Analysis & Computation for Ground States of Degenerate Quantum Gas

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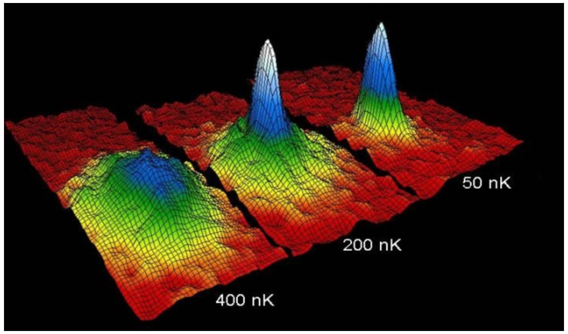
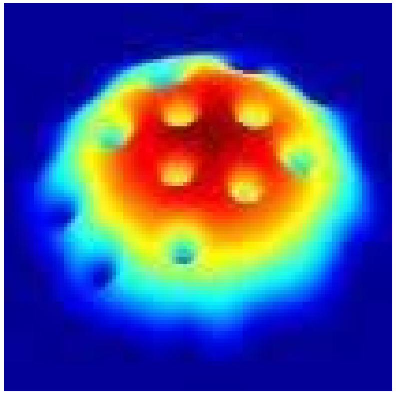
Outline

- Motivation and models –GPE/NLSE
- Ground states -- Mathematical theory
  - Existence, uniqueness & non-existence
- Numerical methods and results
  - Normalized gradient flow method
  - Regularized Newton method
- Extension to
  - Rotation frame, nonlocal interaction & system
- Conclusions

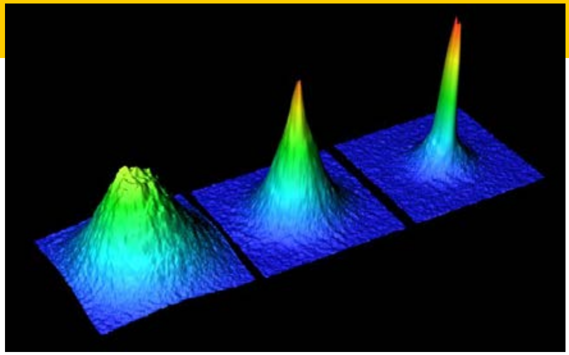


BEC@JILA, 95'

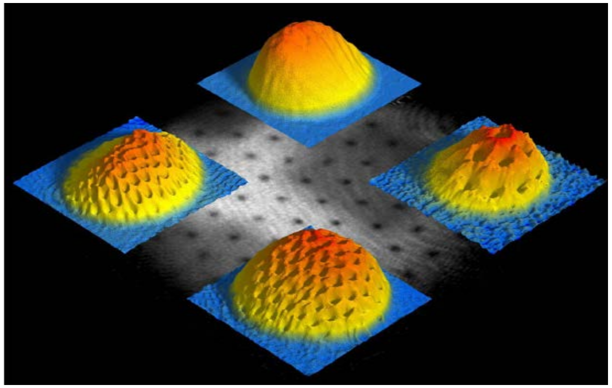


Vortex @ENS

Degenerate Quantum Gas



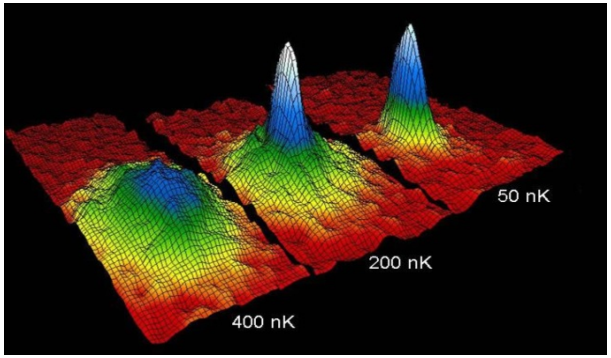
- Typical degenerate quantum gas
  - Liquid Helium 3 & 4
  - Bose-Einstein condensation (BEC)
    - Boson vs Fermion condensation
    - One component, two-component & spin-1
    - Dipolar, spin-orbit, ….



- Typical properties
  - Low (mK) or ultracold (nK) temperature
  - Quantum phase transition & closely related to nonlinear wave
  - Superfluids – flow without friction & quantized vortices

Model for Degenerate Quantum Gas (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 – A. Einstein, 1924' (using S. Bose statistics)
- Experimental realization – JILA 1995'
- 2001 Nobel prize in physics
  - E. A. Cornell, W. Ketterle, C. E. Wieman



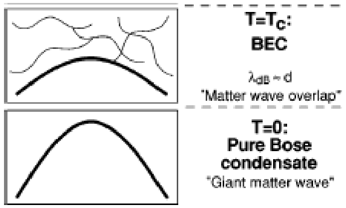
GPE for a BEC – with N identical bosons

- 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



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

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

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

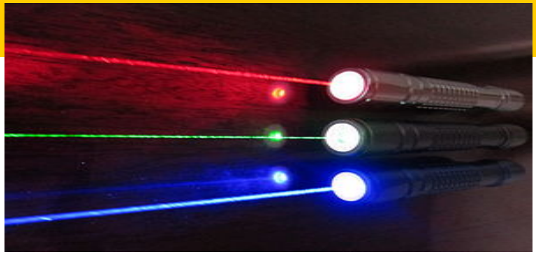
NLSE / GPE

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

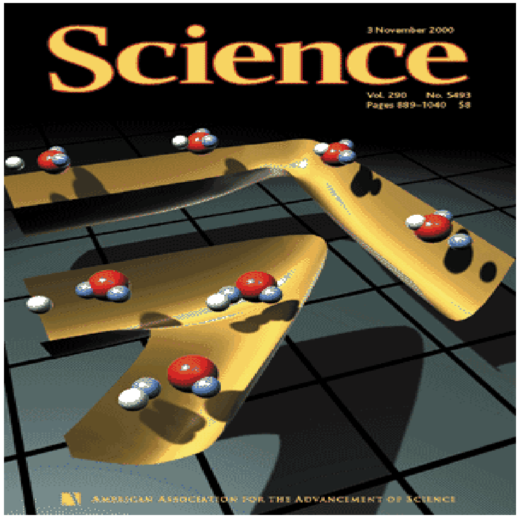
$$i\,\partial_t \psi(\vec{x},t) = -\frac{1}{2}\nabla^2\psi + V(\vec{x})\psi + \beta\,|\psi|^2\,\psi$$

