Mathematical Models & Numerical Simulation for Bose-Einstein Condensation

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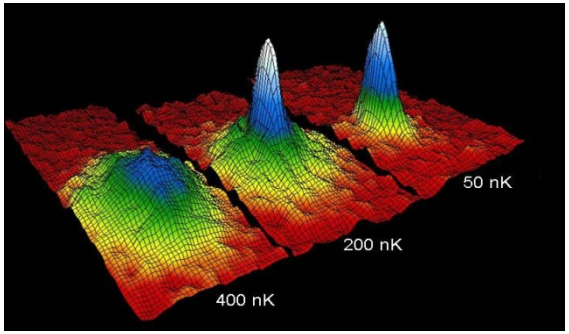
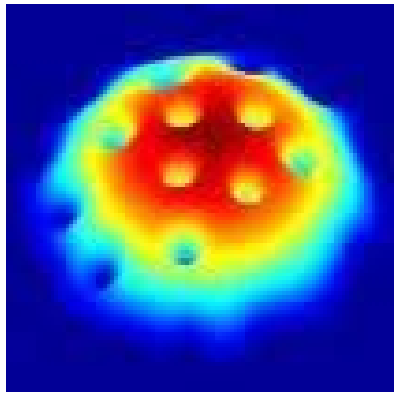


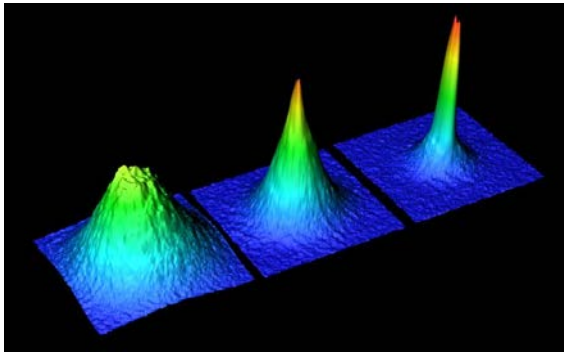
BEC@JILA, 95’



Vortex@ENS

Outline

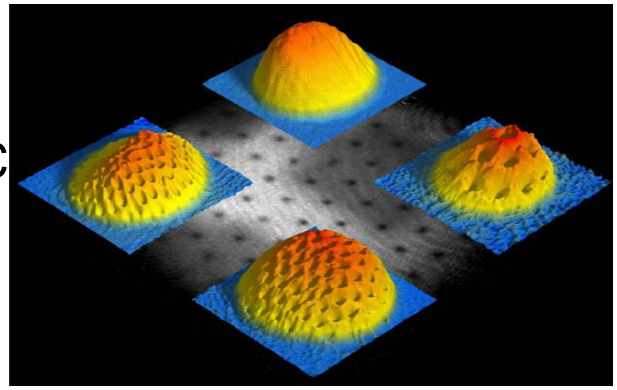
- Part I: Predication, Experiment & Mathematical Models
  - Theoretical predication
  - Physical experiments and results
  - Applications
  - Gross-Pitaevskii equation (GPE)
- Part II: Analysis & Computation for Ground States
  - Existence & uniqueness
  - Energy asymptotics & asymptotic approximation
  - Numerical methods
  - Numerical results



BEC@ETH, 98’

Outline

- Part III: Analysis & Computation for Dynamics of BEC
  - Dynamical laws
  - Numerical methods
  - Numerical results
- Part IV: Rotating BEC & Multi-component BEC
  - BEC in a rotational frame
  - BEC with nonlocal dipole-dipole interac
  - Two-component BEC
  - Spinor BEC
  - Conclusions & Future challenges



BEC@MIT, 00'

Part I

Predication, Experiment

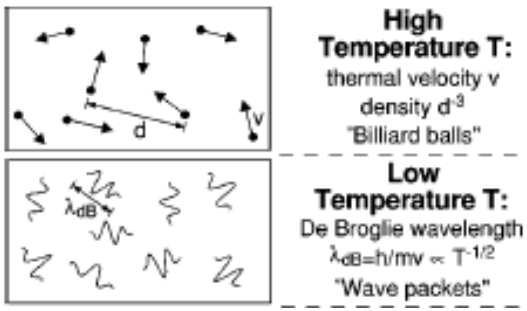
&

Mathematical models

Theoretical predication

- Particles be divided into two big classes
  - Bosons: photons, phonons, etc
    - Integer spin
    - Like in same state & many can occupy one obit
    - Sociable & gregarious
  - Fermions: electrons, neutrons, protons etc
    - Half-integer spin & each occupies a single obit
    - Loners due to Pauli exclusion principle

Theoretical predication

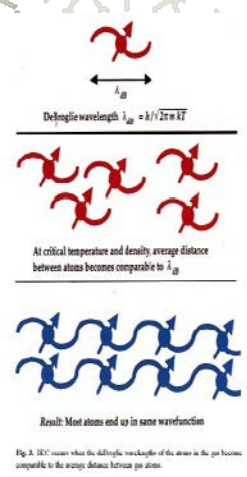


For atoms, e.g. bosons

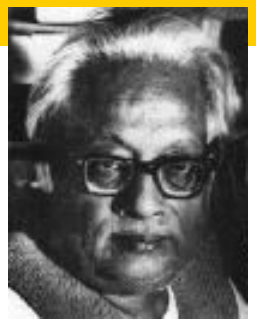
- Get colder:
  - Behave more like waves & less like particles
- Very cold:
  - Overlap with their neighbors

Extremely cold:

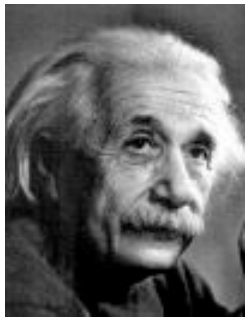
- Most atoms behavior in the same way, i.e gregarious
- quantum mechanical ground state,
- `super-atom' & new matter of wave & fifth state



Theoretical predication of BEC



- S.N. Bose: Z. Phys. 26 (1924)
  - Study black body radiation: object very hot
  - Two photons be counted up as either identical or different
  - Bose statistics or Bose-Einstein statistics



- A. Einstein: Sitz. Ber. Kgl. Preuss. Adad. Wiss. 22 (1924)
  - Apply the rules to atoms in cold temperatures
  - Obtain Bose-Einstein distribution in a cold gas

$$n_i = \frac{1}{e^{(\varepsilon_i - \mu)/k_B T} - 1} := f(\varepsilon_i), \quad j = 0,1,2,\ldots, \quad \mu < \varepsilon_0 < \varepsilon_1 < \cdots$$

$$n_i = \frac{1}{e^{(\varepsilon_i - \mu)/kT} - 1}$$

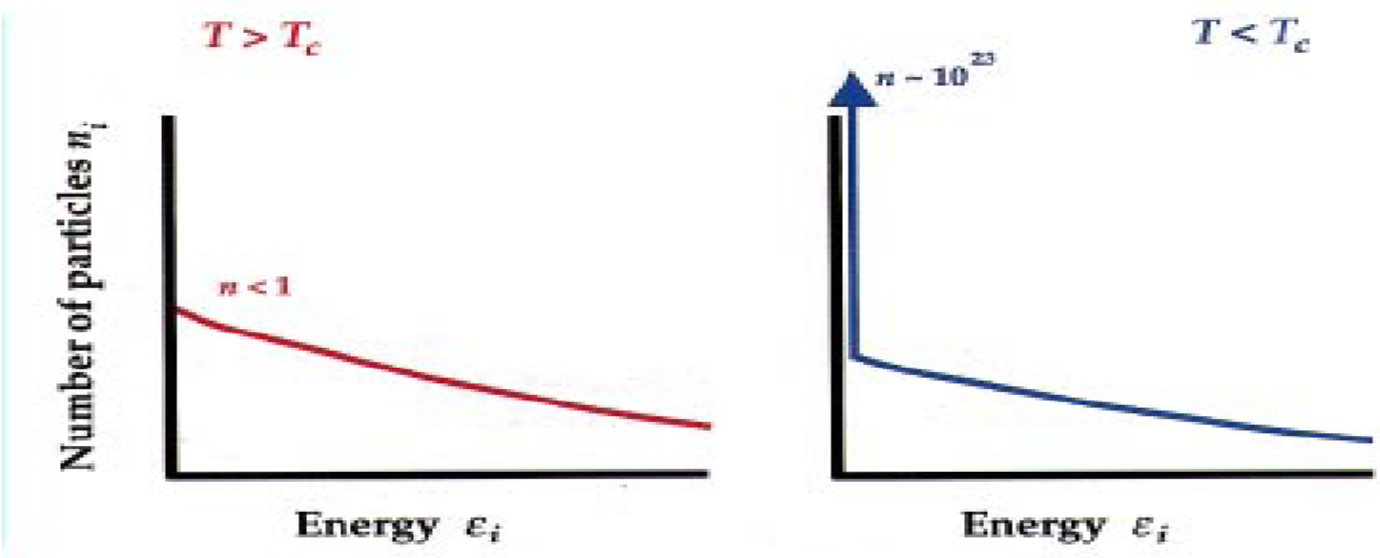


Fig. 2. Schematic diagram of the Bose-Einstein distribution for a system of particles at a temperature T. The formula shows the average number of particles n_i occupying a state i of energy ϵ_i. The parameter μ is the chemical potential, which is the energy required to add an additional particle to the system. The left frame depicts the general behavior of this distribution above the transition temperature T_c; the right panel shows the macroscopic occupancy of the lowest state of the system when $T < T_c$.

- Einstein's prediction on BEC: At zero or `low' temperatures, most particles behavior in the same way (at quantum mechanical ground state)! –gregarious behavior----- quantum phase transition happens at extremely low temperatures --- degenerate quantum gas -- `super atom' –--- fifth matter of state.

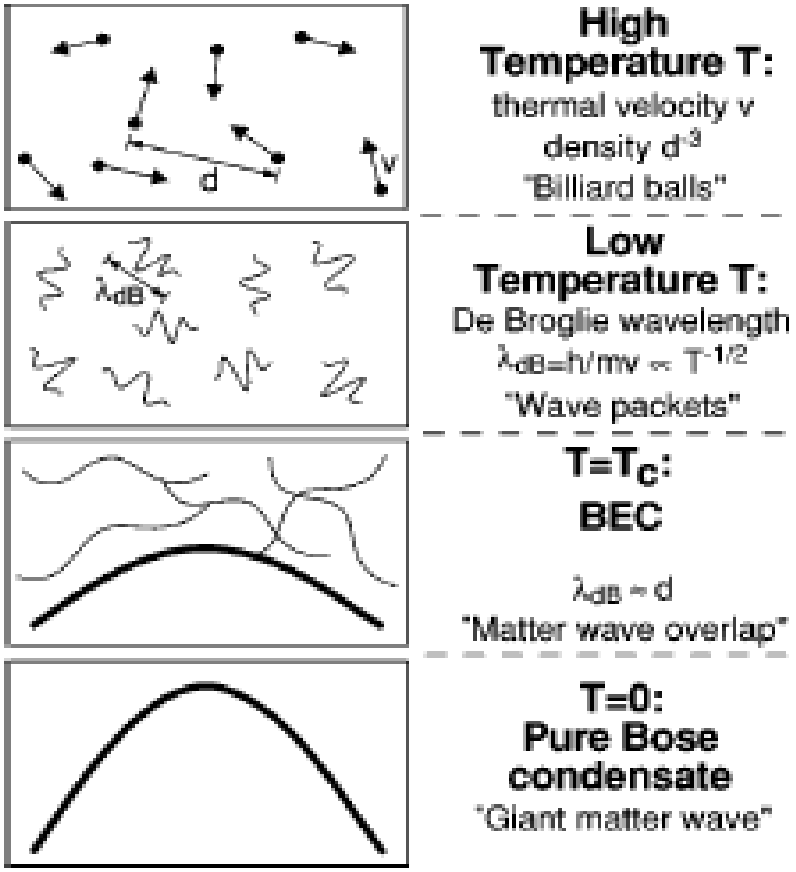


FIG. 2. Criterion for Bose-Einstein condensation. At high temperatures, a weakly interacting gas can be treated as a system of "billiard balls." In a simplified quantum description, the atoms can be regarded as wave packets with an extension of their de Broglie wavelength λ_{dB}. At the BEC transition temperature, λ_{dB} becomes comparable to the distance between atoms, and a Bose condensate forms. As the temperature approaches zero, the thermal cloud disappears, leaving a pure Bose condensate.

Experimental difficulties

- Low temperatures, almost absolutely zero (nK)
- Low density in a gas

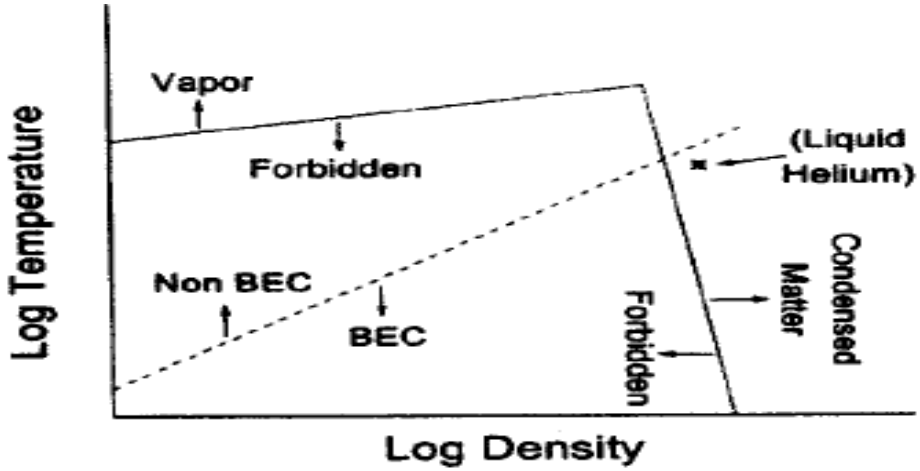
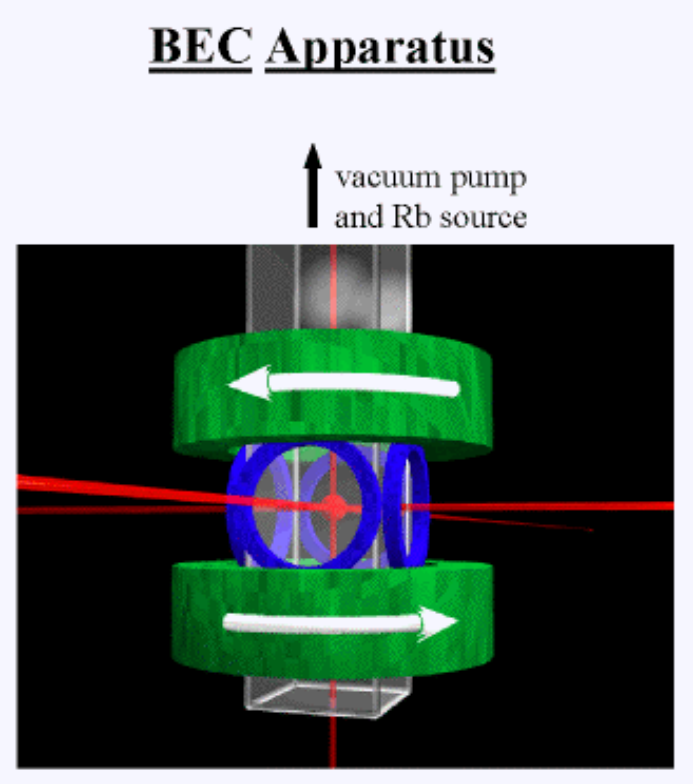


FIG. 1. Generic phase diagram common to all atoms: dotted line, the boundary between non-BEC and BEC; solid line, the boundary between allowed and forbidden regions of the temperature-density space. Note that at low and intermediate densities, BEC exists only in the thermodynamically forbidden regime.

Experimental techniques

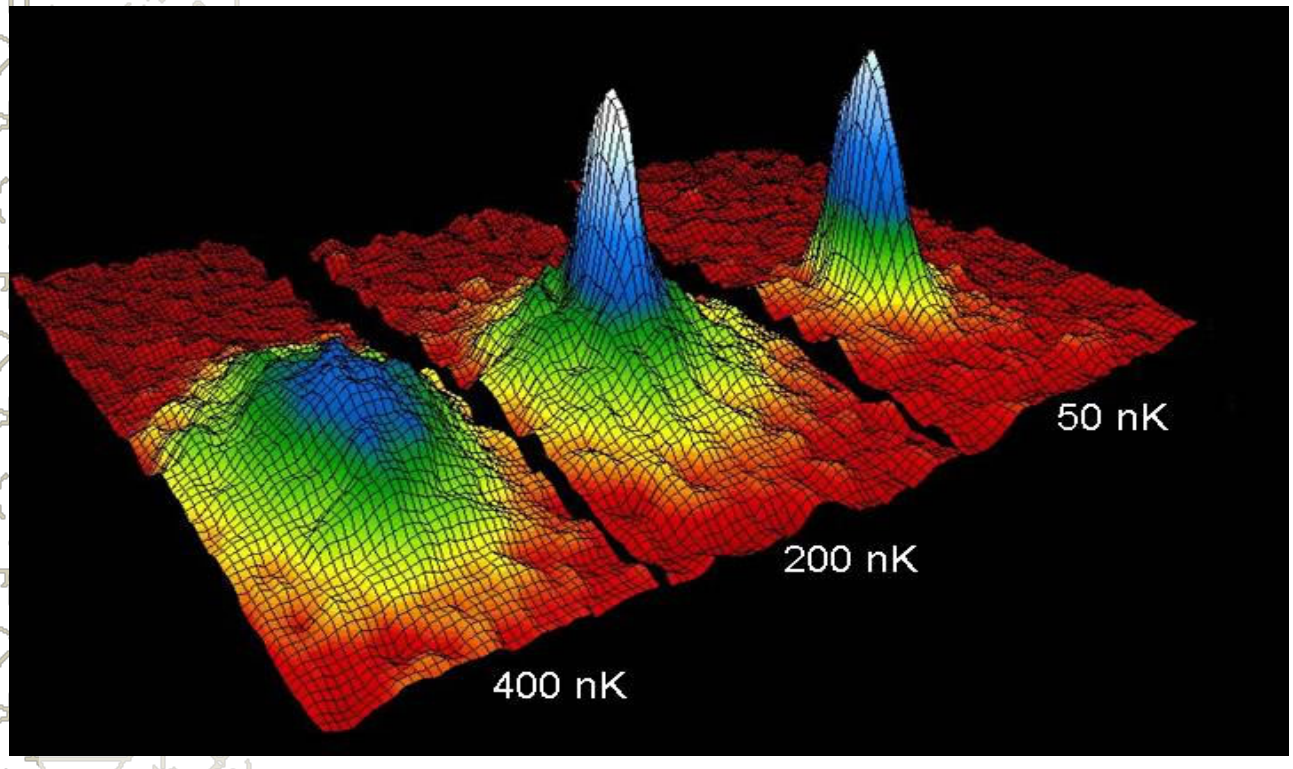
- Laser cooling
- Magnetic trapping
- Evaporative Cooling



($100k—300k)

Experimental results

- JILA (95', Rb, 5,000): Science 269 (1995)



–Anderson et al., Science, 269 (1995), 198: JILA Group; Rb

–Davis et al., Phys. Rev. Lett., 75 (1995), 3969: MIT Group; Rb

–Bradly et al., Phys. Rev. Lett., 75 (1995), 1687, Rice Group; Li

Science AAAS

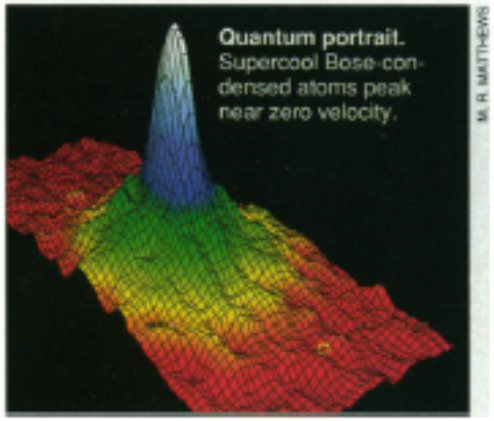
A New Form of Matter Unveiled

Physicists create the long-sought Bose-Einstein condensate, allowing easier exploration of quantum mechanics, while other researchers celebrate a new planet, a gene for eyes, brain images, and more

Back in 1924, Albert Einstein predicted the existence of a new phase of matter, an exotic state in which atoms defied the laws of classical physics and followed only the dictums of quantum mechanics. In 1995, by chilling wisps of gas to ultracold temperatures, physicists finally got their first good look at this state, named the Bose-Einstein condensate after Einstein and Indian physicist Satyendra Bose. This year's work ends an arduous quest and ushers in a new age of exploration in atomic and condensed-matter physics.

We salute the condensate as Molecule of the Year for 1995, but this peculiar form of matter is not a molecule. Indeed, this year's magnificent achievement was to elude the everyday forces that bind atoms together into molecules and so unmask the more subtle powers of quantum mechanics. While atoms in an ordinary gas dart about in all directions, the atoms in the condensate move in lock step, at identical speed and direction. They have relinquished their individual identities to become a single, collective entity, and their organized condition is expected to give rise to bizarre properties.

The condensate's unusual nature makes it an ideal workshop for exploring the counterintuitive realm of quantum mechanics. So



Quantum portrait. Supercool Bose-condensed atoms peak near zero velocity.

M. R. MATTHEWS

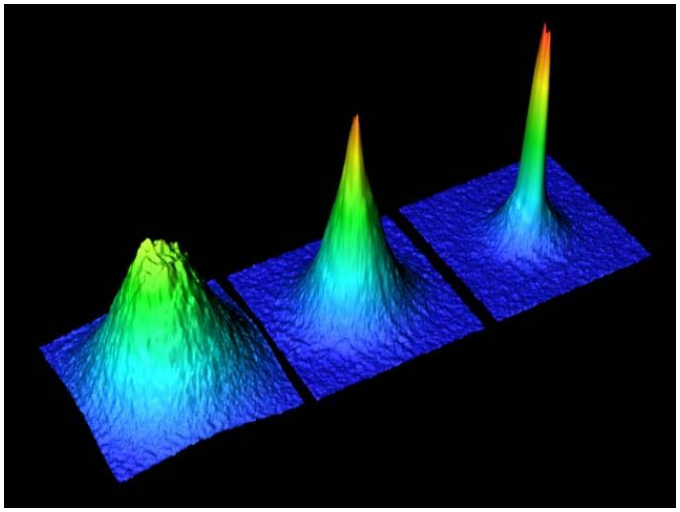
6 months after the first dramatic report, experimentalists are rushing to create and explore this new phase, while theorists calculate its properties. Physicists are already angling to apply the new knowledge, hoping to capitalize on the condensate's unique aspects to create a laser that shoots beams of atoms instead of light. Understanding the laws that govern matter in this cold, coherent state may help physicists understand the mysteries of superconductivity and perhaps even the early universe.

Physicists have glimpsed Bose-Einstein condensation before, but never in a system where they could study all its properties. For example, pairs of electrons and electron holes, known as excitons, have been observed to form condensates in semiconductors, but these last only a few millionths of a second. In ultracold liquid helium, up to 10% of the atoms are thought to be Bose-condensed, and this is intimately linked to startling properties such as superfluidity, which allows this fluid to creep up the sides of a beaker. But in liquid helium, the condensate is modified by the classical forces between atoms, so the quantum-mechanical signature is muddied.

To create a pure condensate, physicists need supercold atoms, where no heat veils the quantum forces. Yet the atoms must be kept in a gaseous phase and prevented from collapsing into a solid or liquid. In July, by cooling atoms of rubidium to within a whisper of absolute zero, researchers at a lab run jointly by the National Institute of Standards and Technology and the University of Colorado managed this feat. In an ultracold cloud of gas, they saw their boldest dreams come true, as a textbook example of Bose-Einstein condensation took shape. When they graphed the distribution of the atoms' velocities, they saw a now-classic portrait, with a dramatic peak close to zero

Experimental results

- Experimental implementation
  - JILA (95'): First experimental realization of BEC in a gas
  - NIST (98'): Improved experiments
  - MIT, ENS, Rice,
  - ETH, Oxford,
  - Peking U., NUS, …
- 2001 Nobel prize in physics:
  - C. Wiemann: U. Colorado
  - E. Cornell: NIST
  - W. Ketterle: MIT



ETH (02', Rb, 300,000)

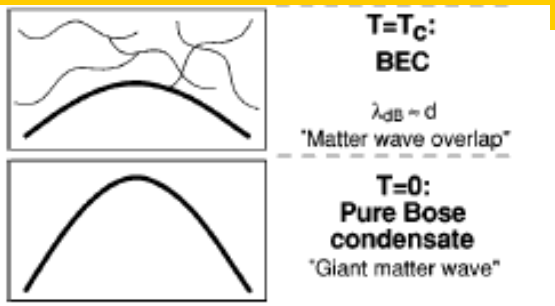
Properties of BEC in experiments

Kinds of atom	^{87}Rb, ^{7}Li, ^{23}Na, ^{52}Cr, ^{4}He,…
Temperatures	$50\text{nK} - - - 2\mu\text{K}$
Density	$10^{11} - - - 10^{15}\text{cm}^{-3}$
# of atoms	$100(^{7}\text{Li}) - - - 10^{6}(^{23}\text{Na}) - - 10^{9}(^{4}\text{He})$
Spatial size	Sphere at diameter 10--15μm cigar-shaped at length 300μm & diameter 15μm
Life span	A few seconds to several minutes

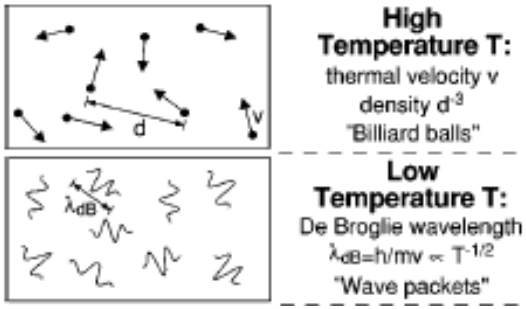
Brief BEC research history

- Milestones
  - 1924 ----- Prediction of BEC by A. Einstein
  - 1938-----London & Tisza linked BEC & superfluidity in liquid helium 4
  - 1995 --- Experiments of BEC in ultracold gas of alkali atoms
  - Since then--- BEC begins a new era in atomic, molecular & optical (AMO) physics & quantum optics; attracts interests of computational, applied & pure mathematicians.
- Some famous physicists in BEC research
  - Nobel Laureates: A. Einstein (1921), L. D. Landau (1961), L. Onsager (1968), R. Feynmann (1965),T.-D. Lee&C.N. Yang (1957), A. Leggett (2003), E. Cornell, C. Weimann&W. Ketterle (2001),
  - Others: S. Bose, F. London, L. Tisza, N. Bogoliubov, R. Penrose, K. Huang, D. Beliaev, L. Pitaevskii, E. Gorss, A. Fetter, P. Zoller, D. Jaksch, I. Bloch, R. Hulet, J. Yngvason, S. Stringari, E.H.. Lieb, …..

Mathematical models



- N-body problem
  - (3N+1)-dim linear Schroedinger equation
- Mean field theory--zeor or `extremely' low temperatures
  - Gross-Pitaevskii equation (GPE): $T < T_c = O(\mathrm{nK})$
  - (3+1)-dim nonlinear Schroedinger equation (NLSE)
- Quantum kinetic theory-- high temperatures
  - High temperature: QBME (3+3+1)-dim
  - Around critical temperature: QBME+GPE
  - Below critical temperature: GPE



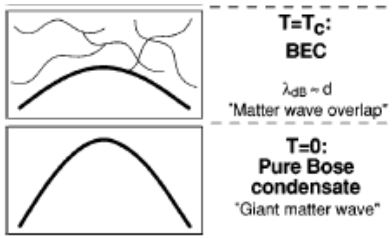
Model for a BEC at zero temperature

– with *N* identical bosons

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

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

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



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

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

Model for a BEC – with *N* identical bosons

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

$$E(\psi)=\int_{\mathbb{R}^3}\left[\frac{\hbar^2}{2m}|\nabla\psi|^2+V(\vec{x})|\psi|^2+\frac{(N-1)g}{2}|\psi|^4\right]d\vec{x}\quad\text{with}\quad\psi:=\psi(\vec{x},t)$$

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

$$i\hbar\partial_t\psi(\vec{x},t)=\frac{\delta E(\psi)}{\delta\overline{\psi}}=\left[-\frac{\hbar^2}{2m}\nabla^2+V(\vec{x})+(N-1)g|\psi|^2\right]\psi,\quad\vec{x}\in\mathbb{R}^3$$

- Proper non-dimensionalization & dimension reduction– GPE/NLSE $\beta=\frac{4\pi(N-1)a_s}{x_s}\approx\frac{4\pi Na_s}{x_s}$

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

Gross-Pitaevskii equation (GPE)

- The 3D Gross-Pitaevskii equation ($\vec{x} = (x, y, z)$)

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

  - V is a harmonic trap potential

$$V(\vec{x}) = \frac{m}{2}\left(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2\right)$$

  - Normalization condition

$$\int_{\mathbb{R}^3} |\psi(\vec{x},t)|^2\, d\vec{x} = 1.$$

Gross-Pitaevskii equation

- Scaling (w.l.o.g. $\omega_x \le \omega_y \le \omega_z$)
  - Dimensionless variables

$$\tilde{t} = \omega_x t, \qquad \tilde{\vec{x}} = \frac{\vec{x}}{x_s}, \qquad \tilde{\psi}(\tilde{\vec{x}},\tilde{t}) = x_s^{3/2}\psi(\vec{x},t), \qquad x_s = \sqrt{\frac{\hbar}{m\omega_x}}$$

  - Dimensionless Gross-Pitaevskii equation

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

  - With

$$V(\vec{x}) = \frac{1}{2}(x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), \qquad \gamma_y = \frac{\omega_y}{\omega_x}, \qquad \gamma_z = \frac{\omega_z}{\omega_x}, \qquad \beta = \frac{4\pi(N-1)a_s}{x_s} \approx \frac{4\pi N a_s}{x_s}$$

Gross-Pitaevskii equation

- Typical parameters ($\hbar = 1.05 \times 10^{-34}$ [Js])
  - $^{87}\mathrm{Rb}$ Used in JILA

$$m = 1.44 \times 10^{-25}\ [\mathrm{kg}], \quad \omega_x = \omega_y = 10 \times 2\pi\ [1/\mathrm{s}], \quad \omega_z = \sqrt{8}\,\omega_x$$

$$a_s = 5.1\,[\mathrm{nm}], \quad x_s = \sqrt{\frac{\hbar}{m\omega_x}} = 0.3407 \times 10^{-5}\ [\mathrm{m}], \quad \beta = \frac{4\pi N a_s}{x_s} = 0.01881N$$

  - $^{23}\mathrm{Na}$ Used in MIT

$$m = 3.8 \times 10^{-26}\ [\mathrm{kg}], \quad \omega_x = \omega_y = 360 \times 2\pi\ [1/\mathrm{s}], \quad \omega_z = 3.5 \times 2\pi\ [1/\mathrm{s}]$$

$$a_s = 2.75\,[\mathrm{nm}], \quad x_s = \sqrt{\frac{\hbar}{m\omega_z}} = 1.1209 \times 10^{-5}\ [\mathrm{m}], \quad \beta = \frac{4\pi N a_s}{x_s} = 0.003083N$$

Gross-Pitaevskii equation

- Reduction to 2D (disk-shaped condensation)
  - Experimental setup $\omega_x \approx \omega_y, \quad \omega_z >> \omega_x \quad \Leftrightarrow \quad \gamma_y \approx 1, \quad \gamma_z >> 1$
  - Assumption: No excitations along z-axis due to large energy

$$\psi(x,y,z,t) = \psi_{12}(x,y,t)\,\phi_3(z) \quad \text{with}$$

$$\phi_3(z) = \left(\int_{\mathbb{R}^2} |\phi_g(x,y,z)|^2\, dxdy\right)^{1/2} \approx \phi_{\text{ho}}(z) = \left(\frac{\gamma_z}{\pi}\right)^{1/4} e^{-\gamma_z z^2/2}$$

- 2D Gross-Pitaevskii equation $\left(\vec{x} = (x,y), \psi = \psi_{12} \right)$

$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = -\frac{1}{2}\Delta\psi + \frac{x^2 + \gamma_y^2 y^2}{2}\psi + \beta_2\, |\psi|^2 \psi,$$

$$\beta_2 = \int_{-\infty}^{\infty} \phi_3^4(z)dz \approx \int_{-\infty}^{\infty} \phi_{\text{ho}}^4(z)dz = \beta\sqrt{\frac{\gamma_z}{2\pi}} := \beta_2^a$$

Mathematical model for BEC—mean field theory

- The Gross-Pitaevskii equation (GPE/NLSE)

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

- 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
- $\beta = 0$:Schrodinger equation (E. Schrodinger 1925')
- $\beta \neq 0$:GPE (E.P. Gross 1961'; L.P. Pitaevskii 1961')

Gross-Pitaevskii equation

- Two kinds of interaction
  - Repulsive (defocusing) interaction

$$a_s > 0 \quad \Rightarrow \quad \beta \geq 0$$

  - Attractive (focusing) interaction

$$a_s < 0 \quad \Rightarrow \quad \beta \leq 0$$

- Four typical interaction regimes:
  - Linear regime: one atom in the condensation

$$\beta = 0$$

  - Weakly interacting condensation

$$|\beta| << 1$$

Gross-Pitaevskii equation

- Strongly repulsive interacting condensation

$$\beta \quad >> \quad 1$$

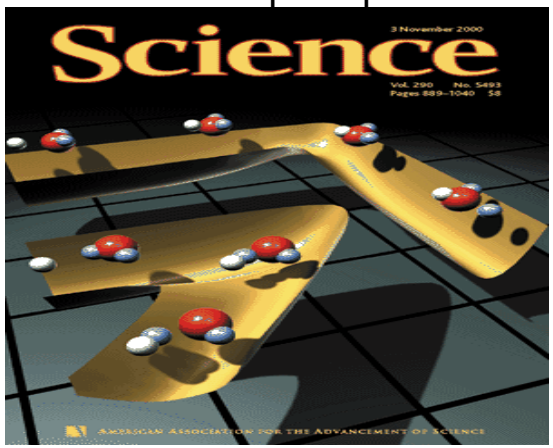
- Strongly attractive interaction

$$\beta < 0 \quad \& \quad |\beta| \quad >> \quad 1$$

- Other potentials
  - Box potential
  - Double-well potential
  - Optical lattice potential
  - On a ring or torus

Other applications of GPE/NLSE

- For laser beam propagation
- In plasma physics: wave interaction between electrons and ions
  - Zakharov system---NLSE +wave equation, …..
- In quantum chemistry: chemical interaction based on the first principle
  - Schrodinger-Poisson system
- In materials science:
  - First principle computation, DFT, …
  - Semiconductor industry
- In nonlinear (quantum) optics
- In biology – protein folding
- In superfluids – flow without friction, liquid $^4\mathrm{He}$



$$2H_2 + O_2 \rightarrow 2H_2O$$

Part II

Analysis & Computation

for

Ground states

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

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

- Energy conservation

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

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.

