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

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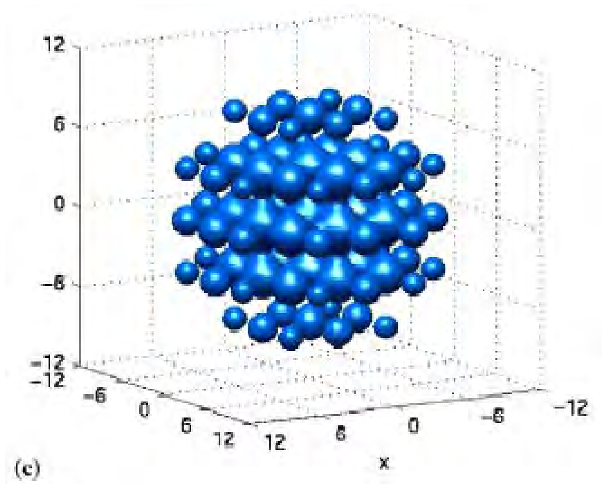
Outline

- 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



NLSE / GPE

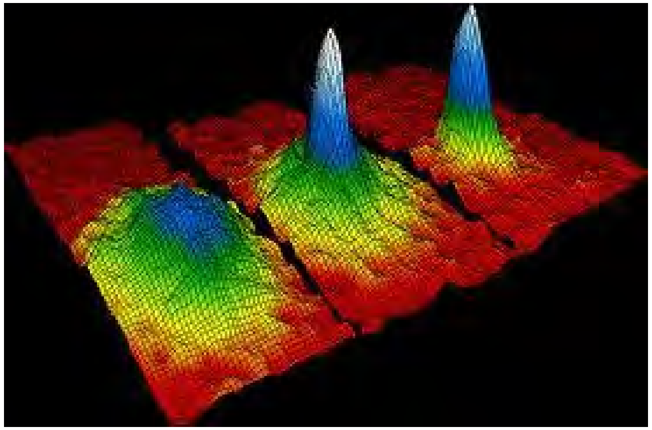
- The nonlinear Schrodinger equation (NLSE) ---1925

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

- 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 Nobel prize in physics
  - E. A. Cornell, W. Ketterle, C. E. Wieman



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

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

GPE 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

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

Laser beam propagation

- Nonlinear wave (or Maxwell) equations

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

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

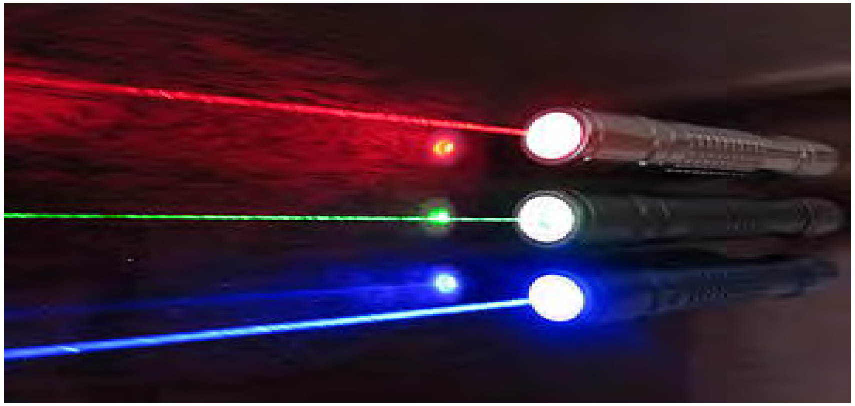
$$\Delta v(\vec{x})+k_0^2 n^2(|v|)v(\vec{x})=0, \quad \vec{x}\in\mathbb{R}^3; \quad k_0=\frac{\omega}{c_0}\gg 1, \quad n(|v|)=\frac{c_0}{c(|v|)}$$

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

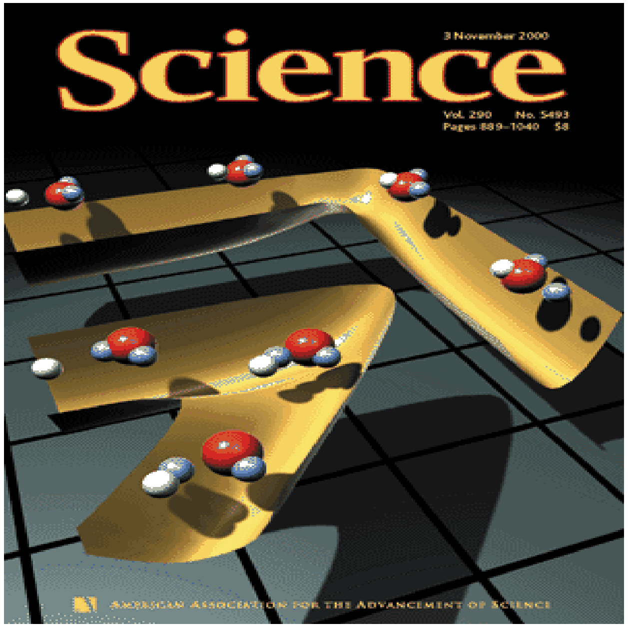
$$i\partial_t\psi(\vec{x},t)=-\frac{1}{2}\Delta\psi-|\psi|^2\psi-\delta\partial_{tt}\psi,\quad \vec{x}\in\mathbb{R}^2\quad \text{with}\quad \delta\ll 1$$

- 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

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

- 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

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

- 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

$$E(\phi_\varepsilon) \overset{\varepsilon \to 0}{\rightarrow} -\infty$$

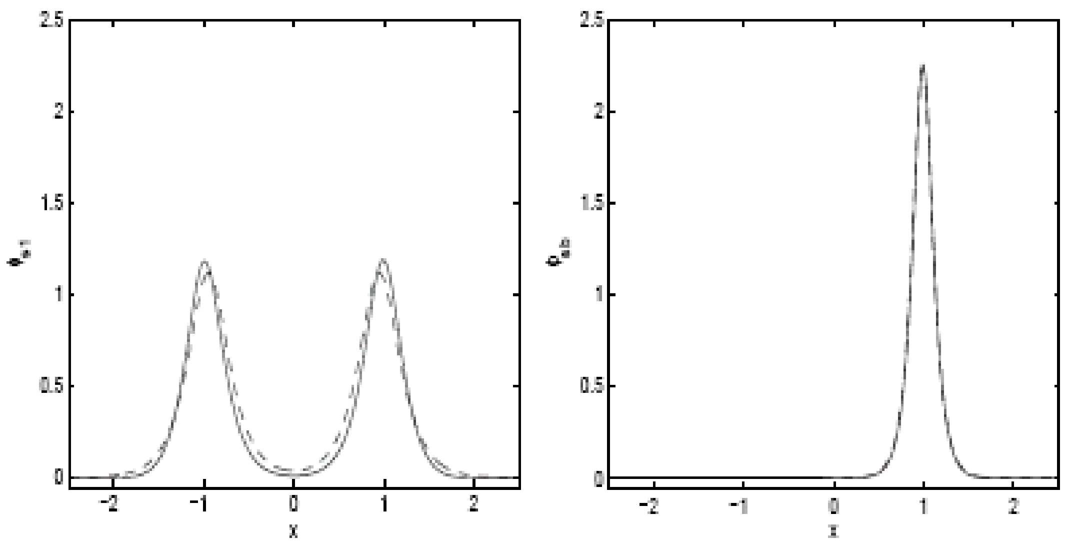
$$\phi_\varepsilon(\vec{x}) = \frac{1}{(2\pi\varepsilon)^{d/4}} \exp\left(-\frac{|\vec{x}|^2}{2\varepsilon} \right), \quad \vec{x} \in \mathbb{R}^d \quad \text{with} \quad \varepsilon \to 0$$

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 ?????

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

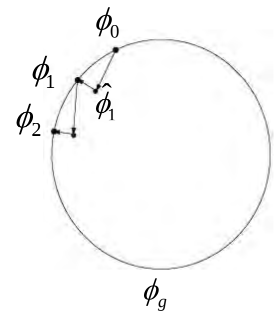
Computing ground states

- 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')

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

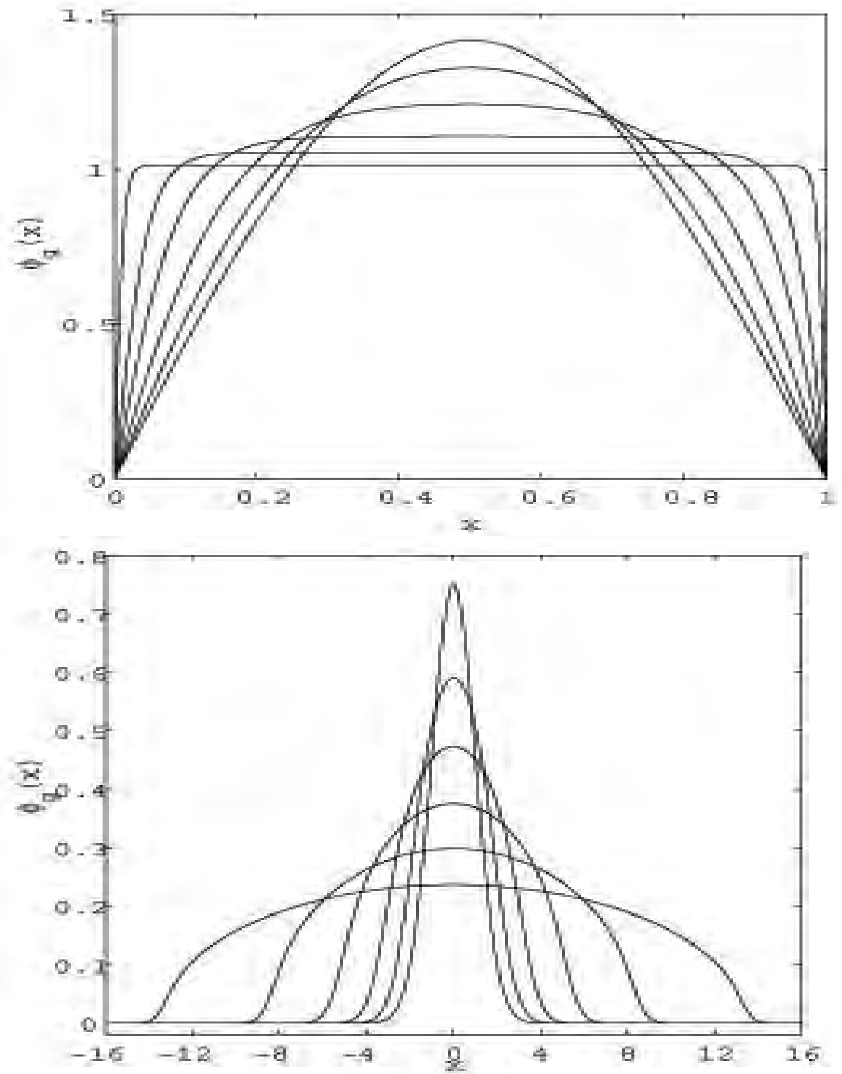
$$\phi(\vec{x},0) = \phi_0(\vec{x}) \qquad \text{with} \qquad \|\phi_0(\vec{x})\| = 1.$$

