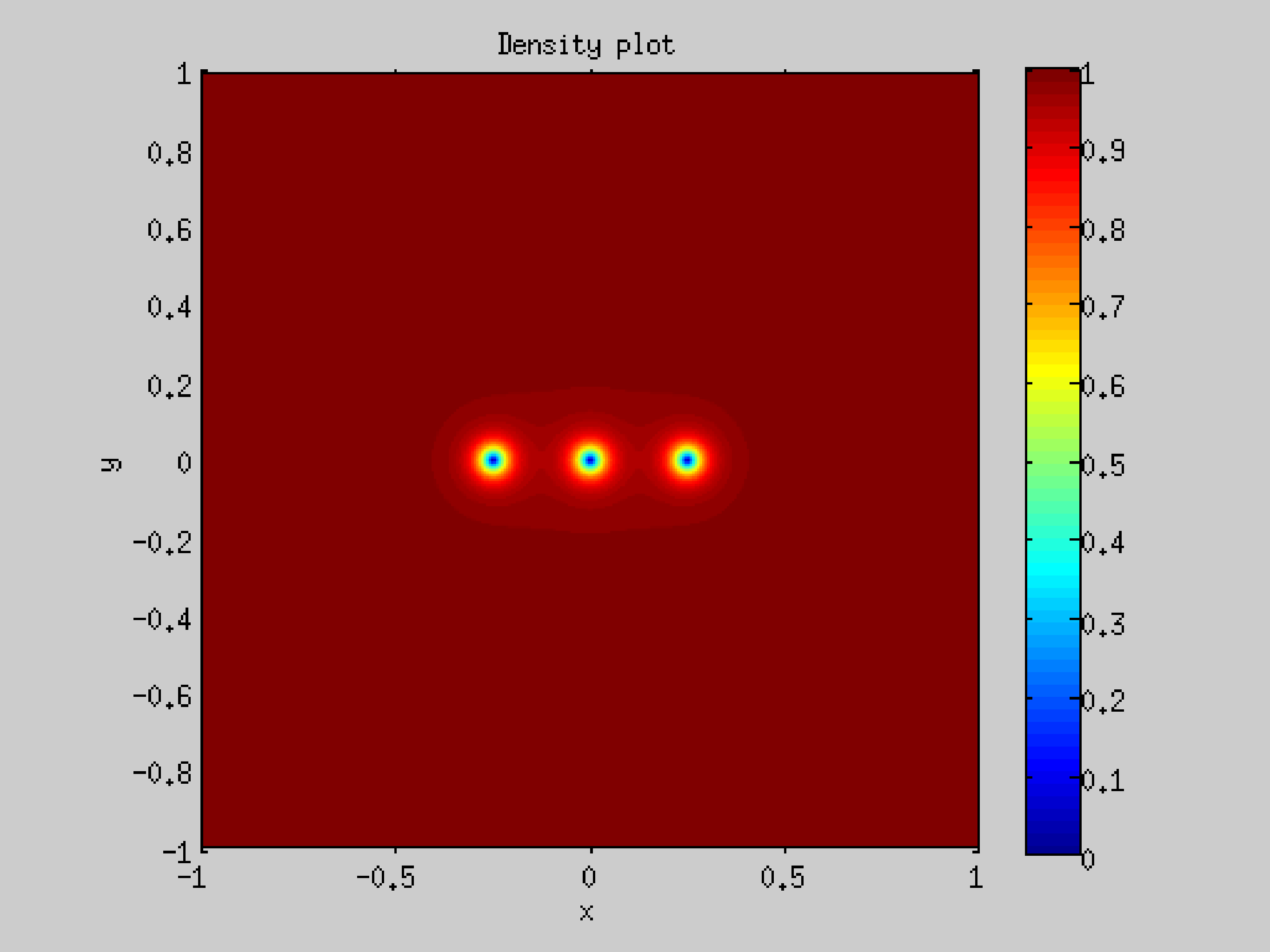
Properties of TSSP

- Explicit & computational cost per time step: $O(M \ln M)$
- Time symmetric: yes
- Time transverse invariant: yes
- Mass conservation: yes
- Stability: yes
- Dispersion relation without potential: yes
- Accuracy
  - Spatial: spectral order; Temporal: 2^{nd} or 4^{th} order
- Best resolution in strong interaction regime: $\beta \gg 1$