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

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

- 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

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

  - 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 $S = \left\{ \rho \,|\, \int_{\mathbb{R}^d} \rho(\vec{x}) d\vec{x} = 1 \ \& \ \tilde{E}(\rho) < \infty \right\}$ is convex in ρ
- Using convex minimization theorem
- Non-existence result

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

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

Excited & central vortex states

- Excited states: $\phi_1, \quad \phi_2, \quad \phi_3, \quad \cdots$
- Central vortex states: $\psi(x,y,t) = e^{-i\,\mu_m\,t}\,\phi_m(x,y) = e^{-i\,\mu_m\,t}\,\phi_m(r)\;e^{im\theta}$

$$\mu_m\,\phi_m(r) = -\frac{1}{2r}\frac{d}{dr}\left(r\,\frac{d\phi_m(r)}{dr}\right) + \left(\frac{m^2}{2r^2} + \frac{r^2}{2}\right)\phi_m(r) + \beta_2\,|\,\phi_m\,|^2\,\phi_m, \qquad 0 < \mathrm{r} < \infty$$

$$2\pi\int_0^\infty |\phi_m(r)|^2\,r\,dr = 1, \qquad \phi_m(0) = 0$$

- Central vortex line states in 3D:
- Open question: (Bao & W. Tang, JCP, 03'; Bao, F. Lim & Y. Zhang, TTSP, 06')

$$\phi_g, \qquad \phi_1, \qquad \phi_2, \qquad \cdots$$

$$E(\phi_g) < E(\phi_1) < E(\phi_2) < \cdots \Rightarrow \mu(\phi_g) < \mu(\phi_1) < \mu(\phi_2) < \cdots \quad ???????$$

- Fundamental gaps

$$\delta_E(\beta) := E(\phi_1) - E(\phi_g) > C_\beta \ge C > 0, \quad \delta_\mu(\beta) := \mu(\phi_1) - \mu(\phi_g) > \tilde{C}_\beta \ge \tilde{C} > 0, \quad \beta \ge 0$$

Approximate ground states

- Three interacting regimes
  - No interaction, i.e. linear case
  - Weakly interacting regime
  - Strongly repulsive interacting regime
- Three different potential
  - Box potential
  - Harmonic oscillator potential
  - BEC on a ring or torus

Energies revisited

- Total energy:

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

  - Kinetic energy: $E_{\text{kin}}(\phi)=\frac{1}{2}\int_{\mathbb{R}^d}|\nabla\phi(\vec{x})|^2\,d\vec{x}$
  - Potential energy: $E_{\text{pot}}(\phi)=\int_{\mathbb{R}^d}V(\vec{x})|\phi(\vec{x})|^2\,d\vec{x}$
  - Interaction energy: $E_{\text{int}}(\phi)=\frac{\beta}{2}\int_{\mathbb{R}^d}|\phi(\vec{x})|^4\,d\vec{x}$
- Chemical potential

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

$$=E(\phi)+E_{\text{int}}(\phi)=E_{\text{kin}}(\phi)+E_{\text{pot}}(\phi)+2E_{\text{int}}(\phi)$$

Box Potential in 1D

- The potential: $V(x) = \begin{cases} 0, & 0 \le x \le 1, \\ \infty, & \text{otherwise.} \end{cases}$
- The nonlinear eigenvalue problem

$$\mu\,\phi(x) = -\frac{1}{2}\phi''(x) + \beta\,|\phi(x)|^2\,\phi(x), \qquad 0 < x < 1,$$

$$\phi(0) = \phi(1) = 0 \qquad \text{with} \qquad \int_0^1 |\phi(x)|^2 dx = 1$$

- Case I: no interaction, i.e. $\beta = 0$
  - A complete set of orthonormal eigenfunctions

$$\phi_l(x) = \sqrt{2}\sin(l\pi x), \qquad \mu_l = \frac{1}{2}l^2\pi^2, \qquad l = 1, 2, 3, \cdots$$

Box Potential in 1D

- Ground state & its energy:

$$\phi_g(x) = \phi_g^0(x) = \sqrt{2}\sin(\pi x), \qquad E_g := E(\phi_g^0) = \frac{\pi^2}{2} = \mu_g := \mu(\phi_g^0)$$

- j-th-excited state & its energy

$$\phi_j(x) = \phi_j^0(x) = \sqrt{2}\sin((j+1)\pi x), \qquad E_j := E(\phi_j^0) = \frac{(j+1)^2\pi^2}{2} = \mu_j := \mu(\phi_j^0)$$

- Case II: weakly interacting regime, i.e. $|\beta| = o(1)$
  - Ground state & its energy:

$$\phi_g(x) \approx \phi_g^0(x) = \sqrt{2}\sin(\pi x), \quad E_g := E(\phi_g) \approx E(\phi_g^0) = \frac{\pi^2}{2} + \frac{3\beta}{2}, \quad \mu_g := \mu(\phi_g) \approx \mu(\phi_g^0) = \frac{\pi^2}{2} + 3\beta$$

  - j-th-excited state & its energy

$$\phi_j(x) \approx \phi_j^0(x) = \sqrt{2}\sin((j+1)\pi x), \quad E_j := E(\phi_j) \approx E(\phi_j^0) = \frac{(j+1)^2\pi^2}{2} + \frac{3\beta}{2},$$

$$\mu_j := \mu(\phi_j) \approx \mu(\phi_j^0) = \frac{(j+1)^2\pi^2}{2} + 3\beta$$

Box Potential in 1D

- Case III: Strongly interacting regime, i.e. $\beta \gg 1$
  - Thomas-Fermi approximation, i.e. drop the diffusion term

$$\mu_g^{\mathrm{TF}}\ \phi_g^{\mathrm{TF}}(x) = \beta\,|\,\phi_g^{\mathrm{TF}}(x)\,|^2\ \phi_g^{\mathrm{TF}}(x), \qquad 0 < x < 1, \qquad \Rightarrow \quad \phi_g^{\mathrm{TF}}(x) = \sqrt{\frac{\mu_g^{\mathrm{TF}}}{\beta}}$$

$$\Downarrow \int_0^1 |\,\phi_g^{\mathrm{TF}}(x)\,|^2\ dx = 1$$

$$\phi_{\mathrm{g}}(\mathrm{x}) \approx \phi_g^{\mathrm{TF}}(x) = 1, \qquad \mathrm{E}_{\mathrm{g}} \approx \mathrm{E}_g^{\mathrm{TF}} = \frac{\beta}{2}, \qquad \mu_{\mathrm{g}} \approx \mu_g^{\mathrm{TF}} = \beta,$$

- Boundary condition is NOT satisfied, i.e. $\phi_g^{\mathrm{TF}}(0) = \phi_g^{\mathrm{TF}}(1) = 1 \neq 0$
- Boundary layer near the boundary

Box Potential in 1D

– Matched asymptotic approximation

- Consider near x=0, rescale $x = \frac{1}{\sqrt{\mu_g}} X, \qquad \phi(x) = \sqrt{\frac{\mu_g}{\beta}}\,\Phi(x)$
- We get

$$\Phi(X) = -\frac{1}{2}\Phi''(X) + \Phi^3(X), \quad 0 \le X < \infty; \qquad \Phi(0) = 0, \quad \lim_{X\to\infty}\Phi(X) = 1$$

- The inner solution

$$\Phi(X) = \tanh(X), \quad 0 \le X < \infty \qquad \Rightarrow \quad \phi_g(x) \approx \sqrt{\frac{\mu_g}{\beta}}\tanh(\sqrt{\mu_g}\,x), \quad 0 \le x = o(1)$$

- Matched asymptotic approximation for ground state

$$\phi_g(x) \approx \phi_g^{\mathrm{MA}}(x) = \sqrt{\frac{\mu_g^{\mathrm{MA}}}{\beta}}\left[\tanh(\sqrt{\mu_g^{\mathrm{MA}}}\,x) + \tanh(\sqrt{\mu_g^{\mathrm{MA}}}(1-x)) - \tanh(\sqrt{\mu_g^{\mathrm{MA}}})\right], \quad 0 \le x \le 1$$

$$1 = \int_0^1 |\phi_g^{\mathrm{MA}}(x)|^2 dx \quad \Rightarrow \quad \mu_g \approx \mu_g^{\mathrm{MA}} = \beta + 2\sqrt{\beta+1} + 2 = \mu_g^{\mathrm{TF}} + 2\sqrt{\beta+1} + 2, \quad \beta \gg 1.$$

Box Potential in 1D

- Approximate energy

$$E_g \approx E_g^{\mathrm{MA}} = \frac{\beta}{2} + \frac{4}{3}\sqrt{\beta+1} + 2, \quad E_{\mathrm{int},g} \approx E_{\mathrm{int},g}^{\mathrm{MA}} = \frac{\beta}{2} + \frac{2}{3}\sqrt{\beta+1},$$

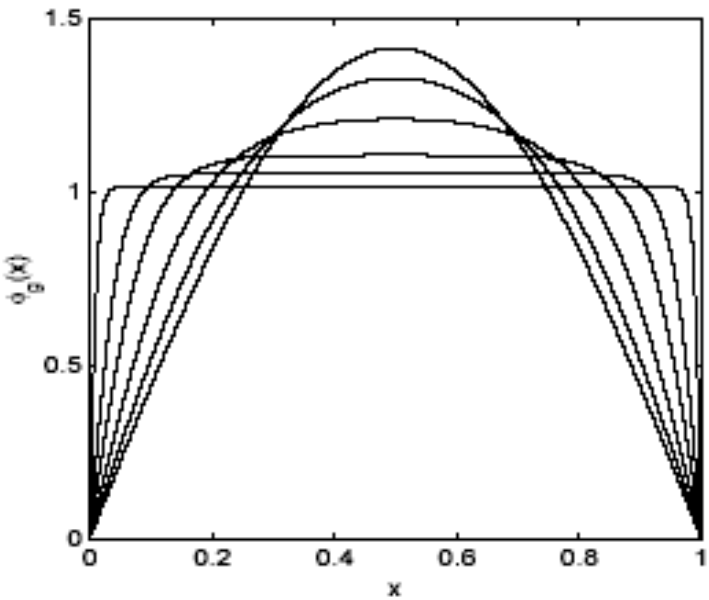
$$E_{\mathrm{kin},g} \approx E_{\mathrm{kin},g}^{\mathrm{MA}} = \frac{2}{3}\sqrt{\beta+1} + 2$$

- Asymptotic ratios:

$$\lim_{\beta\to\infty} \frac{E_g}{\mu_g} = \frac{1}{2}, \qquad \lim_{\beta\to\infty} \frac{E_{\mathrm{int},g}}{E_g} = 1, \qquad \lim_{\beta\to\infty} \frac{E_{\mathrm{kin},g}}{E_g} = 0,$$

- Width of the boundary layer:

$$O(1/\sqrt{\beta})$$



$1/\beta_1$	$4/25$	$2/25$	$1/25$	$1/50$	$1/100$	$1/400$
$\max\lvert\phi_g - \phi_g^{\mathrm{MA}}\rvert$	8.17E-3	9.24E-4	4.67E-5	8E-7	– –	– –
$\lVert\phi_g - \phi_g^{\mathrm{MA}}\rVert_{L^2}$	6.84E-3	8.05E-4	4.11E-5	6E-7	– –	– –
$\lvert E_{\mathrm{kin},g} - E_{\mathrm{kin},g}^{\mathrm{MA}}\rvert$	1.3018	0.9479	0.6464	0.4340	0.2946	0.1399
Rate		0.4577	0.5523	0.5747	0.5589	0.5372
$\lvert E_{\mathrm{int},g} - E_{\mathrm{int,g}}^{\mathrm{MA}}\rvert$	0.5948	0.4608	0.3218	0.2171	0.1473	0.0701
Rate		0.3683	0.5180	0.5678	0.5596	0.5356
$\lvert E_g - E_g^{\mathrm{MA}}\rvert$	0.7071	0.4871	0.3245	0.2171	0.1472	0.0698
Rate		0.5377	0.5860	0.5799	0.5606	0.5382
$\lvert\mu_g - \mu_g^{\mathrm{MA}}\rvert$	0.1124	0.0263	0.0027	0.0001	– –	– –
E_g/μ_g	0.6854	0.6234	0.5813	0.5543	0.5368	0.5175
$E_{\mathrm{int},g}/E_g$	0.4591	0.6042	0.7204	0.8042	0.8628	0.9323
$E_{\mathrm{kin},g}/E_g$	0.5409	0.3958	0.2796	0.1958	0.1372	0.0677

- Numerical observations:

$$\left\|\phi_g - \phi_g^{\mathrm{MA}}\right\|_{L^\infty} = O(e^{-3\sqrt{\beta}/2}), \qquad \left\|\phi_g - \phi_g^{\mathrm{MA}}\right\|_{L^2} = O(e^{-3\sqrt{\beta}/2}), \qquad \mu_g = \mu_g^{\mathrm{MA}} + O(e^{-3\sqrt{\beta}/2})$$

$$E_g = E_g^{\mathrm{MA}} + O(1/\sqrt{\beta}), \qquad E_{\mathrm{kin},g} = E_{\mathrm{kin},g}^{\mathrm{MA}} + O(1/\sqrt{\beta}), \qquad E_{\mathrm{int},g} = E_{\mathrm{int},g}^{\mathrm{MA}} + O(1/\sqrt{\beta})$$

Box Potential in 1D

- Matched asymptotic approximation for excited states

$$\phi_j(x) \approx \phi_j^{\mathrm{MA}}(x) = \sqrt{\frac{\mu_j^{\mathrm{MA}}}{\beta}} \quad [\sum_{l=0}^{[(j+1)/2]} \tanh(\sqrt{\mu_g^{\mathrm{MA}}}(x - \frac{2l}{j+1})) + \sum_{l=0}^{[j/2]} \tanh(\sqrt{\mu_g^{\mathrm{MA}}}(\frac{2l+1}{j+1} - x)) - C_j \tanh(\sqrt{\mu_g^{\mathrm{MA}}})]$$

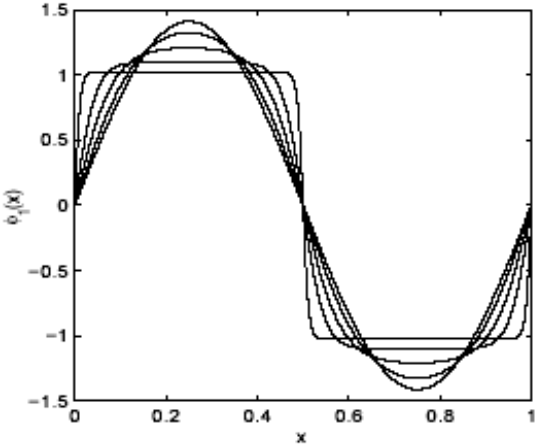
- Approximate chemical potential & energy

$$\mu_j \approx \mu_j^{\mathrm{MA}} = \beta + 2(j+1)\sqrt{\beta + (j+1)^2} + 2(j+1)^2,$$

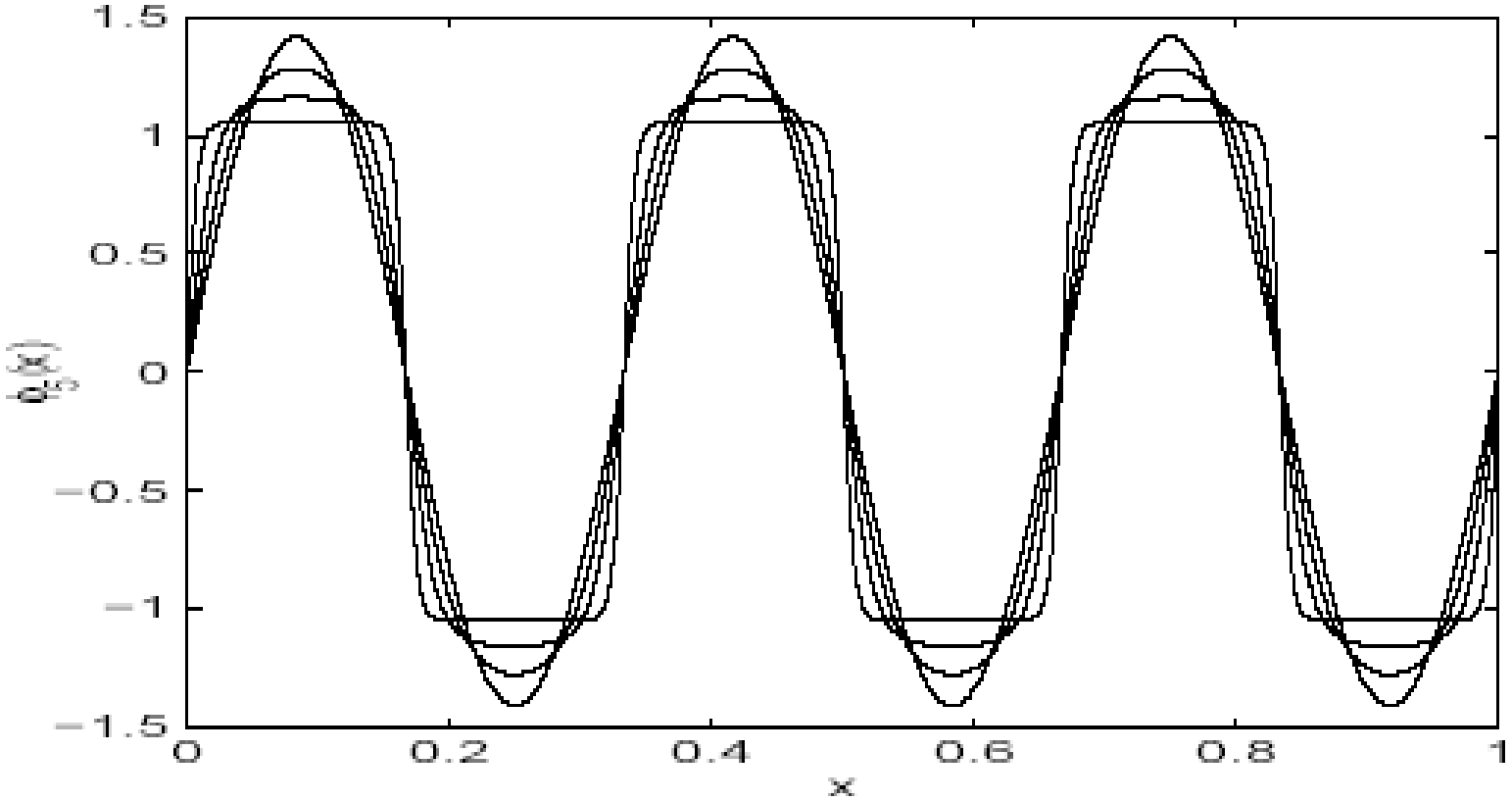
$$E_j \approx E_j^{\mathrm{MA}} = \frac{\beta}{2} + \frac{4}{3}(j+1)\sqrt{\beta + (j+1)^2},$$

$$E_{\mathrm{int},j} \approx E_{\mathrm{int},j}^{\mathrm{MA}} = \frac{\beta}{2} + \frac{2}{3}(j+1)\sqrt{\beta + (j+1)^2},$$

$$E_{\mathrm{kin},j} \approx E_{\mathrm{kin},j}^{\mathrm{MA}} = \frac{2}{3}(j+1)\sqrt{\beta + (j+1)^2} + 2(j+1)^2$$



Fifth excited states



Energy & Chemical potential

β_1	0	25	100	400	1600	6400	25600
E_g	4.9348	21.623	65.547	228.77	855.38	3308.7	13015
E_1	19.739	37.689	86.493	262.19	915.08	3421.5	13235
E_2	44.413	62.765	114.45	300.98	979.42	3538.7	13458
E_3	78.956	97.473	150.76	345.97	1048.8	3660.3	13686
E_4	123.37	141.97	196.17	397.99	1123.5	3786.6	13917
E_5	177.65	196.30	251.06	457.80	1203.9	3917.7	14153
μ_g	4.9348	37.201	122.10	442.05	1682.0	6562.0	25922
μ_1	19.739	54.990	148.80	488.40	1768.2	6728.1	26248
μ_2	44.413	80.758	180.96	539.34	1858.7	6898.3	26578
μ_3	78.956	151.77	219.96	595.21	1953.6	7072.8	26912
μ_4	123.37	160.42	267.06	656.48	2053.1	7251.6	27251
μ_5	177.65	214.83	323.03	723.84	2157.4	7434.7	27593

Box potential in 1D

- Boundary layers & interior layers with width

$$O(1/\sqrt{\beta})$$

- Observations: energy & chemical potential are in the same order

$$E(\phi_g) < E(\phi_1) < E(\phi_2) < \cdots \qquad \Rightarrow \qquad \mu(\phi_g) < \mu(\phi_1) < \mu(\phi_2) < \cdots$$

- Asymptotic ratios:

$$\lim_{\beta\to\infty} \frac{E_j}{\mu_j} = \frac{1}{2}, \qquad \lim_{\beta\to\infty} \frac{E_{\text{int},j}}{E_j} = 1, \qquad \lim_{\beta\to\infty} \frac{E_{\text{kin},j}}{E_j} = 0,$$

$$\lim_{\beta\to\infty} \frac{E_j}{E_g} = 1, \qquad \lim_{\beta\to\infty} \frac{\mu_j}{\mu_g} = 1, \qquad \lim_{\beta\to\infty} \frac{E_j}{\mu_g} = 0,$$

- Extension to high dimensions

Harmonic Oscillator Potential in 1D

- The potential: $V(x) = \frac{x^2}{2}$
- The nonlinear eigenvalue problem

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

- Case I: no interaction, i.e. $\beta = 0$
  - A complete set of orthonormal eigenfunctions

$$\phi_l(x) = (2^l\, l!)^{-1/2} \frac{1}{\pi^{1/4}} e^{-x^2/2}\, H_l(x), \qquad \mu_l = l + \frac{1}{2}, \qquad l = 0, 1, 2, 3, \cdots$$

$$H_l(x) = (-1)^l\, e^{x^2} \frac{d^l e^{-x^2}}{dx^l}: \text{ Hermite polynomials with}$$

$$H_0(x) = 1, \quad H_1(x) = 2x, \quad H_2(x) = 4x^2 - 2, \quad \cdots$$

Harmonic Oscillator Potential in 1D

- Ground state & its energy:

$$\phi_g(x) = \phi_g^0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}, \qquad E_g := E(\phi_g^0) = \frac{1}{2} = \mu_g := \mu(\phi_g^0)$$

- j-th-excited state & its energy

$$\phi_j(x) = \phi_j^0(x) = (2^j \; j!)^{-1/2} \frac{1}{\pi^{1/4}} e^{-x^2/2} \; H_j(x), \qquad E_j := E(\phi_j^0) = \frac{(j+1)}{2} = \mu_j := \mu(\phi_j^0)$$

- Case II: weakly interacting regime, i.e. $|\beta| = o(1)$
  - Ground state & its energy:

$$\phi_g(x) \approx \phi_g^0(x) = \frac{1}{\pi^{1/4}} e^{-x^2/2}, \quad E_g := E(\phi_g) \approx E(\phi_g^0) = \frac{1}{2} + \frac{\beta}{2} C_0, \quad \mu_g := \mu(\phi_g) \approx \mu(\phi_g^0) = \frac{1}{2} + \beta C_0$$

  - j-th-excited state & its energy

$$\phi_j(x) \approx \phi_j^0(x), \quad E_j := E(\phi_j) \approx E(\phi_j^0) = \frac{(j+1)}{2} + \frac{\beta}{2} C_j,$$

$$\mu_j := \mu(\phi_j) \approx \mu(\phi_j^0) = \frac{(j+1)}{2} + \beta C_j \quad \text{with} \quad C_j = \int_{-\infty}^{\infty} |\phi_j^0(x)|^4 \, dx$$

Harmonic Oscillator Potential in 1D

- Case III: Strongly interacting regime, i.e. $\beta \gg 1$
  - Thomas-Fermi approximation, i.e. drop the diffusion term

$$\mu_g^{\mathrm{TF}}\ \phi_g^{\mathrm{TF}}(x) = V(x)\,\phi_g^{\mathrm{TF}}(x) + \beta\,|\phi_g^{\mathrm{TF}}(x)|^2\ \phi_g^{\mathrm{TF}}(x) \quad \Rightarrow \quad \phi_g^{\mathrm{TF}}(x) = \begin{cases} \sqrt{(\mu_g^{\mathrm{TF}} - x^2/2)/\beta}, & |x| \le \sqrt{2\mu_g^{\mathrm{TF}}} \\ 0, & \text{otherwise} \end{cases}$$

$$1 = \int_{-\infty}^{\infty} |\phi_g^{\mathrm{TF}}(x)|^2\, dx = \frac{2(2\mu_g^{\mathrm{TF}})^{3/2}}{3\beta} \qquad \Rightarrow \qquad \mu_g \approx \mu_g^{\mathrm{TF}} = \frac{1}{2}\left(\frac{3\beta}{2}\right)^{2/3}$$

  - Characteristic length: $O(\beta^{1/3})$
  - It is NOT differentiable at $x = \pm\sqrt{2\mu_g^{\mathrm{TF}}}$
  - The energy is infinite by direct definition:

$$E(\phi_g^{\mathrm{TF}}) = \infty, \quad E_{\mathrm{kin}}(\phi_g^{\mathrm{TF}}) = \infty$$

Harmonic Oscillator Potential in 1D

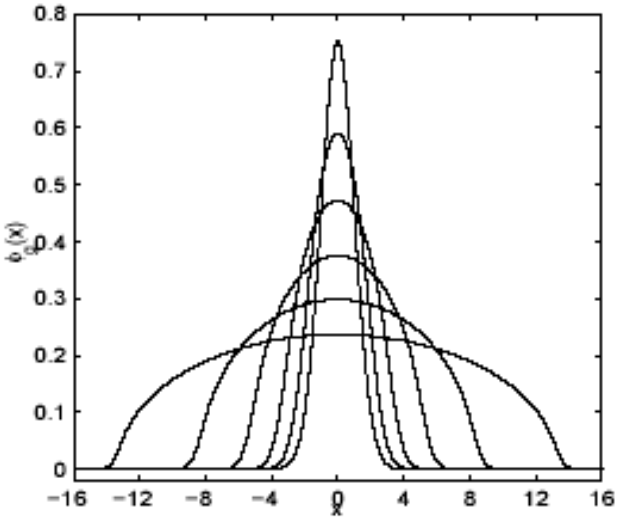
– A new way to define the energy

$$E_{\text{int},g} \approx E_{\text{int},g}^{\text{TF}} = E_{\text{int}}(\phi_g^{\text{TF}}) = \frac{1}{5}\left(\frac{3\beta}{2}\right)^{2/3},$$

$$E_{\text{pot},g} \approx E_{\text{pot},g}^{\text{TF}} = E_{\text{pot}}(\phi_g^{\text{TF}}) = \frac{1}{10}\left(\frac{3\beta}{2}\right)^{2/3}$$

$$E_g = \mu_g - E_{\text{int},g} \approx \mu_g^{\text{TF}} - E_{\text{int},g}^{\text{TF}} = \frac{3}{10}\left(\frac{3\beta}{2}\right)^{2/3} := E_g^{\text{TF}},$$

$$E_{\text{kin},g} \approx E_g^{\text{TF}} - E_{\text{int},g}^{\text{TF}} - E_{\text{pot},g}^{\text{TF}} = 0$$



– Asymptotic ratios

$$\lim_{\beta\to\infty}\frac{E_g}{\mu_g} = \frac{3}{5}, \qquad \lim_{\beta\to\infty}\frac{E_{\text{int},g}}{E_g} = \frac{2}{3}, \qquad \lim_{\beta\to\infty}\frac{E_{\text{pot},g}}{E_g} = \frac{1}{3}, \qquad \lim_{\beta\to\infty}\frac{E_{\text{kin},g}}{E_g} = 0,$$

$1/\beta_1$	$1/100$	$1/200$	$1/400$	$1/800$	$1/1600$	$1/6400$
$\max\lvert\phi_g - \phi_g^{\mathrm{TF}}\rvert$	0.0788	0.0605	0.0464	0.0355	0.0272	0.0159
Rate		0.3807	0.3836	0.3840	0.3852	0.3872
$\lVert\phi_g - \phi_g^{\mathrm{TF}}\rVert_{L^2}$	0.0571	0.04230	0.0312	0.0230	0.0170	0.0092
Rate		0.4350	0.4371	0.4389	0.4404	0.4427
$\lvert E_{\mathrm{pot},g} - E_{\mathrm{pot},g}^{\mathrm{TF}}\rvert$	0.0246	0.0171	0.0118	0.0080	0.0054	0.0023
Rate		0.5238	0.5383	0.5528	0.5687	0.6196
$\lvert E_{\mathrm{int},g} - E_{\mathrm{int},g}^{\mathrm{TF}}\rvert$	0.0204	0.0144	0.0101	0.0070	0.0047	0.0021
Rate		0.4980	0.5167	0.5348	0.5531	0.6051
$E_{\mathrm{kin},g} - 0$	0.0350	0.0245	0.0170	0.0117	0.0080	0.0037
Rate		0.5134	0.5267	0.5381	0.5478	0.5599
$\lvert E_g - E_g^{\mathrm{TF}}\rvert$	0.0392	0.0272	0.0187	0.0128	0.0087	0.0039
Rate		0.5280	0.5394	0.5492	0.5582	0.5725
$\lvert\mu_g - \mu_g^{\mathrm{TF}}\rvert$	0.0188	0.0128	0.0086	0.0058	0.0039	0.0019
Rate		0.5613	0.5651	0.5659	0.5638	0.5329
E_g/μ_g	0.6020	0.6009	0.6004	0.6002	0.6001	0.6000
$E_{\mathrm{int},g}/E_g$	0.6612	0.6643	0.6656	0.6662	0.6665	0.6666
$E_{\mathrm{pot},g}/E_g$	0.3347	0.3339	0.3336	0.3334	0.3334	0.3333

- Numerical observations:

$$\left\|\phi_g - \phi_g^{\mathrm{TF}}\right\|_{L^\infty} = O\left(\frac{\ln\beta}{\beta^{2/5}}\right), \qquad \left\|\phi_g - \phi_g^{\mathrm{MA}}\right\|_{L^2} = O\left(\frac{\ln\beta}{\beta^{2/5}}\right), \qquad \mu_g = \mu_g^{\mathrm{MA}} + O\left(\frac{\ln\beta}{\beta^{2/3}}\right)$$

$$E_g = E_g^{\mathrm{MA}} + O\left(\frac{\ln\beta}{\beta^{2/3}}\right), \qquad E_{\mathrm{kin},g} = E_{\mathrm{kin},g}^{\mathrm{MA}} + O\left(\frac{\ln\beta}{\beta^{2/3}}\right), \qquad E_{\mathrm{int},g} = E_{\mathrm{int},g}^{\mathrm{MA}} + O\left(\frac{\ln\beta}{\beta^{2/3}}\right)$$

Harmonic Oscillator Potential in 1D

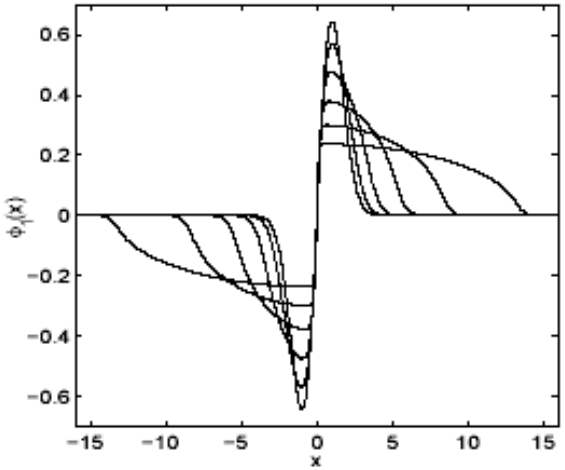
– Thomas-Fermi approximation for first excited state

$$\mu_1^{\mathrm{TF}}\ \phi_1^{\mathrm{TF}}(x) = V(x)\,\phi_1^{\mathrm{TF}}(x) + \beta\,|\phi_1^{\mathrm{TF}}(x)|^2\ \phi_1^{\mathrm{TF}}(x)$$

$$\phi_1^{\mathrm{TF}}(x) = \begin{cases} \mathrm{sign}(x)\sqrt{(\mu_1^{\mathrm{TF}} - x^2/2)/\beta}, & 0 < |x| \le \sqrt{2\mu_1^{\mathrm{TF}}} \\ 0, & \text{otherwise} \end{cases}$$

$$1 = \int_{-\infty}^{\infty} |\phi_1^{\mathrm{TF}}(x)|^2\ dx = \frac{2(2\mu_1^{\mathrm{TF}})^{3/2}}{3\beta} \qquad \Rightarrow \qquad \mu_1 \approx \mu_1^{\mathrm{TF}} = \frac{1}{2}\left(\frac{3\beta}{2}\right)^{2/3}$$