- t : time & $\vec{x}\ (\in \mathbb{R}^d)$: spatial coordinate (d=3,2,1)
- $\psi(\vec{x},t)$: 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'

Other applications



- In nonlinear (quantum) optics
- 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 – electron structure computation
  - First principle computation
  - Semiconductor industry
- 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
- Mass conservation

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

- Energy conservation

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

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)

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

- 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 -- constrained minimization problem -- nonconvex

$$\phi_g = \arg\min_{\phi\in S} E(\phi) \qquad S = \left\{\phi \mid \|\phi\|^2 = \int_{\mathbb{R}^d} |\phi(\vec{x})|^2 \, d\vec{x} = 1, \quad E(\phi) < \infty\right\}$$

  – Euler-Lagrange equation (or first-order optimality condition)

→ nonlinear eigenvalue problem with a constraint

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

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

Different numerical methods

- Methods via nonlinear eigenvalue problems
  – Runge-Kutta method: M. Edwards and K. Burnett, Phys. Rev. A, 95', …
  – Analytical expansion: R. Dodd, J. Res. Natl. Inst. Stan., 96',…
  – Gauss-Seidel iteration method: W.W. Lin et al., JCP, 05', …
  – Continuation method: Chang, Chien & Jeng, JCP, 07'; ……
- Methods via constrained minimization problem
  – Explicit imaginary time method: S. Succi, M.P. Tosi et. al., PRE, 00'; Aftalion & Du, PRA, 01',
  – FEM discretization+ nonlinear solver: Bao & Tang, JCP, 03', …
  – Normalized gradient flow via BEFD Bao&Du, SIAM Sci. Comput., 03'; Bao, Chern& Lim, JCP, 06,...
  – Sobolev gradient method : Garcia-Ripoll,& Perez-Garcia, SISC, 01'; Danaila & Kazemi, SISC, 10'
  – Regularized Newton method via trust-region strategy: Xu, Wen & Bao, 15', …

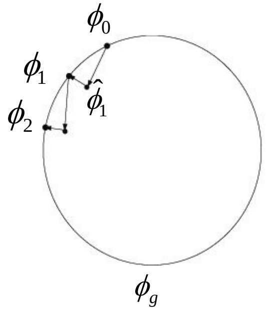
Computing ground states

- Idea: Steepest decent method + Projection – normalized gradient flow

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

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

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



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

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

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

- 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 flow

- 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')
    - GPRLab – Antoine & Duboscq, CPC, 14'