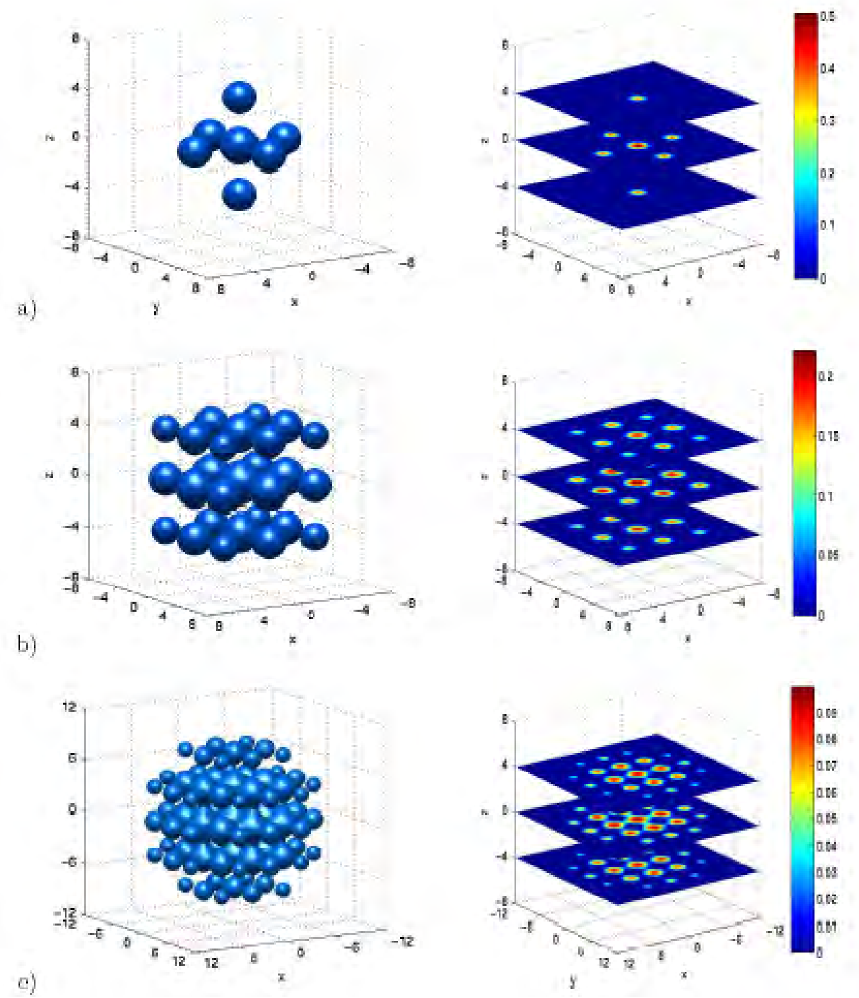
  - Mass conservation & energy diminishing

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

  - 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

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

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

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

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

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

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

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

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

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

Dynamics with no potential

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

- Momentum conservation $\vec{J}(t) := \mathrm{Im} \int_{\mathbb{R}^d} \bar{\psi} \, \nabla \psi \, d\vec{x} \equiv \vec{J}(0) \quad t \ge 0$
- 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

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

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

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

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

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

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

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

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

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

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

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

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

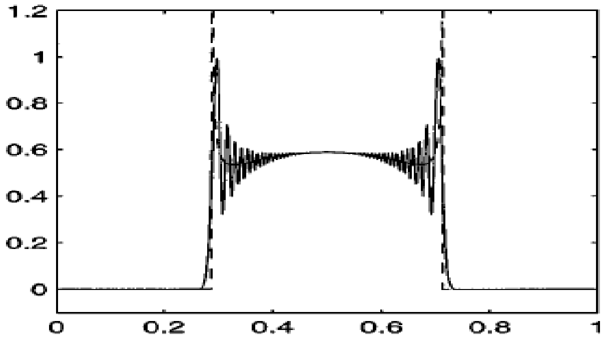
- Mathematical justification: G. B. Whitman, E. Madelung, E. Wigner, P.L. Lious, P. A. Markowich, F.-H. Lin, P. Degond, C. D. Levermore, D. W. McLaughlin, E. Grenier, F. Poupaud, C. Ringhofer, N. J. Mauser, P. Gerand, R. Carles, P. Zhang, P. Marcati, J. Jungel, C. Gardner, S. Kerranni, H.L. Li, C.-K.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

Numerical difficulties for dynamics

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

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

- 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

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

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

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

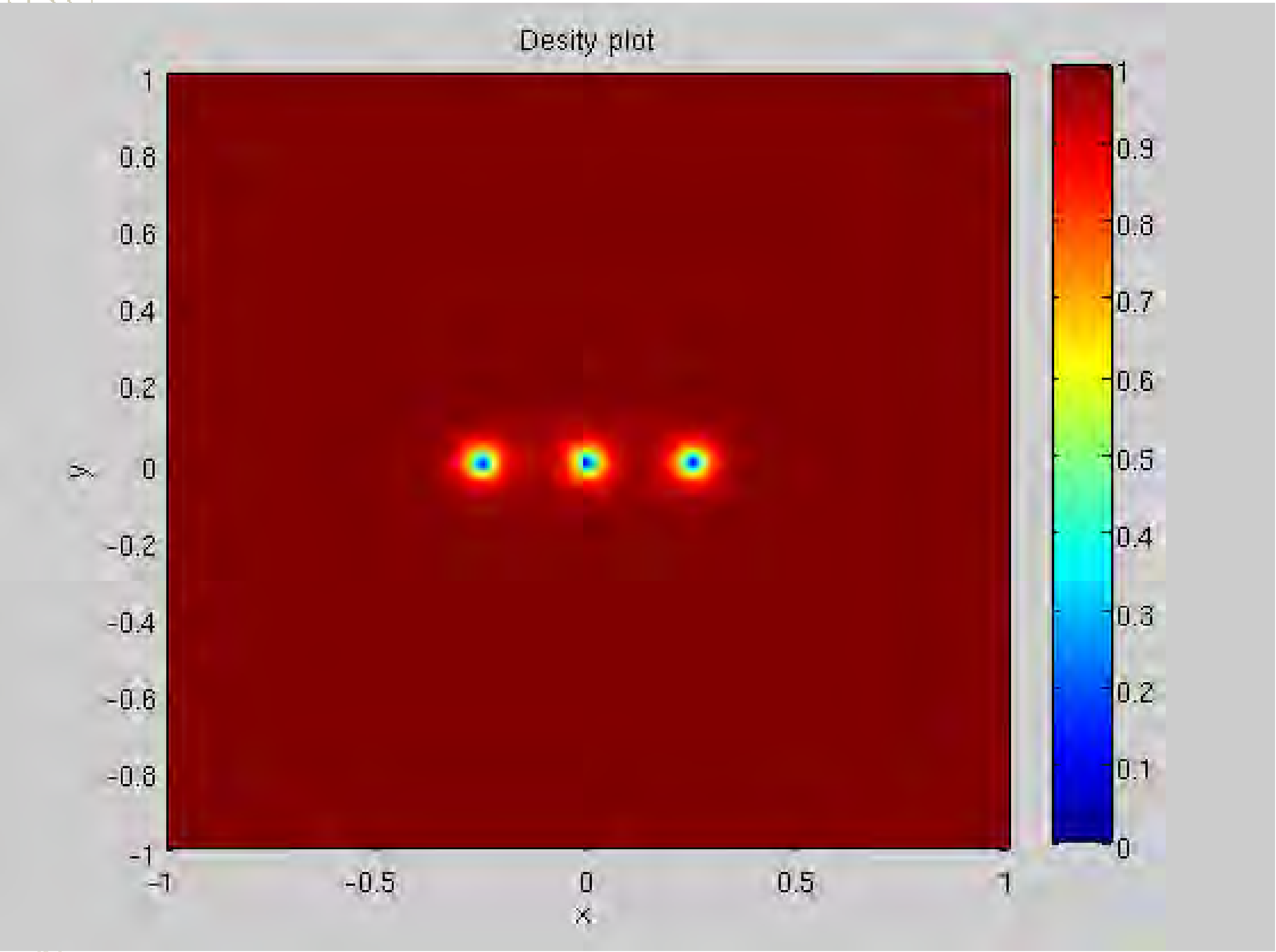
$$\Rightarrow \psi(\vec{x},t) = e^{-i\,(t-t_n)[V(x)+\beta|\psi(\vec{x},t_n)|^2]}\,\psi(\vec{x},t_n)$$