- Jump at x=0!
- Interior layer at x=0



Harmonic Oscillator Potential in 1D

- Matched asymptotic approximation

$$\phi_1^{\mathrm{MA}}(x) = \sqrt{\frac{\mu_1^{\mathrm{MA}}}{\beta}}[\tanh(\sqrt{\mu_1^{\mathrm{MA}}}\,x) - \mathrm{sign}(x)] + \begin{cases} \mathrm{sign}(x)\sqrt{(\mu_1^{\mathrm{MA}} - x^2/2)/\beta}, & 0 < |x| \le \sqrt{2\mu_1^{\mathrm{MA}}} \\ 0, & \text{otherwise} \end{cases}$$

- Width of interior layer:

$$O(1/\sqrt{\mu_1^{\mathrm{MA}}}) = O(1/\beta^{1/3}) \quad \Leftarrow \quad \mu_1^{\mathrm{MA}} = O(\beta^{2/3})$$

- Ordering: $E(\phi_g) < E(\phi_1) \Rightarrow \mu(\phi_g) < \mu(\phi_1)$

β_1	0	25	100	400	1600	6400	25600
E_g	0.5000	3.4402	8.5085	21.360	55.786	135.51	341.46
E_1	1.5000	4.2115	9.2419	22.078	54.497	136.22	342.17
μ_g	0.5000	5.6421	14.134	35.578	89.632	225.85	569.10
μ_1	1.5000	6.3732	14.850	36.288	90.340	226.56	569.80

Harmonic Oscillator Potential

- Extension to high dimensions
- Identity of energies for stationary states in d-dim.

$$2\,E_{\text{kin}} - 2\,E_{\text{pot}} + d\;E_{\text{int}} = 0$$

  - Scaling transformation

$$\psi(\vec{x}) = (1+\nu)^{d/2}\psi_0((1+\nu)\vec{x}) \qquad \text{with} \quad \psi_0(\vec{x})\text{: a stationary state}$$

  - Energy variation vanishes at first order in ν

$$E(\psi(\vec{x})) = (1+\nu)^2 E_{\text{kin}}(\psi_0) + (1+\nu)^{-2} E_{\text{pot}}(\psi_0) + (1+\nu)^d E_{\text{int}}(\psi_0)$$

$$\frac{d}{d\nu} E(\psi(\vec{x}))\,|_{\nu=0} = 0$$

BEC on a ring

- The potential: $V(x) = 0$ on an interal
- The nonlinear eigenvalue problem

$$\mu\,\phi(\theta) = -\frac{1}{2}\phi''(\theta) + \beta\,|\phi(\theta)|^2\,\phi(\theta), \qquad 0 \le \theta \le 2\pi,$$

$$\phi(\theta + 2\pi) = \phi(\theta), \qquad \text{with} \qquad \int_0^{2\pi} |\phi(\theta)|^2 d\theta = 1$$

- For linear case, i.e. $\beta = 0$
  - A complete set of orthonormal eigenfunctions

$$\phi_0(\theta) = \frac{1}{\sqrt{2\pi}}, \quad \phi_{2l}(\theta) = \frac{1}{\sqrt{\pi}}\cos(l\theta), \quad \phi_{2l+1}(\theta) = \frac{1}{\sqrt{\pi}}\sin(l\theta);$$

$$\mu_0 = 0, \quad \mu_{2l} = \mu_{2l+1} = \frac{l^2}{2}, \qquad l = 1, 2, 3, \cdots$$

BEC on a ring

- Ground state & its energy:

$$\phi_g(x) = \phi_g^0(x) = \frac{1}{\sqrt{2\pi}}, \qquad E_g := E(\phi_g^0) = 0 = \mu_g := \mu(\phi_g^0)$$

- j-th-excited state & its energy

$$\phi_j(x) = \phi_j^0(x) = \frac{1}{\sqrt{\pi}}\cos(l\theta), \qquad E_j := E(\phi_j^0) = \frac{j^2}{2} = \mu_j := \mu(\phi_j^0)$$

- Some properties $\qquad |\beta| = o(1)$

- Ground state & its energy

$$\phi_g(x) = \phi_g^0(x) = \frac{1}{\sqrt{2\pi}}, \qquad E_g := E(\phi_g^0) = \frac{\beta}{8\pi}, \quad \mu_g := \mu(\phi_g^0) = \frac{\beta}{4\pi}$$

- With a shift:

$$\phi(\theta) \text{ is a solution } \Rightarrow \phi(\theta + \theta_0) \text{ is also a solution}$$

- Interior layer can be happened at any point in excited states

Numerical methods for ground states

- Runge-Kutta method: (M. Edwards and K. Burnett, Phys. Rev. A, 95')
- Analytical expansion: (R. Dodd, J. Res. Natl. Inst. Stan., 96')
- Explicit imaginary time method: (S. Succi, M.P. Tosi et. al., PRE, 00')
- Minimizing $E(\phi)$ by FEM: (Bao & W. Tang, JCP, 02')
- Normalized gradient flow: (Bao & Q. Du, SIAM Sci. Comput., 03')
  - Backward-Euler + finite difference (BEFD)
  - Backward Euler + spectral method (BESP): (Bao, Chern & Lim, JCP, 06')
- Gauss-Seidel iteration method: (W.W. Lin et al., JCP, 05')
- Spectral method + stabilization: (Bao, I. Chern & F. Lim, JCP, 06')
- Reguarized Newton method: (Bao, Wen & Xu, 15')

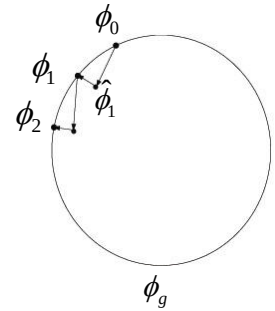
Imaginary time method

- Idea: Steepest decent method + Projection

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

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

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



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

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

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

- Physical institutive in linear case
  - Solution of GPE: $\psi(\vec{x},t) = \sum_{j=0}^{\infty} a_j\ e^{-i\mu_j t}\ \phi_j(\vec{x})$ with $\psi(\vec{x},0) = \psi_0(\vec{x}) = \sum_{j=0}^{\infty} a_j\ \phi_j(\vec{x})$
  - Imaginary time dynamics: $\tau = i\,t$

$$\phi(\vec{x},\tau) = \psi(\vec{x},t) = \sum_{j=0}^{\infty} a_j\ e^{-\mu_j\tau}\ \phi_j(\vec{x}) \overset{\mu_0<\mu_1<\cdots}{\Rightarrow} \frac{\phi(\vec{x},\tau)}{a_0\ e^{-\mu_0\tau}} \overset{\tau\to\infty}{\to} \phi_0(\vec{x}):\ \text{grond state}$$

Normalized gradient flow

- Idea: (Bao & Q. Du, SIAM Sci. Comput., 03')
  - The projection step is equivalent to solve an ODE

$$\phi_t(\vec{x},t) = \mu_\phi(t,\Delta t_n)\phi(\vec{x},t), \quad t_n < t < t_{n+1} \quad \text{with} \quad \mu_\phi(t,k) = -\frac{1}{2\Delta t_n}\ln\left\|\phi(\vec{x},t_{n+1}^-)\right\|^2 \quad \& \quad \phi(\vec{x},t_n^+) = \phi(\vec{x},t_{n+1}^-)$$

  - Gradient flow with discontinuous coefficients:

$$\phi_t(\vec{x},t) = \frac{1}{2}\nabla^2\phi - V(\vec{x})\,\phi - \beta\,|\phi|^2\,\phi + \mu_\phi(t,\Delta t_n)\,\phi, \quad t \ge 0,$$

  - Letting time step go to 0

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

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

  - Mass conservation & Energy diminishing

$$\|\phi(.,t)\| = \|\phi_0\| = 1, \qquad \frac{d}{dt}E(\phi(.,t)) \le 0, \qquad t \ge 0$$

Fully discretization

- Consider in 1D:

$$\phi_t(x,t) = \frac{1}{2}\phi_{xx} - V(x)\phi - \beta|\phi|^2\phi, \quad x \in \Omega = (a,b), \quad t_n \le t < t_{n+1}, \quad \phi(a,t) = \phi(b,t) = 0$$

$$\phi(x,t_{n+1}) = \frac{\phi(x,t_{n+1}^-)}{\|\phi(x,t_{n+1}^-)\|}, \qquad \phi(x,0) = \phi_0(\mathrm{x}) \quad \text{with} \quad \|\phi_0(x)\| = 1.$$

- Different Numerical Discretizations
  - Physics literatures: Crank-Nicolson FD or Forward Euler FD
  - BEFD: Energy diminishing & monotone (Bao & Q. Du, SIAM Sci. Comput., 03')
  - BESP: Spectral accuracy in space & stable (Bao, I. Chern & F. Lim, JCP, 06')
  - Crank-Ncolson FD for continuous normalized gradient flow

Backward Euler Finite Difference

- Mesh and time steps: $h = \Delta x = \dfrac{b-a}{M}; \quad k = \Delta t > 0;$

$$x_j = a + j\,h, \quad j = 0,1,\cdots,M; \quad t_n = n\,k,\ \mathrm{k}=0,1,2,\cdots; \qquad \phi_j^n \approx \phi(\mathrm{x_j},\mathrm{t_n})$$

- BEFD discretization

$$\frac{\phi_j^* - \phi_j^n}{k} = \frac{1}{2h^2}[\phi_{j+1}^* - 2\phi_j^* + \phi_{j-1}^*] - V(x_j)\phi_j^* - \beta(\phi_j^n)^2\phi_j^*, \quad j = 1,\ldots,M-1,$$

$$\phi_0^* = \phi_M^* = 0, \qquad \phi_j^0 = \phi_0(x_j), \quad j = 0,1,\ldots,M, \tag{3.4}$$

$$\phi_j^{n+1} = \frac{\phi_j^*}{\|\phi^*\|}, \quad j = 0,\ldots,M,\ n = 0,1,\ldots,$$

where the norm is defined as $\|\phi^*\|^2 = h\sum_{j=1}^{M-1}(\phi_j^*)^2$.

- 2nd order in space; unconditional stable; at each step, only a linear system with sparse matrix to be solved!

Backward Euler Spectral method

- Discretization $\mu_l = \frac{\pi l}{b-a}, \qquad (\hat{U})_l = \sum_{j=1}^{M-1} U_j \, \sin(\mu_l(x_j - a)), \quad l = 1, 2, \cdots, M-1.$

$$\frac{\phi_j^* - \phi_j^n}{\Delta t} = \frac{1}{2} D_{xx}^s \phi^* |_{x=x_j} - V(x_j)\phi_j^* - \beta |\phi_j^n|^2 \phi_j^*, \quad j = 1, 2, \cdots, M-1,$$

$$\phi_0^* = \phi_M^* = 0, \qquad \phi_j^0 = \phi_0(x_j), \quad j = 0, 1, \cdots, M,$$

$$\phi_j^{n+1} = \frac{\phi_j^*}{\|\phi^*\|}, \qquad j = 0, 1, \cdots, M, \quad n = 0, 1, \cdots ;$$

$$D_{xx}^s U|_{x=x_j} = -\frac{2}{M} \sum_{l=1}^{M-1} \mu_l^2 (\hat{U})_l \, \sin(\mu_l(x_j - a)), \qquad j = 1, 2, \cdots, M-1,$$

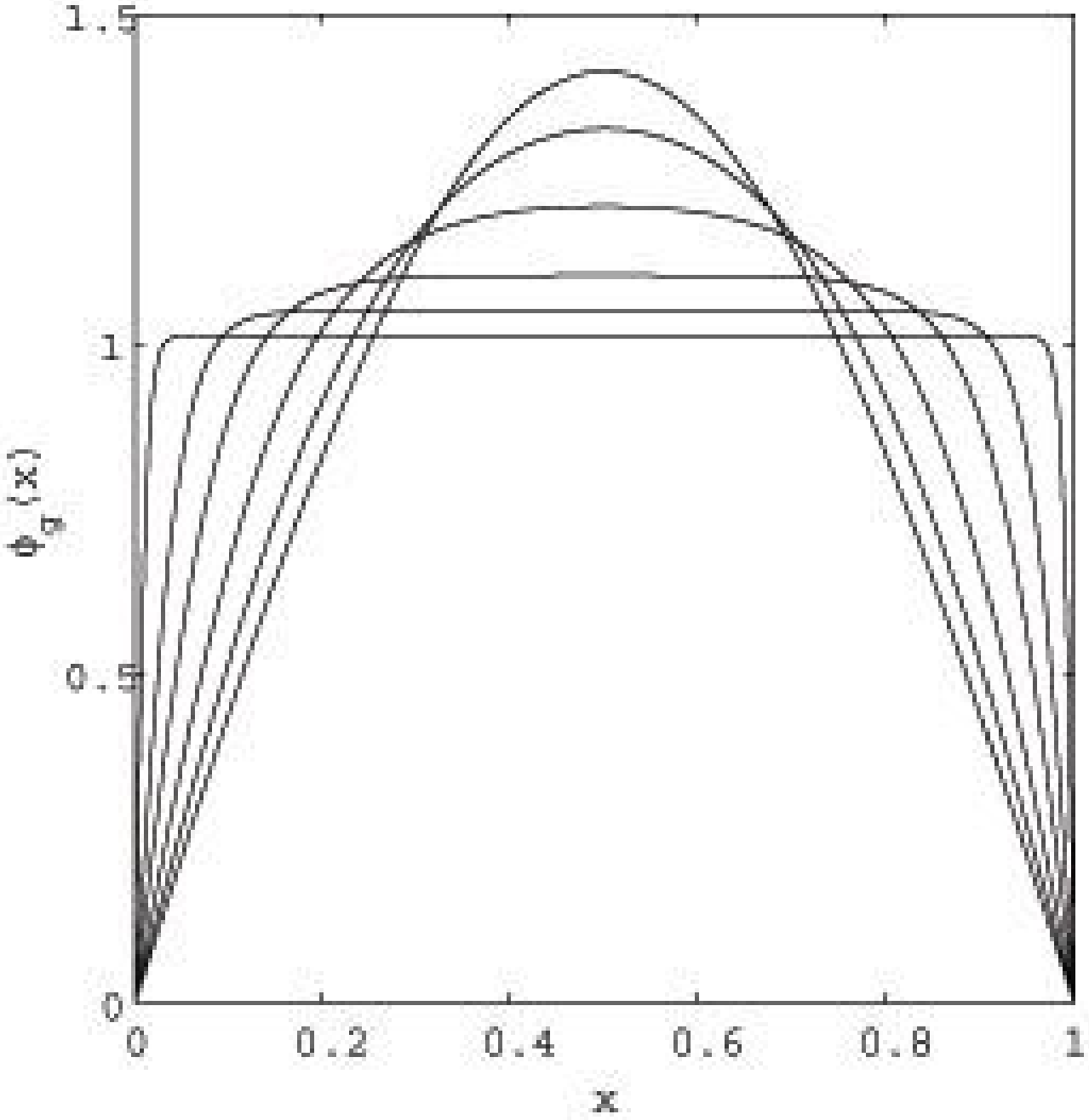
$$\frac{\phi_j^{*,m+1} - \phi_j^n}{\Delta t} = \frac{1}{2} D_{xx}^s \phi^{*,m+1}\Big|_{x=x_j} - \alpha \phi_j^{*,m+1} + \left(\alpha - V(x_j) - \beta |\phi_j^n|^2\right) \phi_j^{*,m}, \; m \geq 0,$$

$$\phi_j^{*,0} = \phi_j^n, \qquad j = 0, 1, \cdots, M;$$

- Spectral order in space; efficient & accurate

Ground states

- Numerical results (Bao&W. Tang, JCP, 03'; Bao, F. Lim & Y. Zhang, TTSP, 06')
  - In 1d
    - Box potential: $V(x) = 0 \quad 0 \le x \le 1; \quad \infty \quad \text{otherwise}$
      - Ground state; excited states: first fifth
    - Harmonic oscillator potential: $V(x) = x^2/2$
      - ground & first excited & Energy and chemical potential
    - Double well potential : $V(x) = (4 - x^2)^2/2$
      - Ground & asymptotic excited state
    - Optical lattice potential: $V(x) = x^2/2 + 12\sin^2(4x)$
      - Ground & asymptotic excited state with potential next



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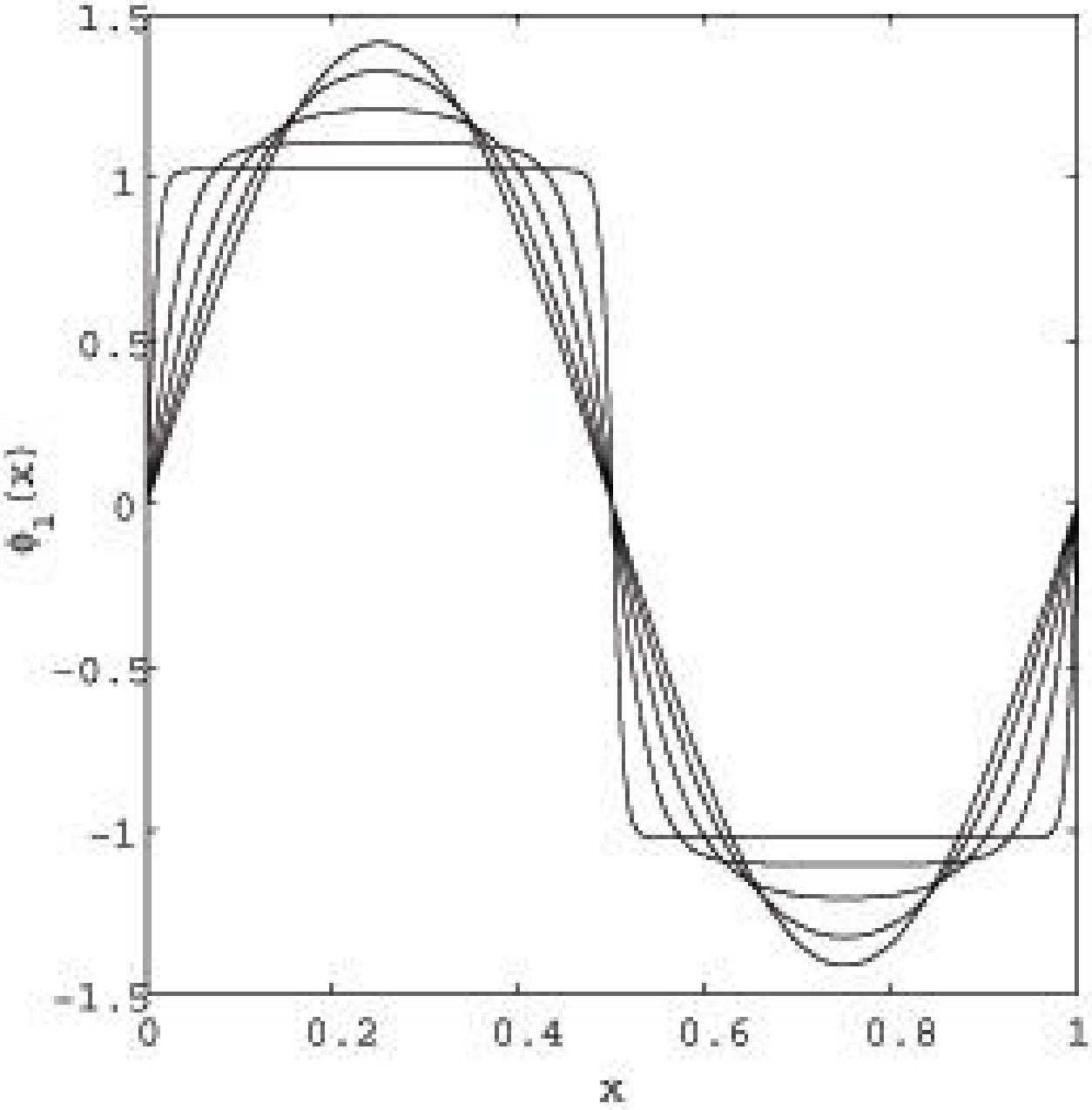

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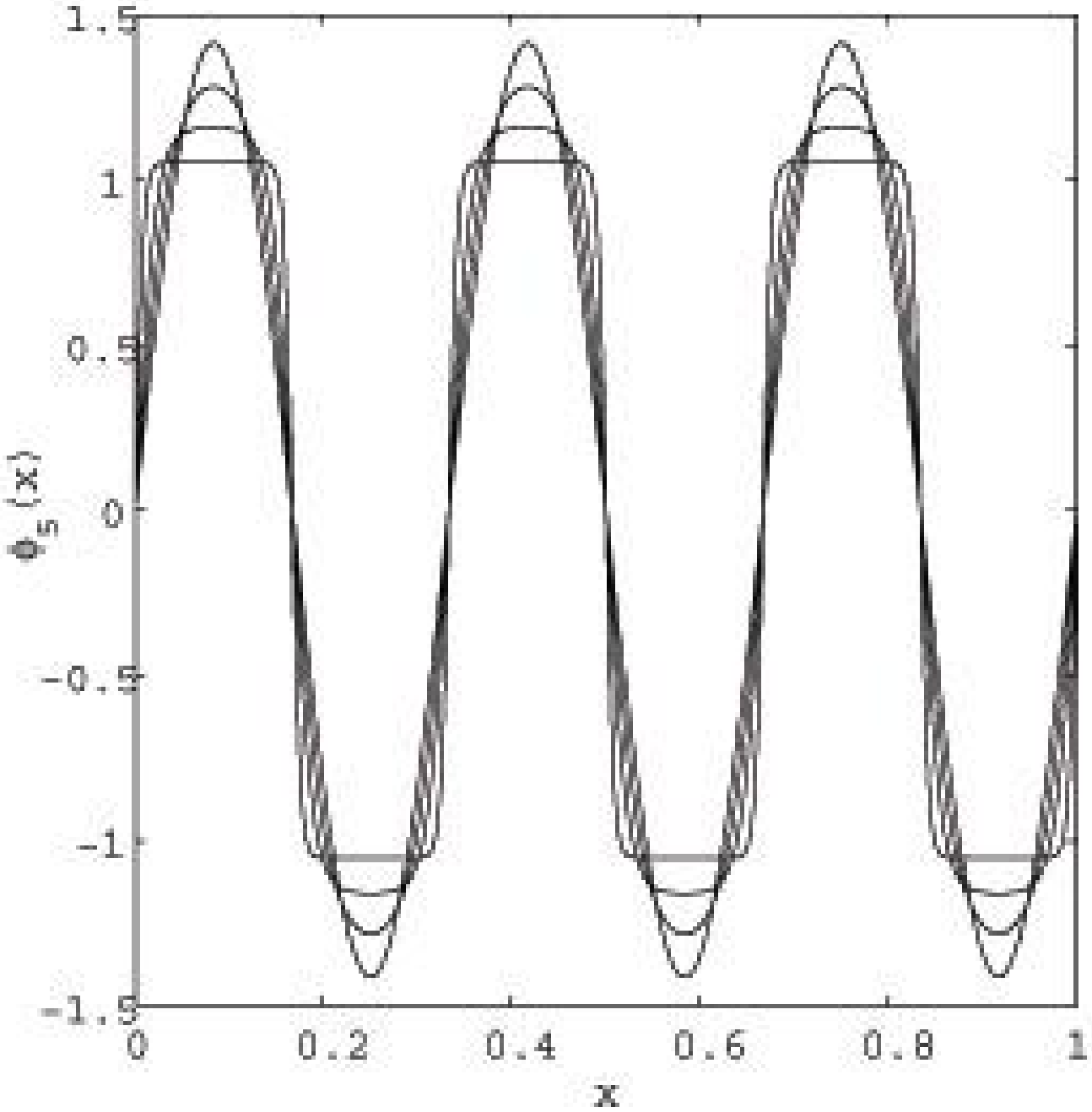

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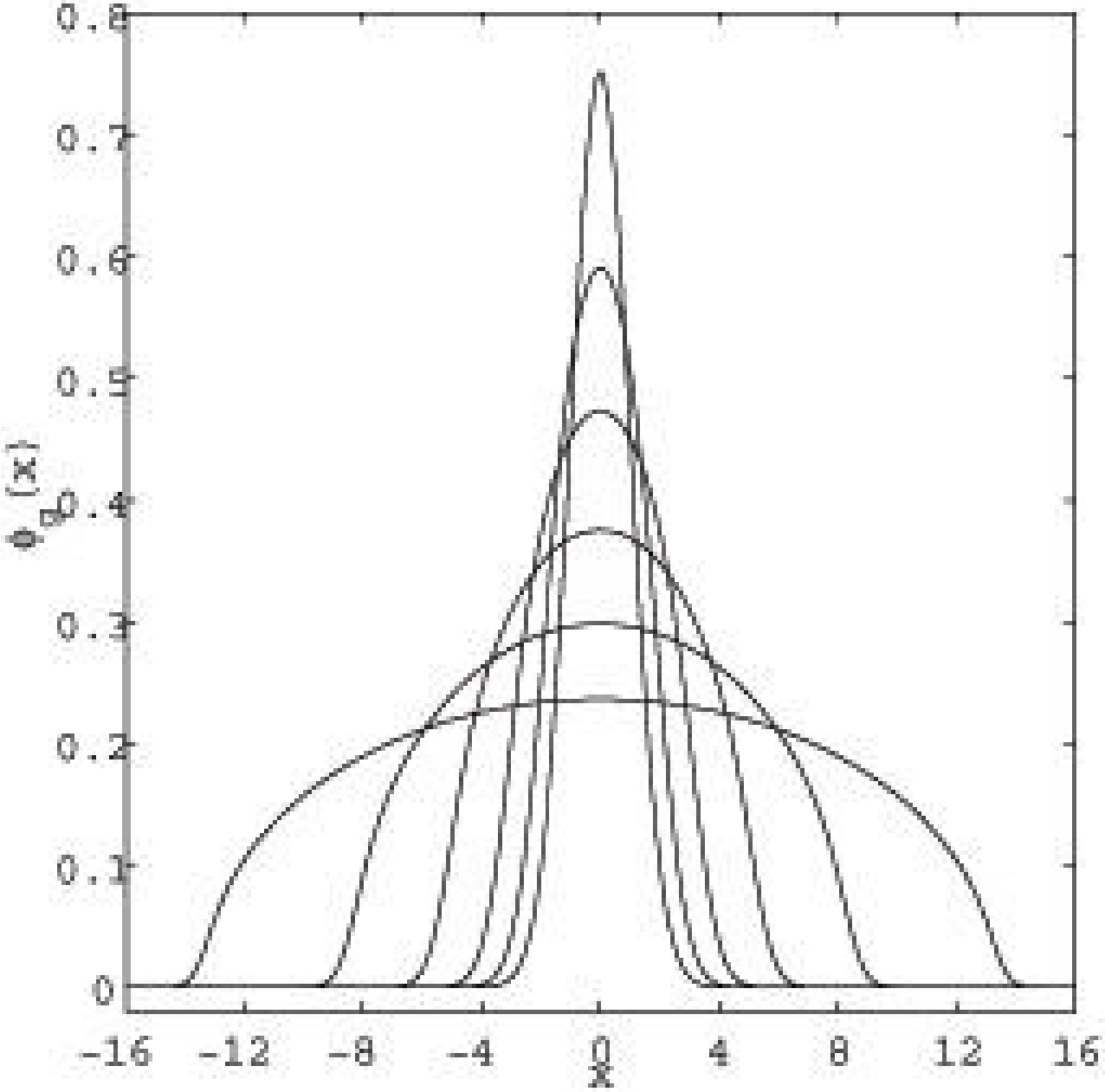

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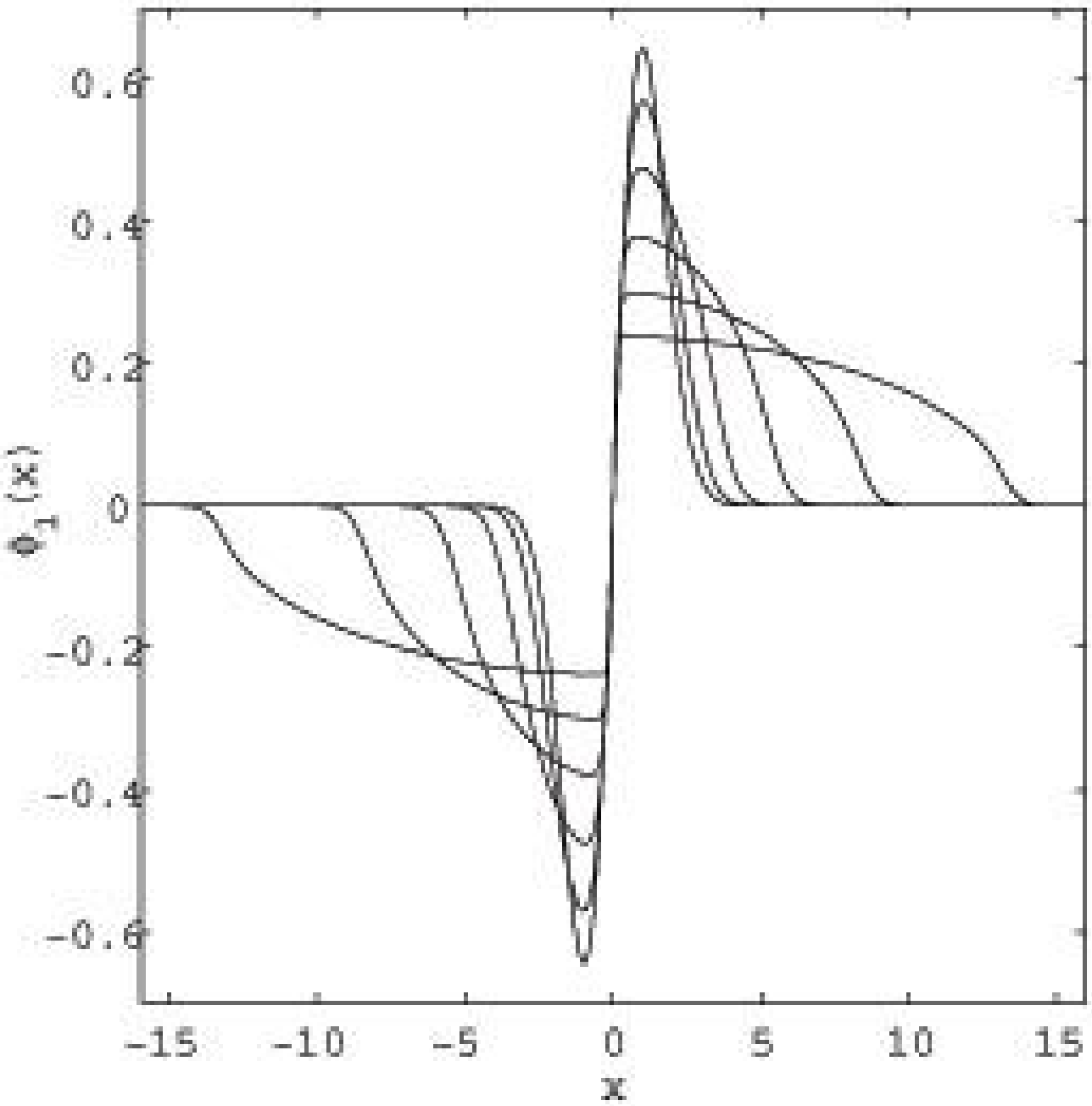

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β	$E(\phi_g)$	$E(\phi_1)$	$E(\phi_2)$	$E(\phi_3)$	$\mu(\phi_g)$	$\mu(\phi_1)$	$\mu(\phi_2)$	$\mu(\phi_3)$
0	0.5000	1.5000	2.5000	3.500	0.5000	1.5000	2.5000	3.500
3.1371	1.0441	1.9414	2.8865	3.8505	1.5266	2.3578	3.2590	4.1919
31.371	3.9810	4.7438	5.5573	6.4043	6.5527	7.2802	8.0432	8.8349
156.855	11.464	12.191	12.944	13.719	19.070	19.784	20.512	21.252
313.71	18.171	18.891	19.629	20.383	30.259	30.971	31.691	32.419

Observations

$E(\phi_g) < E(\phi_1) < E(\phi_2) < \cdots \Rightarrow \quad \mu(\phi_g) < \mu(\phi_1) < \mu(\phi_2) < \cdots,$ for any fixed β

$$\lim_{\beta \to +\infty} \frac{E(\phi_j)}{E(\phi_g)} = 1 \qquad \lim_{\beta \to +\infty} \frac{\mu(\phi_j)}{\mu(\phi_g)} = 1$$