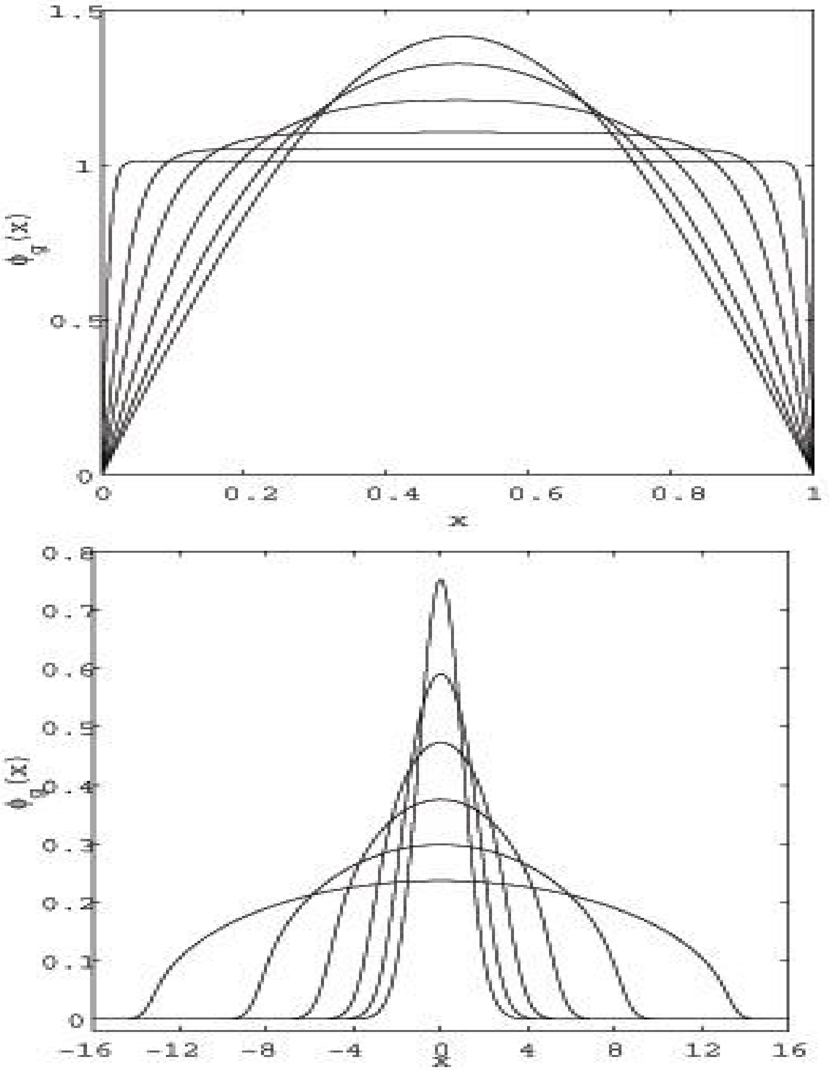
Regularized Newton Method

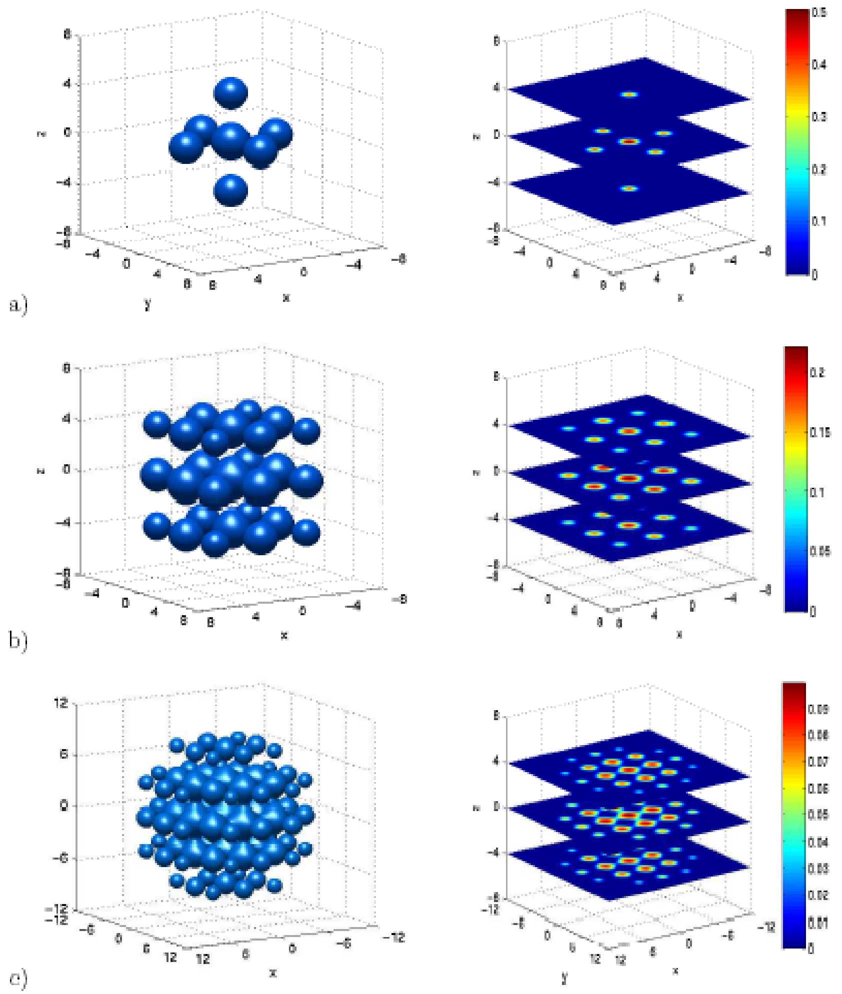
- Discretization--- Xu, Wen & Bao, 15'

$$\phi_g = \arg\min_{\phi \in S} E(\phi) \Rightarrow \min_{X \in \mathbb{R}^N \,\&\, \|X\|=1} F(X) := \frac{1}{2} X^T A X + \alpha \sum_{j=1}^{N} \left| X_j \right|^4$$

  - Construct initial solutions via feasible gradient type method
  - A regularized Newton method via trust-region strategy --- MJD Powell, Y.X. Yuan, RH Byrd, RB Schnabel, GA, Schultz, W. Sun, Z. Wen, ……..
  - Use multigrid method to accelerate convergence
  - Similar method has been developed and used for electronic structure computation – Z. Wen & W. Yin, 13'; Z. Wen, A. Milzarek, Ulbrich & Zhang, SISC, 13', Z Wen & A. Zhou, SISC 14', …..
  - Converge very fast in strong interaction regime & fast rotation

Ground states in 1D & 3D





Extension to GPE with rotation

- GPE / NLSE with an angular momentum rotation

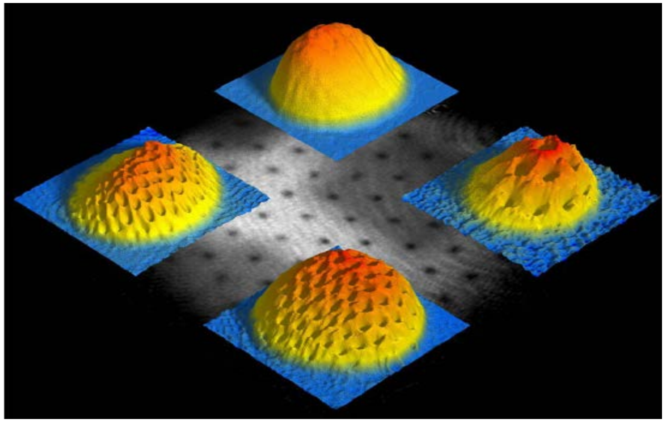
$$i\,\partial_t \psi(\vec{x},t) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta|\psi|^2]\psi, \quad \vec{x}\in\mathbb{R}^d, \quad t>0$$