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

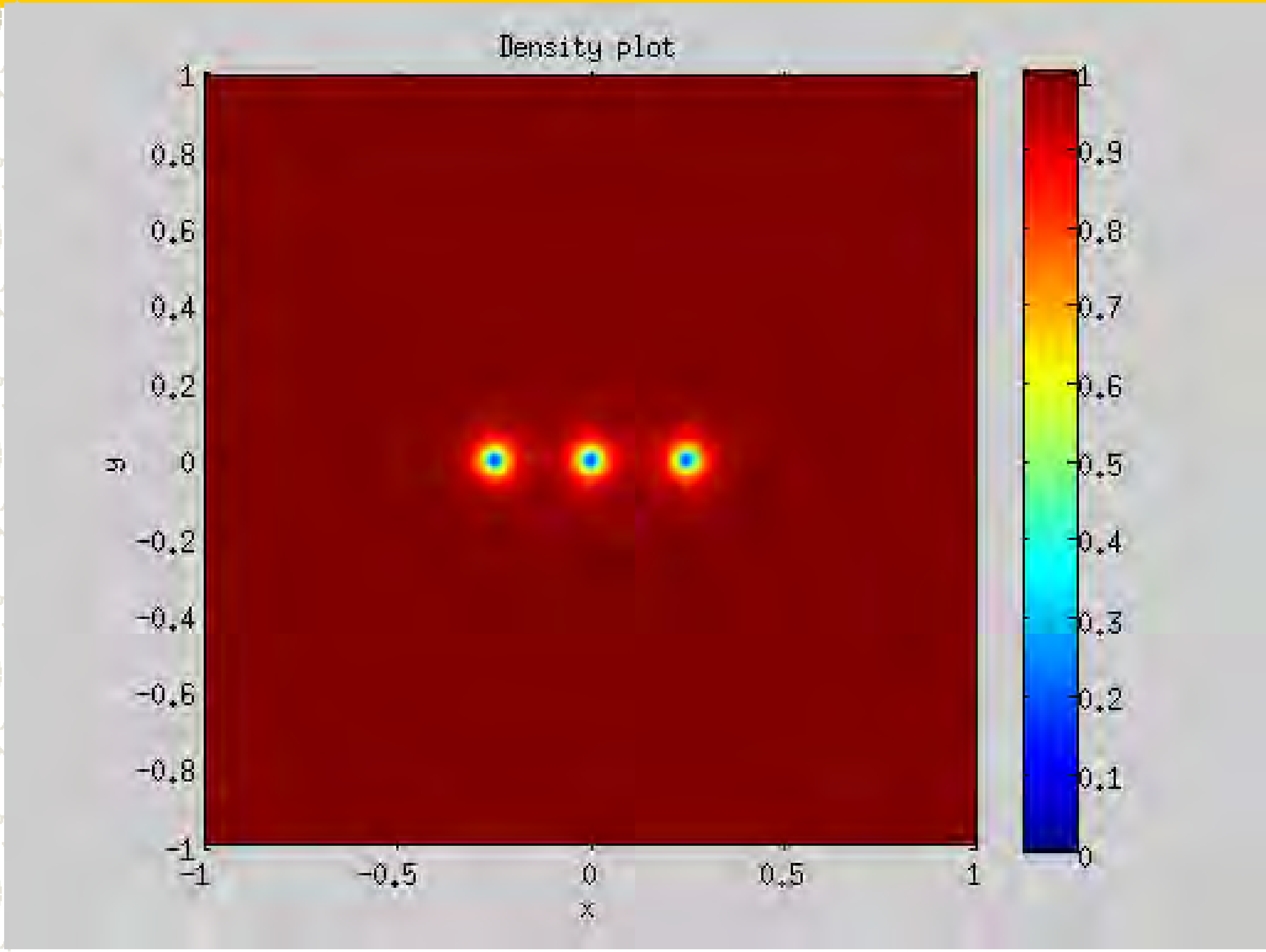
Properties of TSSP

- 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: $\beta \gg 1$

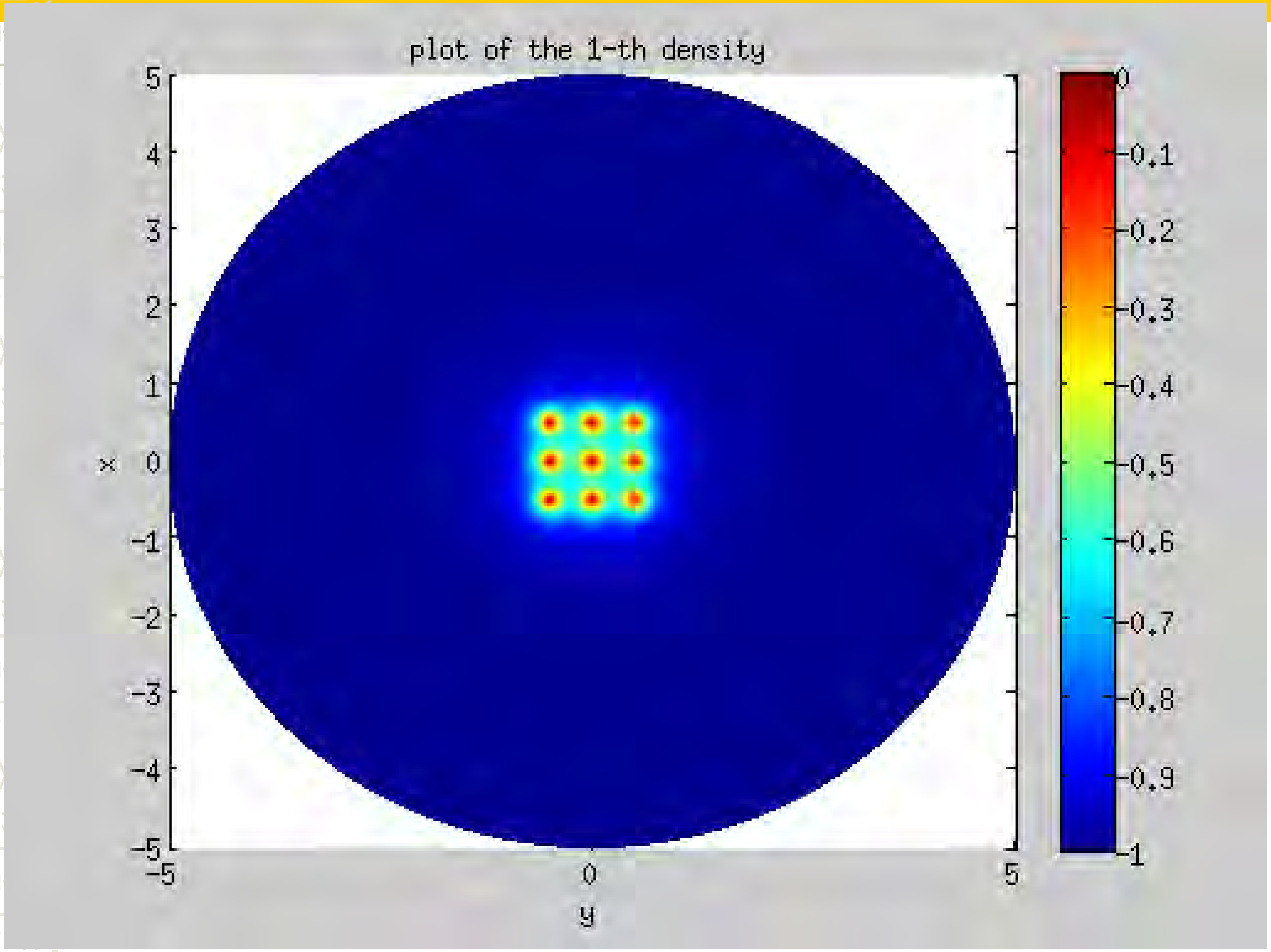
Interaction of 3 like vortices



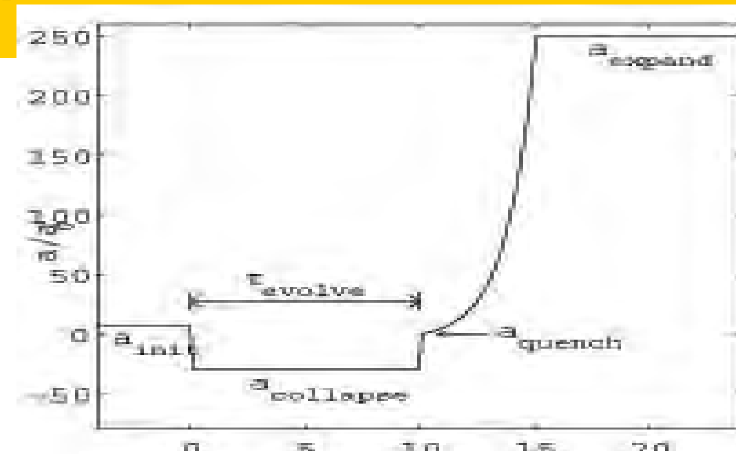
Interaction of 3 opposite vortices



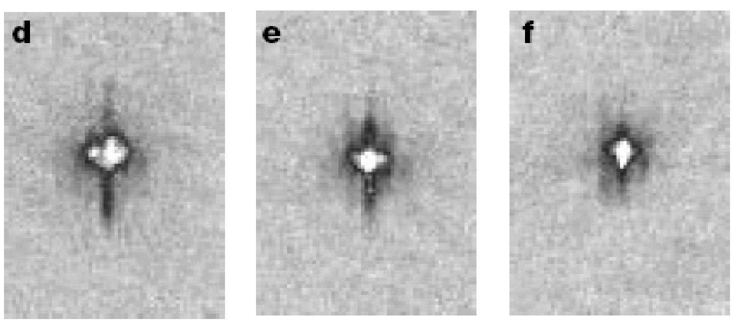
Interaction of a lattice