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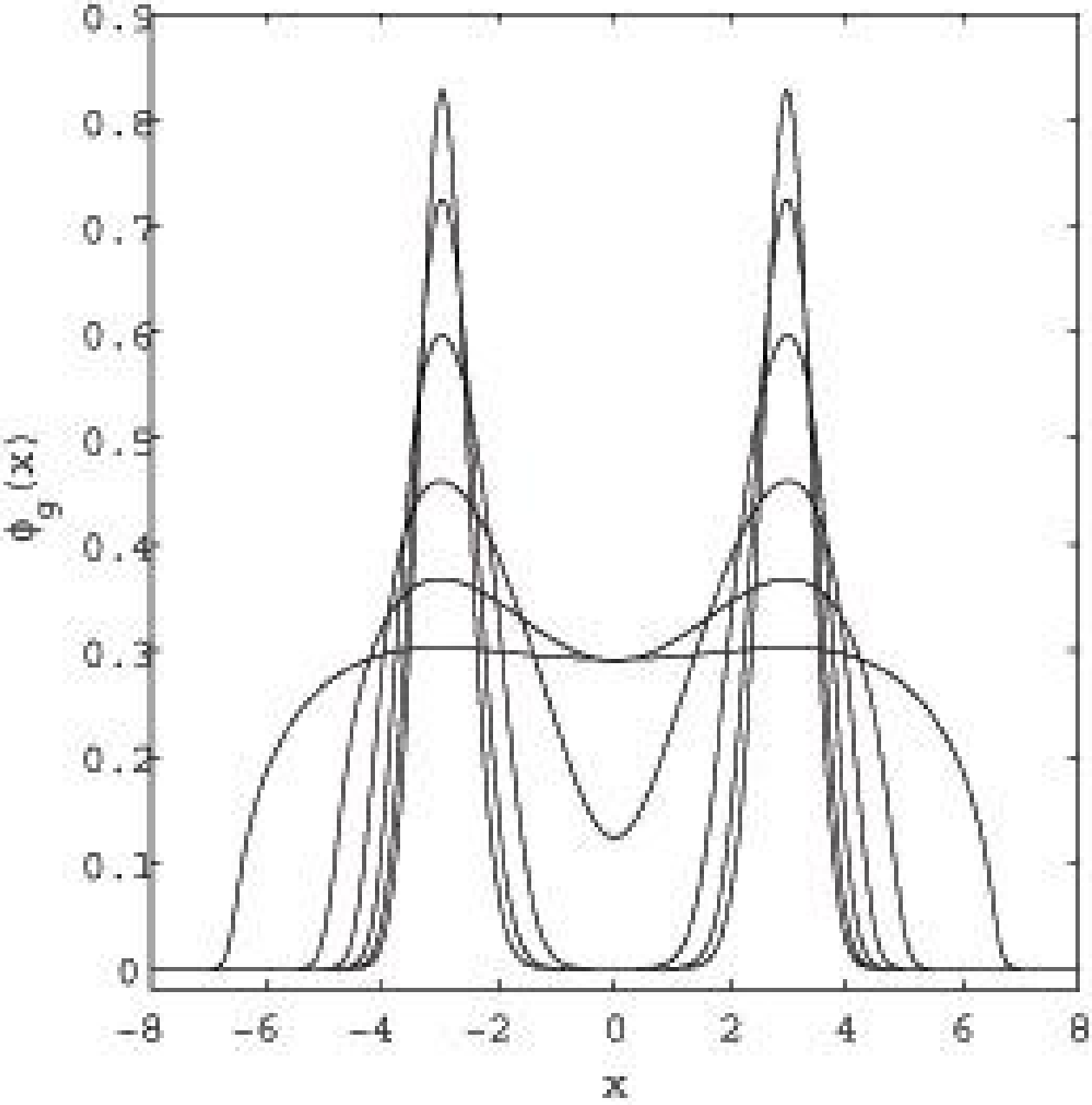

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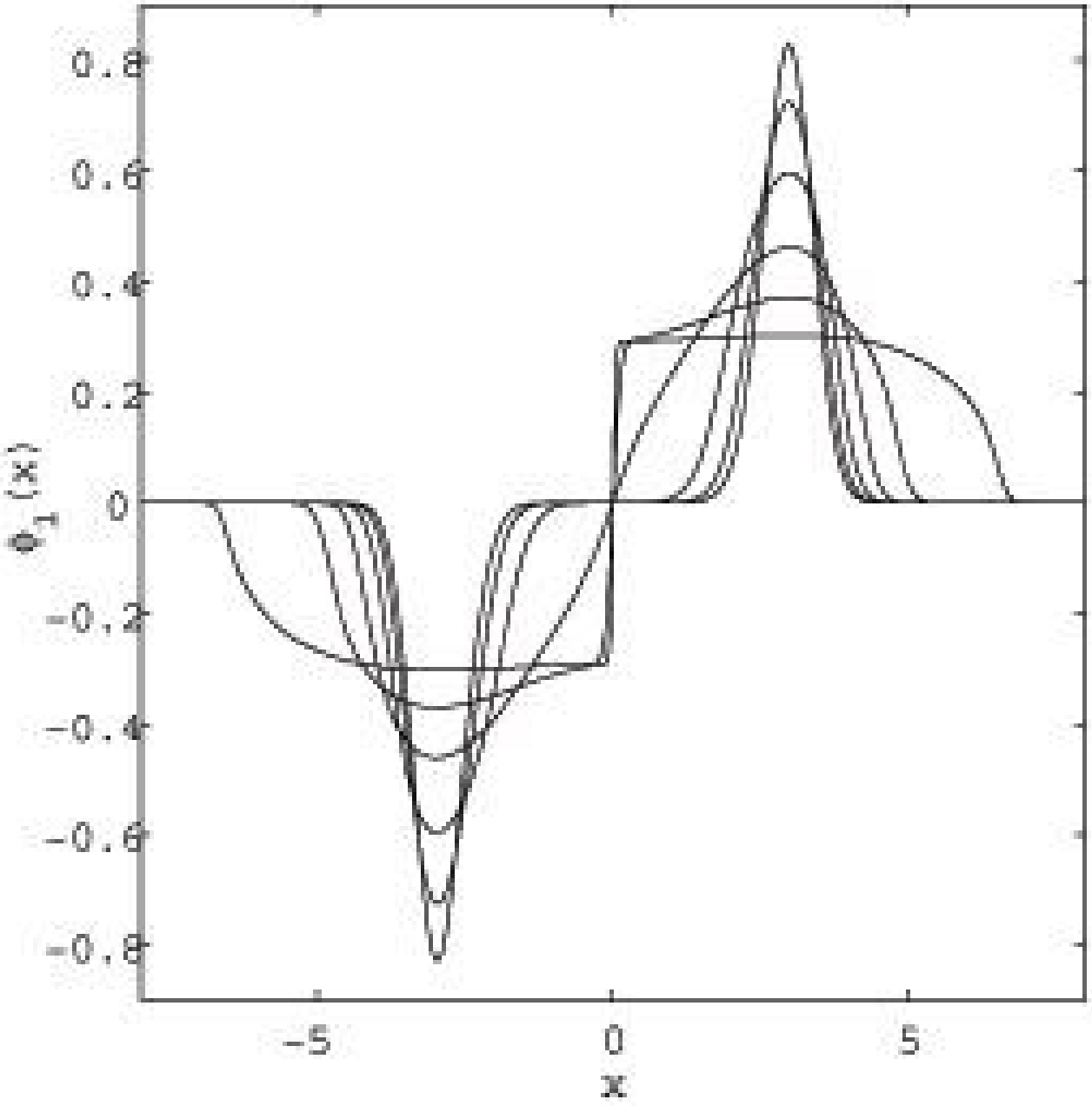

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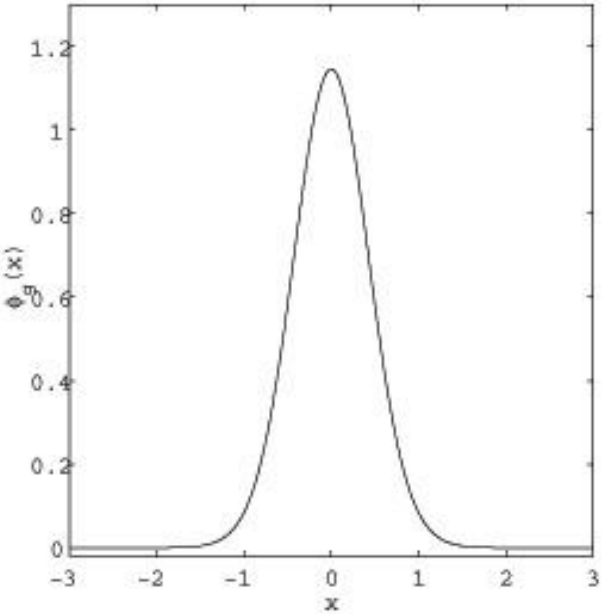
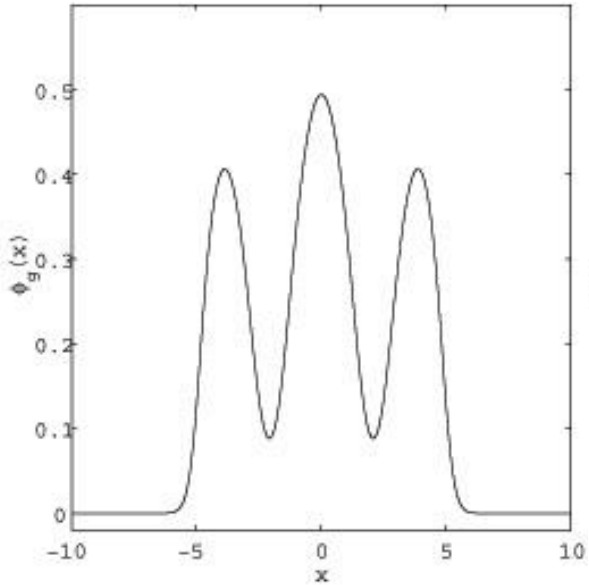
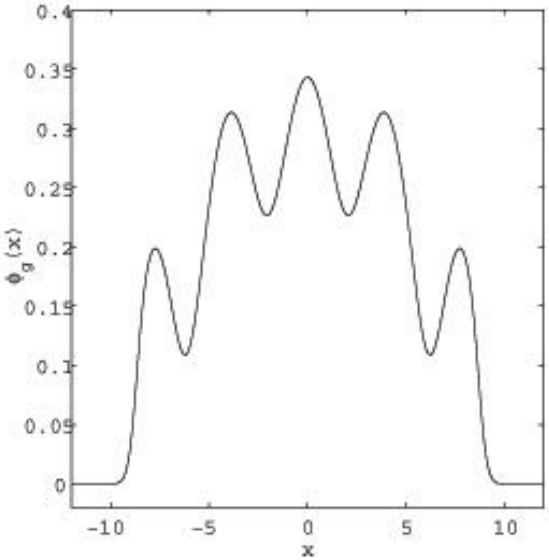


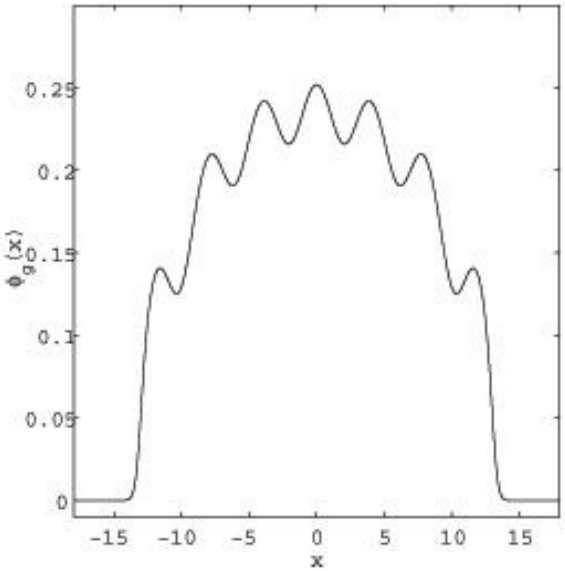
$\phi_g(x)$
x
0
0.2
0.4
0.6
0.8
1
1.2
-3
-2
-1
0
1
2
3



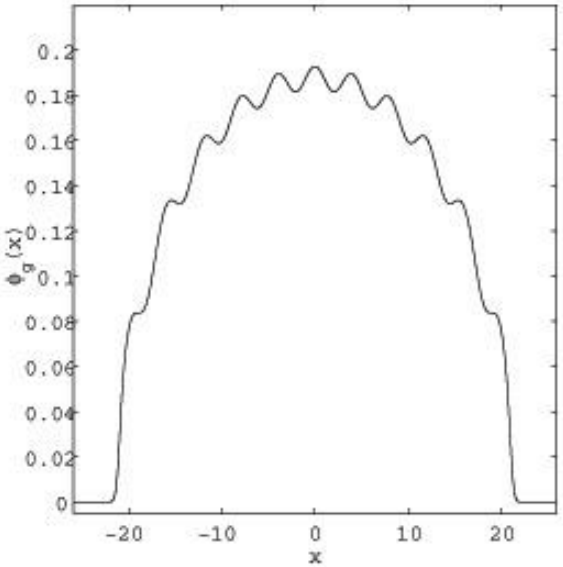
$\phi_g(x)$
x
0
0.1
0.2
0.3
0.4
0.5
-10
-5
0
5
10



$\phi_g(x)$
x
0
0.05
0.1
0.15
0.2
0.25
0.3
0.35
0.4
-10
-5
0
5
10

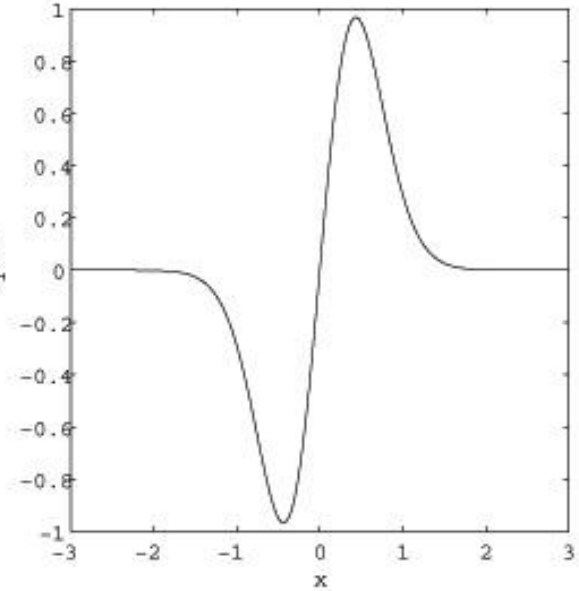


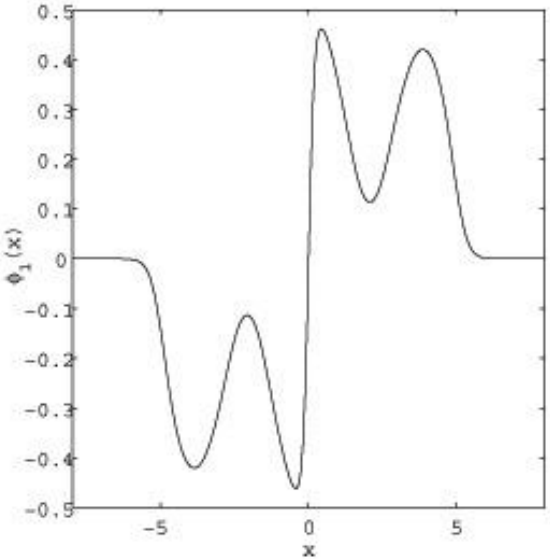
$\phi_g(x)$
x
0
0.05
0.1
0.15
0.2
0.25
-15
-10
-5
0
5
10
15

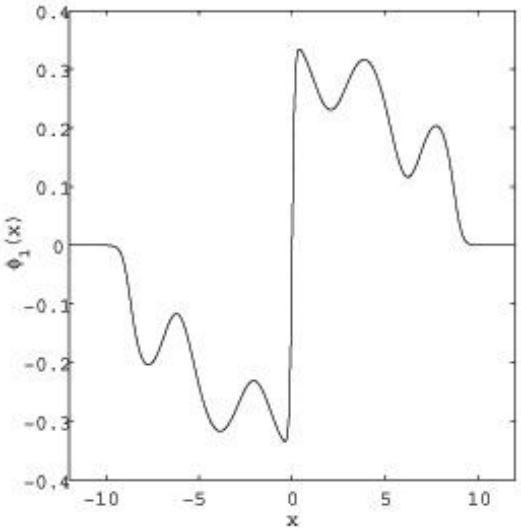


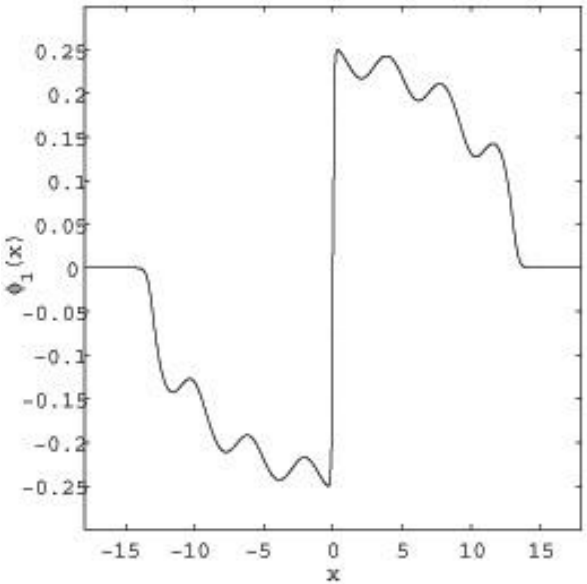
$\phi_g(x)$
x
0
0.02
0.04
0.06
0.08
0.1
0.12
0.14
0.16
0.18
0.2
-20
-10
0
10
20

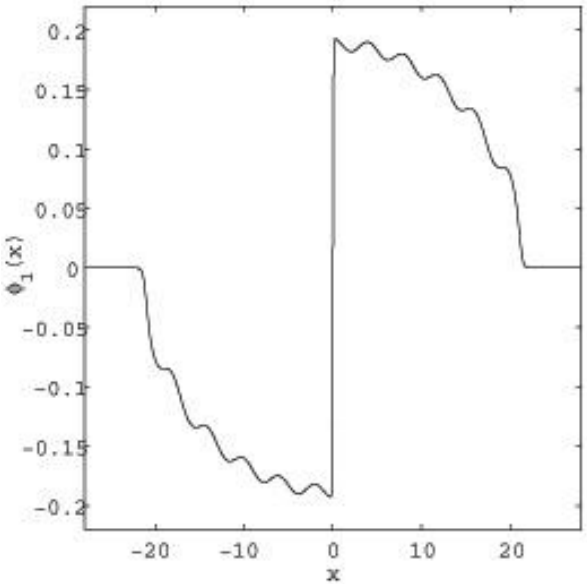
back











ϕ1(x)
x
1
0.8
0.6
0.4
0.2
0
-0.2
-0.4
-0.6
-0.8
-1
-3
-2
-1
0
1
2
3
0.5
0.4
0.3
0.2
0.1
-0.1
-0.2
-0.3
-0.4
-0.5
-5
5
-10
10
0.25
0.15
0.05
-0.05
-0.15
-0.25
-15
15
-20
20

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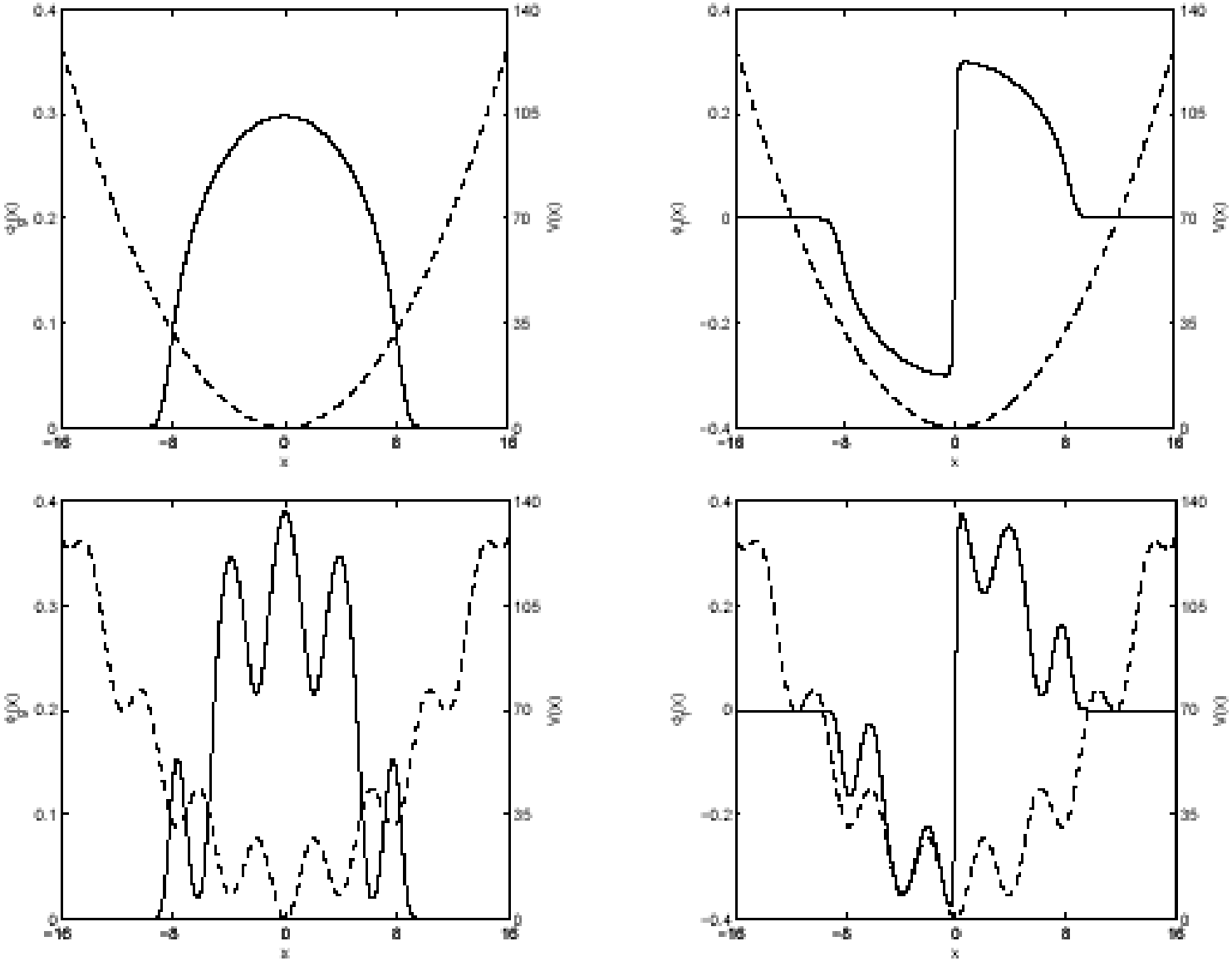
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$V(x)$

back

Ground states

- Numerical results (Bao&W. Tang, JCP, 03'; Bao, F. Lim & Y. Zhang, BIM, 07')
  - In 2d
    - Harmonic oscillator potentials:
      - ground
    - Optical lattice potential:
      - Ground & asymptotic excited states
  - In 3D
    - Optical lattice potential:

ground asymptotic excited states

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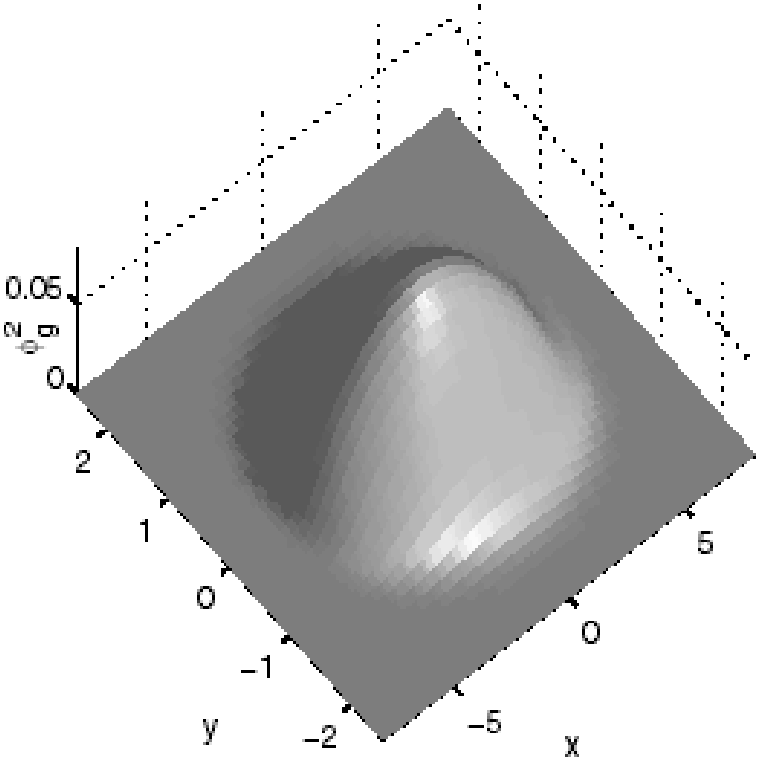

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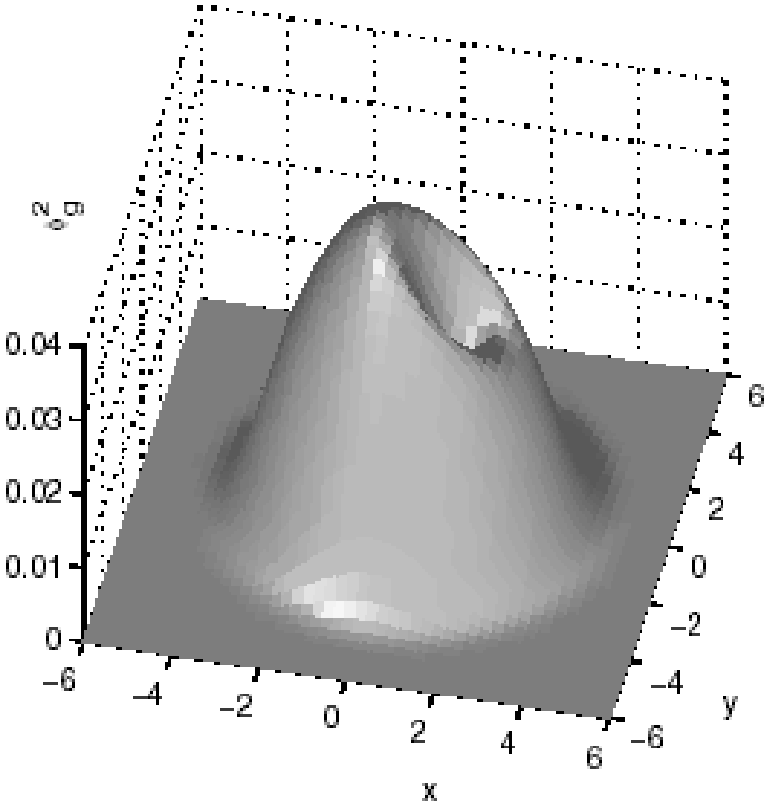

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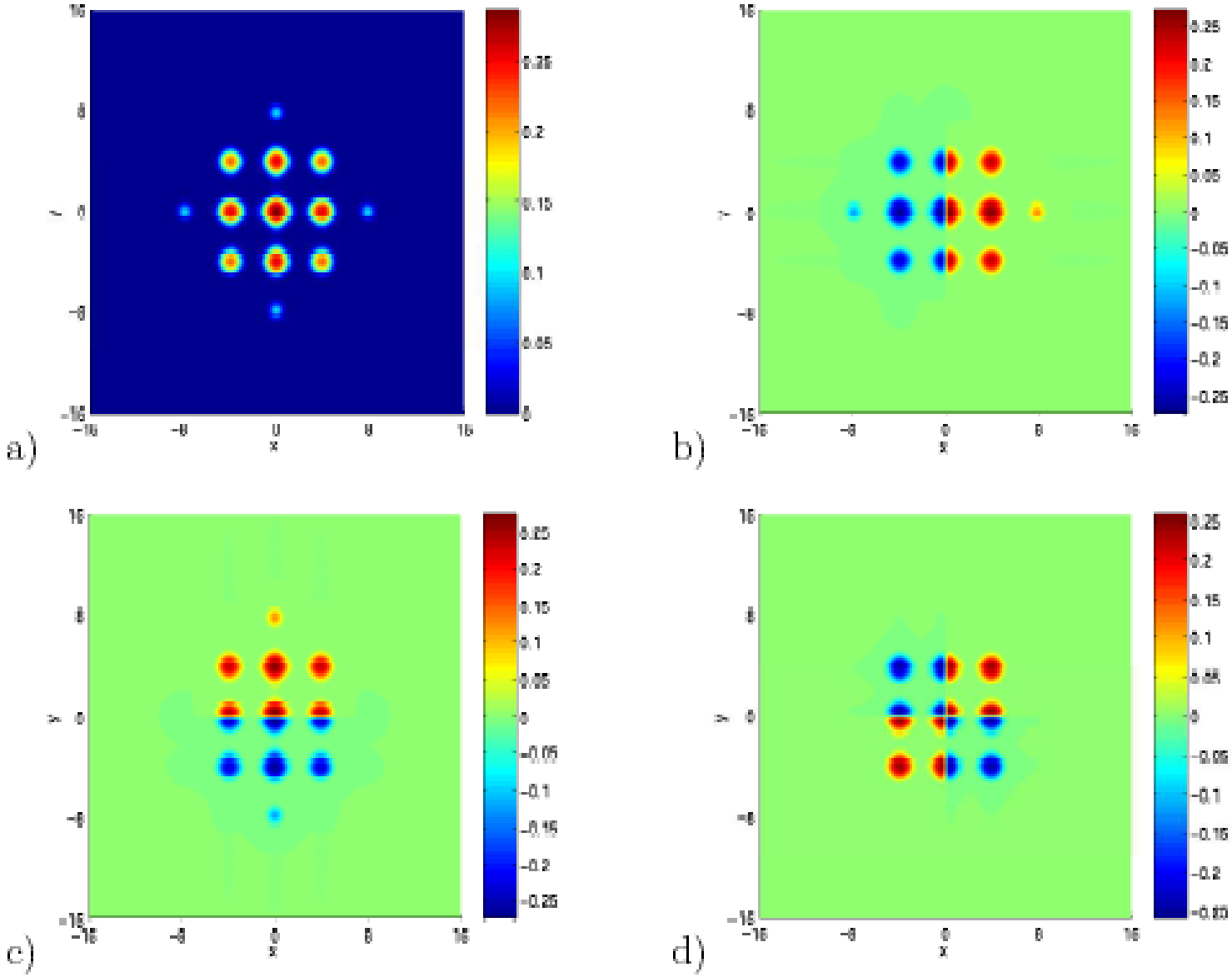

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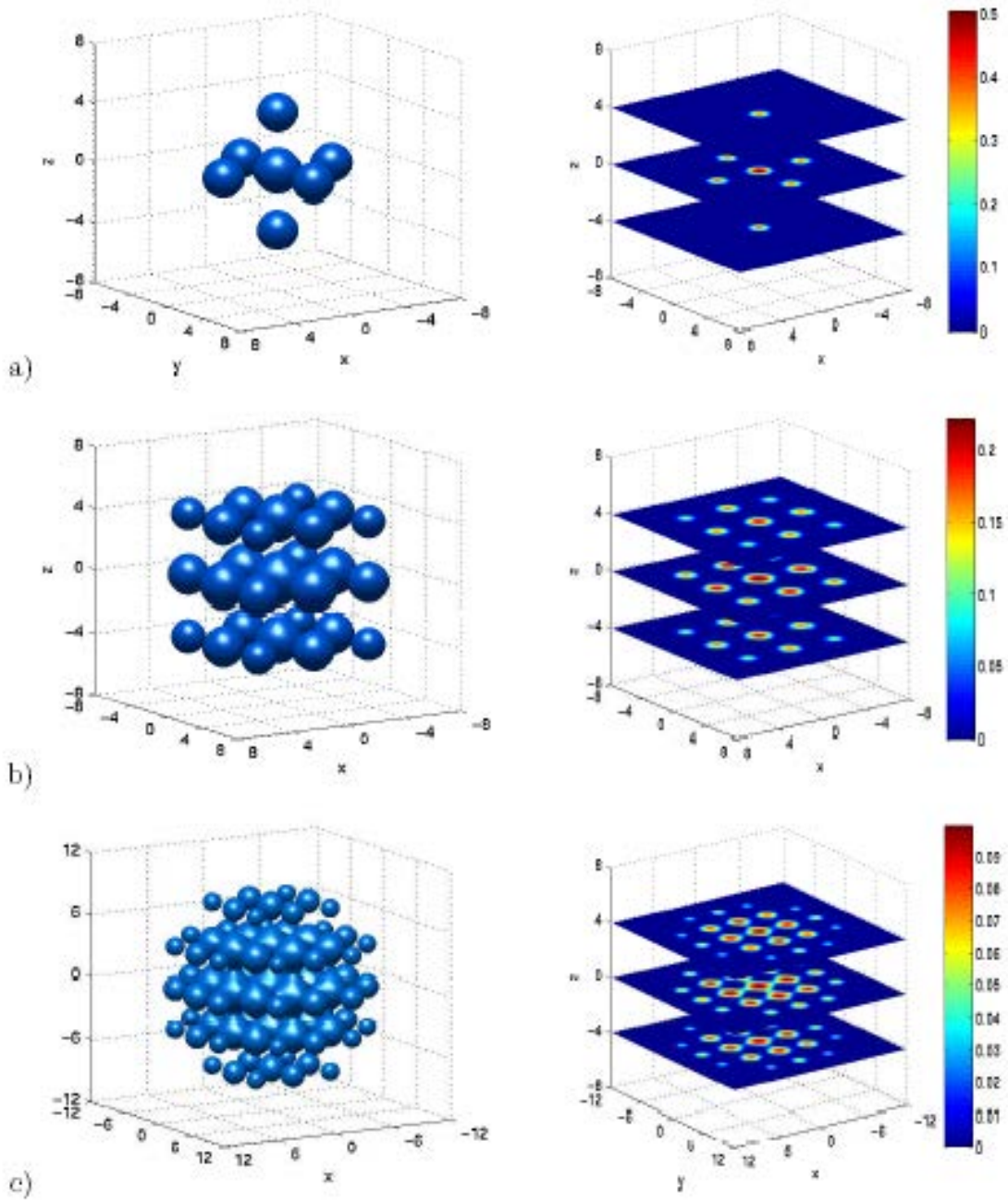