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

- Ground states

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

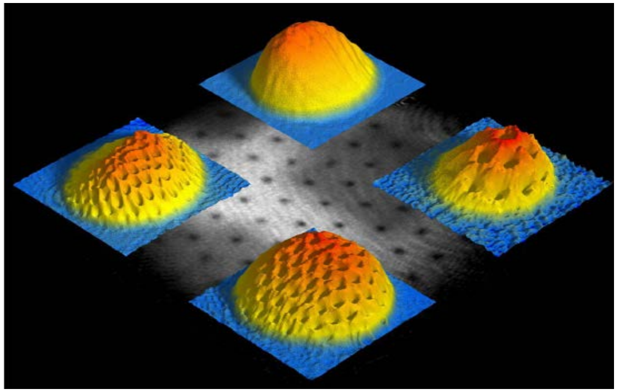
- Energy functional



Vortex @MIT

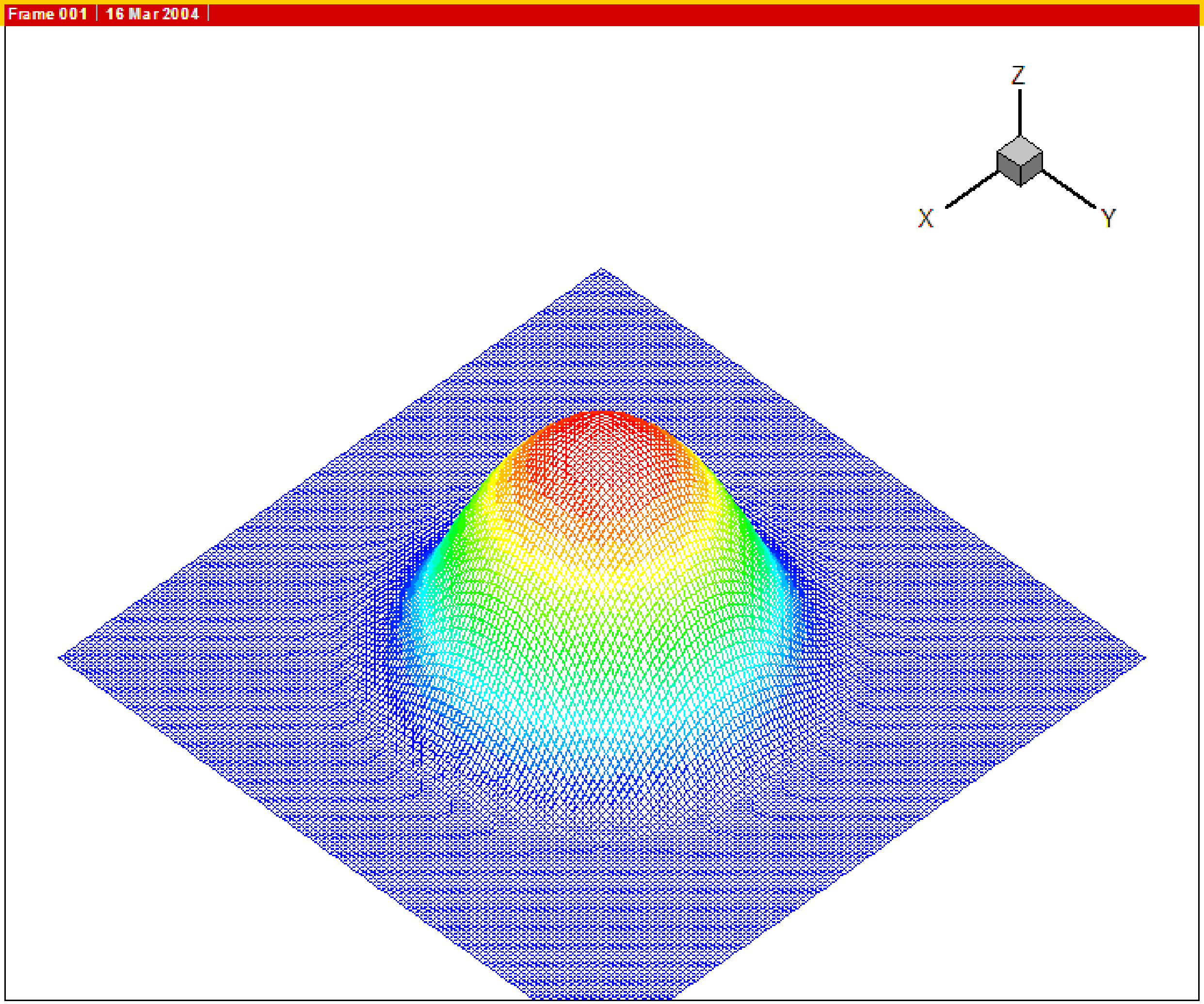
$$E_\Omega(\phi) = \int_{\mathbb{R}^d}\left[\frac{1}{2}|\nabla\phi|^2 + V(x)|\phi|^2 - \Omega\,\bar{\phi}L_z\phi + \frac{\beta}{2}|\phi|^4\right]d\,\vec{x}$$

Ground states

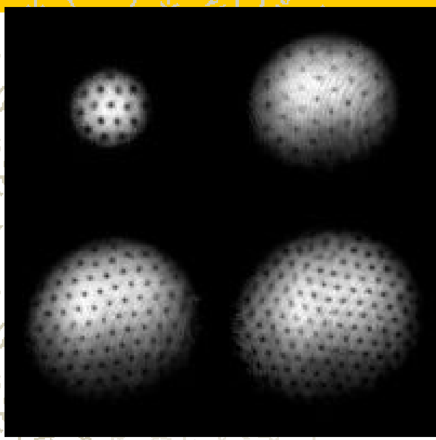


- Constrained Minimization problem
  - Energy functional is non-convex
  - Constraint is non-conex
  - Minimizer is complex instead of real
- Existence & uniqueness – Seiringer, CMP, 02'; Bao,Wang & Markowich, CMS, 05';
  - Exists a ground state when $\beta \geq 0 \,\&\, |\Omega| \leq \min\{\gamma_x, \gamma_y\}$
  - Uniqueness when $|\Omega| < \Omega_c(\beta)$
  - Quantized vortices appear when $|\Omega| \geq \Omega_c(\beta)$
  - Phase transition & bifurcation in energy diagram
- Numerical methods --- NGF via BEFD or BEFP or Newton method