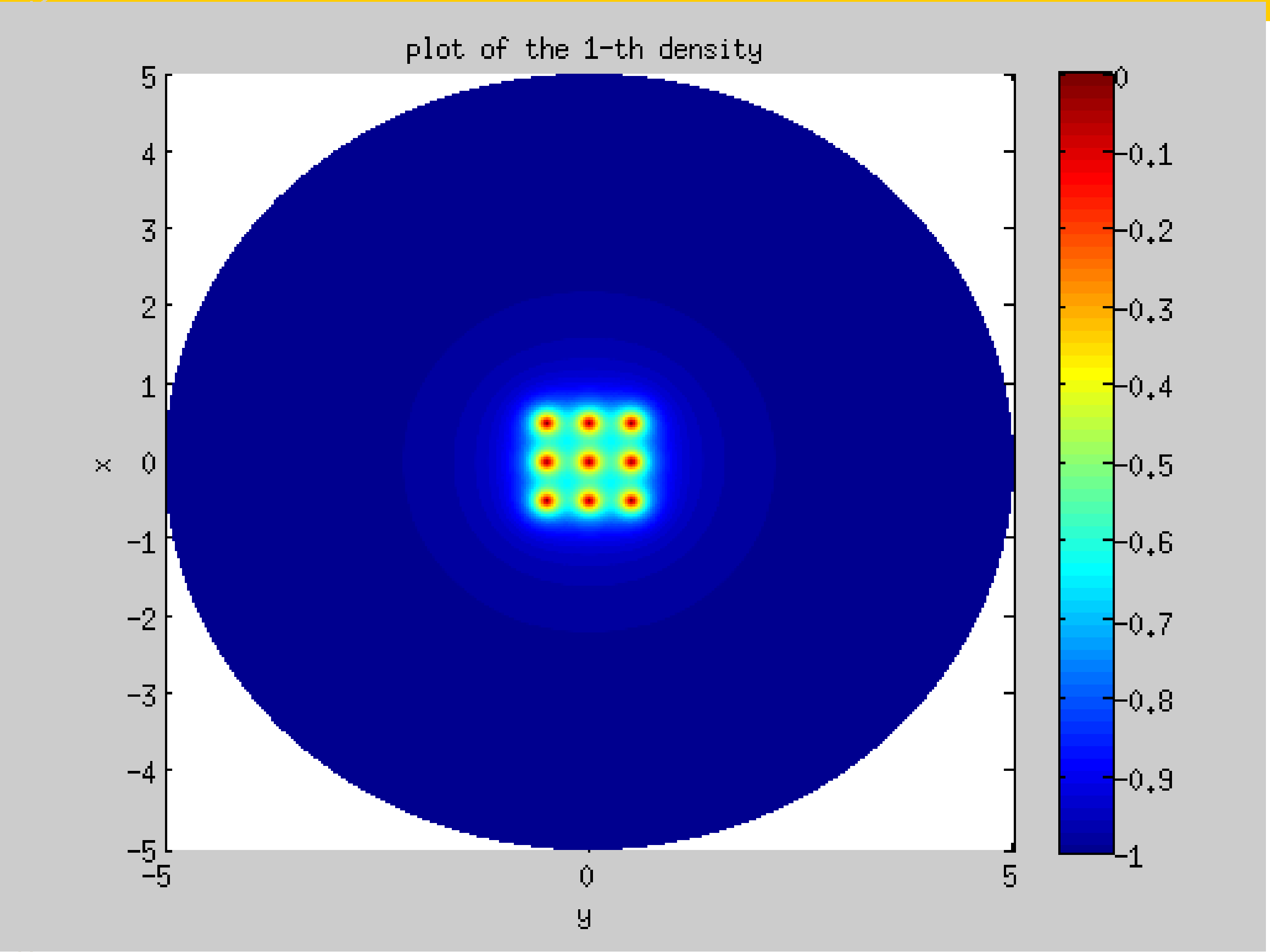
Interaction of 3 like vortices



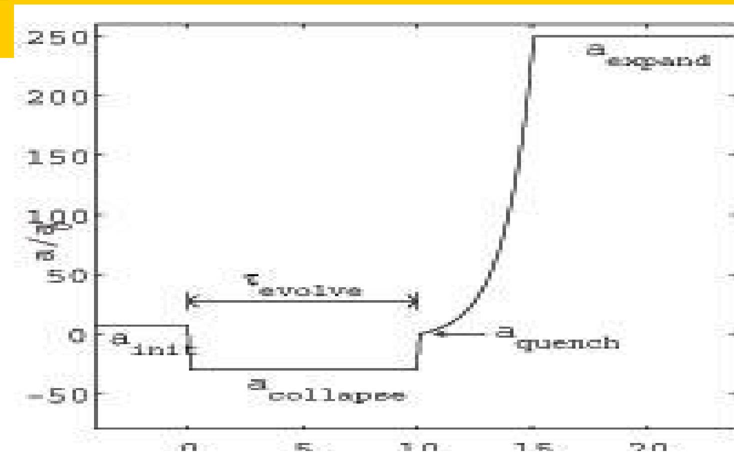
Interaction of 3 opposite vortices



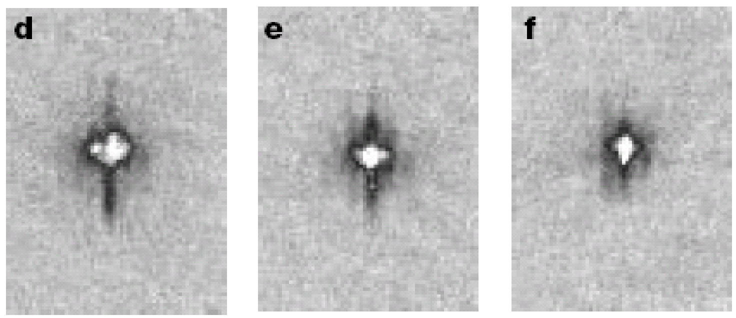
Interaction of a lattice

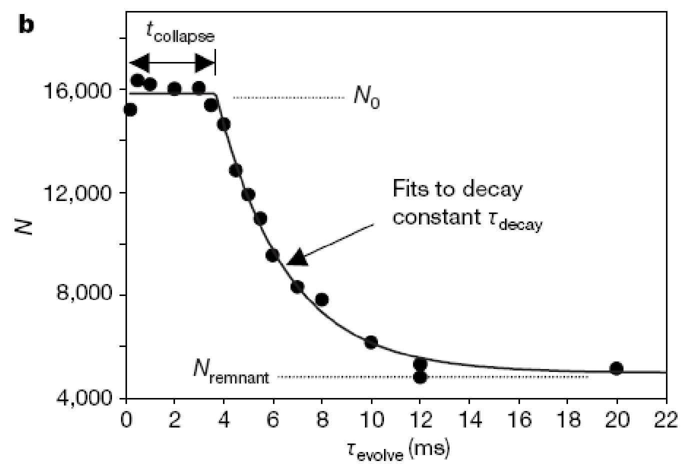