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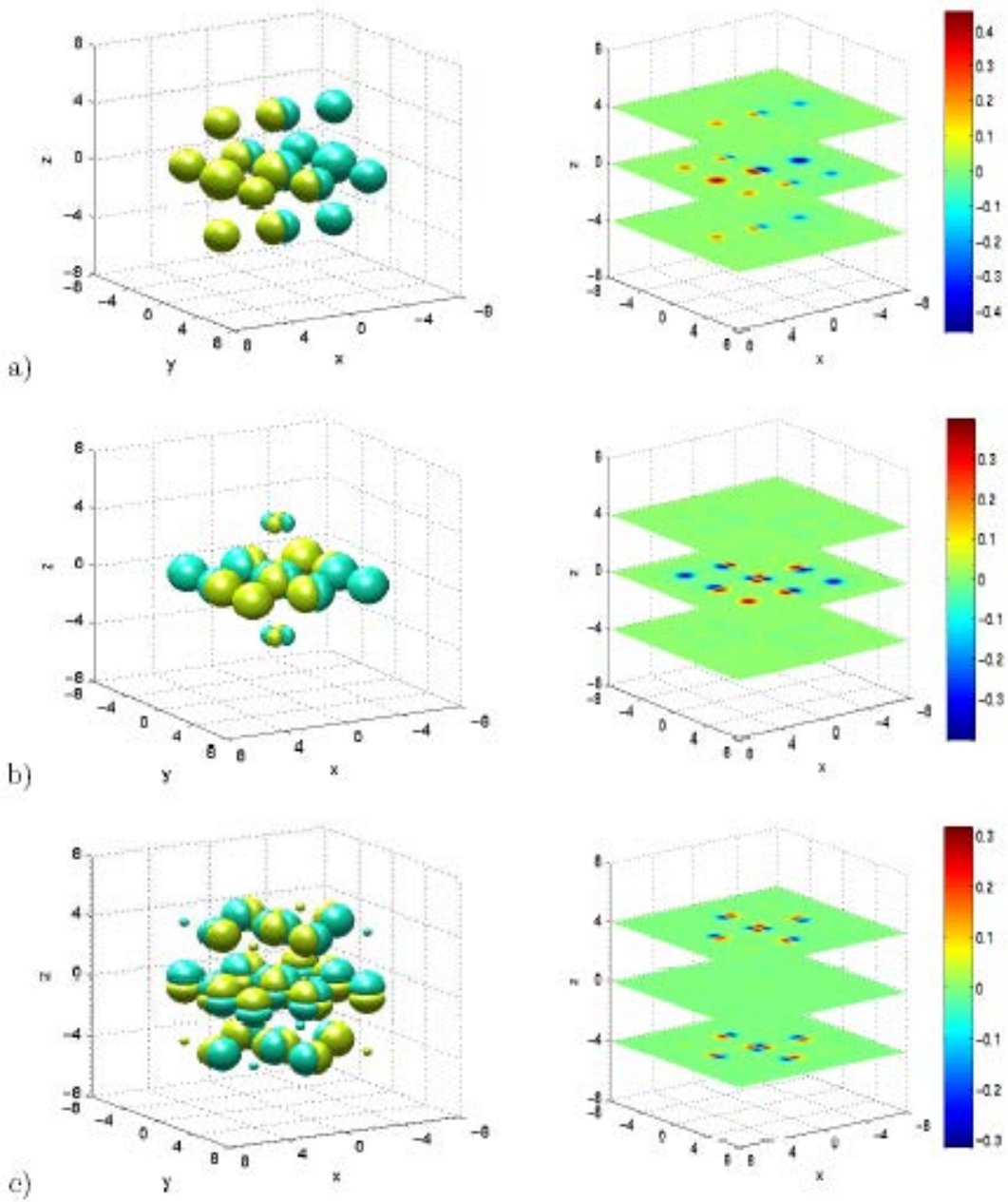


back

Part III

Analysis & Computation

for

Dynamics in BEC

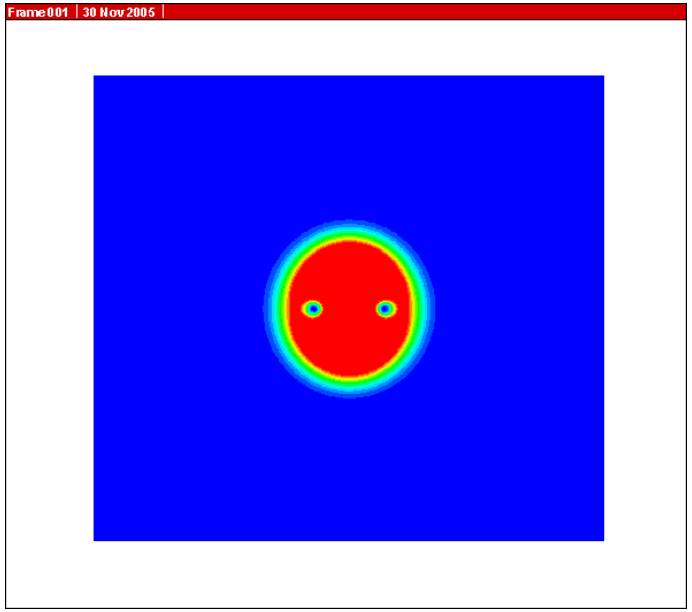
Dynamics of a BEC

- Time-dependent NLSE / GPE

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

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

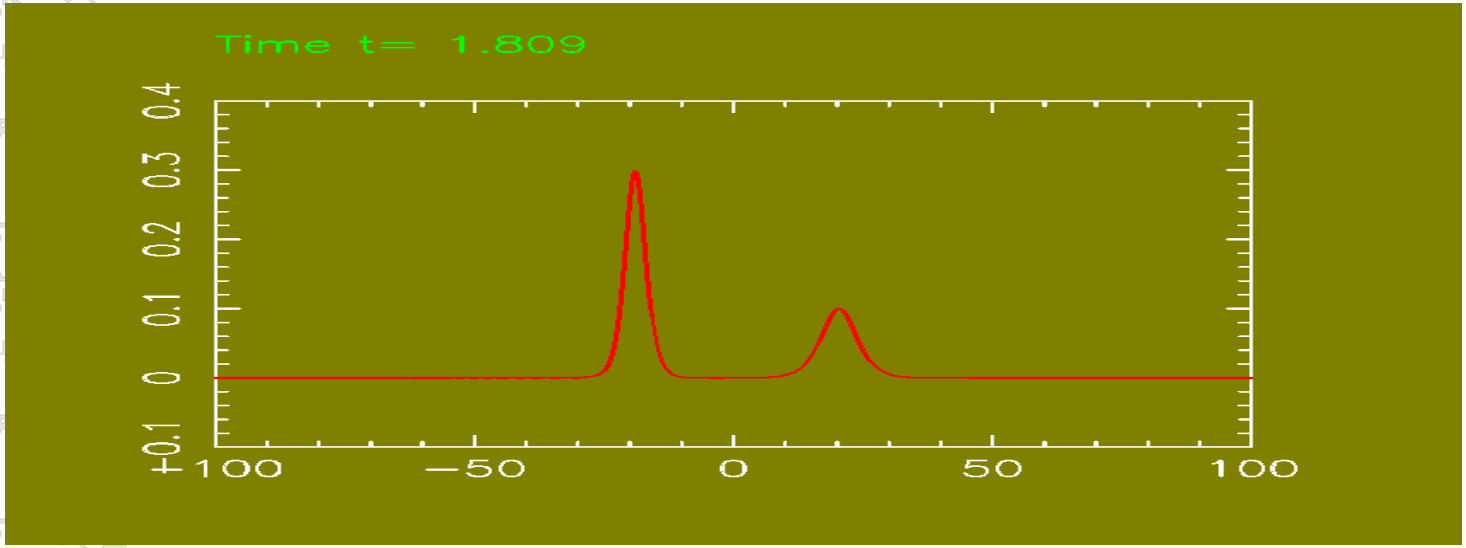
- Well-posedness & dynamical laws
  - Well-posedness & finite time blow-up
  - Dynamical laws
    - Soliton solutions
    - Center-of-mass
    - An exact solution under special initial data
  - Numerical methods and applications



Dynamics with no potential

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

- Momentum conservation $\vec{J}(t) := \mathrm{Im} \int_{\mathbb{R}^d} \bar{\psi}\, \nabla \psi \, d\vec{x} \equiv \vec{J}(0) \quad t \geq 0$
- Dispersion relation $\psi(\vec{x},t) = A e^{i(\vec{k}\bullet\vec{x}-\omega t)} \Rightarrow \omega = \frac{1}{2}\left|\vec{k}\right|^2 + \beta A^2$
- Bright soliton in 1D: $\psi(x,t) = \frac{a}{\sqrt{-\beta}} \mathrm{sech}(a(x - vt - x_0))\, e^{i(vx - \frac{1}{2}(v^2 - a^2)t + \theta_0)}$



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

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

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

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

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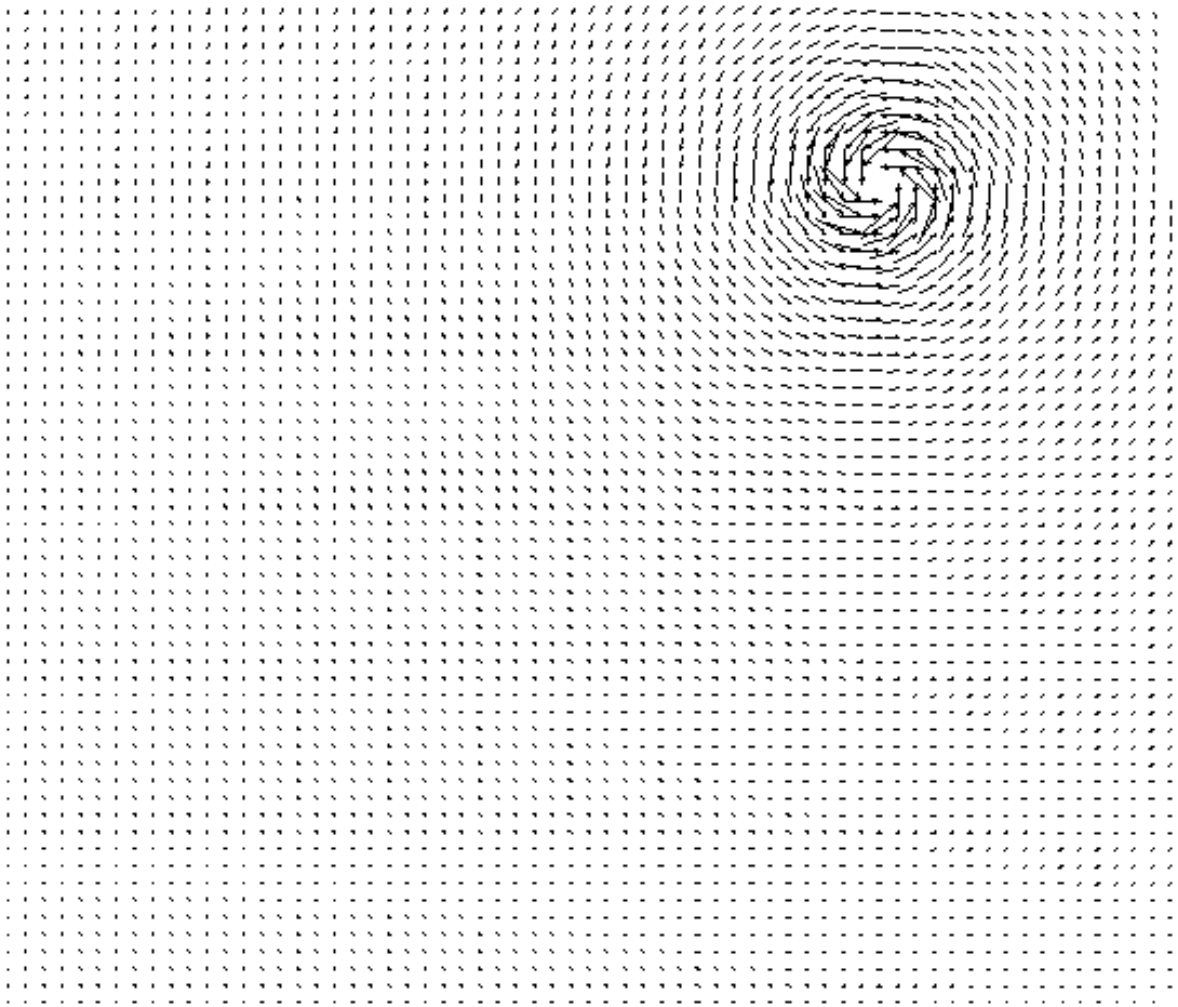


Well-posedenss

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

  - 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

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

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

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

(i) $E(\psi_0) < 0$

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

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

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

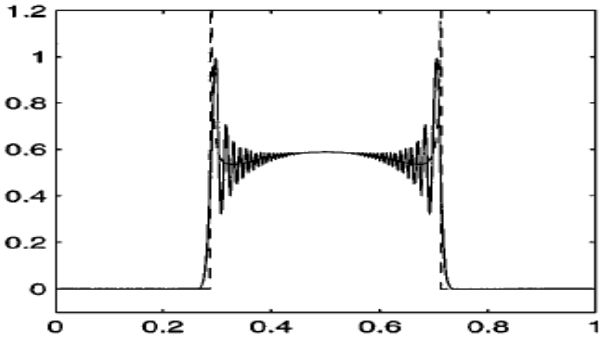
$$\Rightarrow \delta_V(t) \leq d\, E(\psi_0)t^2 + \delta_V'(0)t + \delta_V(0) \Rightarrow \exists 0 < t^* < \infty \;\&\; \delta_V(t^*) = 0!!$$

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 for dynamics

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

Time-splitting spectral method (TSSP)

- Time-splitting:

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

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

$$\Downarrow \quad |\psi(\vec{x},t)| = |\psi(\vec{x},t_n)|$$

$$\psi(\vec{x},t_{n+1}) = e^{-i(V(\vec{x})+\beta|\psi(x,t_n)|^2)\Delta t}\,\psi(\vec{x},t_n)$$

- For non-rotating BEC
  - Trigonometric functions (Bao, D. Jaksck & P. Markowich, J. Comput. Phys., 03')
  - Laguerre-Hermite functions (Bao & J. Shen, SIAM Sci. Comp., 05')

Time-splitting spectral method

$$\psi_j^* = \exp(-\mathrm{i}(x_j^2/2 + \kappa_1|\psi_j^n|^2)k/(2\varepsilon))\psi_j^n,$$

$$\psi_j^{**} = \frac{1}{M}\sum_{l=-M/2}^{M/2-1} \exp(-\mathrm{i}\varepsilon k\mu_l^2/2)\widehat{\psi}_l^* \exp(\mathrm{i}\mu_l(x_j - a)), \quad j = 0, 1, 2, \ldots, M-1,$$

$$\psi_j^{n+1} = \exp(-\mathrm{i}(x_j^2/2 + \kappa_1|\psi_j^{**}|^2)k/(2\varepsilon))\psi_j^{**}, \quad j = 0, 1, 2, \ldots, M-1,$$

where $\widehat{\psi}_l^*$, the Fourier coefficients of ψ^*, are defined as

$$\mu_l = \frac{2\pi l}{b-a}, \quad \widehat{\psi}_l^* = \sum_{j=0}^{M-1} \psi_j^* \exp(-\mathrm{i}\mu_l(x_j - a)), \quad l = -\frac{M}{2}, \ldots, \frac{M}{2} - 1.$$

Properties of TSSP

- Explicit, time reversible & unconditionally stable
- Easy to extend to 2d & 3d from 1d; efficient due to FFT
- Conserves the normalization
- Spectral order of accuracy in space
- 2nd, 4th or higher order accuracy in time
- Time transverse invariant

$$V(\vec{x}) \quad \rightarrow \quad V(\vec{x}) + \alpha \qquad \Rightarrow \qquad |\psi(\vec{x},t)|^2 \quad \text{unchanged}$$

- 'Optimal' resolution in semicalssical regime

$$h = O(\varepsilon), \qquad k = O(\varepsilon), \qquad \varepsilon = 1/\beta^{2/(2+d)}$$

Crank-Nicolson finite difference (CNFD) method

- Crank-Nicolson finite difference (CNFD)method

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

CNFD

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

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

- Error estimate: Yes

Error estimates for CNFD

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

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

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

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

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

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

Dynamics of Ground states

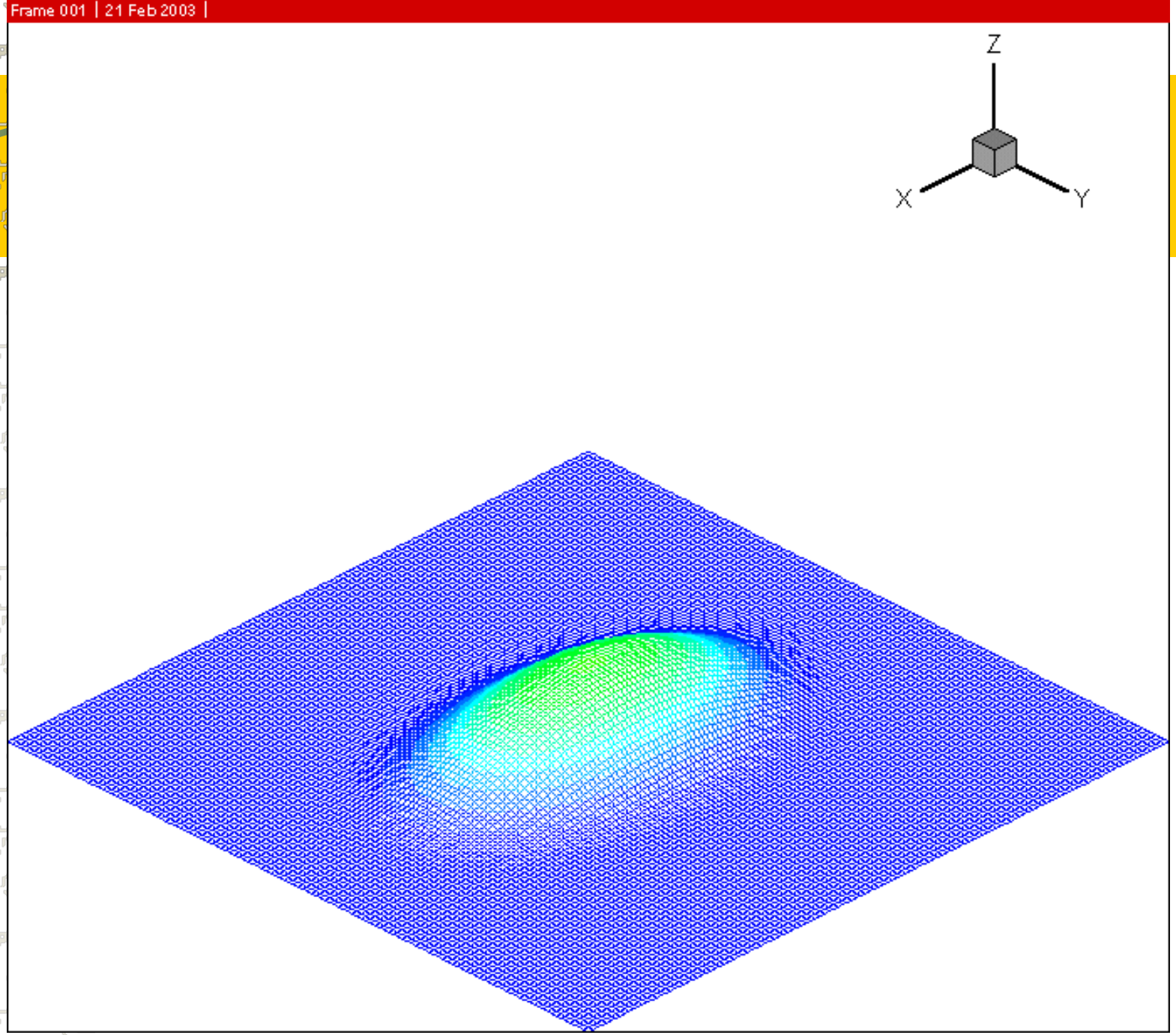
- 1d dynamics: $\beta = 100$ at $t = 0$, $\omega_x \to 4\omega_x$
- 2d dynamics of BEC (Bao, D. Jaksch & P. Markowich, J. Comput. Phys., 03')
  - Defocusing: $\beta = 20$, at $t = 0$ $\omega_x \to 2\omega_x$, $\omega_y \to 2\omega_y$
  - Focusing (blowup): At $t = 0$ $\beta = 40 \to -50$
- 3d collapse and explosion of BEC (Bao, Jaksch & Markowich,J. Phys B, 04')
  - Experiment setup leads to three body recombination loss

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

  - Numerical results:
    - Number of atoms , central density Jets formation & Movie

next

back



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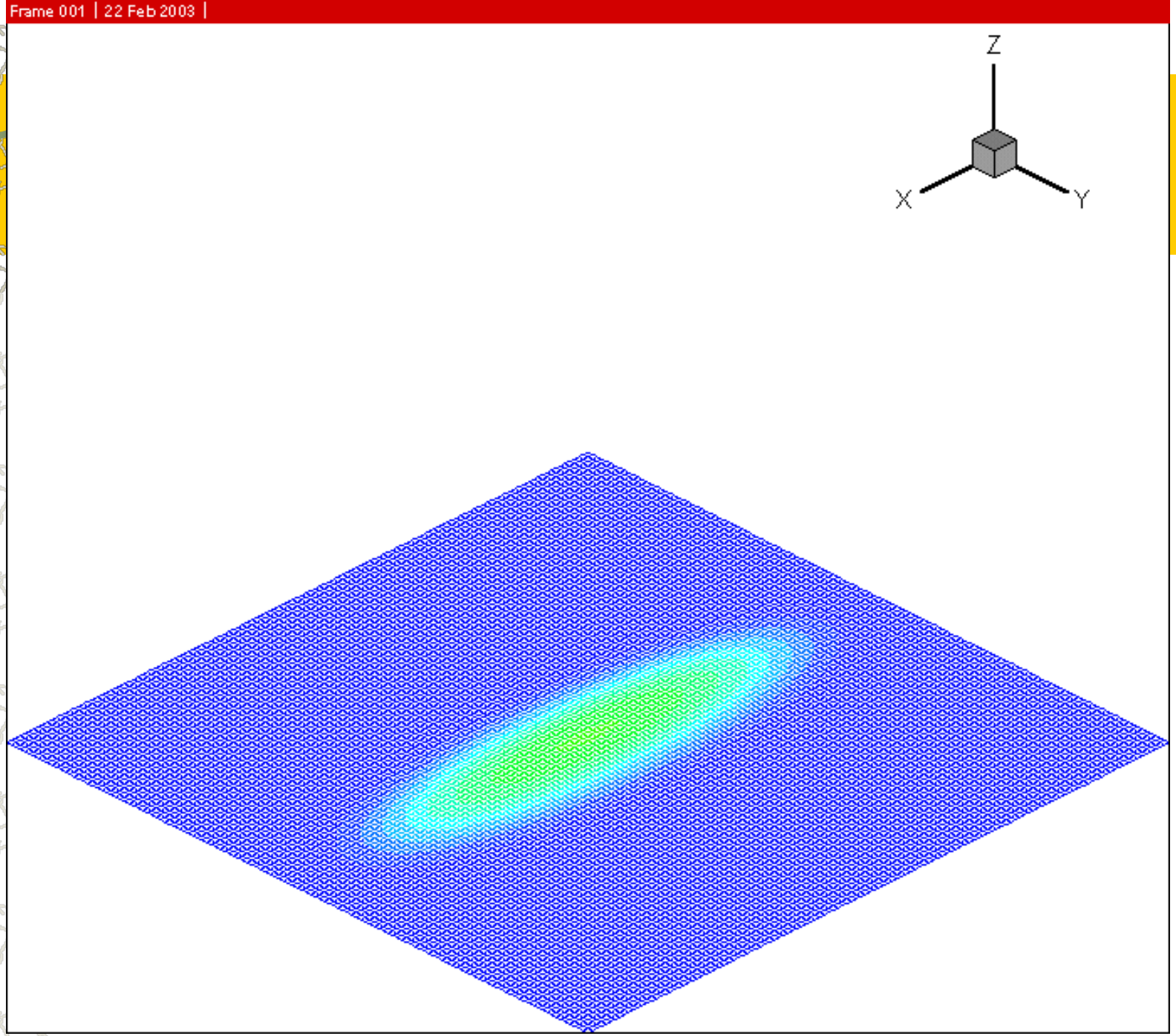
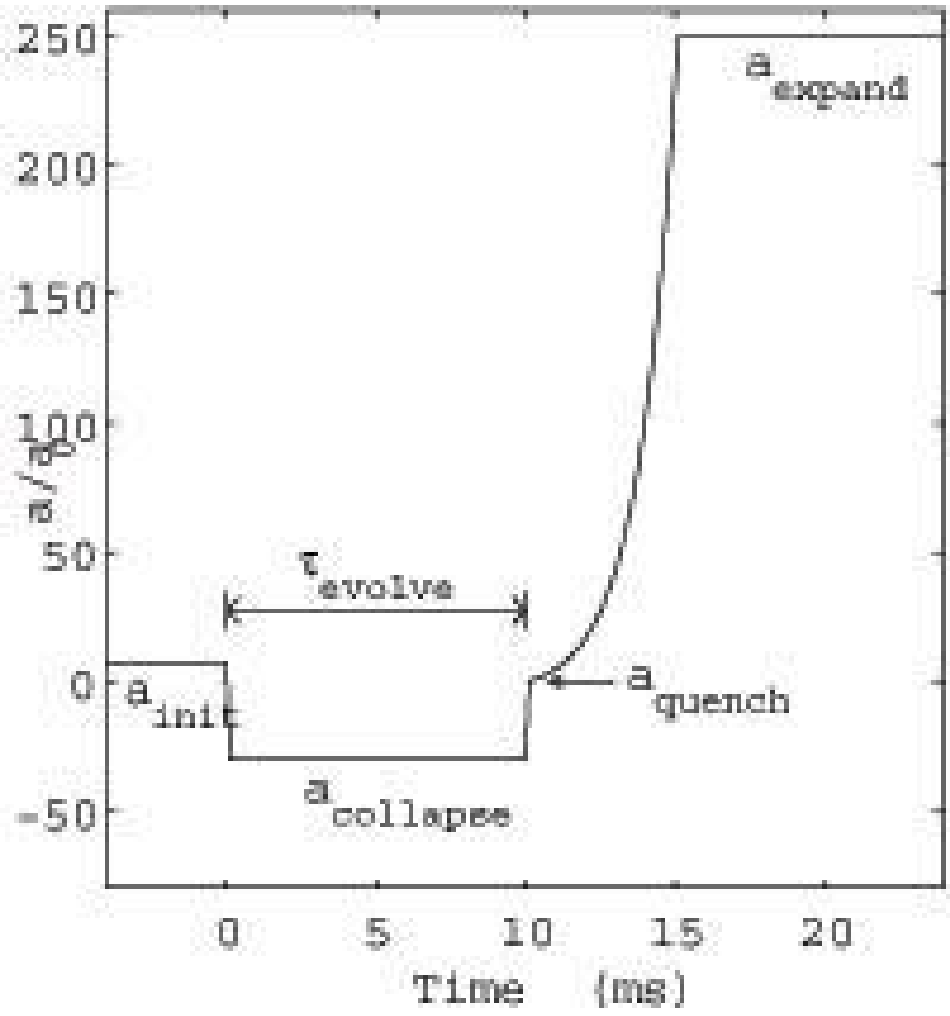


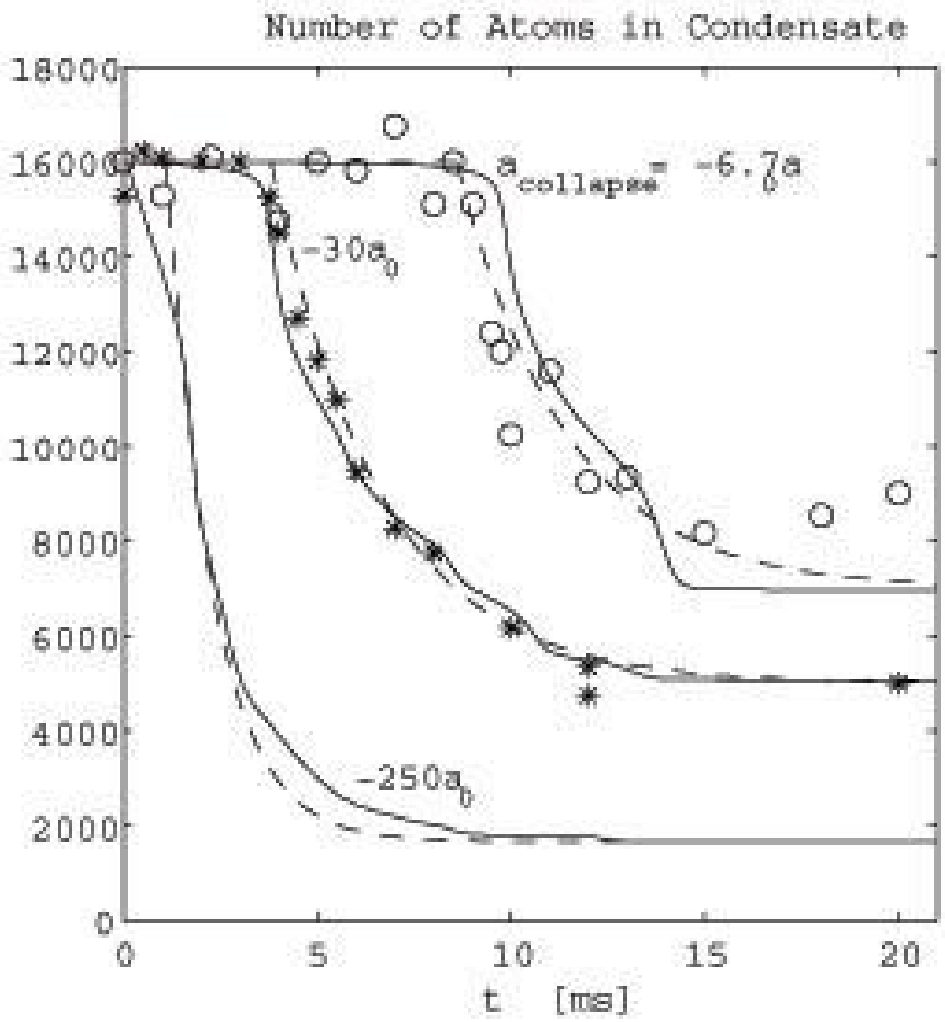
back

Collapse and Explosion of BEC



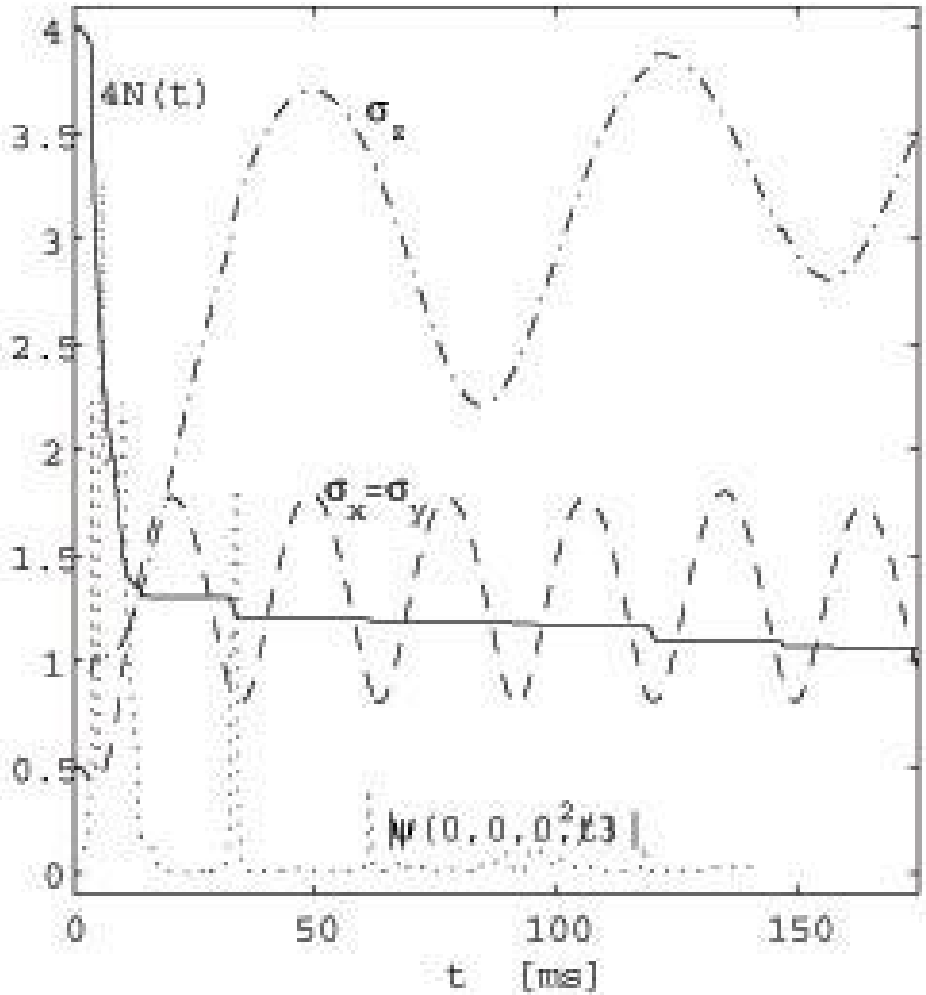
back

Number of atoms in condensate



back

Central density



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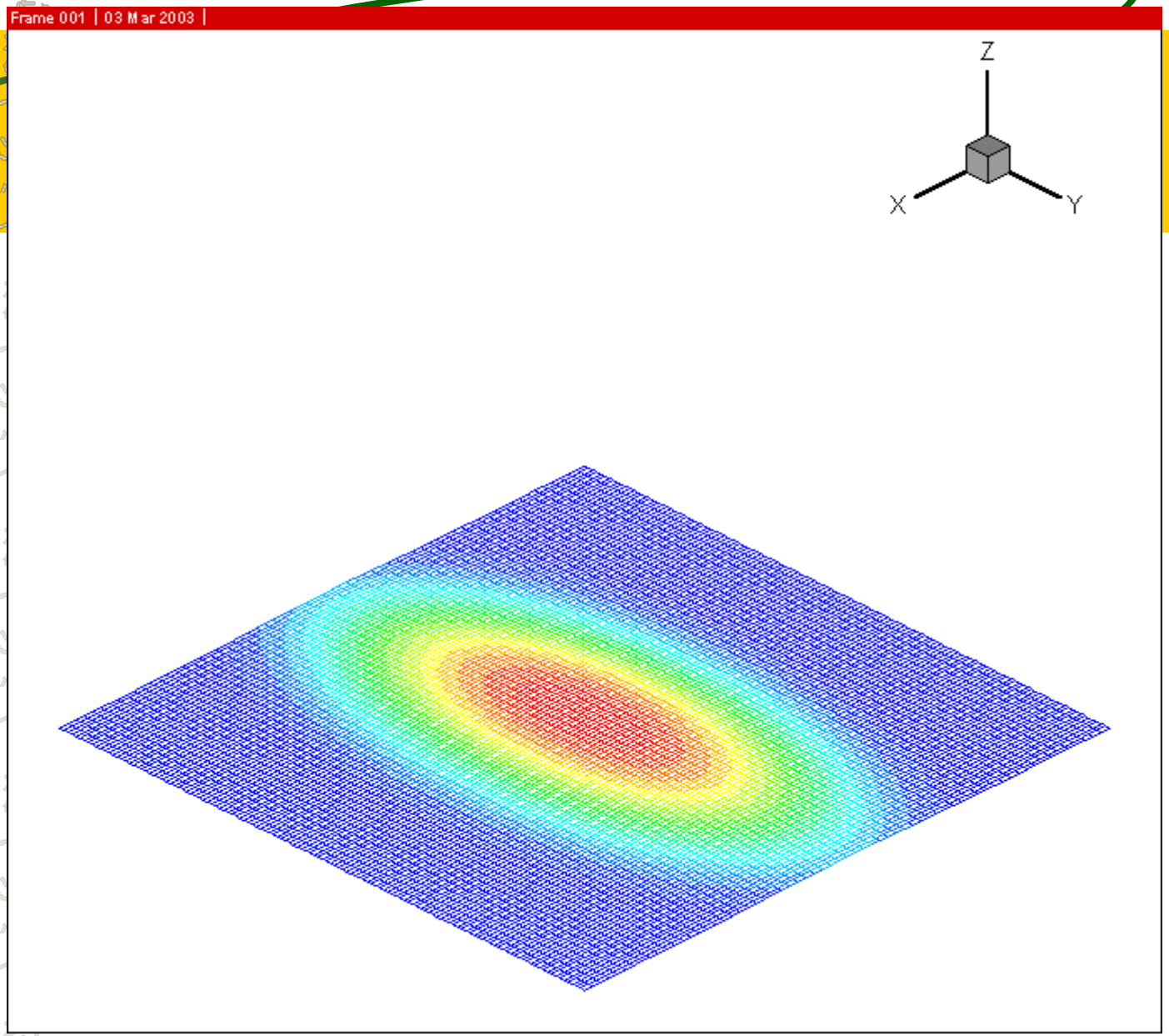