Ground states with different Ω



Ground states of rapid rotation



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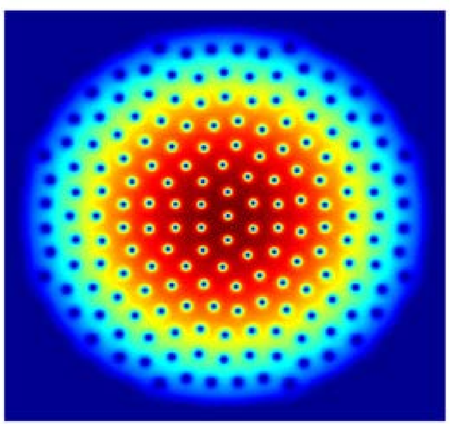
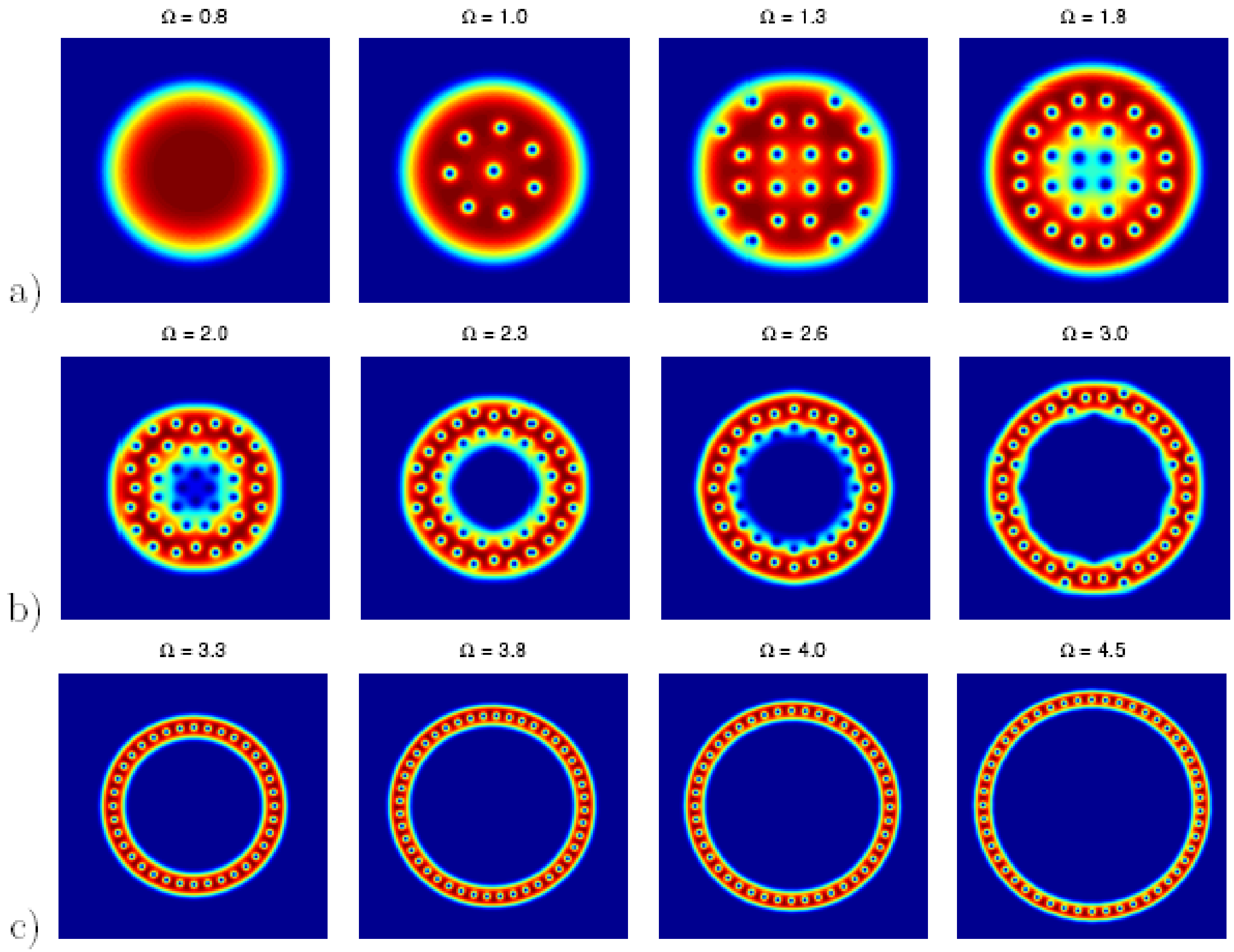
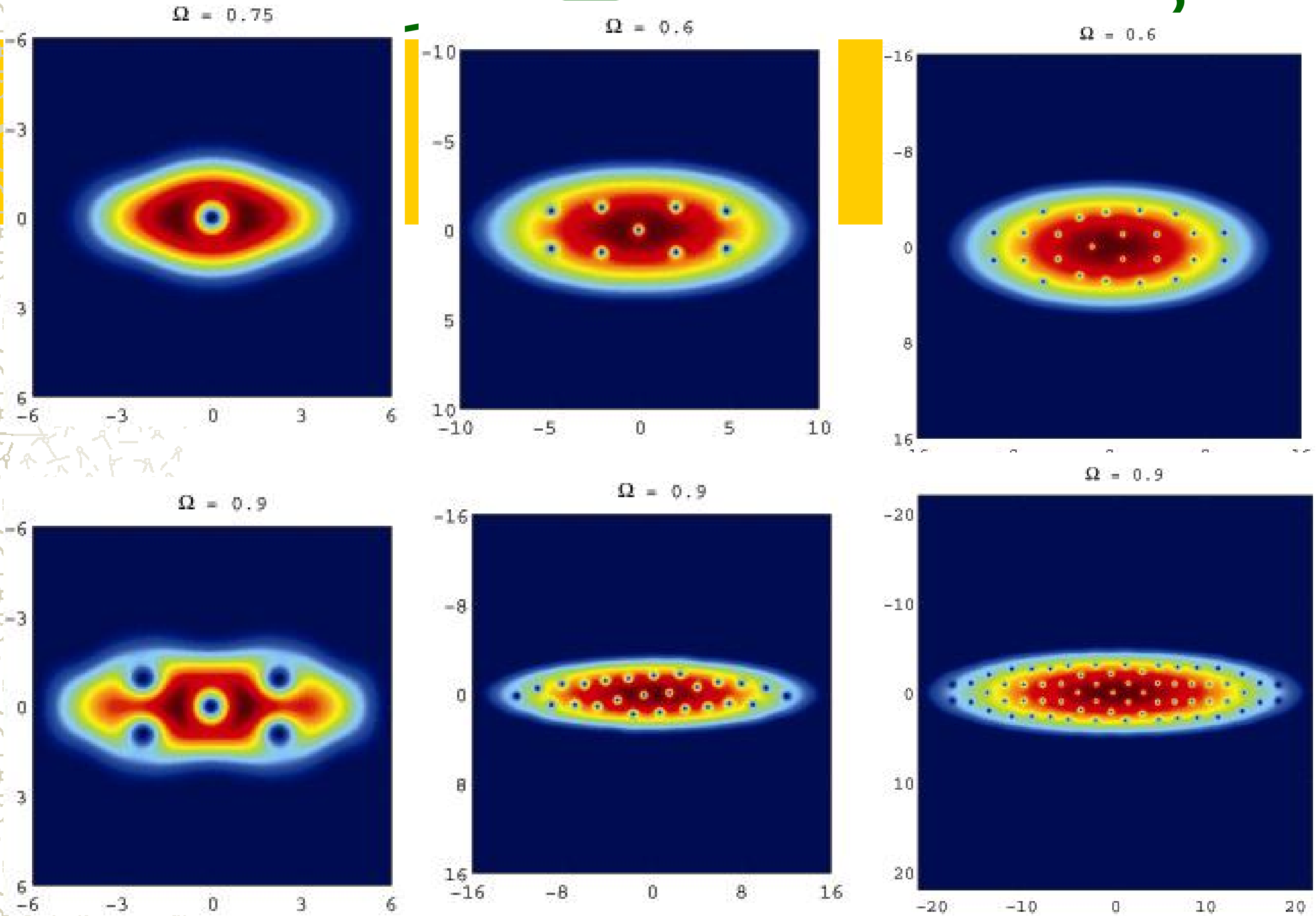
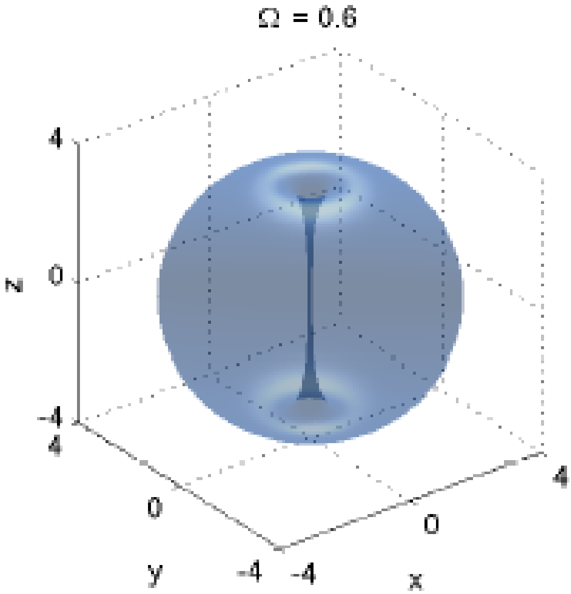
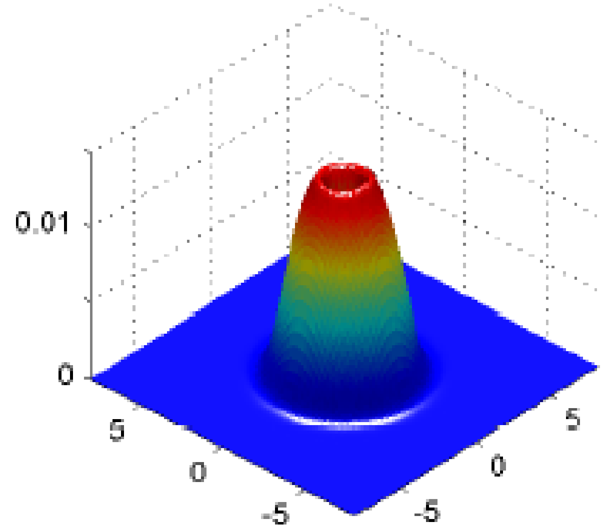
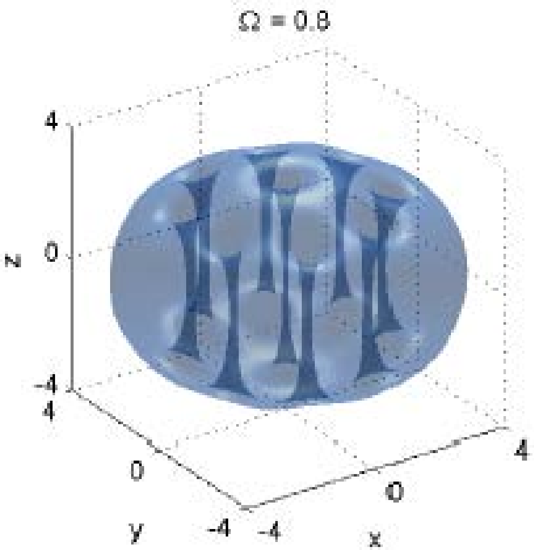