3D collapse & explosion of BEC



- 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

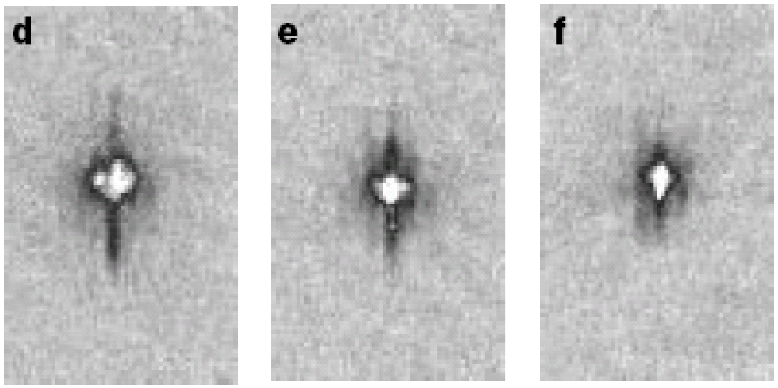


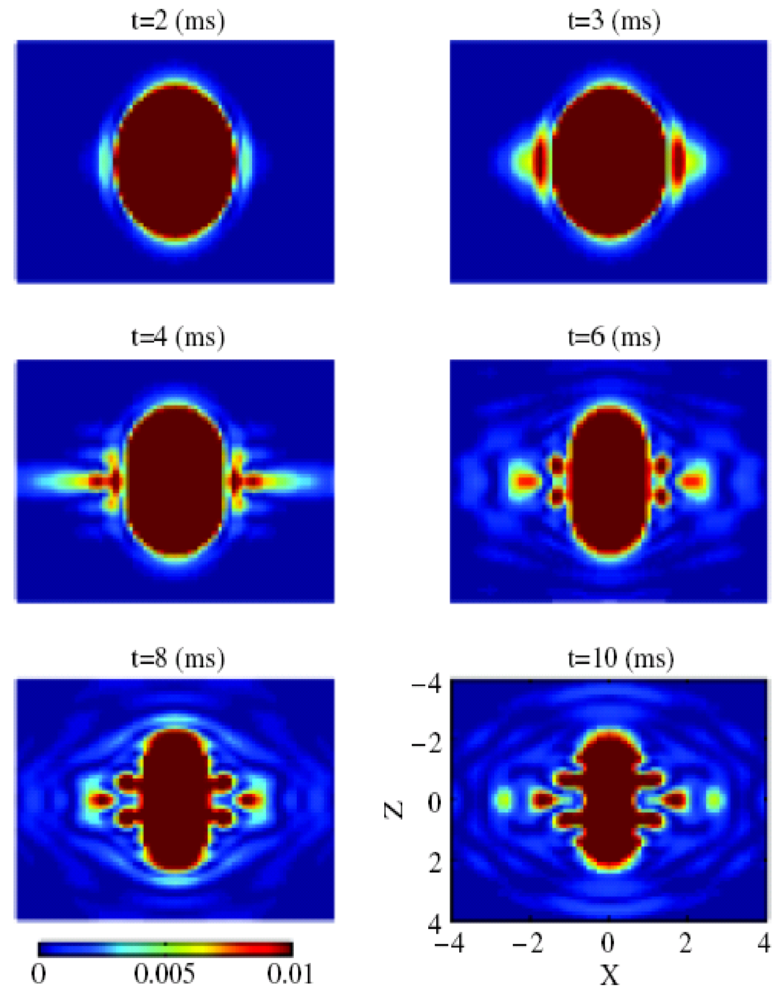


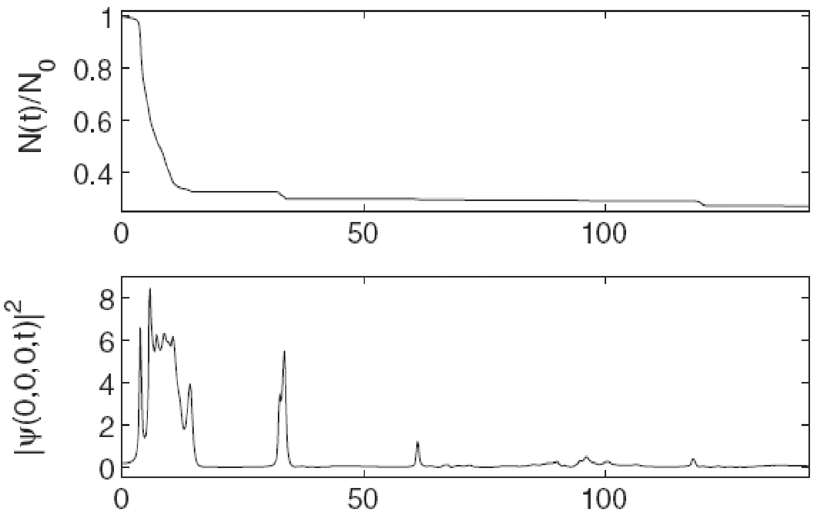
- Mathematical model (Duine & Stoof, PRL, 01')