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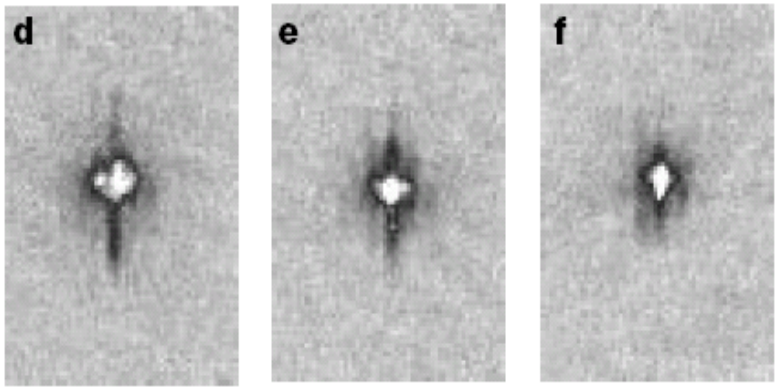
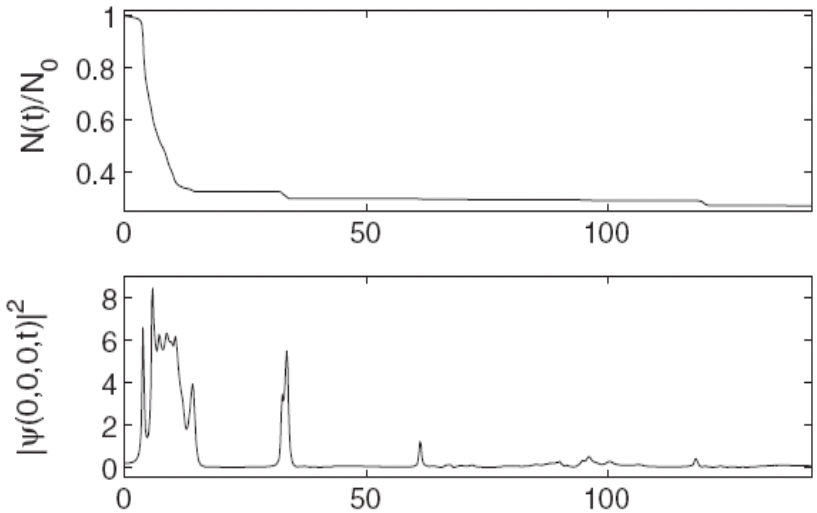
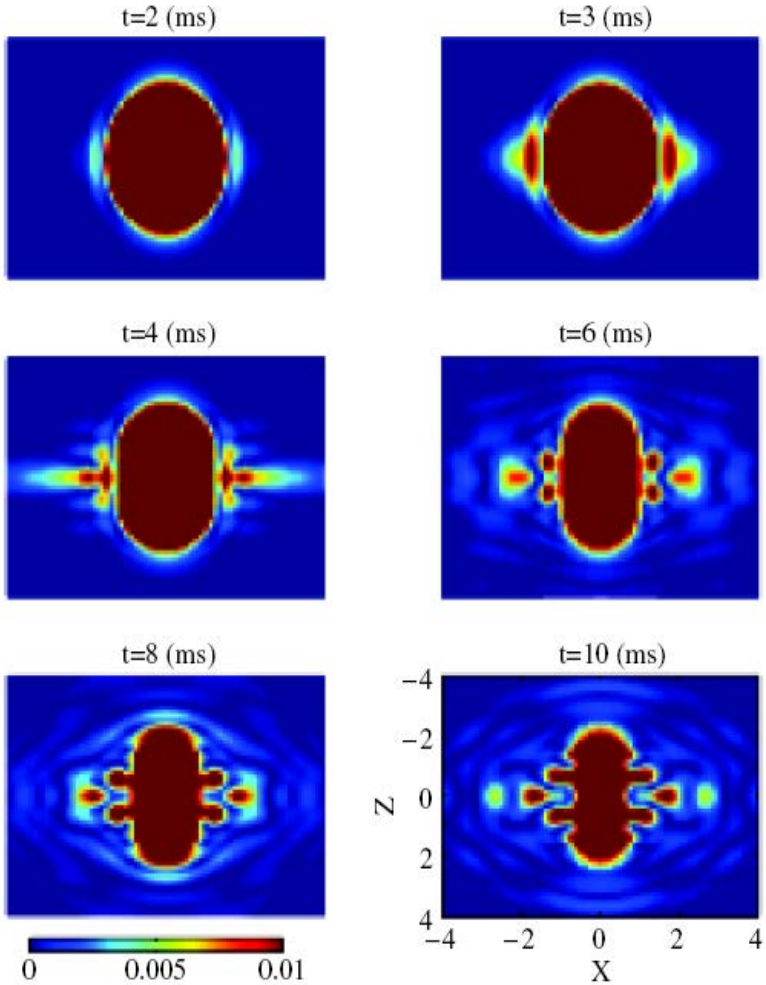
Numerical results (Bao et., J Phys. B, 04)







Jet formation

back

Semiclassical scaling

- When $\beta >> 1$, re-scaling $\vec{x} \to \vec{x}\,\varepsilon^{-1/2}$ $\psi = \psi^{\varepsilon}\varepsilon^{d/4}$ $\varepsilon = 1/\beta^{2/(d+2)}$

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

With

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

- Leading asymptotics (Bao & Y. Zhang, Math. Mod. Meth. Appl. Sci., 05')

$$E(\psi) = \varepsilon^{-1}E^{\varepsilon}(\psi^{\varepsilon}) = O\left(\varepsilon^{-1}\right) = O\left(\beta^{2/(d+2)}\right)$$

$$\mu(\psi) = \varepsilon^{-1}\mu^{\varepsilon}(\psi^{\varepsilon}) = O\left(\varepsilon^{-1}\right) = O\left(\beta^{2/(d+2)}\right)$$

Comparison of two scaling

Quanties	Thomas-Fermi scaling	Semiclassical scaling
t_s	$1/\omega_x$	$1/\omega_x$
x_s	$x_s = \sqrt{\hbar / m\omega_x}$	$x_s \varepsilon^{-1/2} = x_s \beta^{1/(d+2)} = x_s (\frac{4\pi N a_s}{x_s})^{1/(d+2)}$
ψ_s	$x_s^{-3/2}$	$x_s^{-3/2} \varepsilon^{d/4}$
E_s	$\hbar\omega_x := \frac{m x_s^2}{t_s^2}$	$\hbar\omega_x \varepsilon^{-1}$
Energy E	$O\left(\beta^{2/(d+2)}\right)$	$O(1)$
Chemical potential μ	$O\left(\beta^{2/(d+2)}\right)$	$O(1)$
length of wave function	$O\left(\beta^{1/(d+2)}\right) = O(\sqrt{2\mu})$	$O(1)$
height of wave function	$O\left(\beta^{-d/2(d+2)}\right) = O(\sqrt{\mu/\beta})$	$O(1)$

Semiclassical limits

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

$$\psi := \psi^\varepsilon \qquad \psi^\varepsilon(\vec{x},0) := \psi_0^\varepsilon(\vec{x}) = \sqrt{\rho_0^\varepsilon(\vec{x})}\, e^{iS_0^\varepsilon(\vec{x})/\varepsilon}$$

- 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

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

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

From QM to fluid dynamics

- Quantum Hydrodynamics (QHD): Euler +3rd dispersion

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

$$\partial_t (\vec{J}^\varepsilon) + \nabla \bullet (\frac{\vec{J}^\varepsilon \otimes \vec{J}^\varepsilon}{\rho^\varepsilon}) + \nabla P(\rho^\varepsilon) + \rho^\varepsilon \nabla V = \frac{\varepsilon^2}{4} \nabla (\rho^\varepsilon \Delta \ln \rho^\varepsilon)$$

- Formal Limits --- Euler equations for fluids

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

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

- 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

Part IV

Rotating BEC

&

multi-component BEC

Rotating BEC

- The Schrodinger equation ($\vec{x} = (x, y, z)$)

$$i\hbar \frac{\partial \psi(\vec{x}, t)}{\partial t} = \frac{\delta H(\psi)}{\delta \psi^*}$$

  - The Hamiltonian:

$$H(\psi) = \int \psi^*(\vec{x}, t) [-\frac{\hbar^2 \nabla^2}{2m} + V(\vec{x}) - \Omega L_z] \psi(\vec{x}, t)\, d\vec{x}$$

$$+ \frac{1}{2} \int \psi^*(\vec{x}, t)\, \psi^*(\vec{x}', t)\ \ \Phi(\vec{x} - \vec{x}')\, \psi(\vec{x}', t)\, \psi(\vec{x}, t)\, d\vec{x}\, d\vec{x}'$$

  - The interaction potential is taken as in Fermi form

$$\Phi(\vec{x}) = (N-1)\, U_0\, \delta(\vec{x}), \qquad U_0 = 4\pi \hbar^2 a_s / m .$$

Rotating BEC

- The 3D Gross-Pitaevskii equation ($\vec{x} = (x, y, z)$)

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{x},t) = [-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) - \Omega L_z + N U_0 |\psi|^2]\psi$$

  - Angular momentum rotation

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

  - V is a harmonic trap potential

$$V(\vec{x}) = \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)$$

  - Normalization condition

$$\int_{\mathbb{R}^3} |\psi(\vec{x},t)|^2 \, d\vec{x} = 1$$

Rotating BEC

- General form of GPE ($\vec{x} \in \mathrm{R}^d$)

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

with $L_z := -i(x\partial_y - y\partial_x) \equiv -i\partial_\theta$

$$\beta = \begin{cases} \beta\int_{-\infty}^{\infty}\varphi_3^4(z)\,dz \approx \beta\sqrt{\frac{\gamma_z}{2\pi}}, \\ \beta, \end{cases} \qquad V(\vec{x}) = \begin{cases} \frac{1}{2}(x^2 + \gamma_y^2 y^2), & d = 2 \\ \frac{1}{2}(x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2), & d = 3 \end{cases}$$

Normalization condition

$$\int_{\mathbb{R}^d} |\psi(\vec{x},t)|^2\, d\vec{x} = 1.$$

Rotating BEC

- Conserved quantities
  - Normalization of the wave function

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

  - Energy

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

$$= E_\Omega(\psi(0))$$

- Chemical potential

$$\mu_\Omega(\psi(t)) = \int_{\mathbb{R}^d} [\frac{1}{2}|\nabla\psi|^2 + V(\vec{x})|\psi|^2 - \Omega\psi^* L_z\psi + \beta\,|\psi|^4] \, d\vec{x}$$

Stationary states

- Stationary solutions of GPE

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

- Nonlinear eigenvalue problem with a constraint

$$\mu\,\phi(\vec{x}) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega\,L_z + \beta\,|\phi(\vec{x})|^2]\,\phi(\vec{x}),$$

$$\int_{\mathbb{R}^d} |\phi(\vec{\mathrm{x}})|^2\,d\vec{x} = 1$$

- Relation between eigenvalue and eigenfunction

$$\mu = \mu_\Omega(\phi) = E_\Omega(\phi) + \frac{\beta}{2}\int_{\mathbb{R}^d} |\phi(\vec{\mathrm{x}})|^4\,d\vec{x}$$

Ground state

- Ground state:

$$E_\Omega(\phi_g) = \min_{\|\phi\|=1} E_\Omega(\phi), \quad \mu_g = \mu_\Omega(\phi_g) = E_\Omega(\phi_g) + \frac{\beta}{2}\int_{\mathbb{R}^d} |\phi_g(\vec{x})|^4 \, d\vec{x}$$

- Existence: $|\Omega| < 1 \;\&\; \beta_d \geq 0$
  - Seiringer (CMP, 02')
- Uniqueness of positive solution: $\Omega = 0 \;\&\; \beta_d \geq 0$
  - Lieb et al. (PRA, 00')
- Energy bifurcation: $0 < \Omega_\beta^c \leq 1$
  - Aftalion & Du (PRA, 01'); B., Markowich & Wang 04'

Numerical results

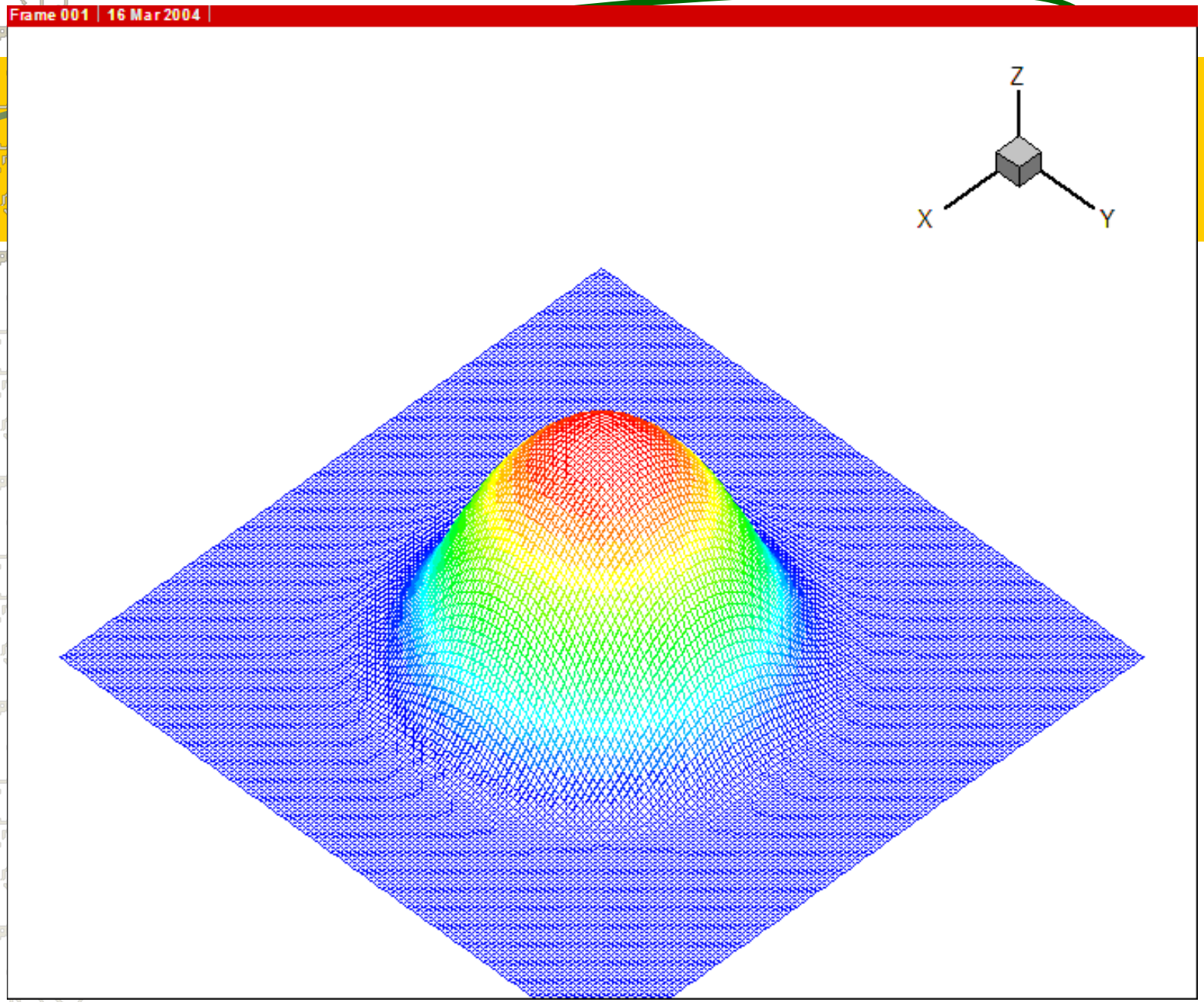
- Ground states:

  in 2D in 3D isosurface

- Vortex lattice
  - Symmetric trapping anisotropic trapping

next

- Giant vortex
  - In 2D In 3D



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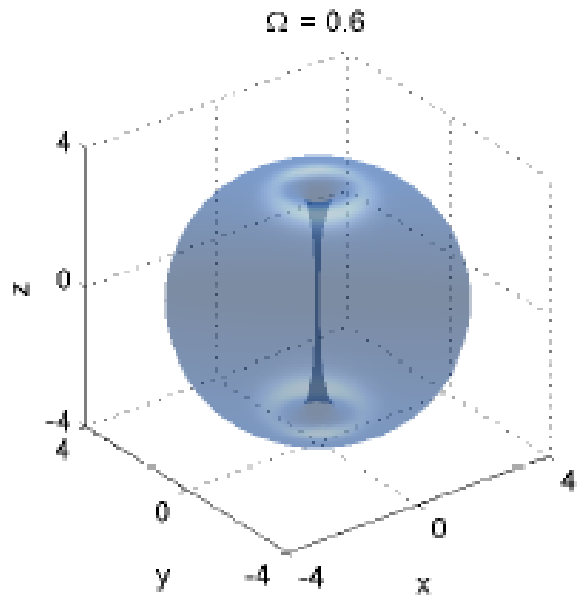
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y
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0
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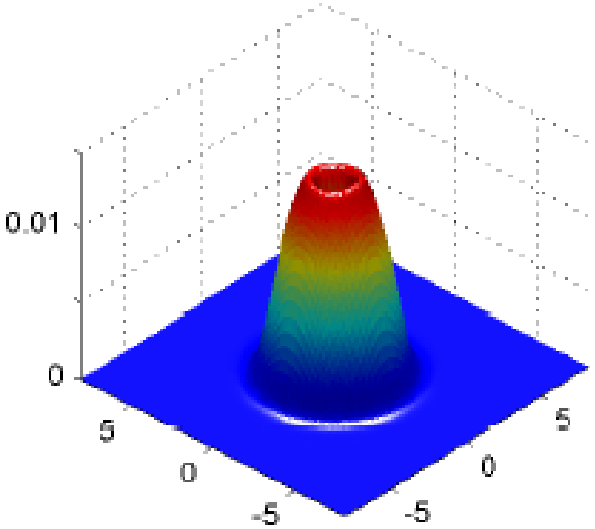
x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0
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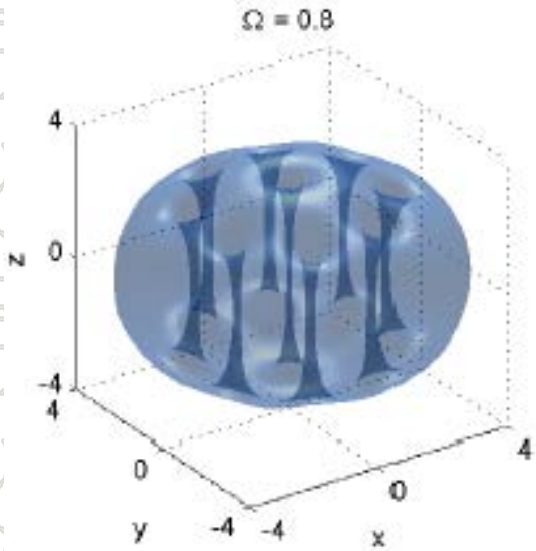
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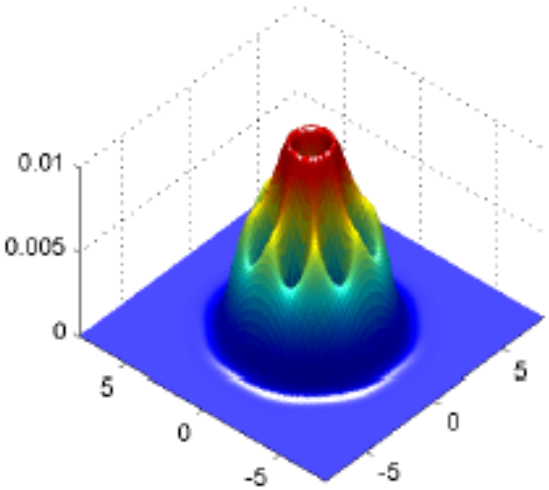
x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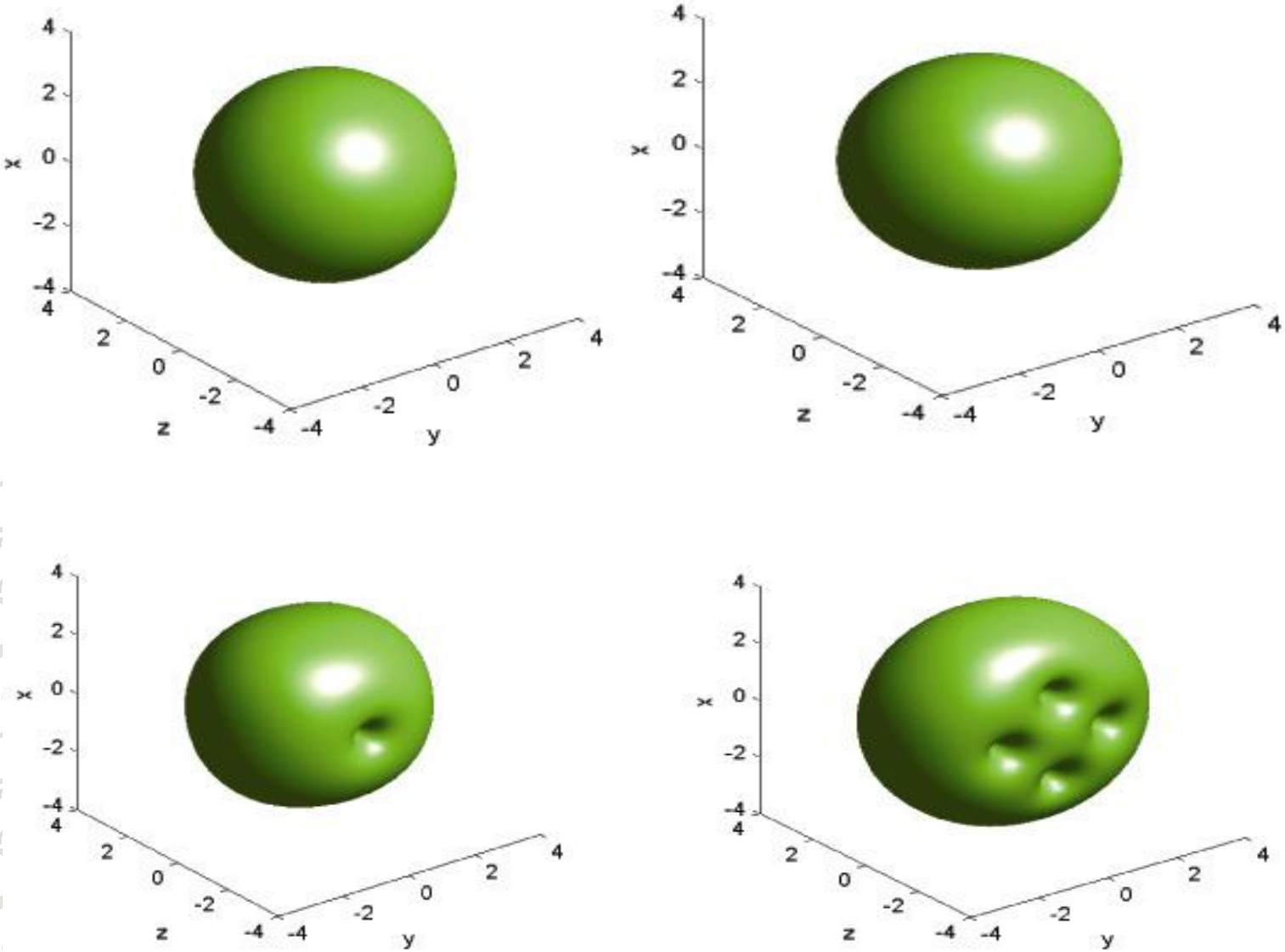

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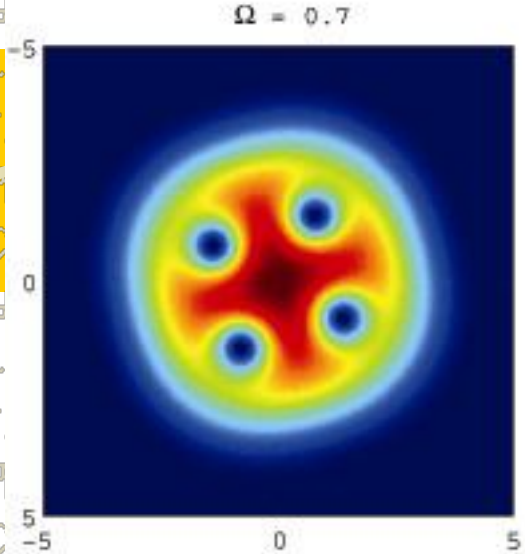
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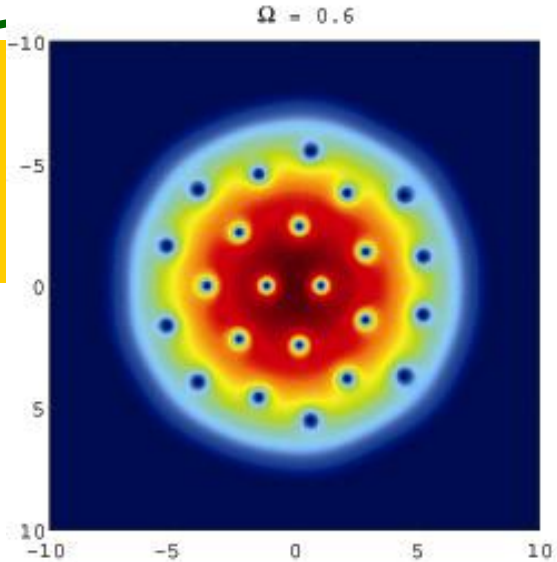
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-5
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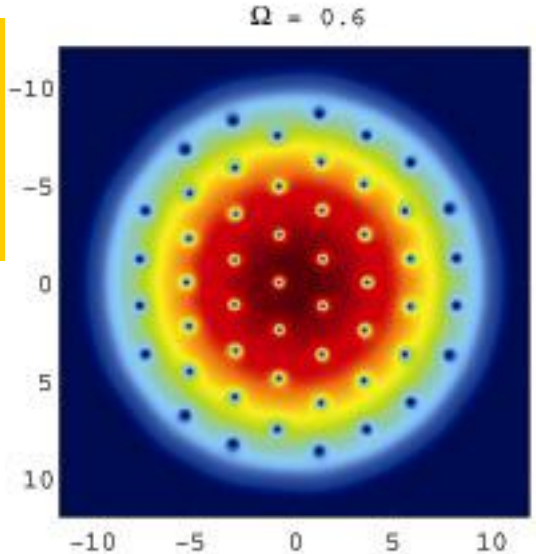
5
10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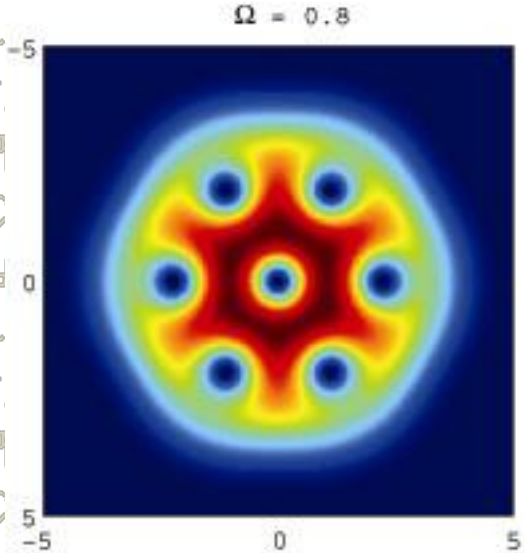
5
10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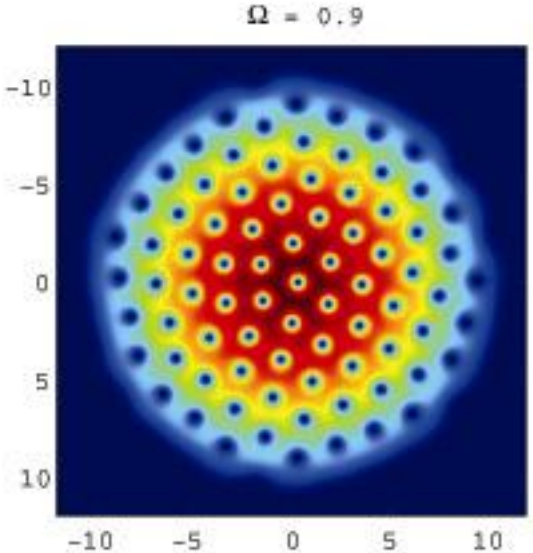
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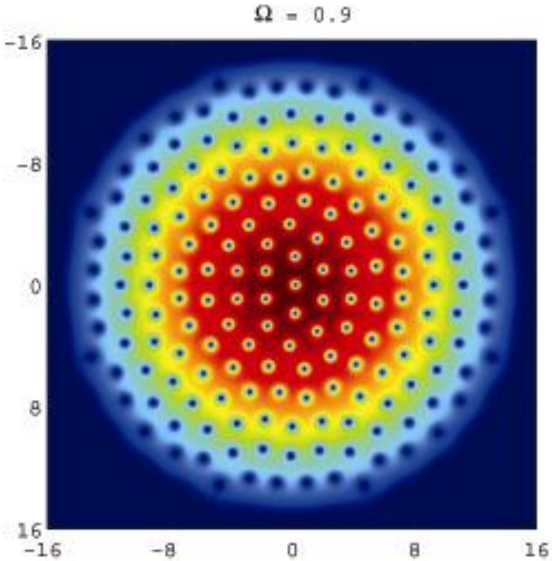
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8
16

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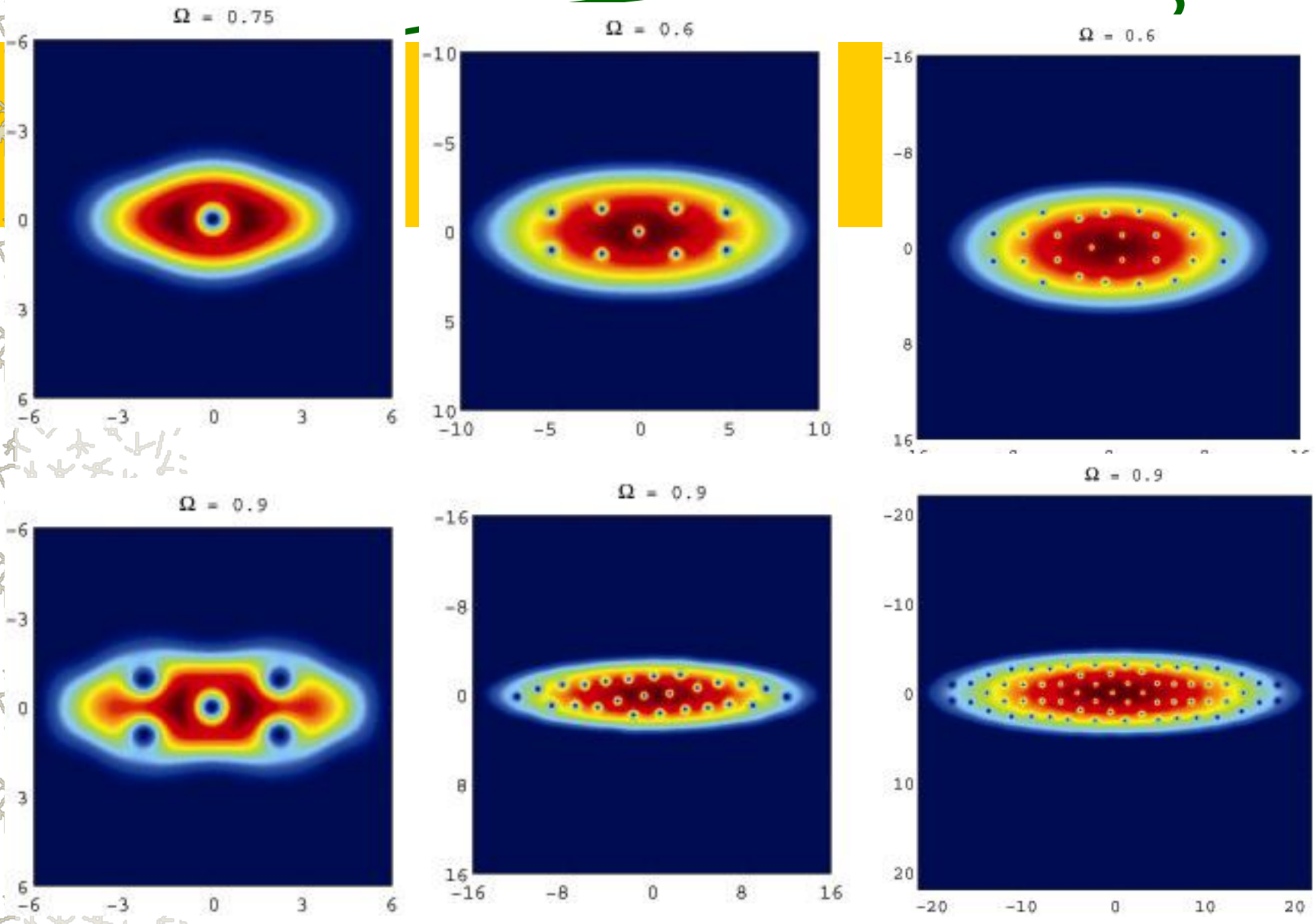