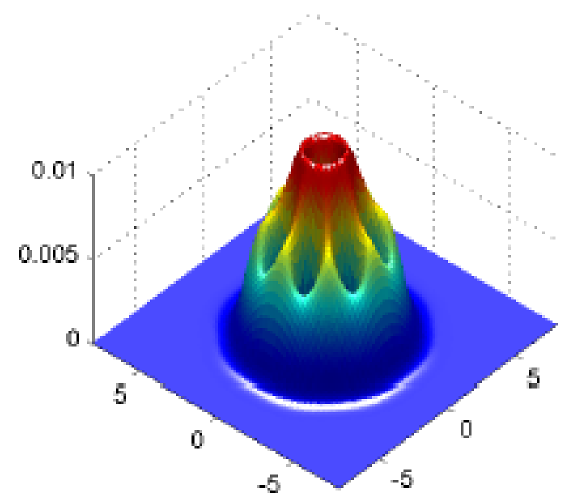



Ω = 0.75
-6 -3 0 3 6
Ω = 0.6
-10 -5 0 5 10
Ω = 0.6
-16 -8 0 8 16
Ω = 0.9
-6 -3 0 3 6
Ω = 0.9
-16 -8 0 8 16
Ω = 0.9
-20 -10 0 10 20


Ω = 0.6
4
0
-4
z
4
0
-4
y
-4
0
4
x


0.01
0
5
0
-5
5
0
-5


Ω = 0.8
4
0
-4
z
4
0
-4
y
-4
0
4
x


0.01
0.005
0
5
0
-5
5
0
-5

Dipolar quantum gas (BEC)

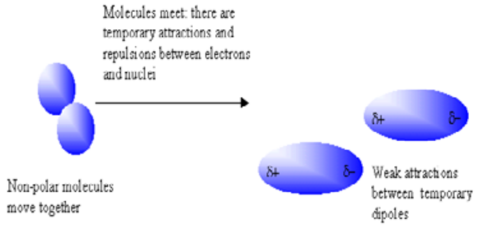
$$\psi = \psi(\vec{x},t) \qquad \vec{x} \in \mathbb{R}^3$$

- GPE with long-range anisotropic DDI

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

  - 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

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



  - Energy

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

- 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

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

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

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

A New Formulation

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

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

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

- Ground state

$$\phi_g=\arg\min_{\phi\in S} E(\phi)$$

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

- Model in 2D

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

Ground State Results

- Theorem (Existence, uniqueness & nonexistence) (Carles, Markowich& Sparber, 08'; Bao, Cai & Wang, JCP, 10')
  - Assumptions

$$V_{\text{ext}}(\vec{x}) \geq 0, \quad \forall \vec{x} \in \mathbb{R}^3 \qquad \& \qquad \lim_{|\vec{x}|\to\infty} V_{\text{ext}}(\vec{x}) = +\infty \quad \text{(confinement potential)}$$

  - Results
    - There exists a ground state $\phi_g \in S$ if $\beta \geq 0 \quad \& \quad -\frac{\beta}{2} \leq \lambda \leq \beta$
    - Positive ground state is unique $\phi_g = e^{i\theta_0}|\phi_g| \quad \text{with} \quad \theta_0 \in \mathbb{R}$
    - Nonexistence of ground state, i.e. $\lim_{\phi\in S} E(\phi) = -\infty$
      - Case I: $\beta < 0$
      - Case II: $\beta \geq 0 \quad \& \quad \lambda > \beta \text{ or } \lambda < -\frac{\beta}{2}$
- Numerical method for DDI via NUFFT (Jiang, Greengard, Bao, SISC,14'; Bao, Tang& Zhang, 15')