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

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

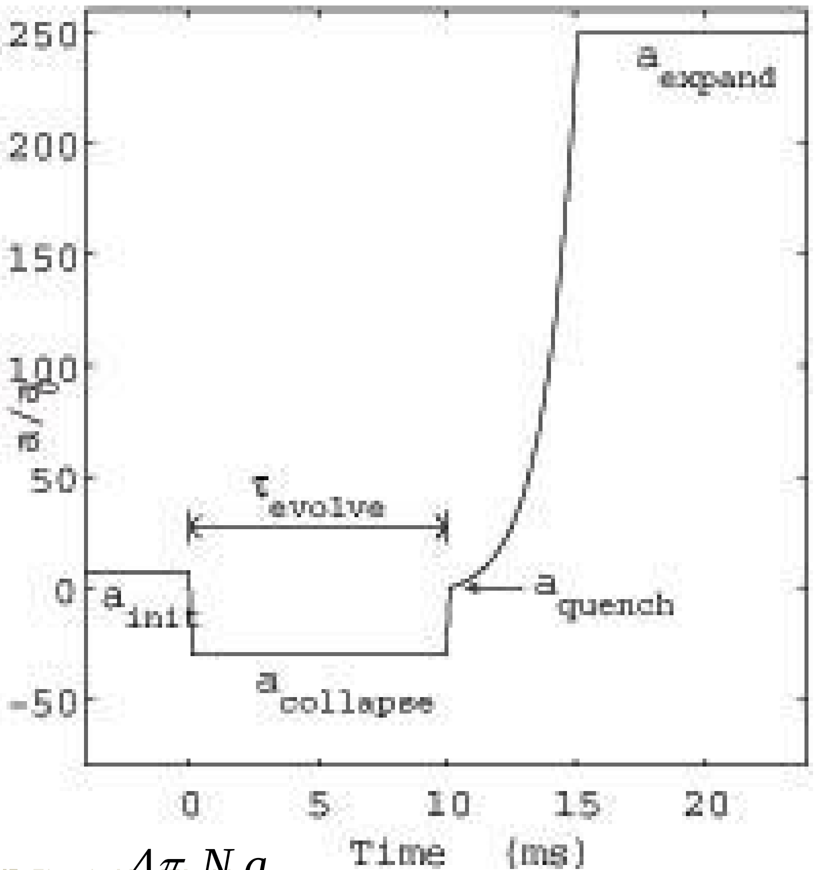


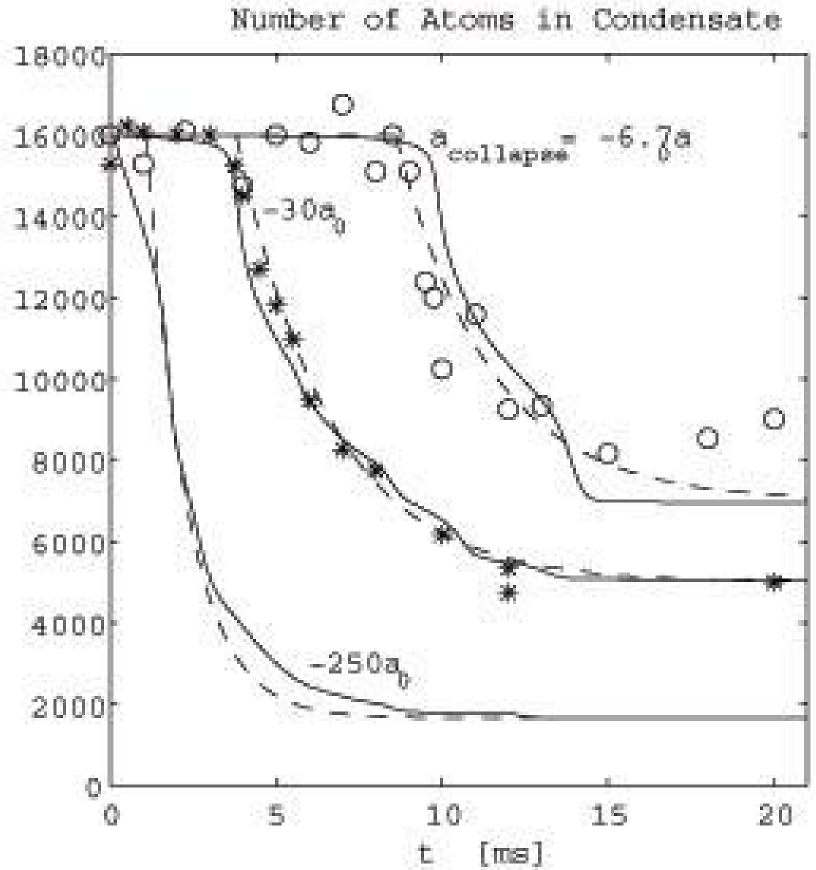




Jet formation

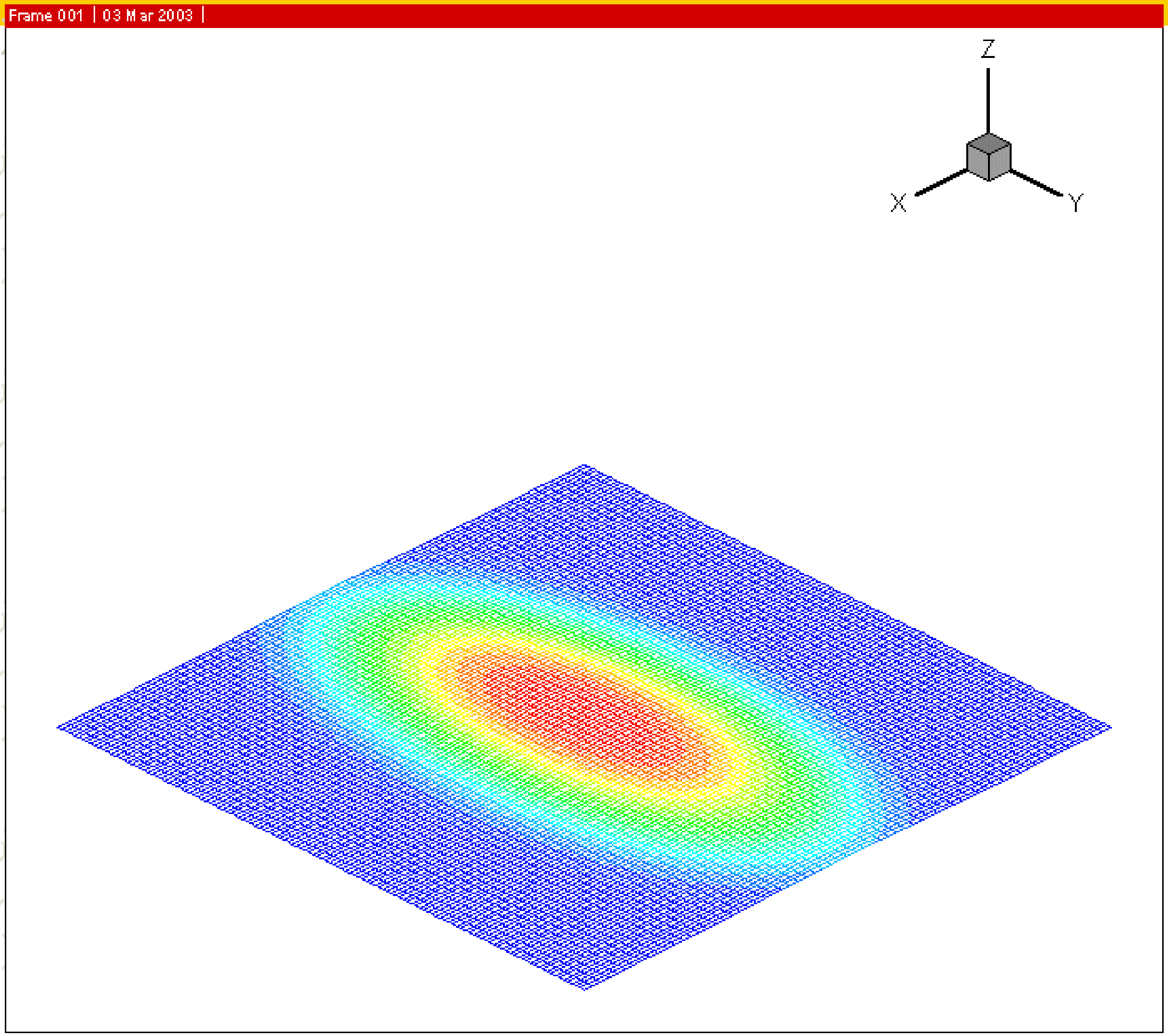
3D Collapse and explosion in BEC





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

3D Collapse and explosion in BEC



Extension to GPE with rotation

- GPE / NLSE with an angular momentum rotation

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

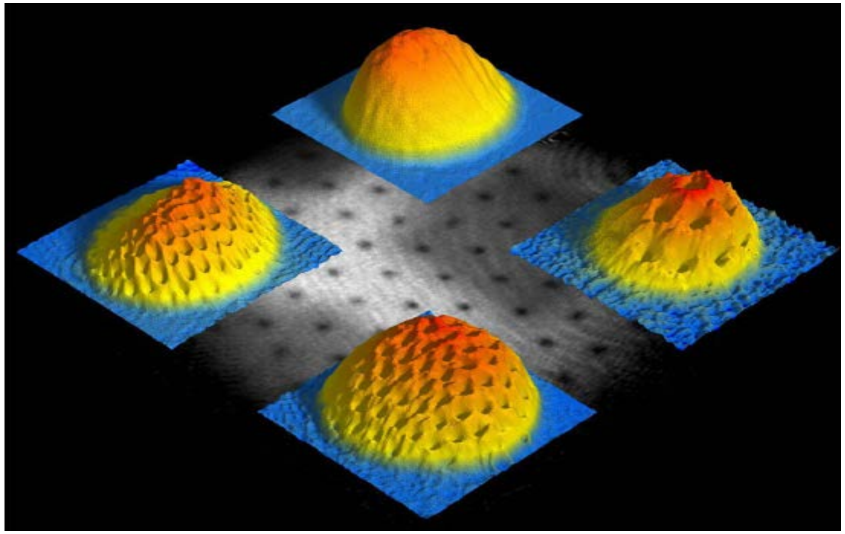