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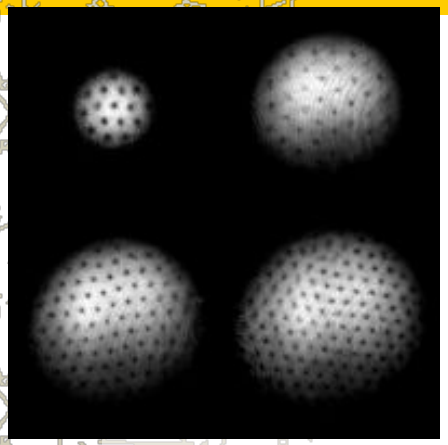
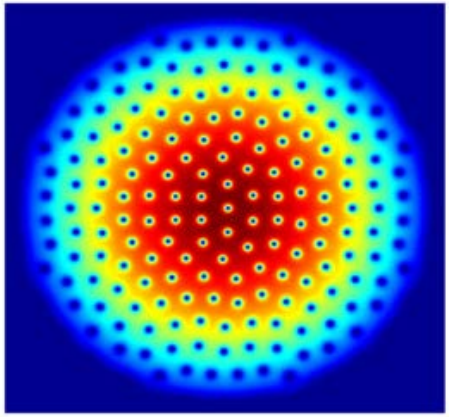
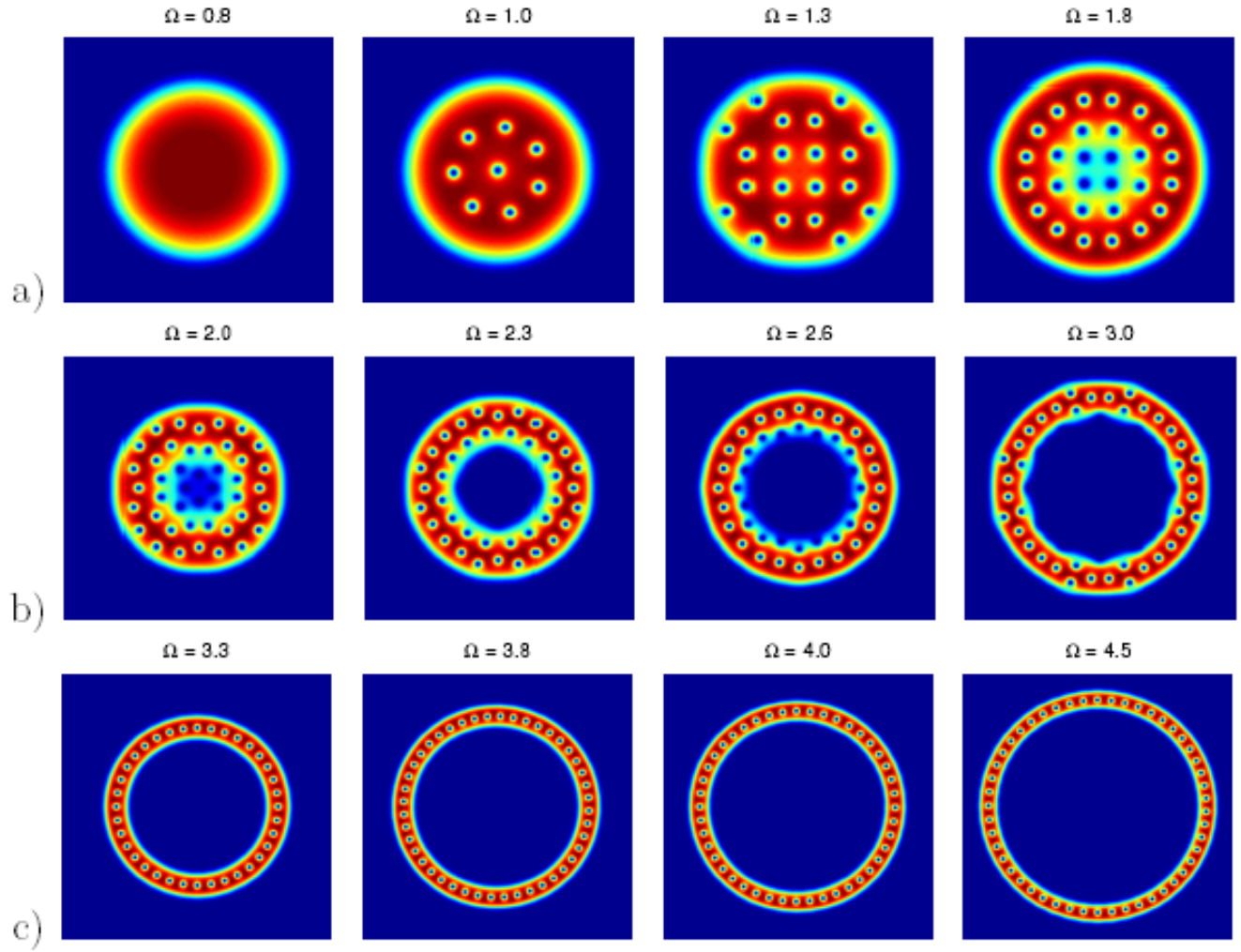
Ground states of rapid rotation



BEC@MIT





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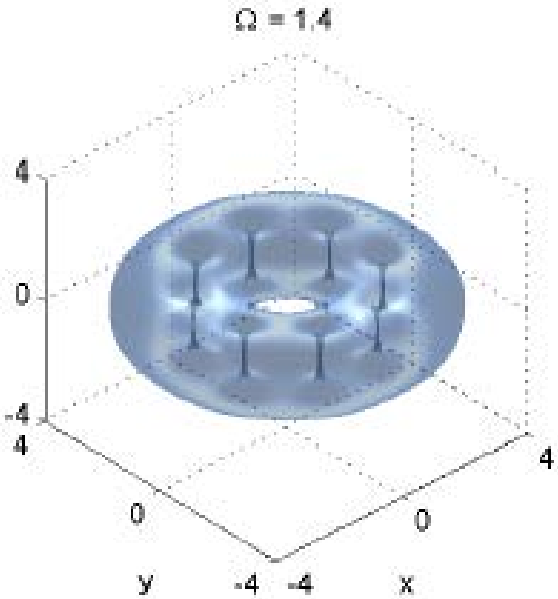
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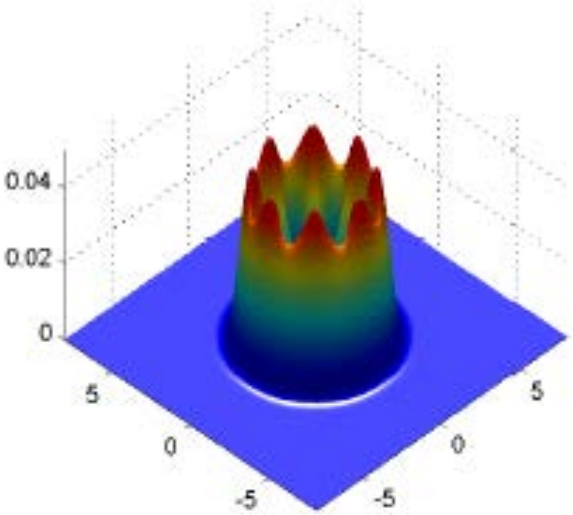
4
x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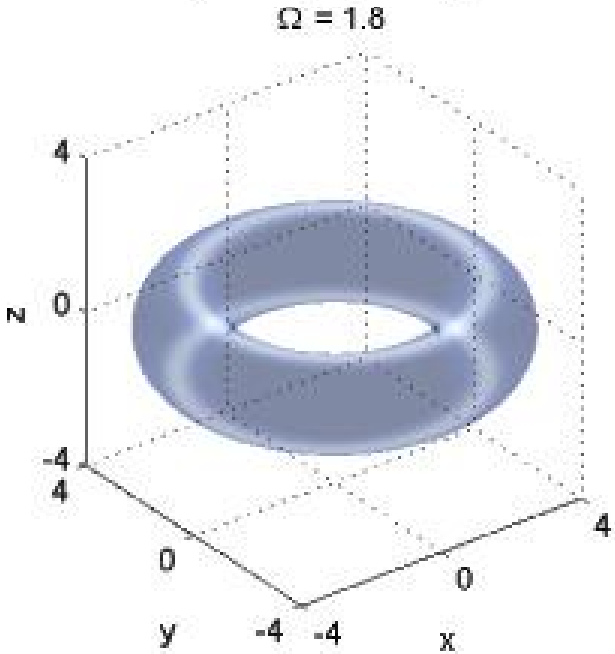
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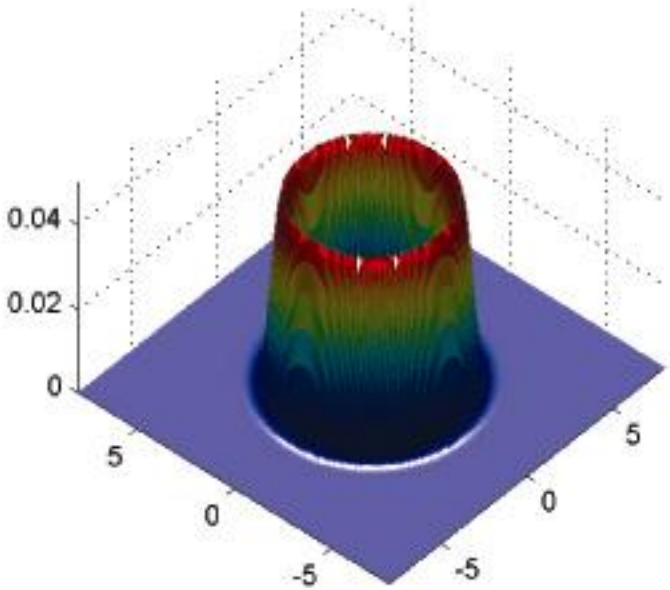
0.04
0.02
0
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0
-5
-5
0
5

back

Dynamical laws of rotating BEC

- Time-dependent Gross-Pitaevskii equation

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

$$\psi(\vec{x},0)=\psi_0(\vec{x}), \qquad L_z:=-i(x\partial_y-y\partial_x)=-i\partial_\theta$$

- Dynamical laws
  - Time reversible & time transverse invariant
  - Conservation laws
  - Well-posedness & finite-time
  - Dynamics of a stationary state with its center shifted
- Numerical methods & results

Numerical Methods

- Time-splitting pseudo-spectral method (TSSP)

Step 1: $$i\,\psi_t(\vec{x},t) = -\frac{1}{2}\nabla^2\psi - \Omega L_z\psi, \qquad L_z := -i(x\partial_y - y\partial_x) = -i\partial_\theta$$

Step 2: $$i\,\psi_t(\vec{x},t) = V_d(\vec{x})\psi(\vec{x},t) + \beta_d\,|\psi(\vec{x},t)|^2\,\psi(\vec{x},t) \quad \Rightarrow \quad |\psi(\vec{x},t)| = |\psi(\vec{x},t_n)|$$

  - Use polar coordinates (B., Q. Du & Y. Zhang, SIAP 06')
  - Time-splitting + ADI technique (B. & H. Wang, JCP, 06')
  - Generalized Laguerre-Hermite functions (B., H. Li &J . Shen, SISC 09')

- A method via rotating Lagrange coordinate (B., et al. SISC, 13')

TSFP for rotating BEC

- Numerical Method one: (Bao, Q. Du & Y. Zhang, SIAM, Appl. Math. 06')
  - Ideas
    - Time-splitting
    - Use polar coordinates: angular momentum becomes constant coefficient
    - Fourier spectral method in transverse direction + FD or FE in radial direction
    - Crank-Nicolson in time
  - Features
    - Time reversible
    - Time transverse invariant
    - Mass Conservation in discretized level
    - Implicit in 1D & efficient to solve
    - Accurate & unconditionally stable

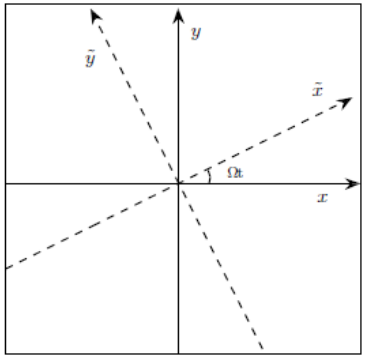
TSFP for rotating BEC

- Numerical Method two: (Bao & H. Wang, J. Comput. Phys. 06')
  - Ideas
    - Time-splitting
    - ADI technique: Equation in each direction become constant coefficient
    - Fourier spectral method
  - Features
    - Time reversible
    - Time transverse invariant
    - Mass Conservation in discretized level
    - Explicit & unconditionally stable
    - Spectrally accurate in space

TSLHP for rotating BEC

- Numerical Method three: (Bao, LI & Shen, SISC 09')
  - Ideas
    - Time-splitting
    - Polar/cylindrical coordinates in 2D/3D, respectively
    - Lagurre + Fourier basis in 2D
    - Lagurre + Fourier +Hermite in 3D
  - Features
    - Time reversible
    - Time transverse invariant
    - Mass Conservation in discretized level
    - Explicit & unconditionally stable
    - Spectrally accurate in space

- 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:

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

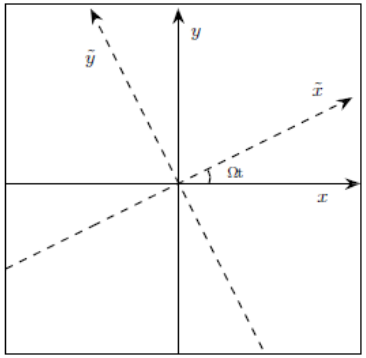
  - GPE in rotating Lagrange coordinates

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

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

A Method via Rotating Lagrange Coordinate

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



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  - 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 ground state

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

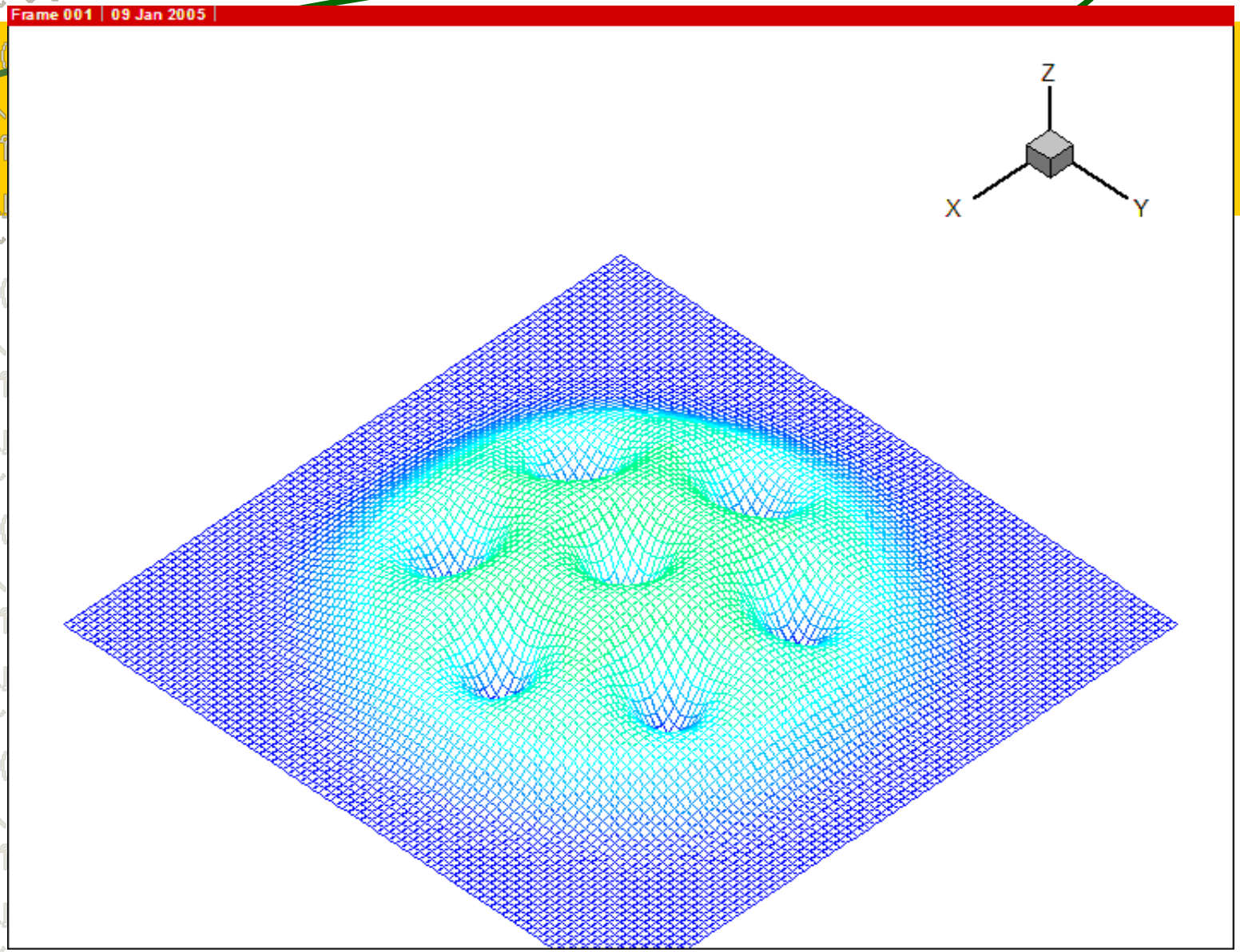
  $\psi_0(\vec{x}) = \phi_g(\vec{x})$: ground state

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

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

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

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



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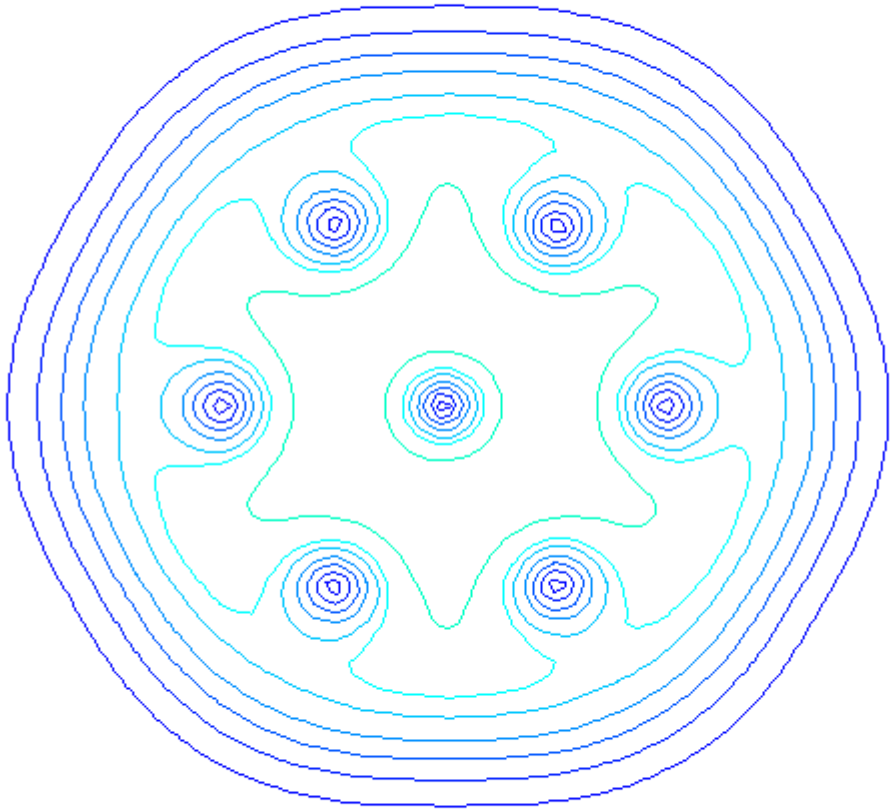

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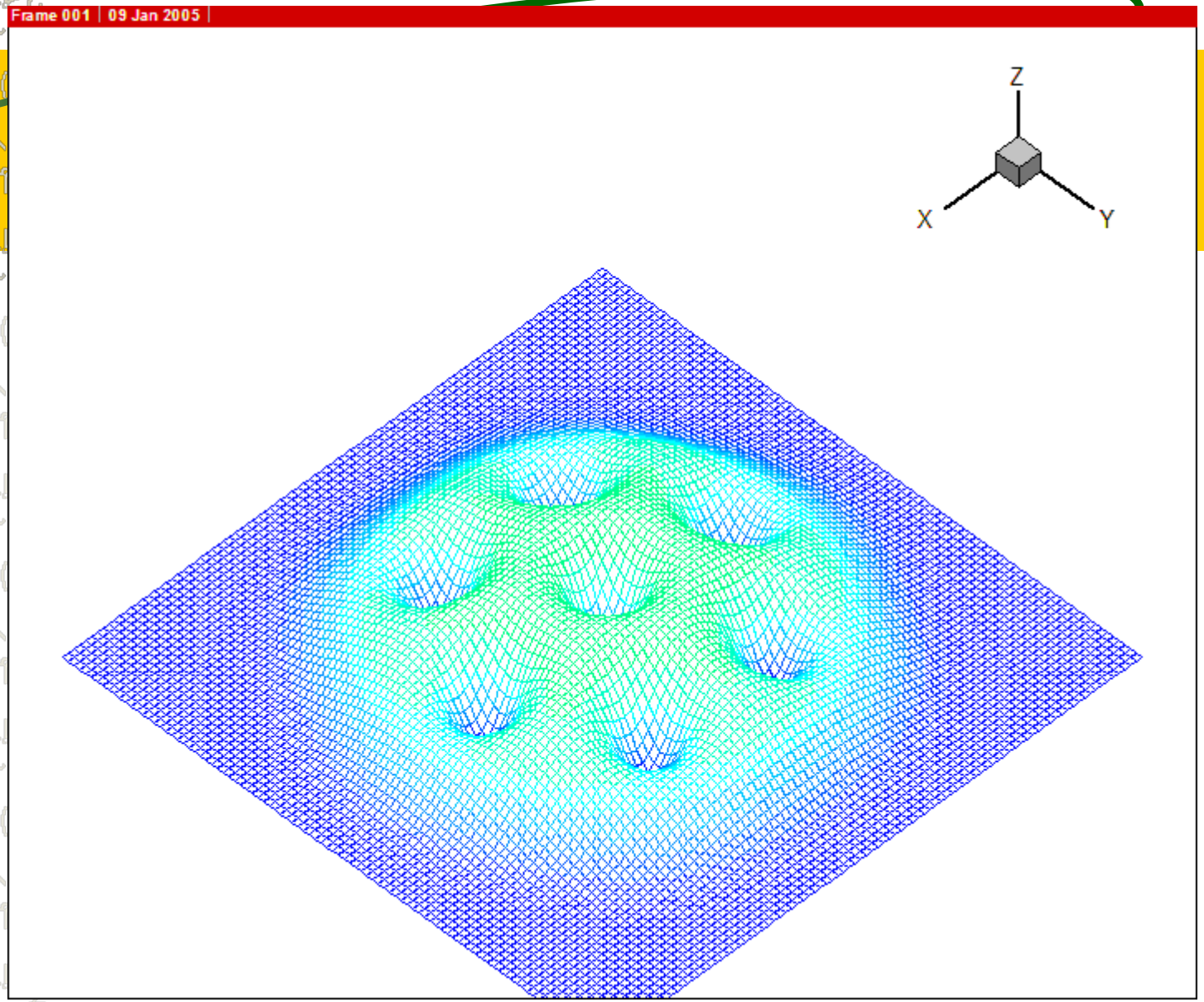

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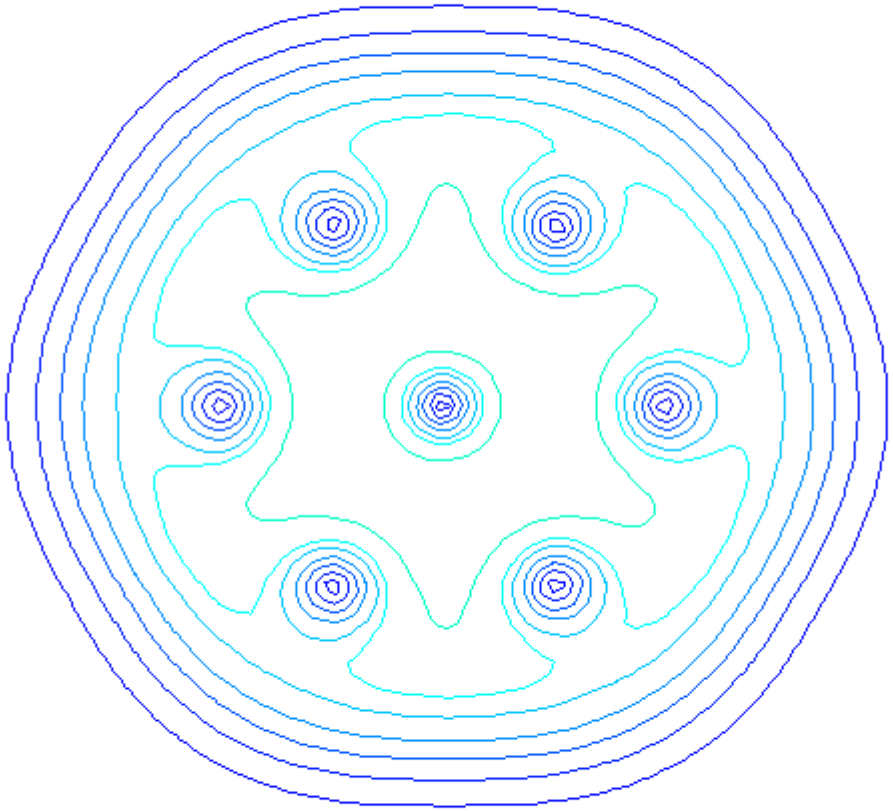

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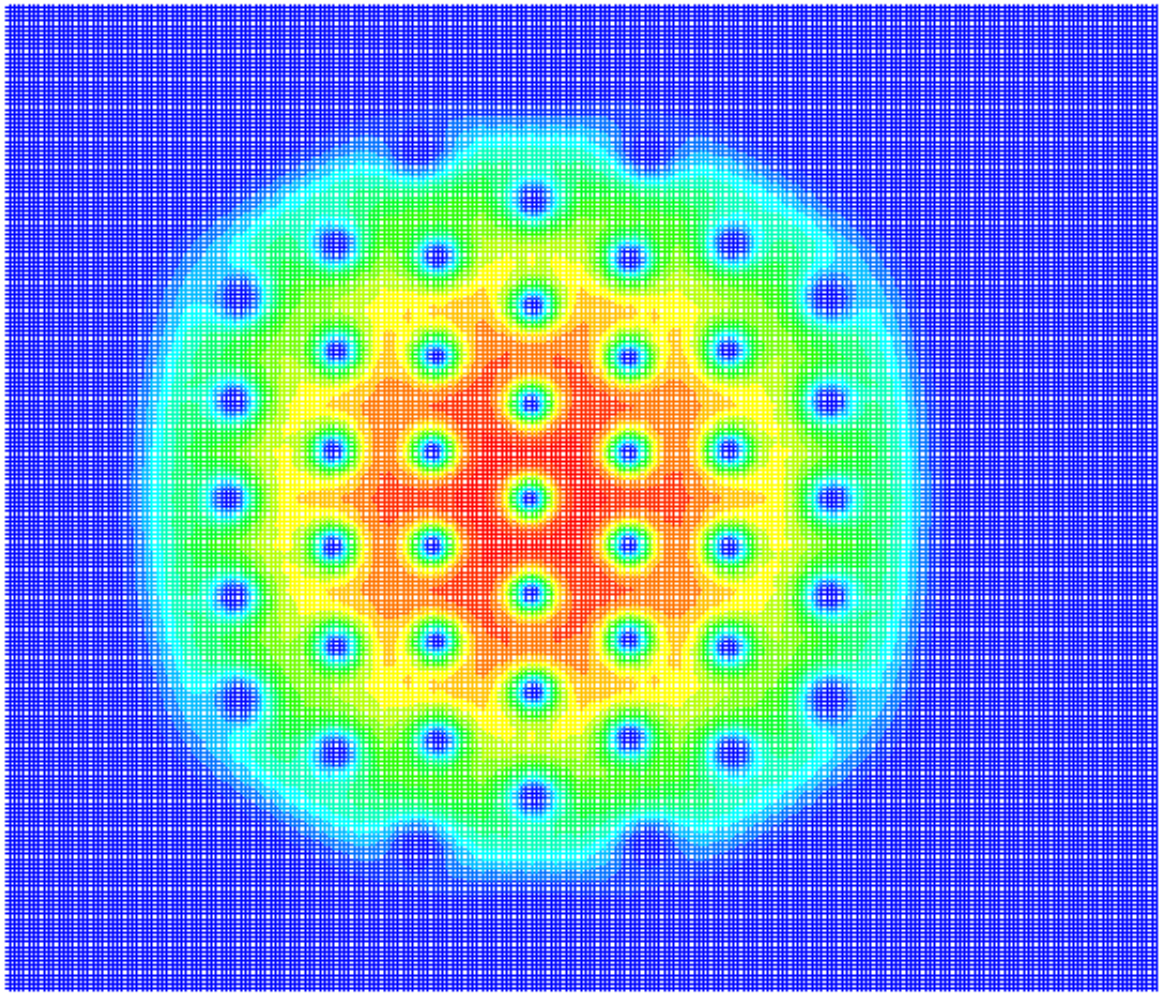

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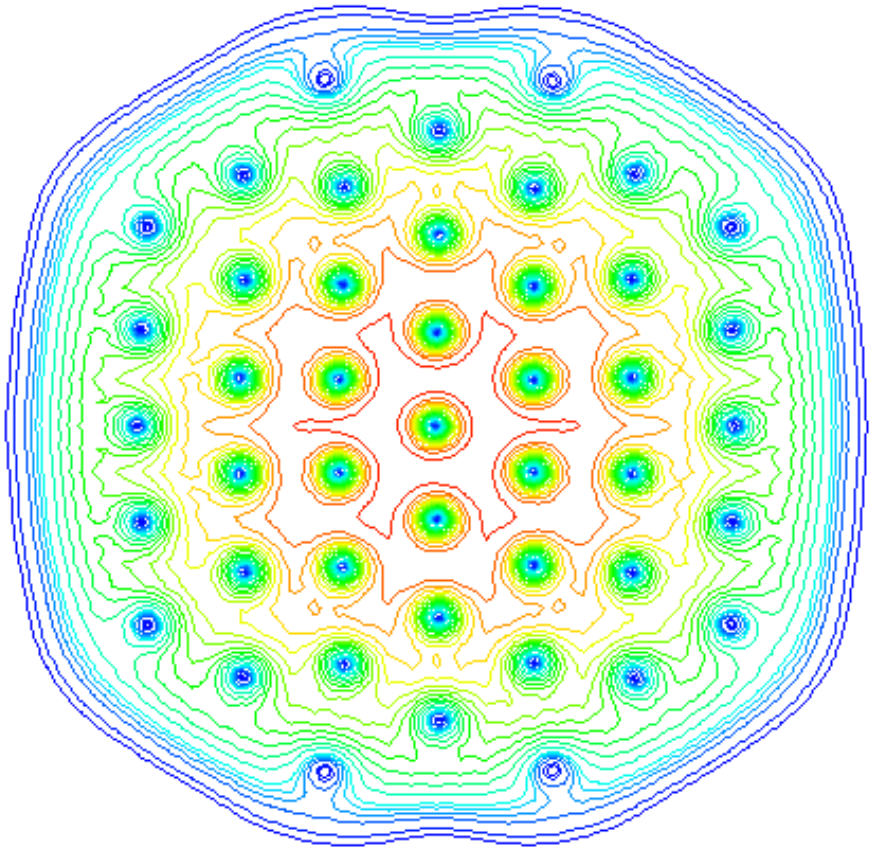


back

Semiclassical scaling

- When $\beta >> 1$, re-scaling $\vec{x} \to \varepsilon^{-1/2}\vec{x} \quad \psi = \psi^{\varepsilon}\varepsilon^{d/4} \quad \varepsilon = 1/\beta^{2/(d+2)}$

$$i\,\varepsilon\frac{\partial}{\partial t}\psi^{\varepsilon}(\vec{x},t) = [-\frac{\varepsilon^2}{2}\nabla^2 + V(\vec{x}) - \varepsilon\,\Omega\,L_z + |\psi^{\varepsilon}|^2]\psi^{\varepsilon}$$

With

$$E_{\varepsilon,\Omega}(\psi^{\varepsilon}) = \int_{\mathrm{R}^d} [\frac{\varepsilon^2}{2}|\nabla\psi^{\varepsilon}|^2 + V(\vec{x})|\psi^{\varepsilon}|^2 - \varepsilon\,\Omega(\psi^{\varepsilon})^* L_z\,\psi^{\varepsilon} + \frac{1}{2}|\psi^{\varepsilon}|^4]\,d\vec{x}$$
$$= O(1)$$