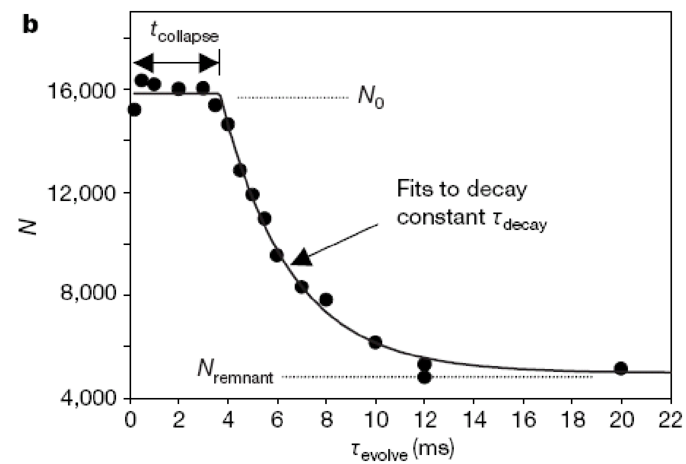


3D collapse & explosion of BEC



- 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



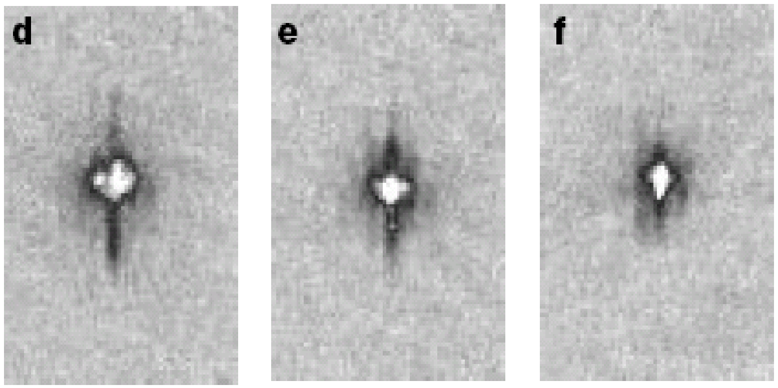


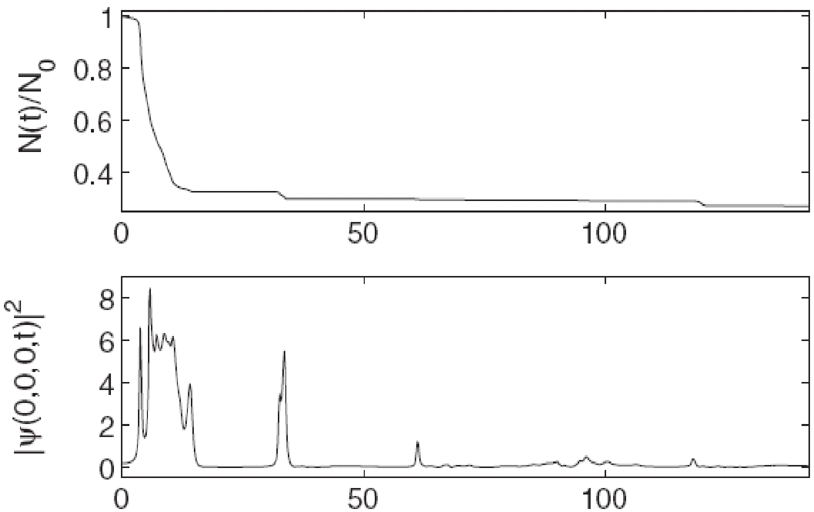
- Mathematical model (Duine & Stoof, PRL, 01')

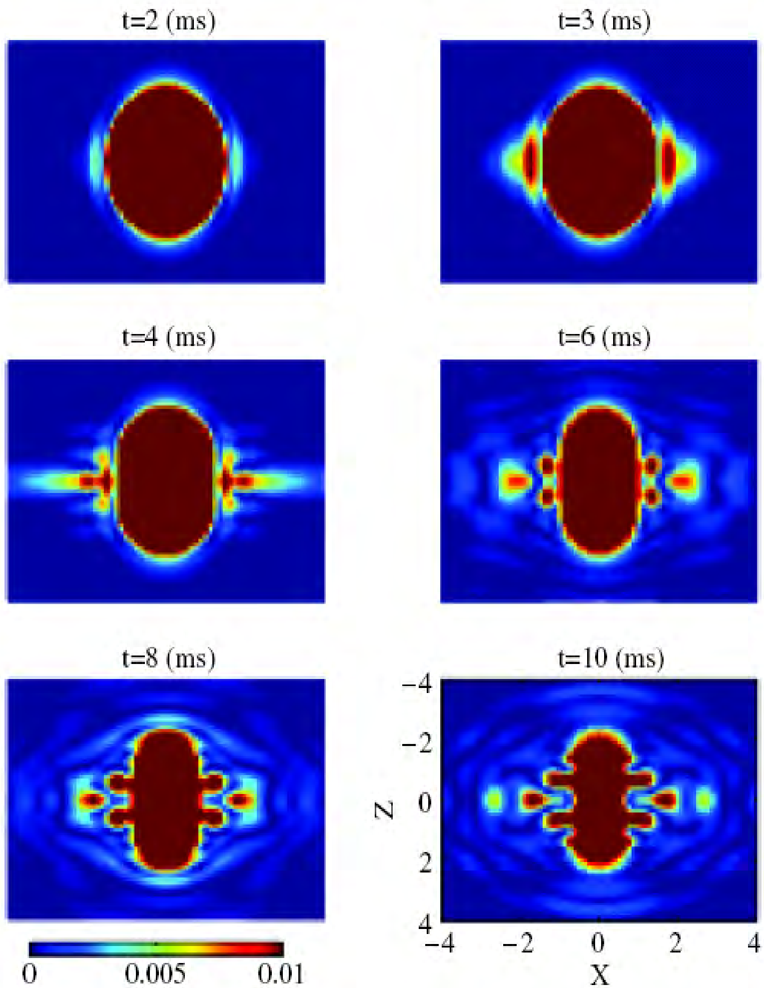
$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x})\psi + \beta|\psi|^2\psi - i\delta_0\beta^2|\psi|^4\psi$$