$$L_z := xp_y - yp_x = -i(x\partial_y - y\partial_x)\equiv -i\partial_\theta,\quad L=\vec{x}\times\vec{P},\quad \vec{P}=-i\nabla$$

- Mass conservation

$$N(t)=\int_{\mathbb{R}^d}|\psi(\vec{x},t)|^2 d\vec{x}$$

- Energy conservation

$$E_\Omega(\psi):=\int_{R^d}\left[\frac{1}{2}|\nabla\psi|^2+V(x)|\psi|^2-\Omega\,\bar{\psi}L_z\psi+\frac{\beta}{2}|\psi|^4\right]d\,\vec{x}$$

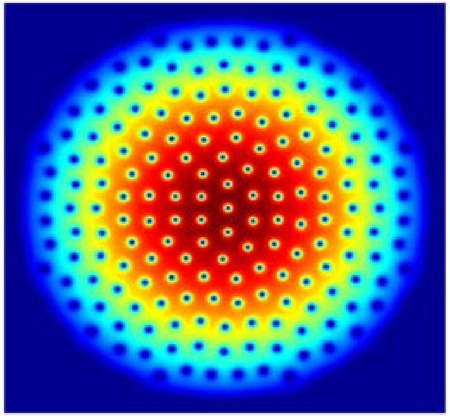


Vortex @MIT

Ground states

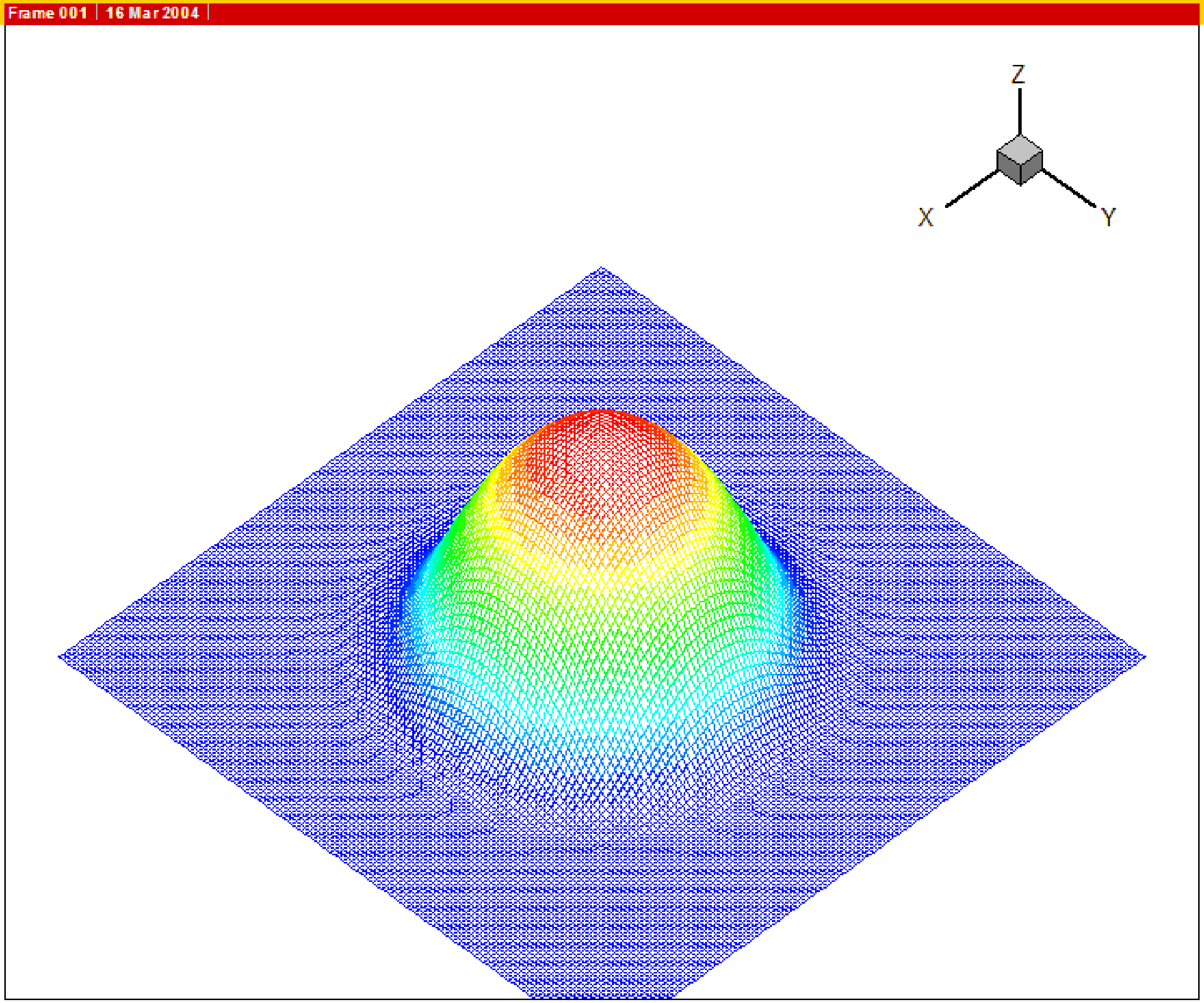
- Ground states – Seiringer, CMP, 02'; Bao,Wang & Markowich, CMS, 05'; …..