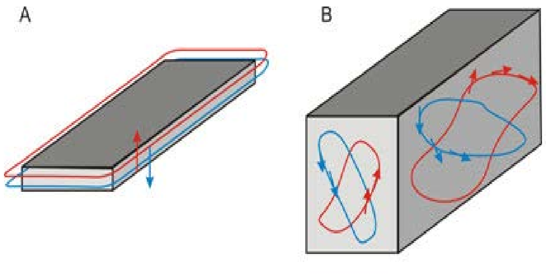
$$\widehat{U}_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2} \qquad P(\vec{x}) = U_{\text{dip}} * \rho = \int_{\mathbb{R}^3} \widehat{\rho}(\xi) e^{i\xi\cdot\vec{x}} \widehat{U}_{\text{dip}}(\xi) d\xi = \int \widehat{\rho}(\xi) e^{i\xi\cdot\vec{x}} [|\xi|^2 \widehat{U}_{\text{dip}}(\xi)] \ldots d|\xi|$$

Degenerate quantum gas (BEC) with spin-orbit-coupling

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

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

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



- Experiments: Lin, et al, Nature, 471(2011), 83.
- Applications ----Topological insulator
- Ground states (Bao & Cai, SIAP,15') --- existence, asymptotic behavior, numerical methods

$$\Phi_g=\arg\min_{\Phi\in S} E(\Phi)$$

$$S=\left\{\Phi=(\phi_1,\phi_2)\,|\,\|\Phi\|^2=\|\phi_1\|^2+\|\phi_2\|^2=1, E(\Phi)<\infty\right\}$$

$$E(\Phi)=\int_{\mathbb{R}^d}[\sum_{j=1}^{2}\left(\frac{1}{2}|\nabla\phi_j|^2+V_j(\vec{x})|\phi_j|^2\right)+\frac{\delta}{2}\left(|\phi_1|^2-|\phi_2|^2\right)+ik_0\left(\bar{\phi}_1\partial_x\phi_1-\bar{\phi}_2\partial_x\phi_2\right)+\Omega\,\mathrm{Re}\left(\phi_1\bar{\phi}_2\right)+\frac{1}{2}\left(\beta_{11}|\phi_1|^4+2\beta_{12}|\phi_1|^2|\phi_2|^2+\beta_{22}|\phi_2|^4\right)]d\vec{x}$$

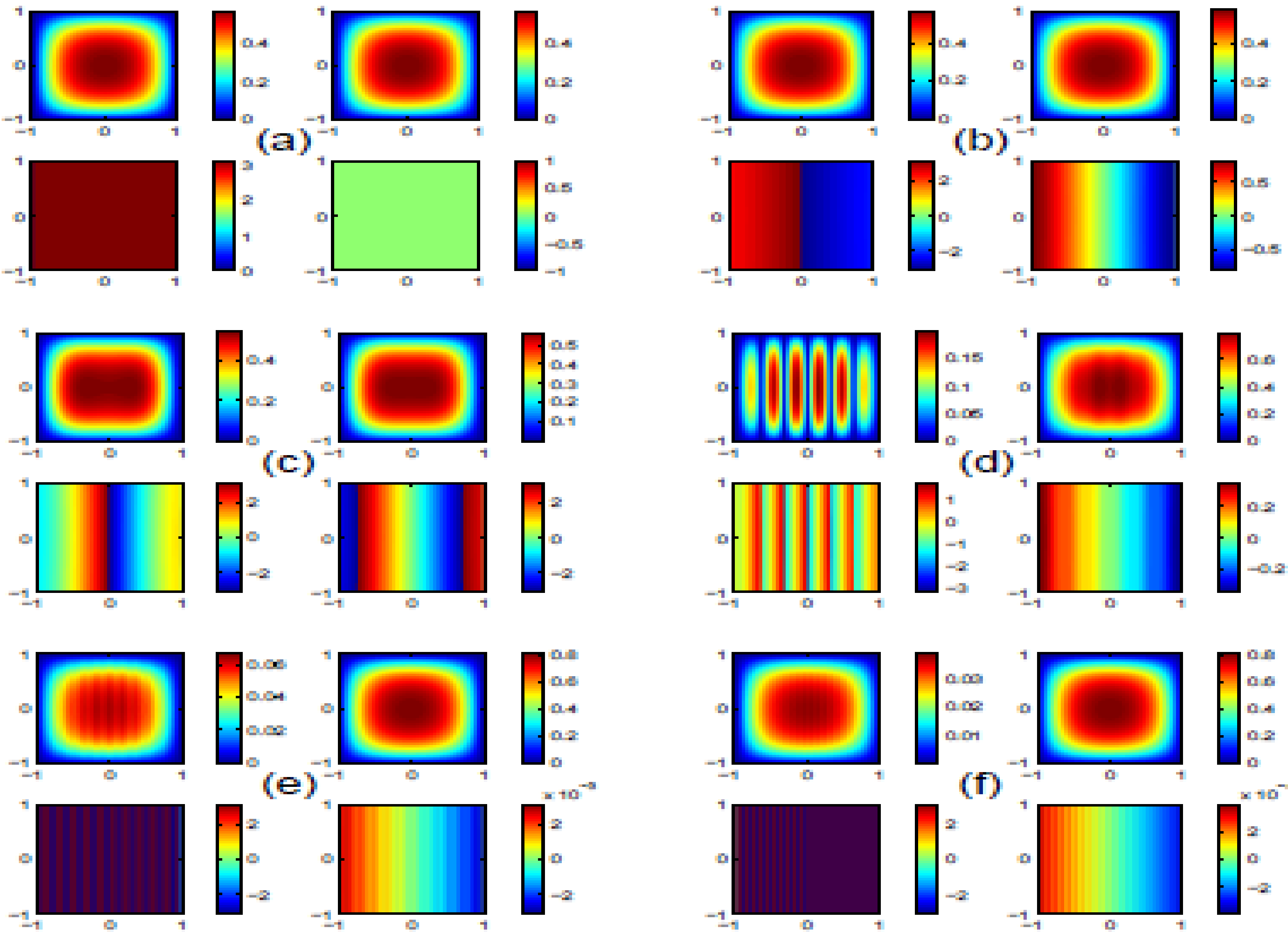


FIG. 3.1. *Ground states* $\tilde{\Phi}_g = (\tilde{\phi}_1^g, \tilde{\phi}_2^g)^T$ *for a SO-coupled BEC in 2D with* $\Omega = 50$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ *for: (a)* $k_0 = 0$, *(b)* $k_0 = 1$, *(c)* $k_0 = 5$, *(d)* $k_0 = 10$, *(e)* $k_0 = 50$, *and (f)* $k_0 = 100$. *In each subplot, top panel shows densities and bottom panel shows phases of the ground state* $\tilde{\phi}_1^g$ *(left column) and* $\tilde{\phi}_2^g$ *(right column).*