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

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

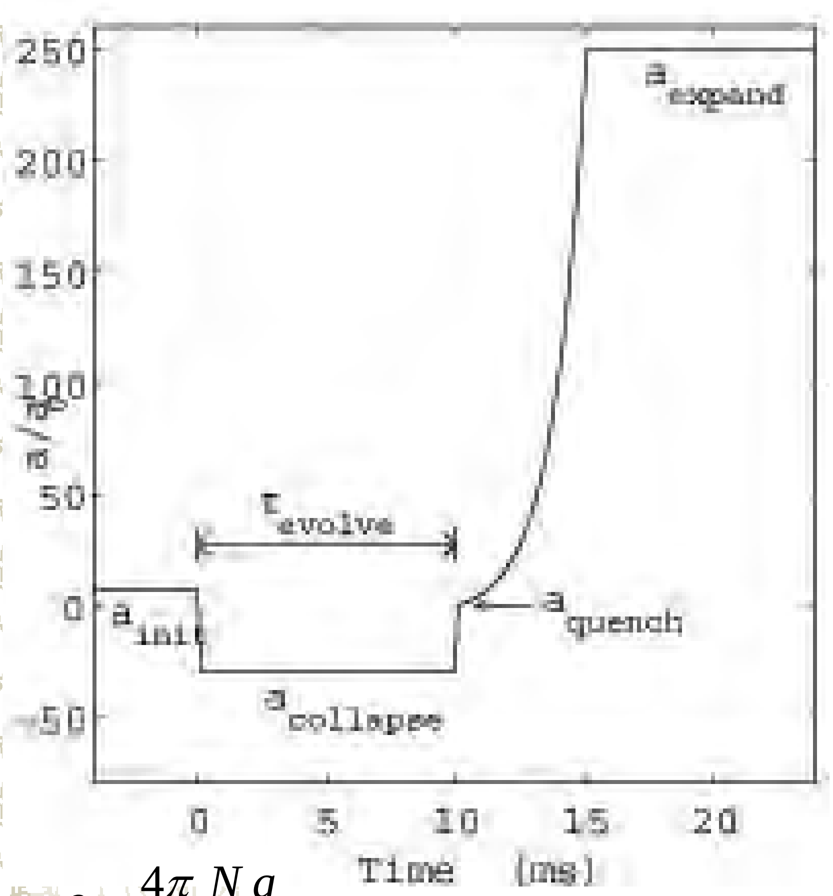


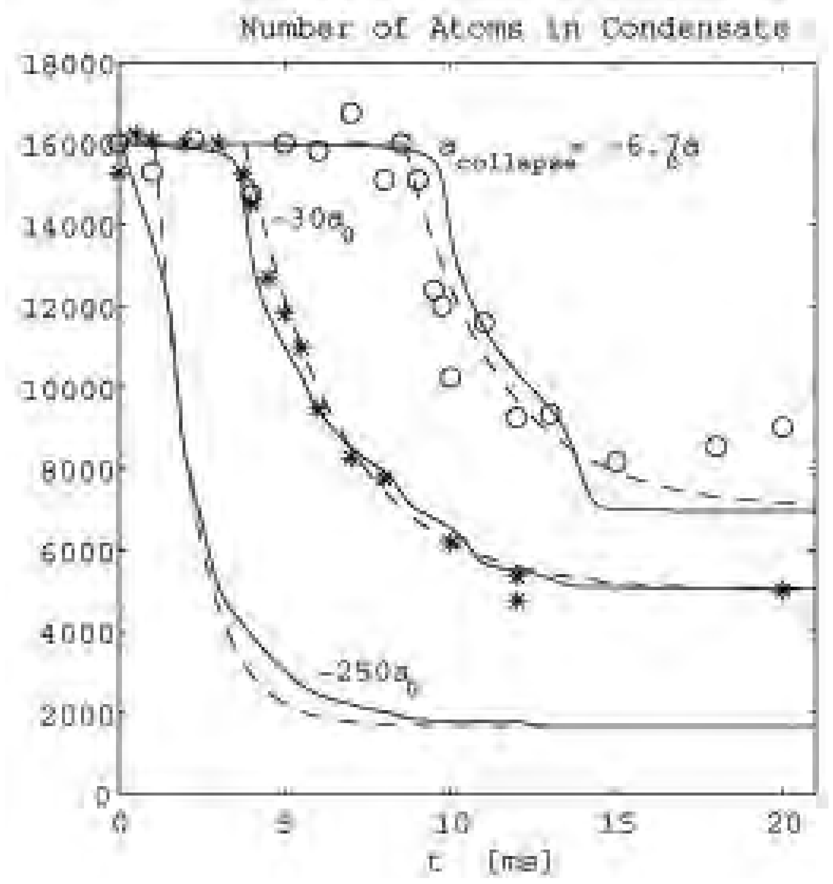




Jet formation

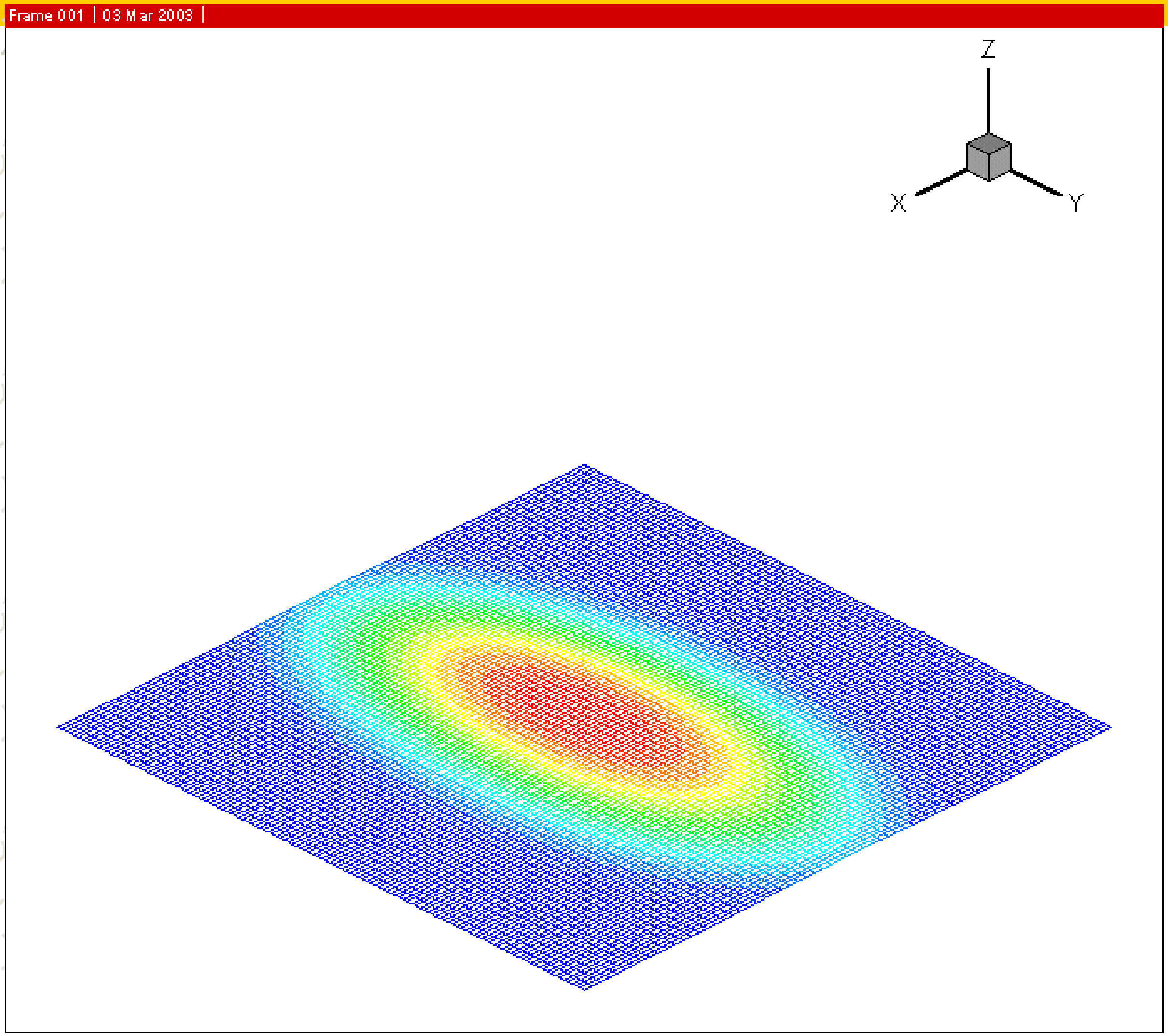
3D Collapse and explosion in BEC





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

3D Collapse and explosion in BEC



Extension to GPE with rotation

- GPE / NLSE with an angular momentum rotation

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

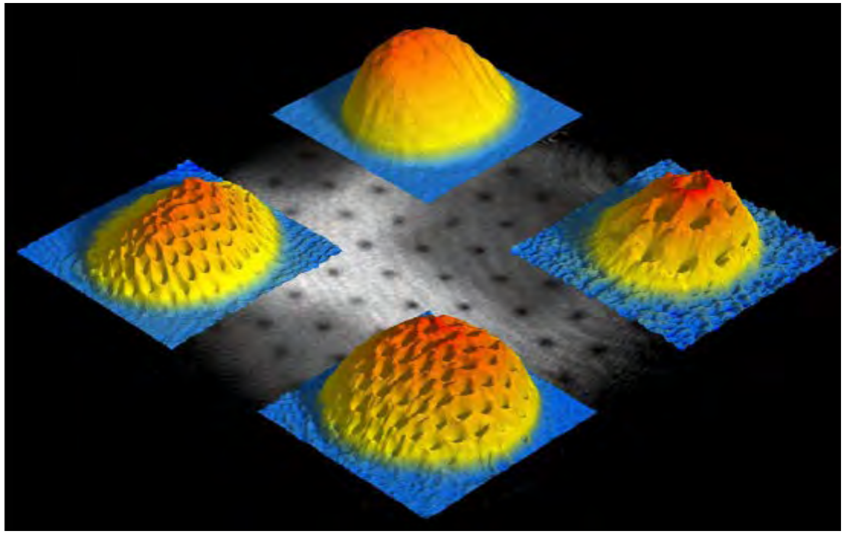
$$L_z := xp_y - yp_x = -i(x\partial_y - y\partial_x) \equiv -i\partial_\theta, \quad L = \vec{x}\times\vec{P}, \quad \vec{P} = -i\nabla$$

- Mass conservation

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

- Energy conservation

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

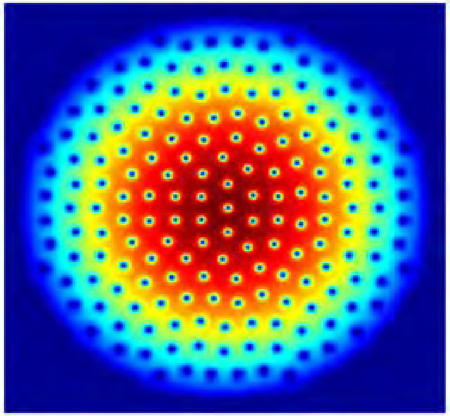


Vortex @MIT

Ground states

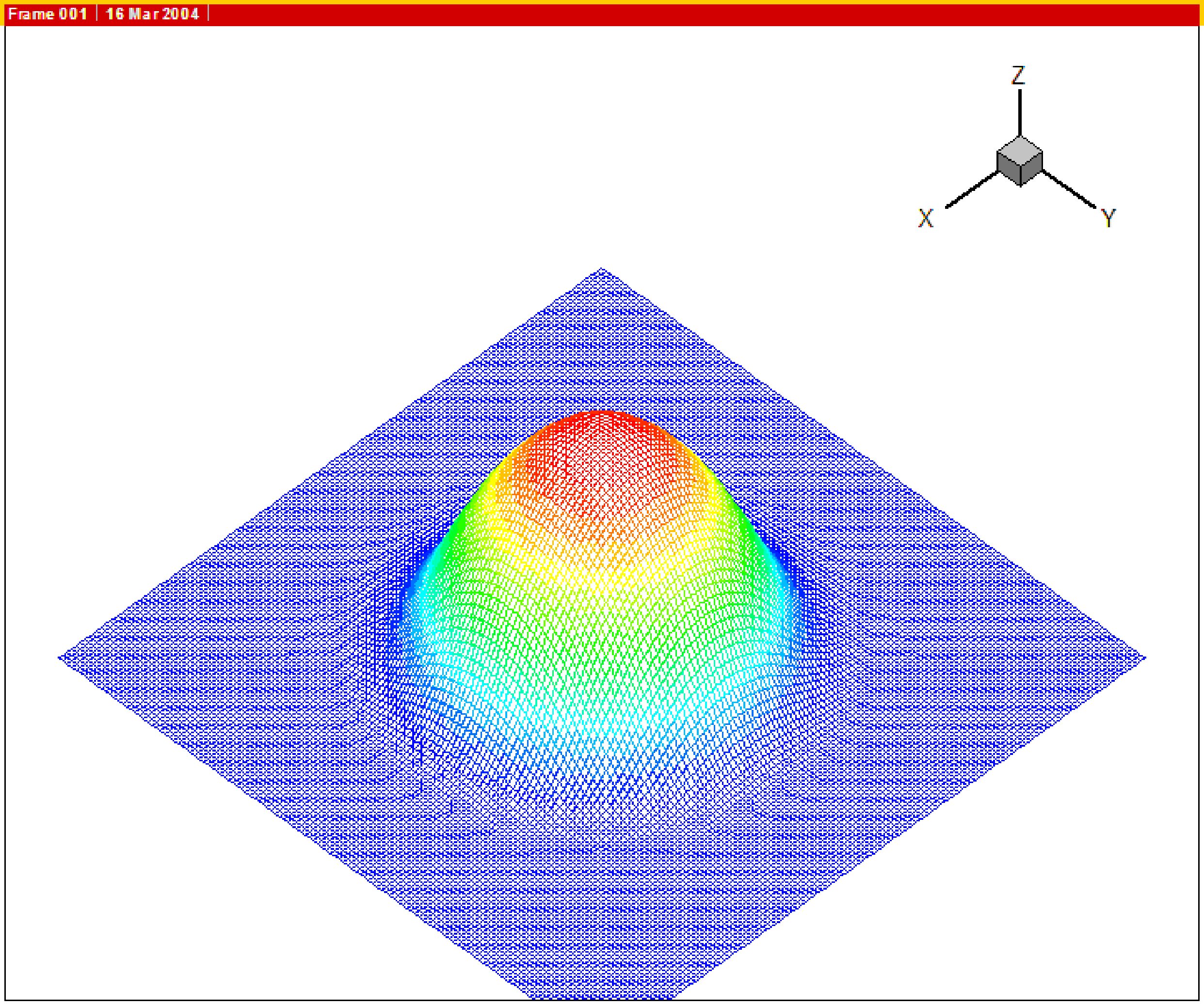
- Ground states – Seiringer, CMP, 02'; Bao,Wang & Markowich, CMS, 05'; …..