$$\min_{\phi \in S} E_{\Omega}(\phi)$$

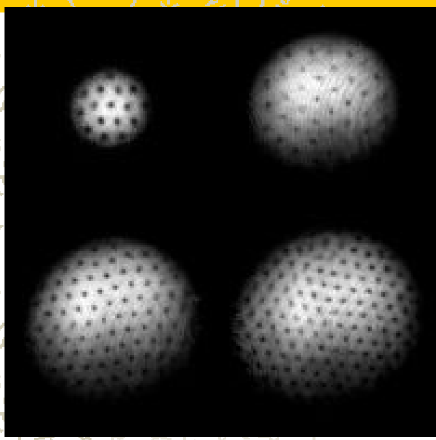


- Existence & uniqueness
  - Exists a ground state when $\beta \geq 0 \;\&\; |\Omega| \leq \min\{\gamma_x, \gamma_y\}$
  - Uniqueness when $|\Omega| < \Omega_c(\beta)$
  - Quantized vortices appear when $|\Omega| \geq \Omega_c(\beta)$
  - Phase transition & bifurcation in energy diagram
- Numerical methods --- GFDN & BEFD or BEFP

Ground states with different Ω



Ground states of rapid rotation



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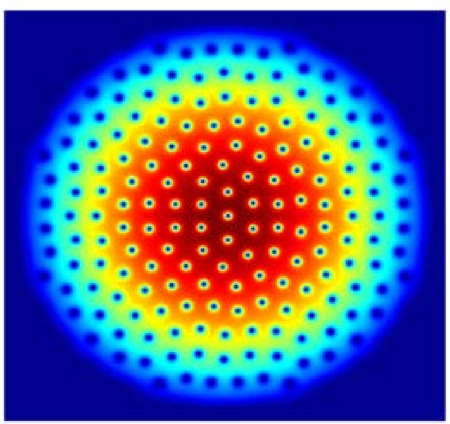
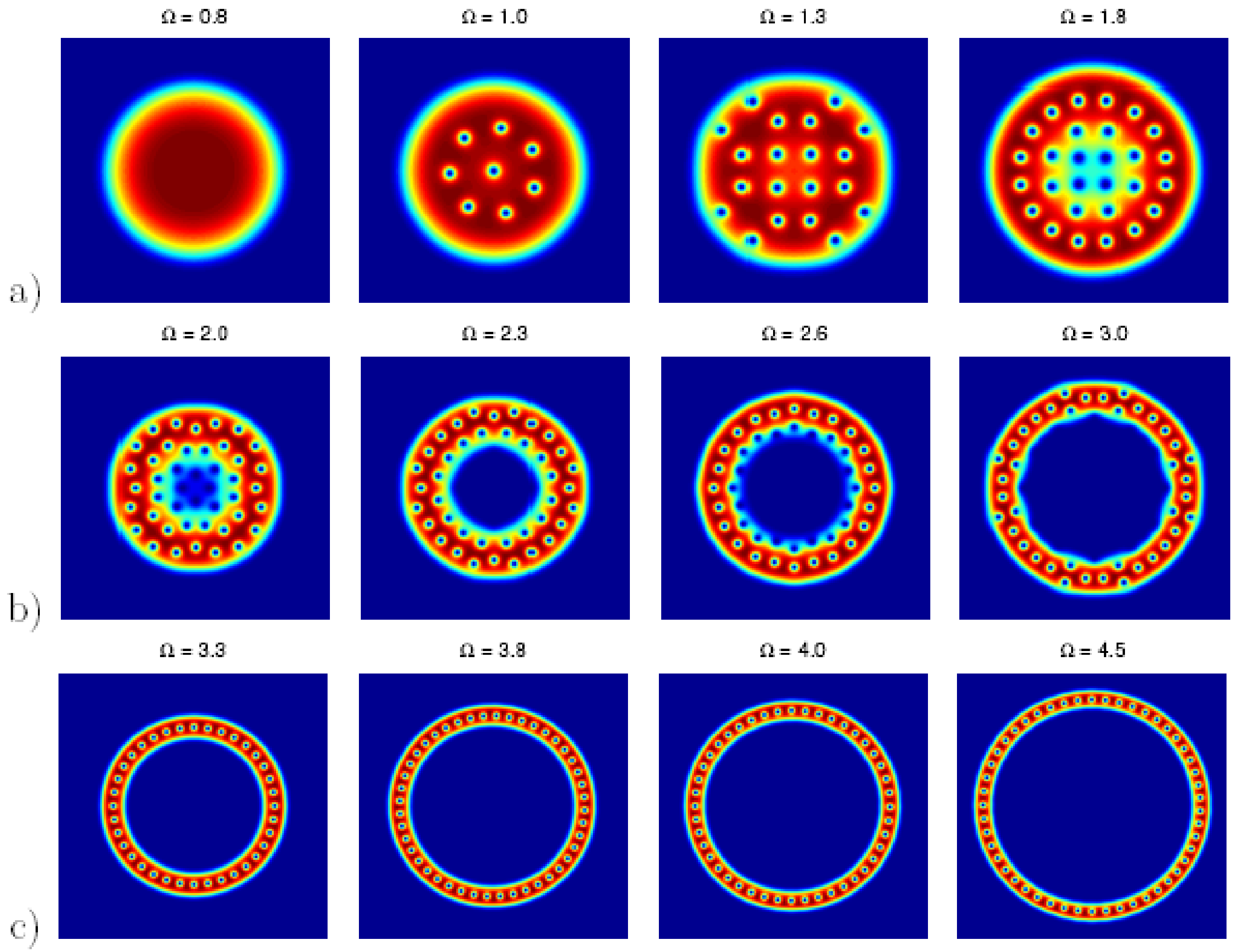
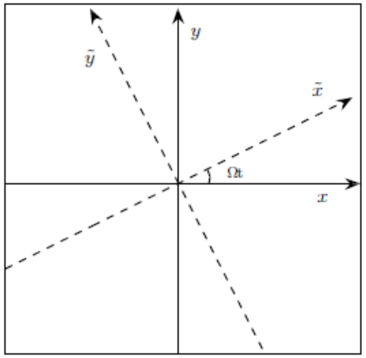