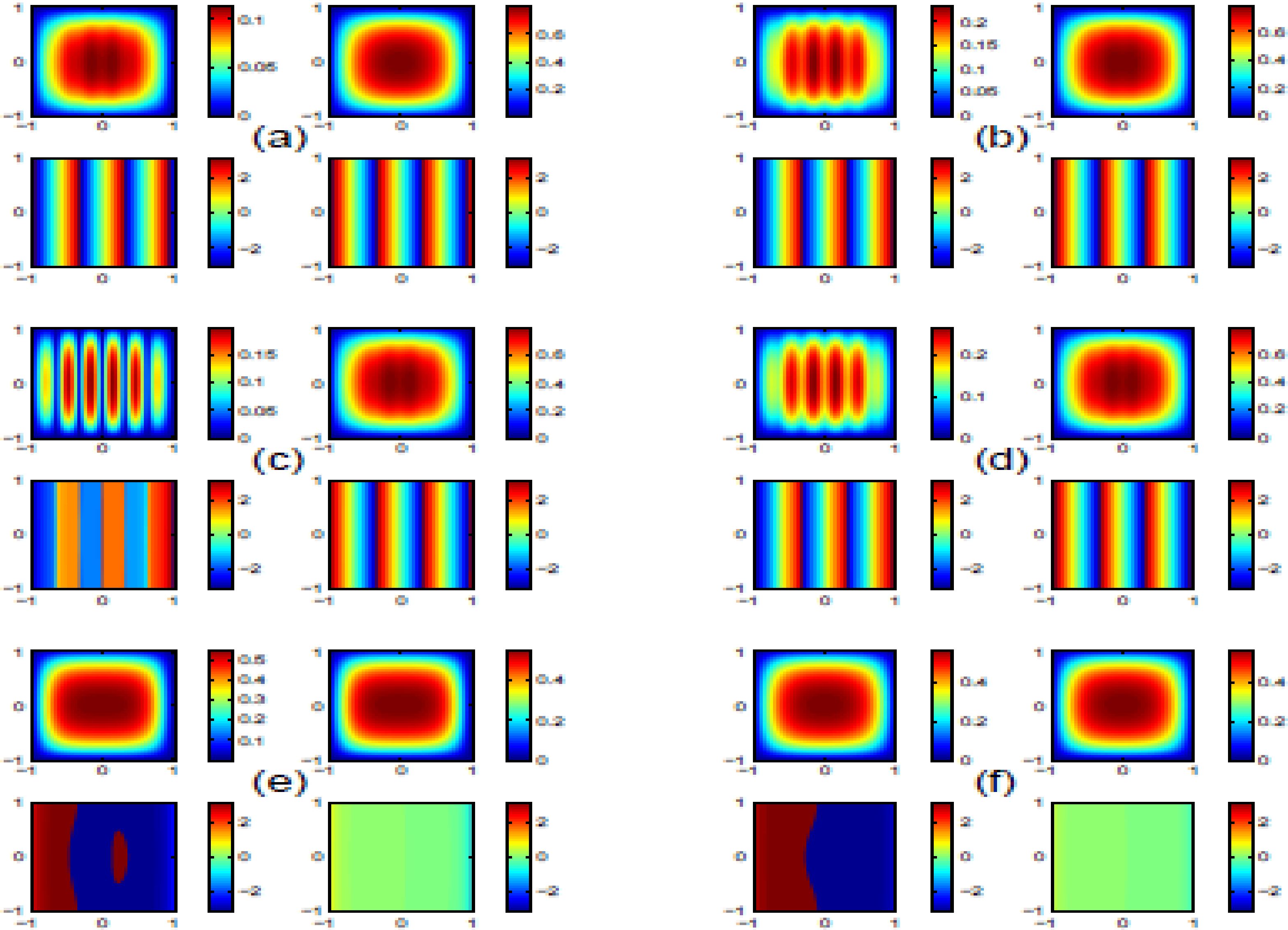


FIG. 3.2. *Ground states* $\Phi_g = (\phi_1^g, \phi_2^g)^T$ *for a SO-coupled BEC in 2D with* $k_0 = 10$, $\delta = 0$, $\beta_{11} = 10$, $\beta_{12} = \beta_{21} = \beta_{22} = 9$ *for: (a)* $\Omega = 1$, *(b)* $\Omega = 10$, *(c)* $\Omega = 50$, *(d)* $\Omega = 200$, *(e)* $\Omega = 300$, *and (f)* $\Omega = 500$. *In each subplot, top panel shows densities and bottom panel shows phases of the ground state* ϕ_1^g *(left column) and* ϕ_2^g *(right column).*

Spinor (F=1) degenerate quantum gas

- Coupled GPEs

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

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

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

- Ground states
  - with

$$\Phi_g=\arg\min_{\Phi\in S}E(\Phi)$$

$$S=\left\{\Phi=(\phi_1,\phi_0,\phi_{-1})\,|\,\|\Phi\|^2=1,\|\phi_1\|^2-\|\phi_{-1}\|^2=M,\,E(\Phi)<\infty\right\},\quad \rho_j=|\phi_j|^2,\quad \rho=\rho_1+\rho_0+\rho_{-1}$$

$$E(\Phi)==\int_{\mathbb{R}^d}[\sum_{j=-1}^{1}\left(\frac{1}{2}|\nabla\phi_j|^2+V(\vec{x})|\phi_j|^2\right)+\frac{\beta_n}{2}\rho^2+\frac{\beta_s}{2}\left((\rho_1-\rho_{-1})^2+2\rho_0(\rho_1+\rho_{-1})\right)+\beta_s\left(\bar{\phi}_{-1}\phi_0^2\bar{\phi}_1+\phi_{-1}\bar{\phi}_0^2\phi_1\right)]d\vec{x}$$

  - Theory – Cao & Wei, 08'; Chern & Lin, 13'
  - Numerical methods and results –Zhang, Yi & You, PRA, 05'; Bao & Wang, SIAM J. Numer. Anal., 07'; Bao & Lim, SISC, 08'; PRE, 08', Ueda, 10'

Conclusions & Future Challenges

- Conclusions:
  - NLSE / GPE – brief derivation
  - Ground states
    - Existence, uniqueness, non-existence
    - Numerical methods: Gradiend flow method via BEFD or Regularized Newton method via trust-region strategy
- Future Challenges
  - Nonlocal high-order interaction & system, e.g. spin-2 BEC
  - Bogoliubov excitation --- linear response;
  - Excited states – constrained min-max problems
- Modeling + Numerical PDE + Optimization → materials science & quantum physics, chemistry

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