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

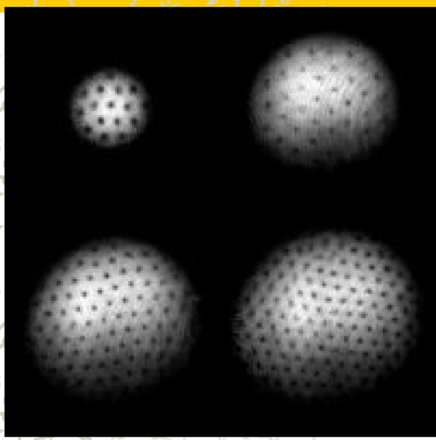


- Existence & uniqueness
  - Exists a ground state when $\beta \geq 0 \,\&\, |\Omega| \leq \min\{\gamma_x, \gamma_y\}$
  - Uniqueness when $|\Omega| < \Omega_c(\beta)$
  - Quantized vortices appear when $|\Omega| \geq \Omega_c(\beta)$
  - Phase transition & bifurcation in energy diagram
- Numerical methods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

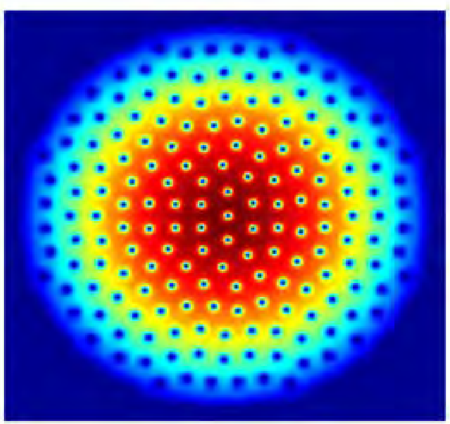
Ground states with different Ω

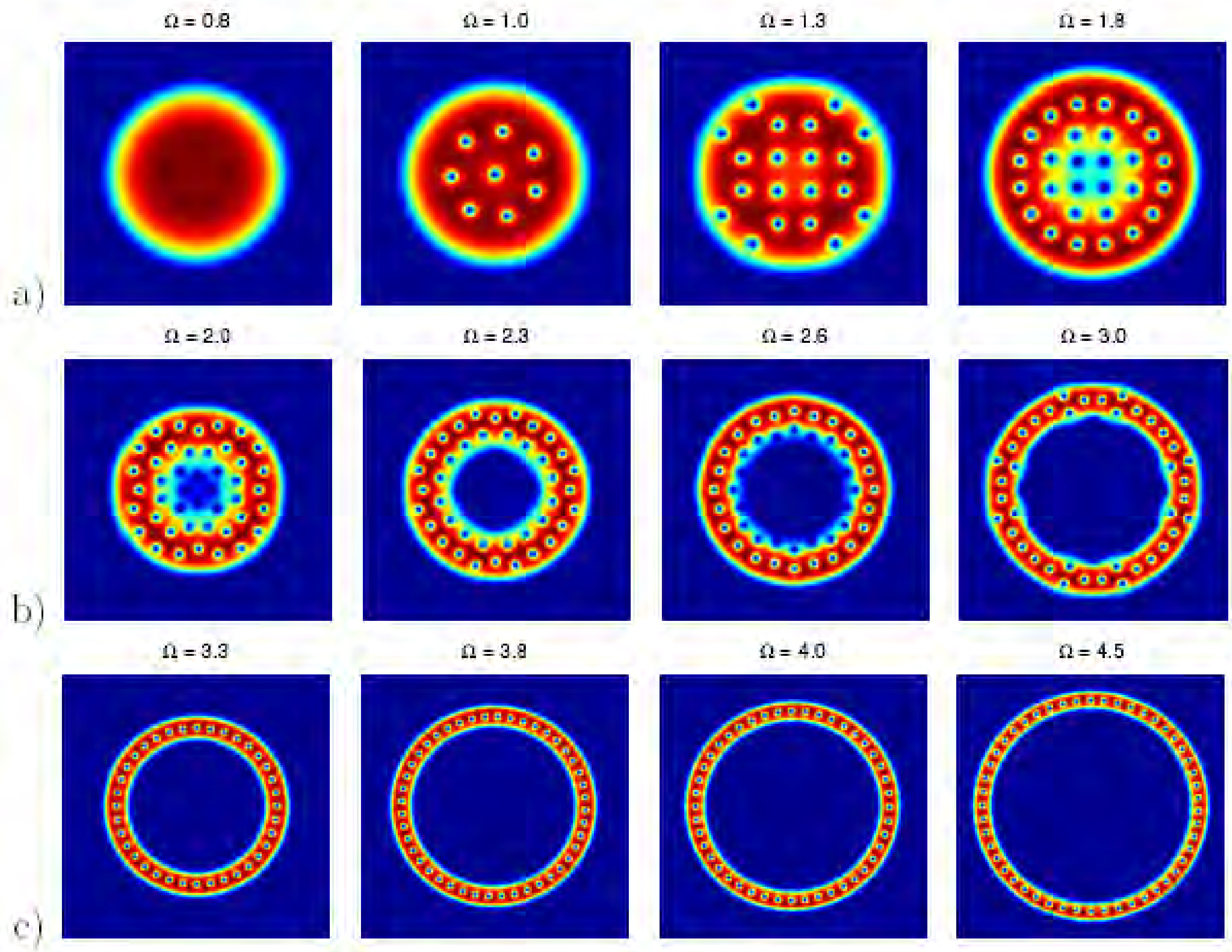


Ground states of rapid rotation



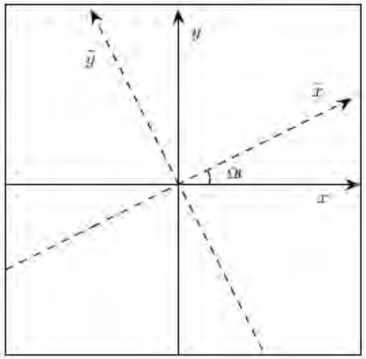
BEC@MIT





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

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



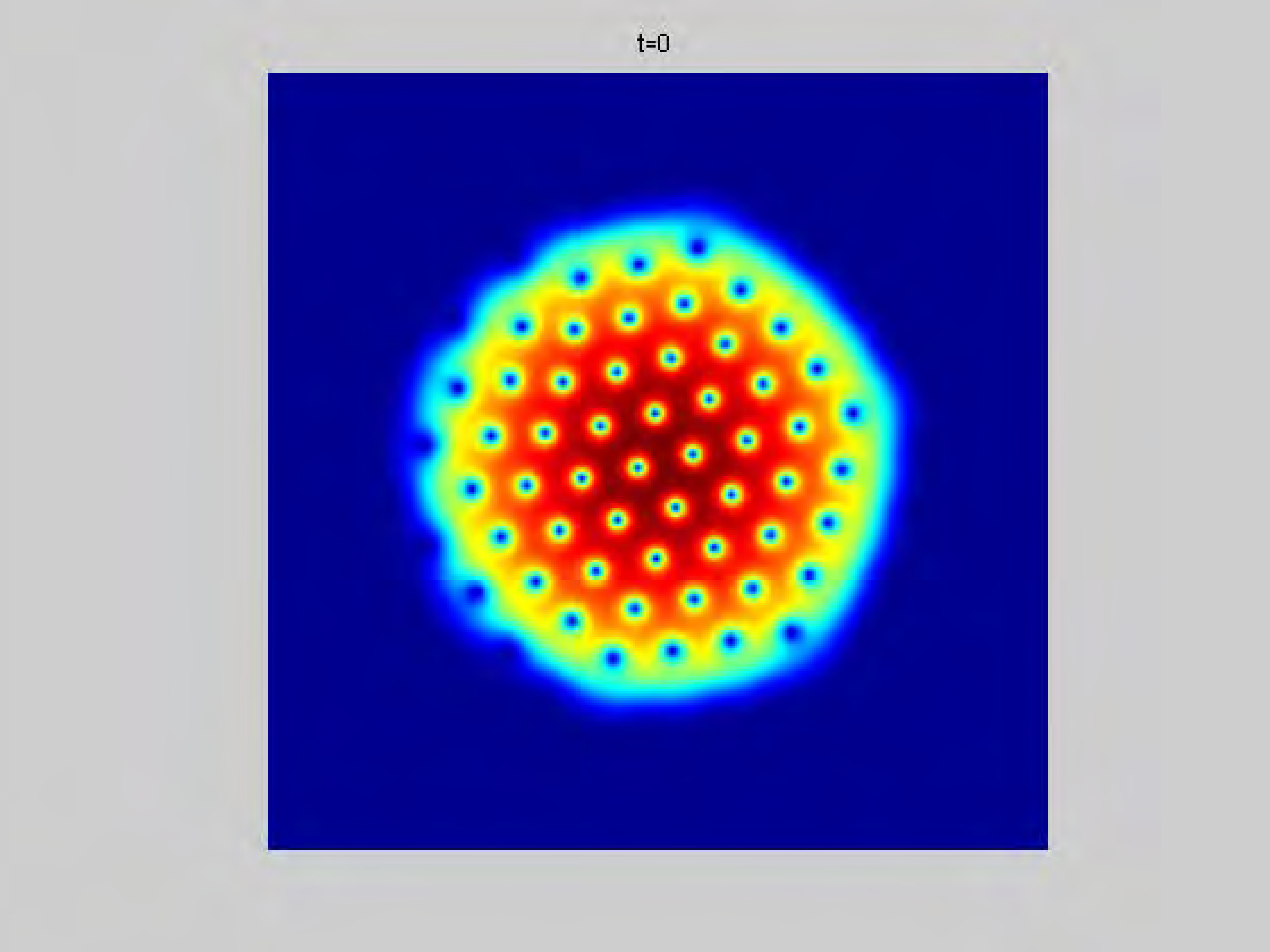
$$A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) \\ -\sin(\Omega t) & \cos(\Omega t) \end{bmatrix} \quad \text{for } d = 2; \quad A(t) = \begin{bmatrix} \cos(\Omega t) & \sin(\Omega t) & 0 \\ -\sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{for } d = 3$$

  - GPE in rotating Lagrange coordinates

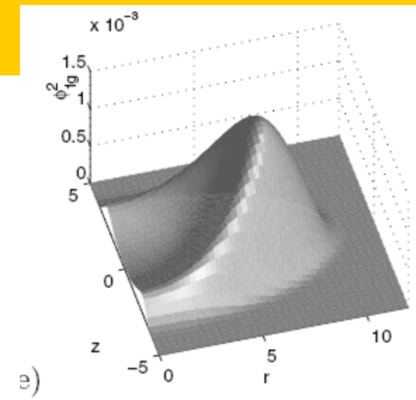
$$i\,\partial_t\,\phi(\tilde{\vec{x}},t) = [-\frac{1}{2}\nabla^2 + V(A(t)\tilde{\vec{x}}) + \beta\,|\phi|^2]\,\phi, \quad \tilde{\vec{x}} \in \mathbb{R}^d, \quad t > 0$$