Dynamics – Bao, Du & Zhang, SIAP, 05'; Bao & Cai, KRM, 13'; ……

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



  – A rotating Lagrange coordinate:

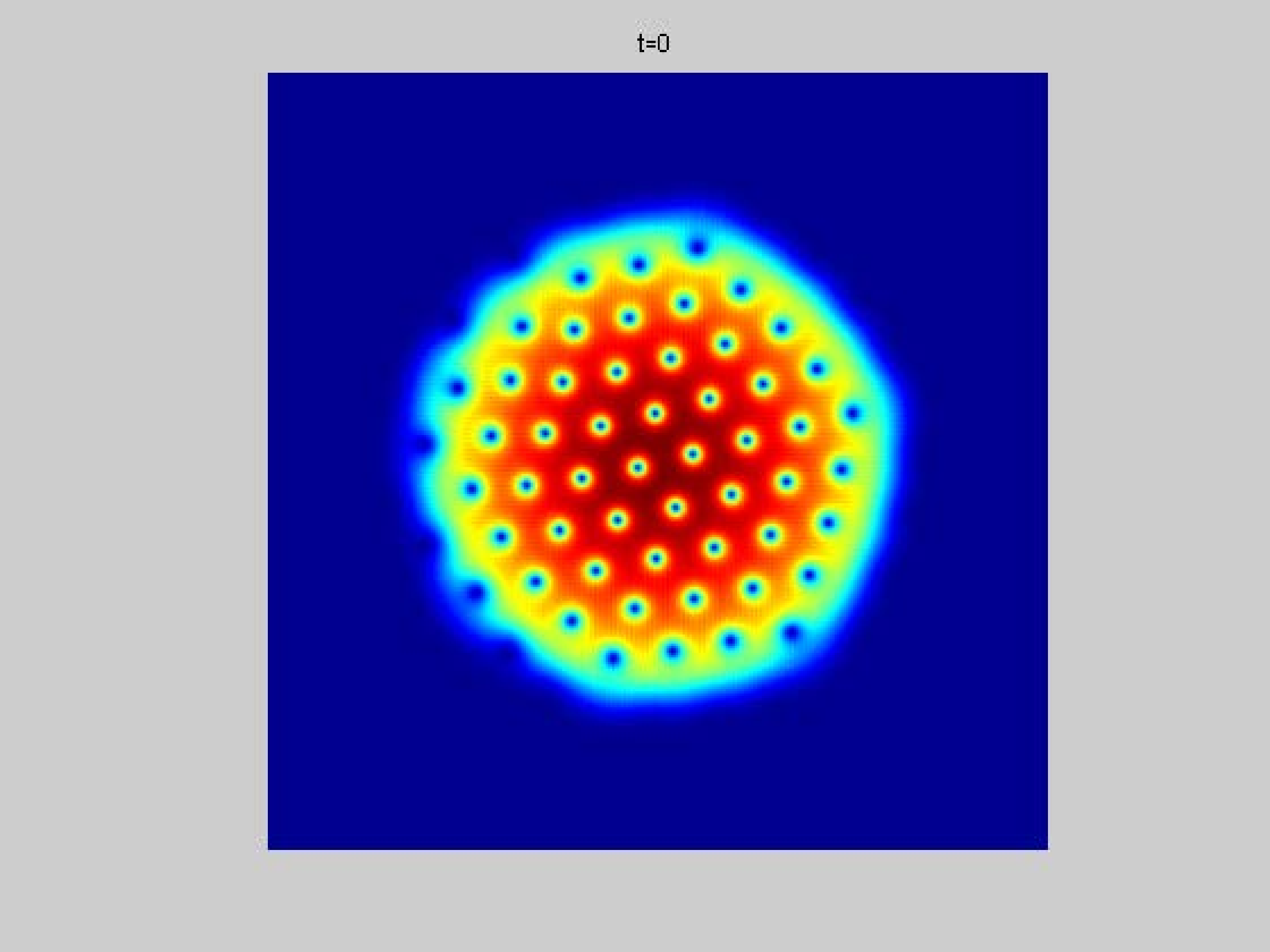
$$A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) \\ -\sin(\Omega t) & \cos(\Omega t) \end{bmatrix} \quad \text{for } d = 2; \quad A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{for } d = 3$$

  – GPE in rotating Lagrange coordinates

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

  – Analysis & numerical methods -- Bao & Wang, JCP6'; Bao, Li & Shen, SISC, 09'; Bao, Marahrens, Tang & Zhang, 13', …….

Dynamics of a vortex lattice



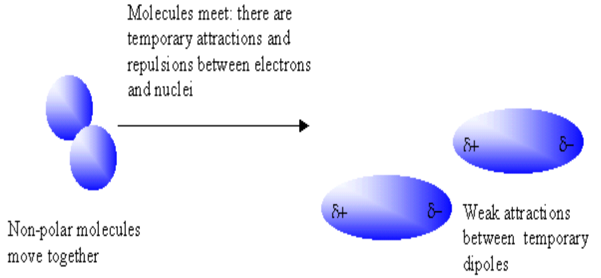
Extension to dipolar quantum gas

- 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

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

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

A New Formulation

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

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

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

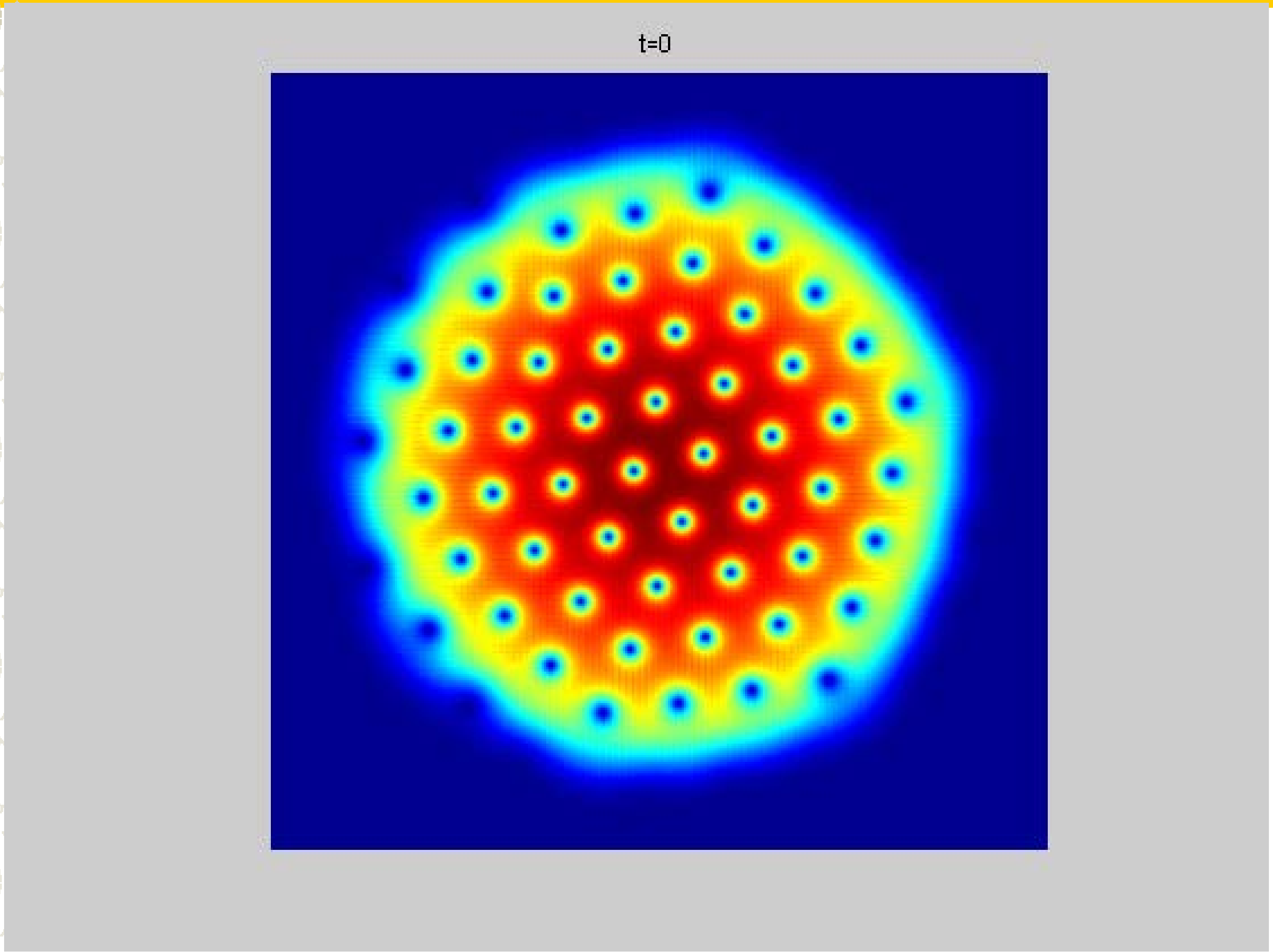
  – Energy

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

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

- Ground state – Bao, Cai & Wang, JCP, 10'; Bao, Ben Abdallah & Cai, SIMA, 12'
- Dynamics – Bao, Cai & Wang, JCP, 10'; Bao & Cai, KRM, 13' $\quad \beta\ge 0\ \&\ -\frac{\beta}{2}\le\lambda\le\beta$
- Dimension reduction – Cai, Rosenkranz, Lei & Bao, PRA, 10'; Bao & Cai, KRM, 13'

Dynamics of a vortex lattice



Coupled GPEs

- Spinor F=1 BEC

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

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

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

- 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

- Analysis & numerical methods:
  - For ground state (Bao & Wang, SIAM J. Numer. Anal., 07'; Bao & Lim, SISC, 08'; PRE, 08')
  - For Dynamics (Bao, Markowich, Schmeiser & Weishaupl, M3AS, 05')

Conclusions & Future Challenges

- Conclusions:
  - NLSE / GPE – brief derivation
  - Ground states
    - Existence, uniqueness, non-existence
    - Numerical methods -- BEFD
  - Dynamics
    - Well-posedness & dynamical laws
    - Numerical methods -- TSSP
- Future Challenges
  - System of NLSE/GPE; with random potential; high dimensions
  - Coupling GPE & Quantum Boltzmann equation (QBE)

Collaborators

- In Mathematics
  - External: P. Markowich (KAUST, Vienna, Cambridge); Q. Du (PSU); J. Shen (Purdue); S. Jin (UW-Madison); L. Pareshi (Italy); P. Degond (France); N. Ben Abdallah (Toulouse), W. Tang (Beijing), I.-L. Chern (Taiwan), Y. Zhang (MUST), H. Wang (China), Y. Cai (UW/UM), H.L. Li (Beijing), T.J. Li (Peking), …….
  - 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), …..
  - Local: B. Li, J. Gong, B. Xiong, W. Ji, F. Y. Lim (IHPC), M.H. Chai (NUSHS), ………
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