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

Dynamics of a vortex lattice



Extension to two-component



- Two-component (Bao, MMS, 04')

$$i\partial_t \psi_1(\vec{x},t) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2]\psi_1$$

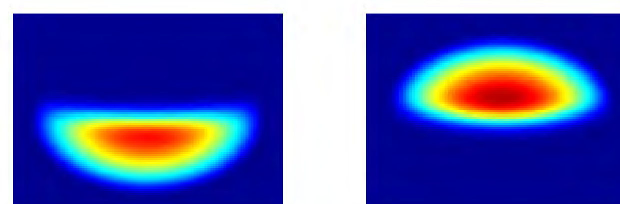
$$i\partial_t \psi_2(\vec{x},t) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2]\psi_2$$

$$\|\psi_1\|^2 = \int_{\Re^d} |\psi_1(\vec{x},t)|^2 \, d\vec{x} = \alpha, \quad \|\psi_2\|^2 = \int_{\Re^d} |\psi_2(\vec{x},t)|^2 \, d\vec{x} = 1-\alpha \qquad 0 \le \alpha \le 1$$

- Ground state

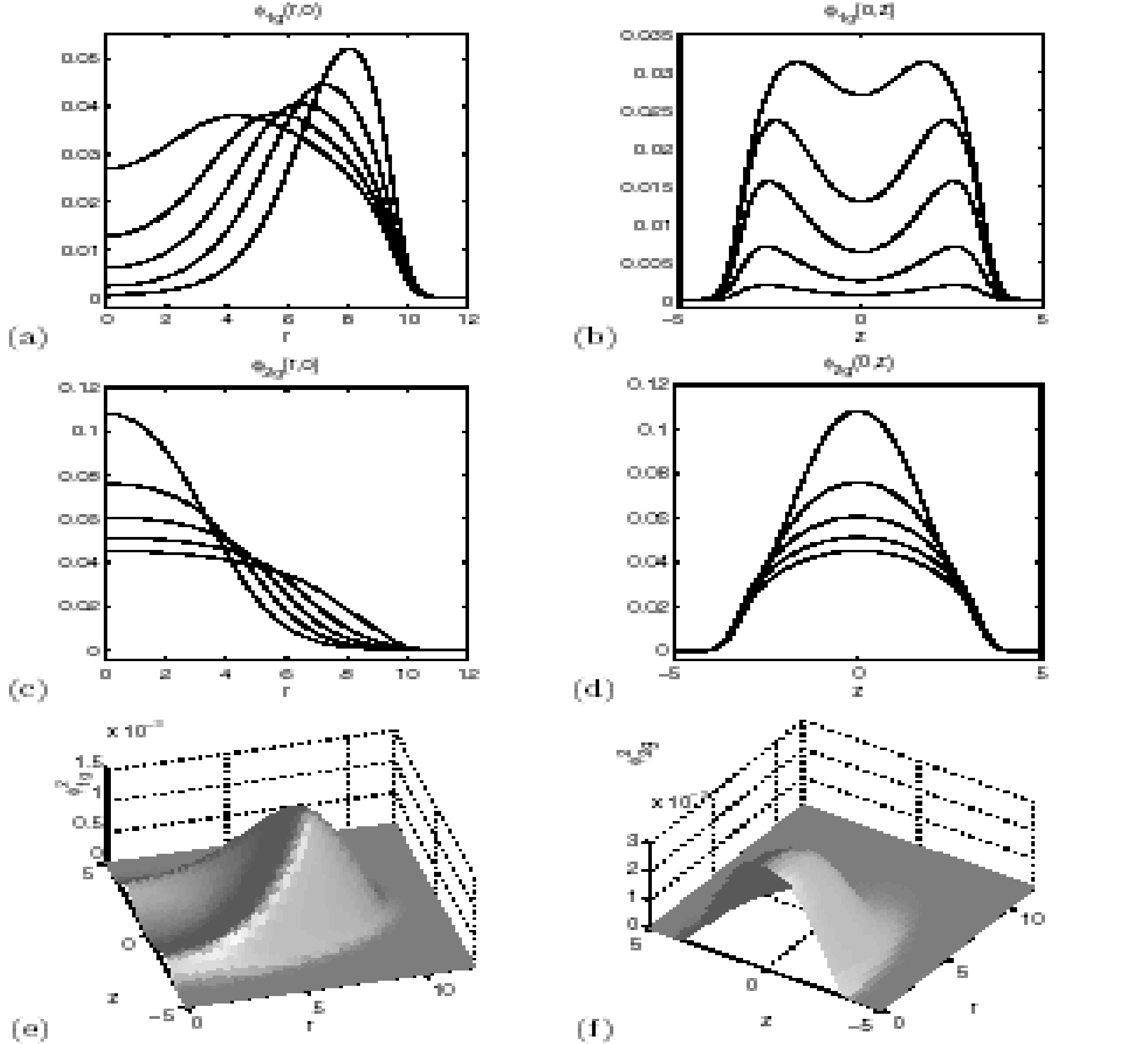
$$E_g := E(\Phi_g) = \min_{\Phi \in S_\alpha} E(\Phi), \qquad S_\alpha = \{\Phi = (\phi_1,\phi_2) \,|\, \|\phi_1\| = \alpha, \|\phi_2\| = 1-\alpha, E(\Phi) < \infty\}$$

  - Existence & uniqueness
  - Quantized vortices & fractional index
  - Numerical methods & results: Crarter & domain



Results

- Theorem (Bao&Cai, EAJAM, 10')
  - Assumptions
    - No rotation $\Omega = 0$ & Confining potential $\lim_{|\vec{x}|\to\infty} V(\vec{x}) = \infty$
    - Repulsive interaction $\beta_{11}, \beta_{12}, \beta_{22} \geq 0$ or $\beta_{11} \geq 0 \,\&\, \beta_{11}\beta_{22} - \beta_{12}^2 \geq 0$
  - Results
    - Existence & Positive minimizer is unique
  - No minimizer in 3D when $\beta_{11} < 0$ or $\beta_{22} < 0$
- Nonuniquness in attractive interaction in 1D
- Quantum phase transition in rotating frame



(a)
r
(b)
z
(c)
r
(d)
z
(e)
r
z
(f)
r
z

Two-component with an external driving field

- Two-component (Bao & Cai, EAJAM 10')

$$i\partial_t \psi_1(\vec{x},t) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2]\psi_1 + \lambda\psi_2$$

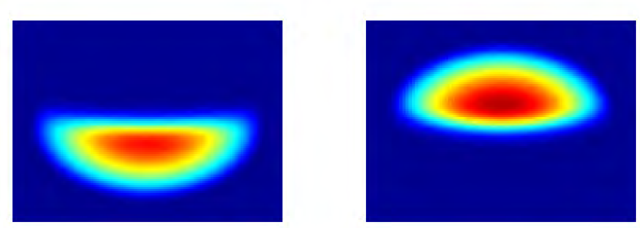
$$i\partial_t \psi_2(\vec{x},t) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2]\psi_2 + \lambda\psi_1$$

$$\|\psi_1\|^2 + \|\psi_2\|^2 = \int_{\Re^d} [|\psi_1(\vec{x},t)|^2 + |\psi_2(\vec{x},t)|^2] d\vec{x} = 1$$

- Ground state

$$E_g := E(\Phi_g) = \min_{\Phi\in S} E(\Phi), \qquad S = \{\Phi = (\phi_1,\phi_2) \mid \|\Phi\| = 1, E(\Phi) < \infty\}$$

  - Existence & uniqueness (Bao & Cai, EAJAM 09')
  - Limiting behavior & Numerical methods
  - Numerical results: Crarter & domain wall



Theorem (Bao & Cai, EAJAM 10')

- No rotation & confining potential &

  $$\beta_{11}, \beta_{12}, \beta_{22} \geq 0 \quad \text{or} \quad \beta_{11} \geq 0 \;\&\; \beta_{11}\beta_{22} - \beta_{12}^2 \geq 0$$

- Existence of ground state!!
- Uniqueness in the form $\Phi_g = (|\phi_1^g|, -\text{sign}(\lambda)|\phi_2^g|)$ under

  $$\beta_{11} > 0 \;\&\; \beta_{11}\beta_{22} - \beta_{12}^2 > 0 \quad \text{or} \quad \beta_{12} > \beta_{11} = \beta_{22} \;\&\; \delta \neq 0$$

- At least two different ground states under– quantum phase transition

  $$\delta = 0 \;\&\; \beta_{12} > \beta_{11} = \beta_{22} \geq 0 \;\&\; \lambda \in (-\Lambda_0, \Lambda_0) \quad \text{for} \quad \Lambda_0 > 0$$

- Limiting behavior

  $$|\lambda| \to +\infty \quad \Rightarrow \quad |\phi_1^g| \;\&\; |\phi_2^g| \to \varphi^g$$

  $$\delta \to +\infty \quad \Rightarrow \quad |\phi_1^g| \to 0 \quad \& \quad |\phi_2^g| \to \phi^g$$

  $$\delta \to -\infty \quad \Rightarrow \quad |\phi_1^g| \to \phi^g \quad \& \quad |\phi_2^g| \to 0$$

Spin-orbit-coupled BEC (Nature, 471 (2011),83-86)

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

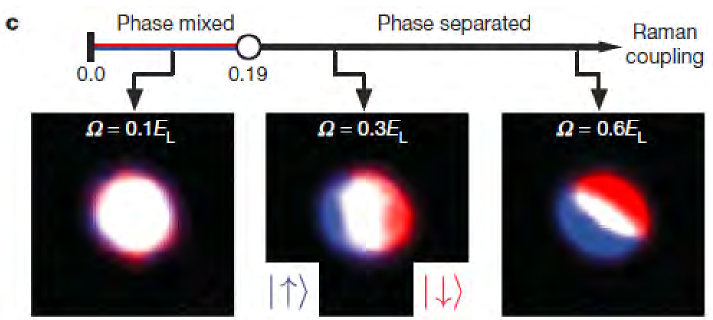
$$i\partial_t\psi_2(\vec{x},t)=[-\frac{1}{2}\nabla^2+V(\vec{x})-ik_0\partial_x-\delta+\beta_{21}|\psi_1|^2+\beta_{22}|\psi_2|^2]\psi_2+\lambda\psi_1$$

$$\|\psi_1\|^2+\|\psi_2\|^2=\int_{\mathfrak{R}^d}[|\psi_1(\vec{x},t)|^2+|\psi_2(\vec{x},t)|^2]d\vec{x}=1$$

- Ground state

$$E_g := E(\Phi_g)=\min_{\Phi\in S}E(\Phi), \qquad S=\left\{\Phi=(\phi_1,\phi_2)\,|\,\|\Phi\|=1, E(\Phi)<\infty\right\}$$

  - Existence & uniqueness
  - Limiting behavior & Numerical methods
  - Numerical results: symmetry breaking



Coupled GPEs

- Spinor F=1 BEC

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

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

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

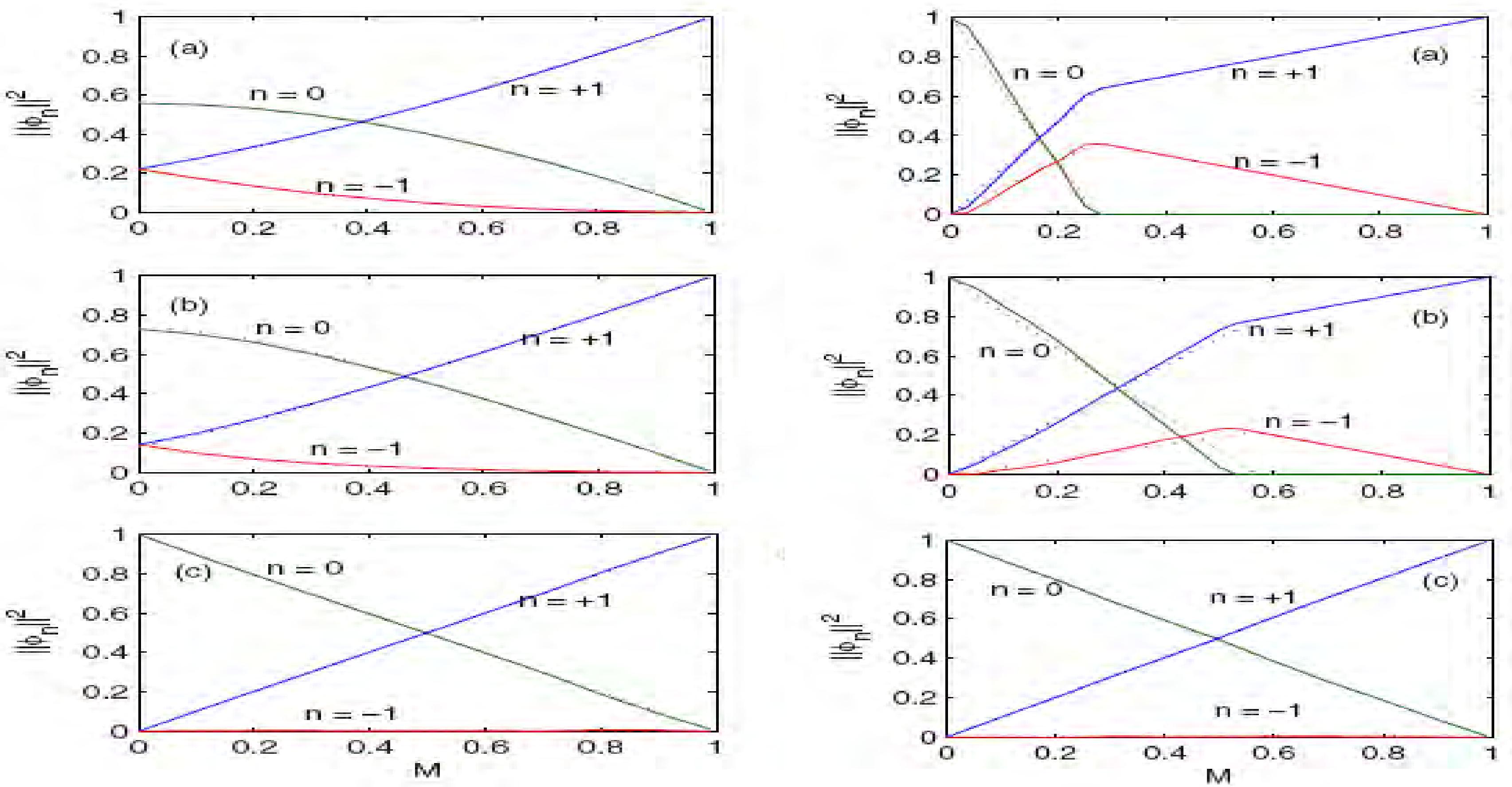
- With

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

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')

Quantum phase transition



Ferromagnetic $g_s < 0$

Antiferromagnetic $g_s > 0$

Extension to dipolar quantum gas

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

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

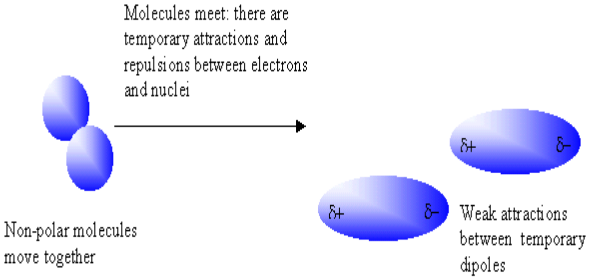
  – Trap potential $V(\vec{x}) = \frac{1}{2}\left(\gamma_x^2\,x^2 + \gamma_y^2\,y^2 + \gamma_z^2\,z^2\right)$

  – 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')

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

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

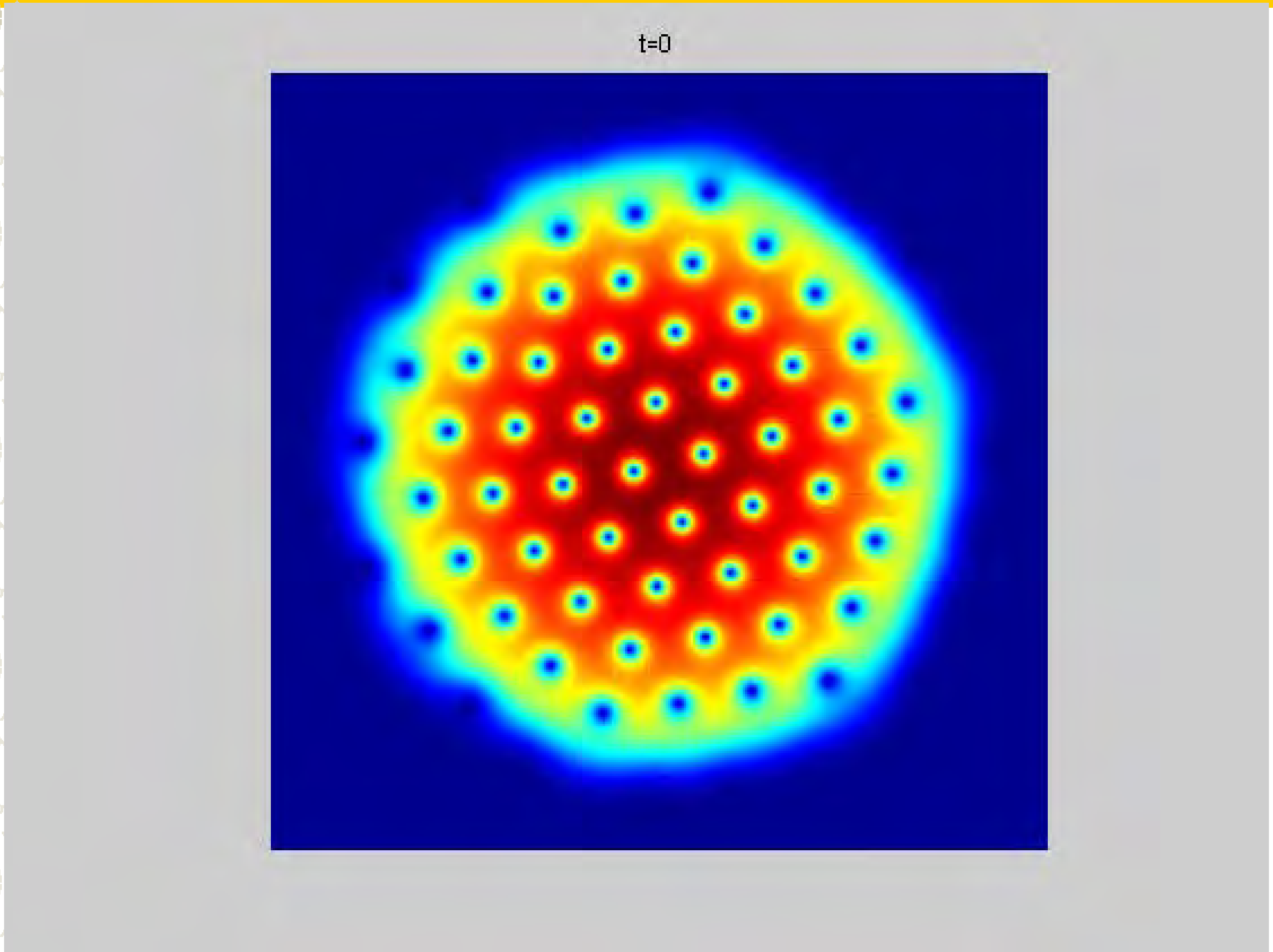
  - Energy

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

  - 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' $\beta\ge 0\ \&\ -\frac{\beta}{2}\le\lambda\le\beta$
- Dimension reduction – Cai, Rosenkranz, Lei & Bao, PRA, 10'; Bao & Cai, KRM, 13'

Dynamics of a vortex lattice



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)

New numerical methods for DDI

- How to compute nonlocal DDI $\quad \phi := U_{\text{dip}} * |\psi|^2$
  - FFT (fast Fourier transform) $\quad \widehat{U}_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2}$
  - DST (discrete sine transform)

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

  - Nonuniform FFT

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

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

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