- Leading asymptotics

$$E_{\Omega}(\psi) = \varepsilon^{-1}E_{\varepsilon,\Omega}(\psi^{\varepsilon}) = O\left(\varepsilon^{-1}\right) = O\left(\beta^{2/(d+2)}\right), \quad \mu_{\Omega}(\psi) = O\left(\beta^{2/(d+2)}\right)$$

Quantum Hydrodynamics

- Set $\psi^\varepsilon = \sqrt{\rho^\varepsilon}\, e^{iS^\varepsilon/\varepsilon}, \quad \vec{v}^\varepsilon = \nabla S^\varepsilon, \quad \vec{J}^\varepsilon = \rho^\varepsilon \vec{v}^\varepsilon, \quad \varepsilon = 1/\beta^{2/(d+2)}$
- Geometrical Optics: (Transport + Hamilton-Jacobi)

$$\partial_t \rho^\varepsilon + \nabla \bullet (\rho^\varepsilon \nabla S^\varepsilon) + \Omega \hat{L}_z \rho^\varepsilon = 0, \qquad \hat{L}_z := (x\partial_y - y\partial_x) \equiv \partial_\theta$$

$$\partial_t S^\varepsilon + \frac{1}{2}\left|\nabla S^\varepsilon\right|^2 + V(\vec{x}) + \rho^\varepsilon + \Omega \hat{L}_z S^\varepsilon = \frac{\varepsilon^2}{2}\frac{1}{\sqrt{\rho^\varepsilon}}\Delta\sqrt{\rho^\varepsilon}$$

- Quantum Hydrodynamics (QHD): (Euler +3rd dispersion)

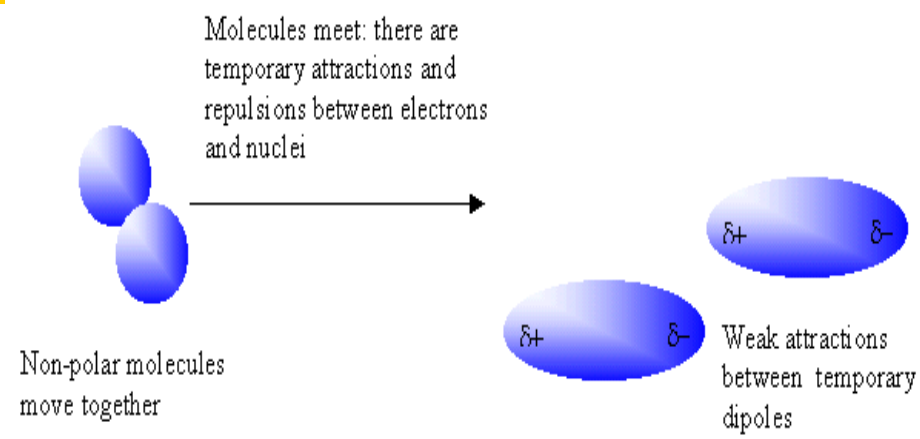
$$\partial_t \rho^\varepsilon + \nabla \bullet (\rho^\varepsilon \vec{v}^\varepsilon) + \Omega \hat{L}_z \rho^\varepsilon = 0$$

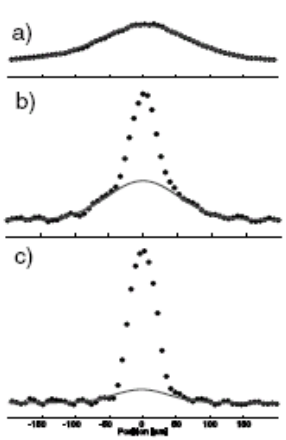
$$\partial_t(\vec{J}^\varepsilon) + \nabla \bullet \left(\frac{\vec{J}^\varepsilon \otimes \vec{J}^\varepsilon}{\rho^\varepsilon}\right) + \nabla P(\rho^\varepsilon) + \rho^\varepsilon \nabla V + \Omega \hat{L}_z \vec{J}^\varepsilon + \Omega A\, \vec{J}^\varepsilon = \frac{\varepsilon^2}{4}\nabla(\rho^\varepsilon \Delta \ln \rho^\varepsilon)$$

$$P(\rho) = \rho^2/2, \qquad \vec{\mathrm{J}}^\varepsilon = \rho^\varepsilon \vec{v}^\varepsilon, \qquad \mathrm{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

Dipolar Quantum Gas

- Experimental setup
  - Molecules meet to form dipoles
  - Cool down dipoles to ultracold
  - Hold in a magnetic trap
  - Dipolar condensation
  - Degenerate dipolar quantum gas
- Experimental realization
  - Chroimum (Cr52)
  - 2005@Univ. Stuttgart, Germany
  - PRL, 94 (2005) 160401
- Big-wave in theoretical study





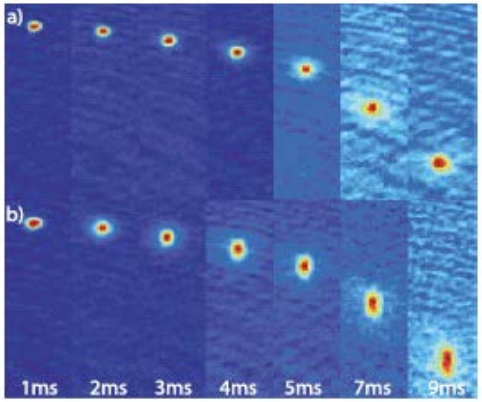


FIG. 3 (color). Time of flight series of absorption images with expansion times from 1 to 9 ms. (a) BEC released from an almost isotropic trap; (b) BEC released from an anisotropic trap.

A. Griesmaier,et al., PRL, 94 (2005)160401

BEC with strong DDI

^{164}Dy

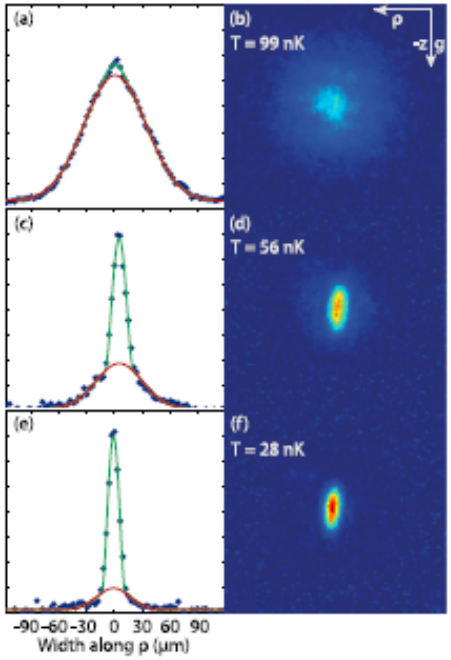


FIG. 2 (color online). TOF profiles of the spin-purified Dy gas for three evaporation time constants, with $\tau = 15$ s in (e) and (f). (a),(c),(e) Data at centers are fit to a parabolic profile (upper curve), which underestimates the condensate fraction, whereas the distributions' wings are fit to a Gaussian profile (lower curve). (b),(d),(f) Absorption images of the emerging BEC. (b) The transition temperature is 99(5) nK, with condensate fraction 2.0(4)%; (d) 44(2)% condensate fraction at 56(3) nK; (f) a BEC of condensate fraction of 73(4)% and $1.5(2) \times 10^4$ atoms forms at 28(2) nK with density 10^{14} cm^{-3}.

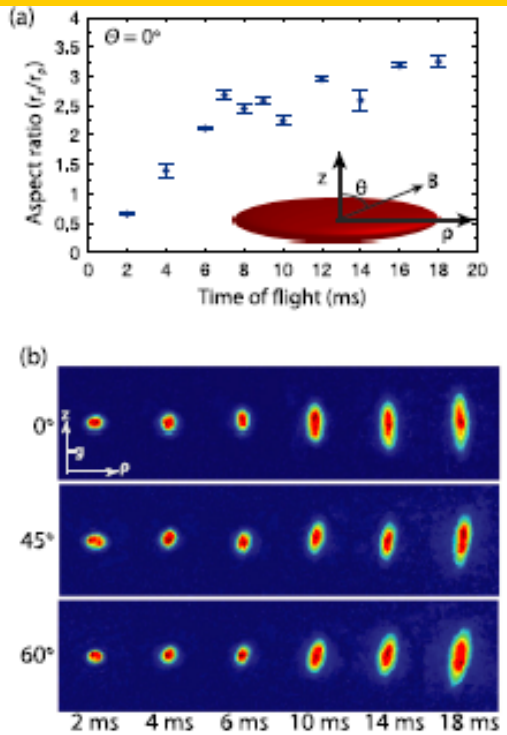


FIG. 3 (color online). Anisotropic expansion profile versus time after trap release. (a) r_z and r_ρ are the dimensions of the parabolic profile fit to the BEC for $\theta = 0°$. Inset: Schematic of the oblate trap and magnetic-field orientation. (b) Images of the expanding condensate after trap release. The condensate rotates by 7(1)° [9.4(6)°] with respect to the $\theta = 0°$ expansion orientation for $\theta = 45°$ [$\theta = 60°$]. No BEC forms for $\theta = 90°$.

Lu, Burdick, Youn & Lev, PRL 107 (2011), 190401.

Mathematical Model

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

$$i\frac{\partial}{\partial t}\psi(\vec{x},t) = \left[-\frac{1}{2}\Delta + V_{\text{ext}}(\vec{x}) + \beta\,|\psi|^2 + \lambda\left(U_{\text{dip}} * |\psi|^2\right)\right]\psi(\vec{x},t)$$

  - Trap potential $V_{\text{ext}}(z) = \frac{1}{2}\left(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2\right)$
  - Interaction constants $\beta = \frac{4\pi N a_s}{a_0}$ (short-range), $\lambda = \frac{mN\mu_0\mu_{\text{dip}}^2}{3\hbar^2 a_0}$ (long-range)
  - Long-range dipole-dipole interaction kernel

$$U_{\text{dip}}(\vec{x}) = \frac{3}{4\pi}\frac{1-3(\vec{n}\cdot\vec{x})^2/|\vec{x}|^2}{|\vec{x}|^3} = \frac{3}{4\pi}\frac{1-3\cos^2(\theta)}{|\vec{x}|^3}, \qquad \vec{n} \in \mathbb{R}^3 \text{ fixed \& satisfies } |\vec{n}| = 1$$

- 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

Mathematical Model

- Mass conservation (Normalization condition)

$$N(t) := \|\psi(\cdot,t)\|^2 = \int_{\mathbb{R}^3} |\psi(x,t)|^2 \, d\vec{x} \equiv \int_{\mathbb{R}^3} |\psi(x,0)|^2 \, d\vec{x} = 1$$

- Energy conservation

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla \psi|^2 + V_{\text{ext}}(x) |\psi|^2 + \frac{\beta}{2} |\psi|^4 + \frac{\lambda}{2} (U_{\text{dip}} * |\psi|^2) |\psi|^2 \right] d\vec{x} \equiv E(\psi_0)$$

- Long-range interaction kernel:
  - It is highly singular near the origin !! At $O\left(\frac{1}{|\vec{x}|^3}\right)$ singularity near the origin !!
  - Its Fourier transform reads
    - No limit near origin in phase space !! $\hat{U}_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2} \qquad \xi \in \mathbb{R}^3$
    - Bounded & no limit at far field too !!
    - Physicists simply drop the second singular term in phase space near origin!!
    - Locking phenomena in computation !!

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)

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

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

- Dipole-dipole interaction becomes

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

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

A New Formulation

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

$$i\frac{\partial}{\partial t}\psi(\vec{x},t)=\left[-\frac{1}{2}\Delta+V_{\text{ext}}(\vec{x})+(\beta-\lambda)|\psi|^2-3\lambda\partial_{\vec{n}\vec{n}}\varphi\right]\psi(\vec{x},t)$$

$$-\Delta\varphi(\vec{x},t)=|\psi(\vec{x},t)|^2,\qquad \lim_{|\vec{x}|\to\infty}\varphi(\vec{x},t)=0$$

- Energy

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

Ground State

- Non-convex minimization problem

$$E(\phi_g) := \min_{\phi \in S} E(\phi) \quad \text{with} \quad S = \left\{ \phi \,|\, \|\phi\| = 1 \,\&\, E(\phi) < \infty \right\}$$

- Nonlinear Eigenvalue problem (Euler-Language eq.)

$$\mu\, \phi(\vec{x}) = \left[-\frac{1}{2}\Delta + V_{\text{ext}}(\vec{x}) + (\beta - \lambda)\,|\phi|^2 - 3\lambda\, \partial_{\vec{n}\vec{n}}\varphi \right] \phi(\vec{x})$$

$$-\Delta\varphi(\vec{x}) = |\phi(\vec{x})|^2, \qquad \lim_{|\vec{x}| \to \infty} \varphi(\vec{x}) = 0, \qquad \|\phi\| = 1$$

- Chemical potential

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

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

Ground State Results

- Theorem (Existence, uniqueness & nonexistence) (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 $\quad \phi_g = e^{i\theta_0} |\phi_g| \quad \text{with} \quad \theta_0 \in \mathbb{R}$
    - Nonexistence of ground state, i.e. $\lim_{\phi \in S} E(\phi) = -\infty$
      - Case I: $\beta < 0$
      - Case II: $\beta \geq 0 \quad \& \quad \lambda > \beta \text{ or } \lambda < -\frac{\beta}{2}$

Key Techniques in Proof

- Estimate on the Poisson equation

$$-\Delta\varphi = |\phi|^2 := \rho \quad \& \quad \lim_{|\vec{x}|\to\infty} \varphi(\vec{x}) = 0 \quad \Rightarrow \quad \|\partial_{\vec{n}}\nabla\varphi\| \le \|\nabla(\nabla\varphi)\| = \|\Delta\varphi\| = \|\rho\| = \|\phi\|_4^2$$

- Positivity & semi-lower continuous

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

- The energy $E(\sqrt{\rho})$ is strictly convex in ρ if

$$\beta \ge 0 \quad \& \quad -\frac{\beta}{2} \le \lambda \le \beta$$

- Confinement potential
- Non-existence result

$$\phi_{\varepsilon_1,\varepsilon_2}(\vec{x}) = \frac{1}{(2\pi\varepsilon_1)^{1/2}} \frac{1}{(2\pi\varepsilon_2)^{1/4}} \exp\left(-\frac{x^2+y^2}{2\varepsilon_1}\right) \exp\left(-\frac{z^2}{2\varepsilon_2}\right), \quad \vec{x} \in \mathbb{R}^3$$

Numerical Method for Ground State

- Gradient flow with discrete normalization

$$\frac{\partial}{\partial t}\phi(\vec{x},t)=\left[\frac{1}{2}\Delta-V_{\text{ext}}(\vec{x})-(\beta-\lambda)|\phi|^2+3\lambda\,\partial_{\vec{n}\vec{n}}\varphi\right]\phi(\vec{x},t),$$

$$-\Delta\varphi(\vec{x},t)=|\phi(\vec{x},t)|^2,\quad \lim_{|\vec{x}|\to\infty}\varphi(\vec{x},t)=0,\qquad \vec{x}\in\Omega\ \&\ t_n\le t<t_{n+1},$$

$$\phi(\vec{x},t_{n+1}):=\phi(\vec{x},t_{n+1}^{+})=\frac{\phi(\vec{x},t_{n+1}^{-})}{\left\|\phi(\vec{x},t_{n+1}^{-})\right\|},\qquad \vec{x}\in\Omega\ \&\ n\ge 0,$$

$$\phi(\vec{x},t)|_{\vec{x}\in\partial\Omega}=\varphi(\vec{x},t)|_{\vec{x}\in\partial\Omega}=0,\ t\ge 0;\quad \phi(\vec{x},0)=\phi_0(\vec{x})\ge 0,\quad \vec{x}\in\Omega,\ \text{with}\ \ \|\phi_0\|=1.$$

- Full discretization
  - Backward Euler sine pseudospectral (BESP) method
  - Avoid to use zero-mode in phase space via DST !!

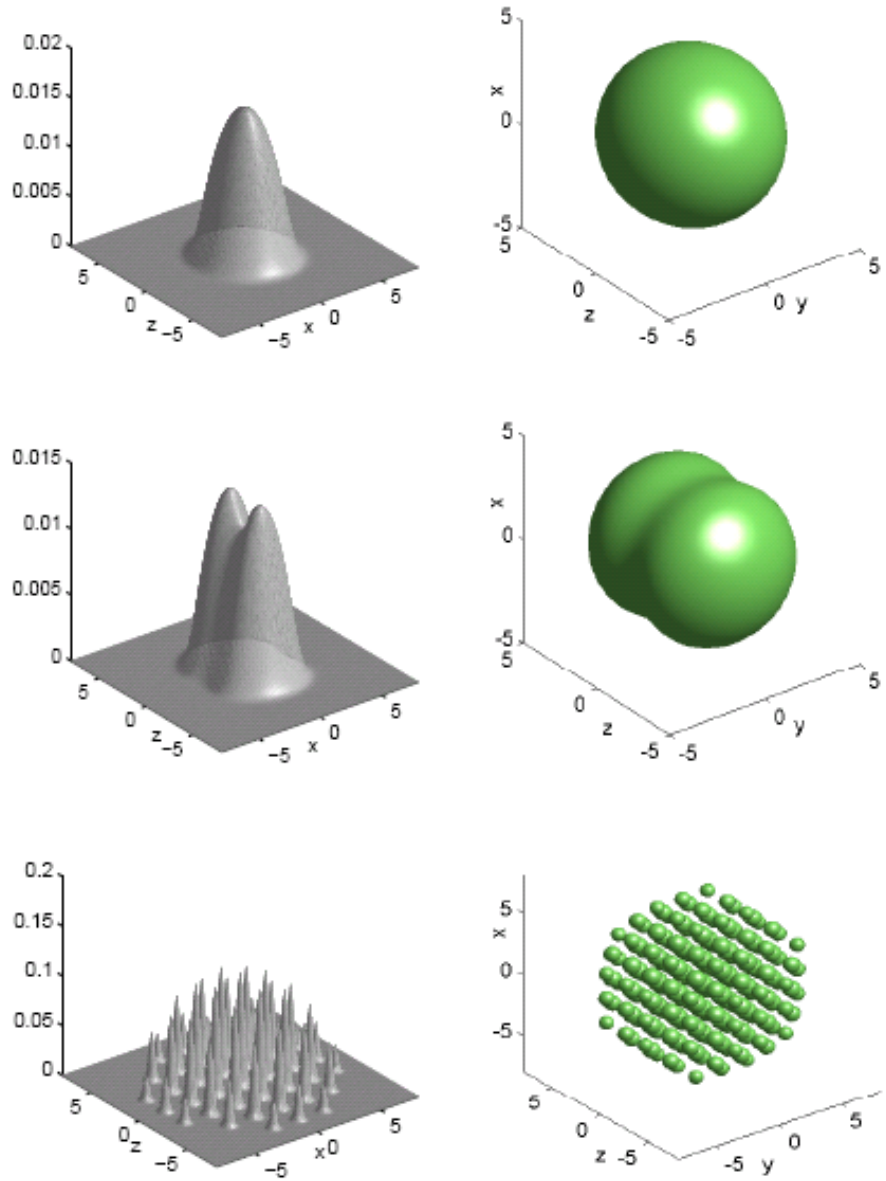


Figure 1: Surface plots of $|\phi_g(x,0,z)|^2$ (left column) and isosurface plots of $|\phi_g(x,y,z)| = 0.01$ (right column) for the ground state of a dipolar BEC with $\beta = 401.432$ and $\lambda = 0.16\beta$ for harmonic potential (top row), double-well potential (middle row) and optical lattice potential (bottom row).

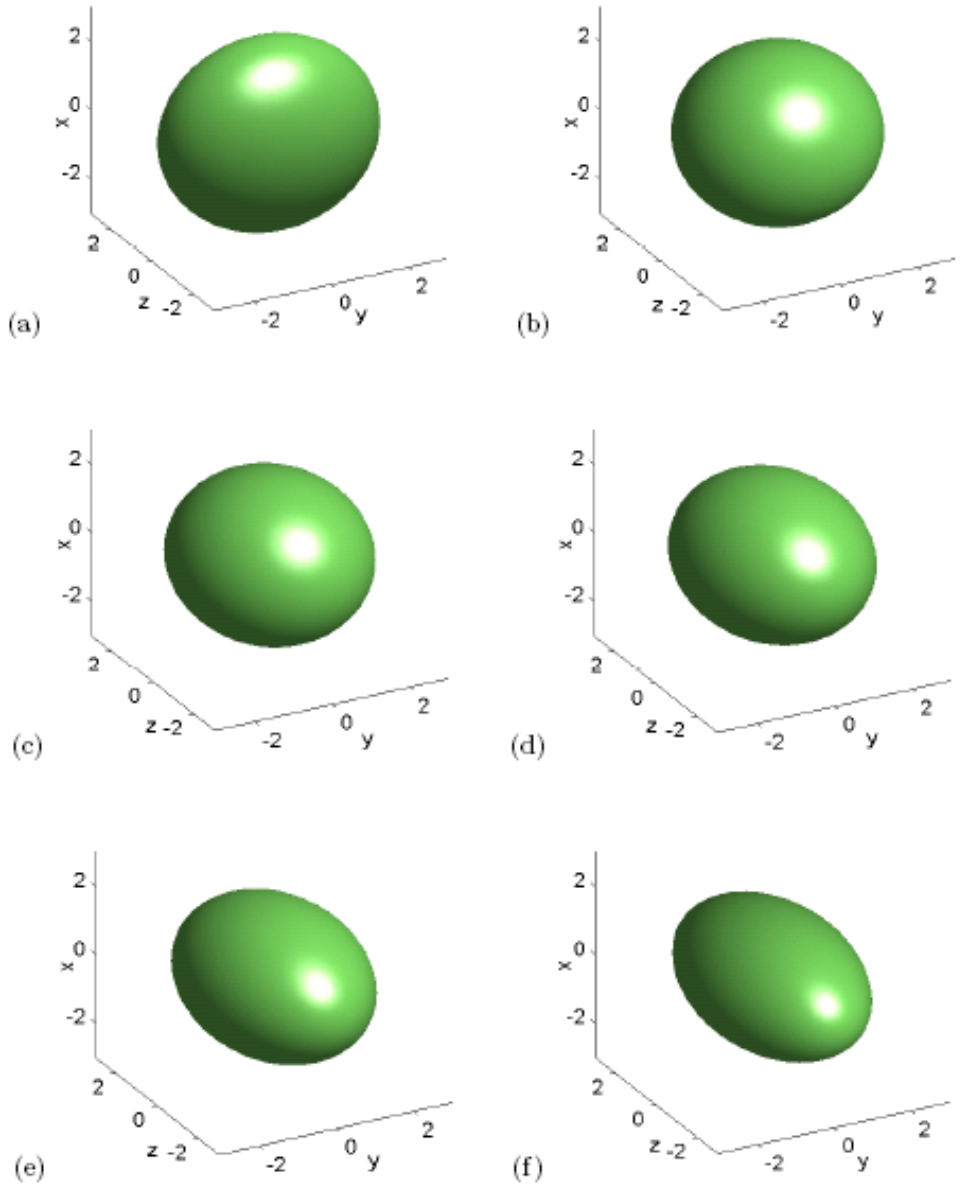


Figure 2: Isosurface plots of the ground state $|\phi_g(\mathrm{x})| = 0.08$ of a dipolar BEC with the harmonic potential $V(\mathrm{x}) = \frac{1}{2}\left(x^2 + y^2 + z^2\right)$ and $\beta = 207.16$ for different values of $\frac{\lambda}{\beta}$: (a) $\frac{\lambda}{\beta} = -0.5$; (b) $\frac{\lambda}{\beta} = 0$; (c) $\frac{\lambda}{\beta} = 0.25$; (d) $\frac{\lambda}{\beta} = 0.5$; (e) $\frac{\lambda}{\beta} = 0.75$; (f) $\frac{\lambda}{\beta} = 1$.

Dynamics and its Computation

- The Problem

$$i\frac{\partial}{\partial t}\psi(\vec{x},t)=\left[-\frac{1}{2}\Delta+V_{\text{ext}}(\vec{x})+(\beta-\lambda)\,|\psi|^2-3\lambda\,\partial_{\vec{n}\vec{n}}\varphi\right]\psi(\vec{x},t)$$

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

$$\psi(\vec{x},0)=\psi_0(\vec{x}),\qquad \vec{x}\in\mathbb{R}^3,$$

- Mathematical questions
  - Existence & uniqueness & finite time blow-up???
- Existing results
  - Carles, Markowich & Sparber, Nonlinearity, 21 (2008), 2569-2590
  - Antonelli & Sparber, 09, preprint --- existence of solitary waves.

Well-posedenss Results

- Theorem (well-posedness) (Bao, Cai & Wang, JCP, 10')
  - Assumptions

    (i) $V_{\text{ext}}(\vec{x}) \in C^{\infty}(\mathbb{R}^3), \quad V_{\text{ext}}(\vec{x}) \geq 0, \forall \vec{x} \in \mathbb{R}^3 \quad \& \quad D^{\alpha} V_{\text{ext}}(\vec{x}) \in L^{\infty}(\mathbb{R}^3) \quad |\alpha| \geq 2$

    (ii) $\psi_0 \in X = \left\{ u \in H^1(\mathbb{R}^3) \,|\, \|u\|_X^2 = \|u\|_{L^2}^2 + \|\nabla u\|_{L^2}^2 + \int_{\mathbb{R}3} V_{\text{ext}}(\vec{x}) u(\vec{x}) d\,\vec{x} < \infty \right\}$
  - Results
    - Local existence, i.e.

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

    - If $\beta \geq 0 \quad \& \quad -\frac{\beta}{2} \leq \lambda \leq \beta$ global existence, i.e. $T_{\max} = +\infty$

Finite Time Blowup Results

- **Theorem** (finite time blowup) (Bao, Cai & Wang, JCP, 10')
  - **Assumptions** (i) $\beta<0$ or $\beta \geq 0 \;\&\; \lambda < -\dfrac{\beta}{2}$ or $\lambda>\beta$

    (ii) $3V_{\text{ext}}(\vec{x}) + \vec{x}\cdot\nabla V_{\text{ext}}(\vec{x}) \geq 0, \quad \forall \vec{x} \in \mathbb{R}^3$
  - **Results**:
    - For any $\psi_0(\vec{x}) \in X$, there exists finite time blowup, i.e. $T_{\max} < +\infty$
    - If one of the following conditions holds

(i) $E(\psi_0) < 0$

(ii) $E(\psi_0) = 0 \quad \& \quad \operatorname{Im} \int_{\mathbb{R}^3} \overline{\psi}_0(x)\,(\vec{x}\cdot\nabla\psi_0(\vec{x}))\,d\,\vec{x} < 0$

(iii) $E(\psi_0) > 0 \quad \& \quad \operatorname{Im} \int_{\mathbb{R}^3} \overline{\psi}_0(x)\,(\vec{x}\cdot\nabla\psi_0(\vec{x}))\,d\,\vec{x} < -\sqrt{3E(\psi_0)}\,\|\vec{x}\,\psi_0\|_{L^2}$

Numerical Method for dynamics

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

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

  - Step 2: solve the nonlinear ODE analytically

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

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

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

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

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

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

New numerical methods for DDI

- How to compute nonlocal DDI

$$\phi := U_{\text{dip}} * |\psi|^2$$

  - FFT (fast Fourier transform)
  - DST (discrete sine transform)

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

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

  - Nonuniform FFT

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

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

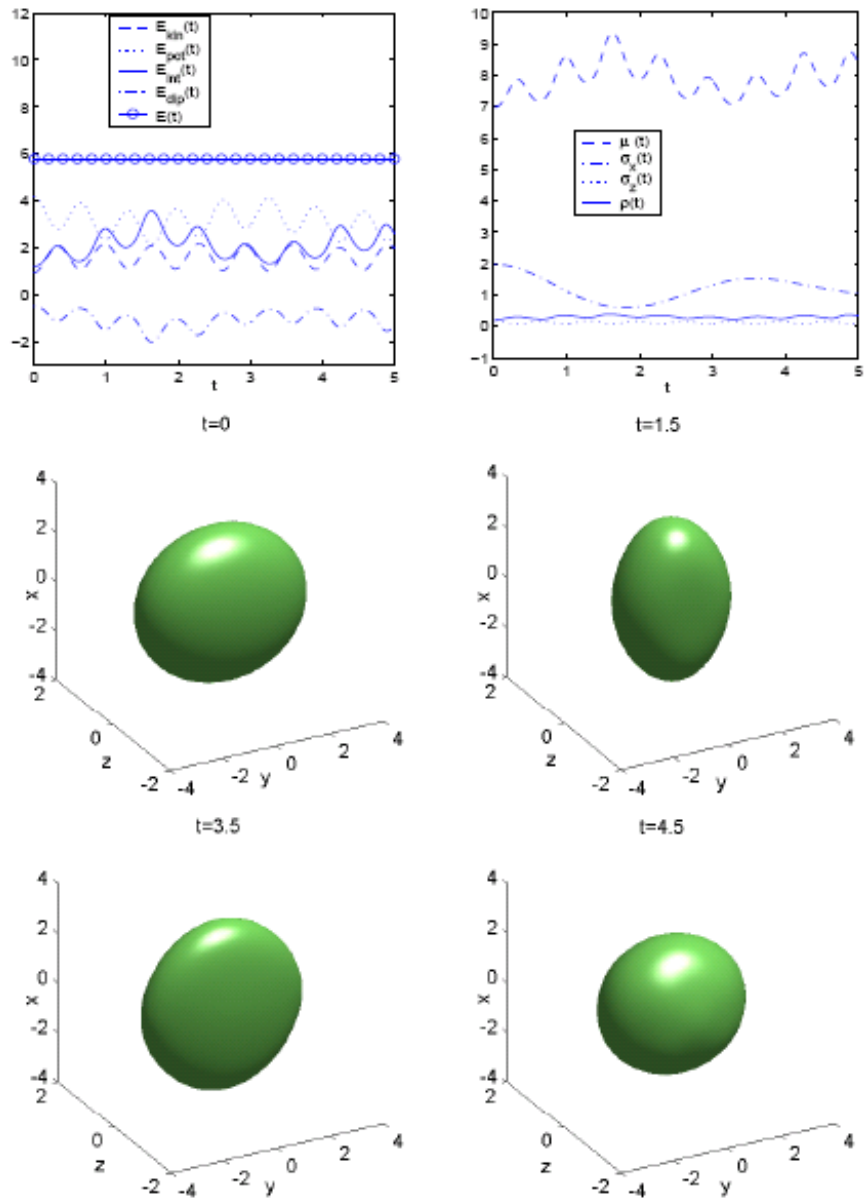


Figure 3: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar direction is suddenly changed from $\mathbf{n} = (0,0,1)^T$ to $(1,0,0)^T$ at time $t = 0$.

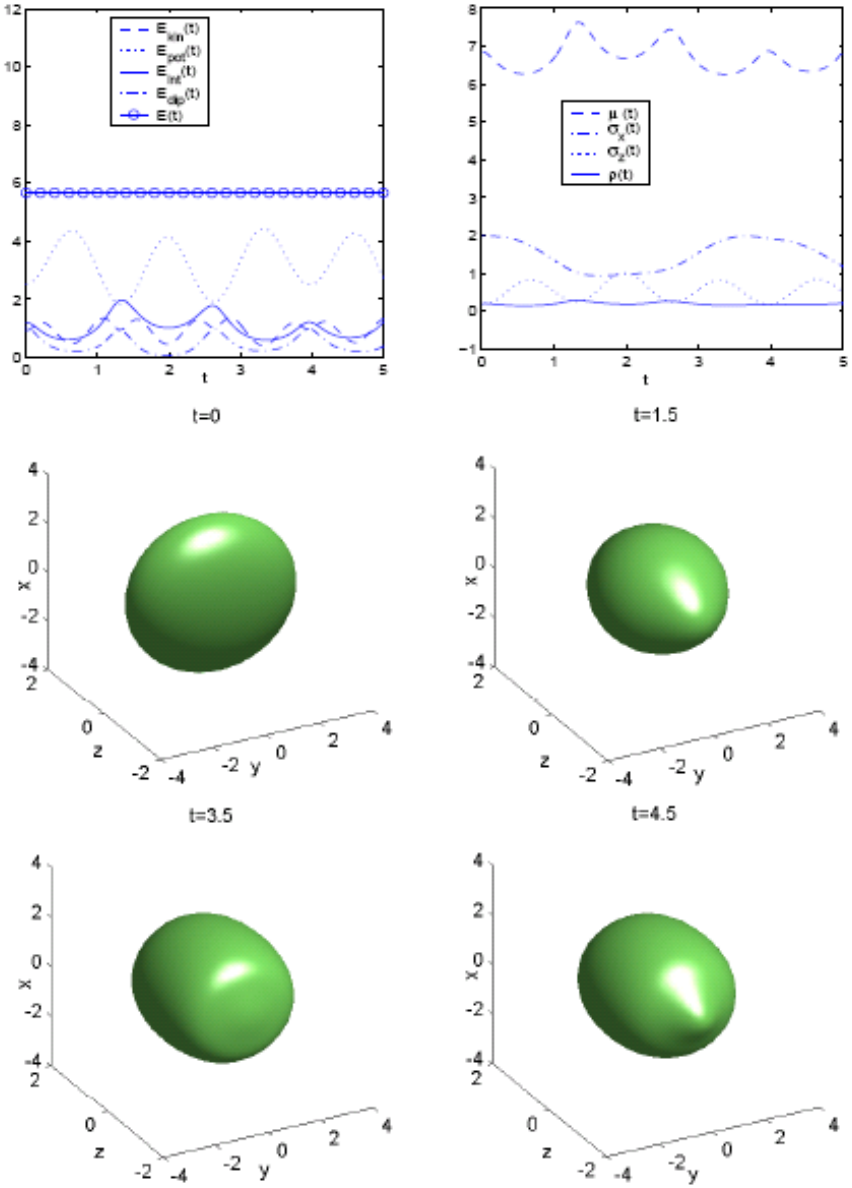


Figure 4: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the trap potential is suddenly changed from from $\frac{1}{2}(x^2+y^2+25z^2)$ to $\frac{1}{2}(x^2+y^2+\frac{25}{4}z^2)$ at time $t=0$.

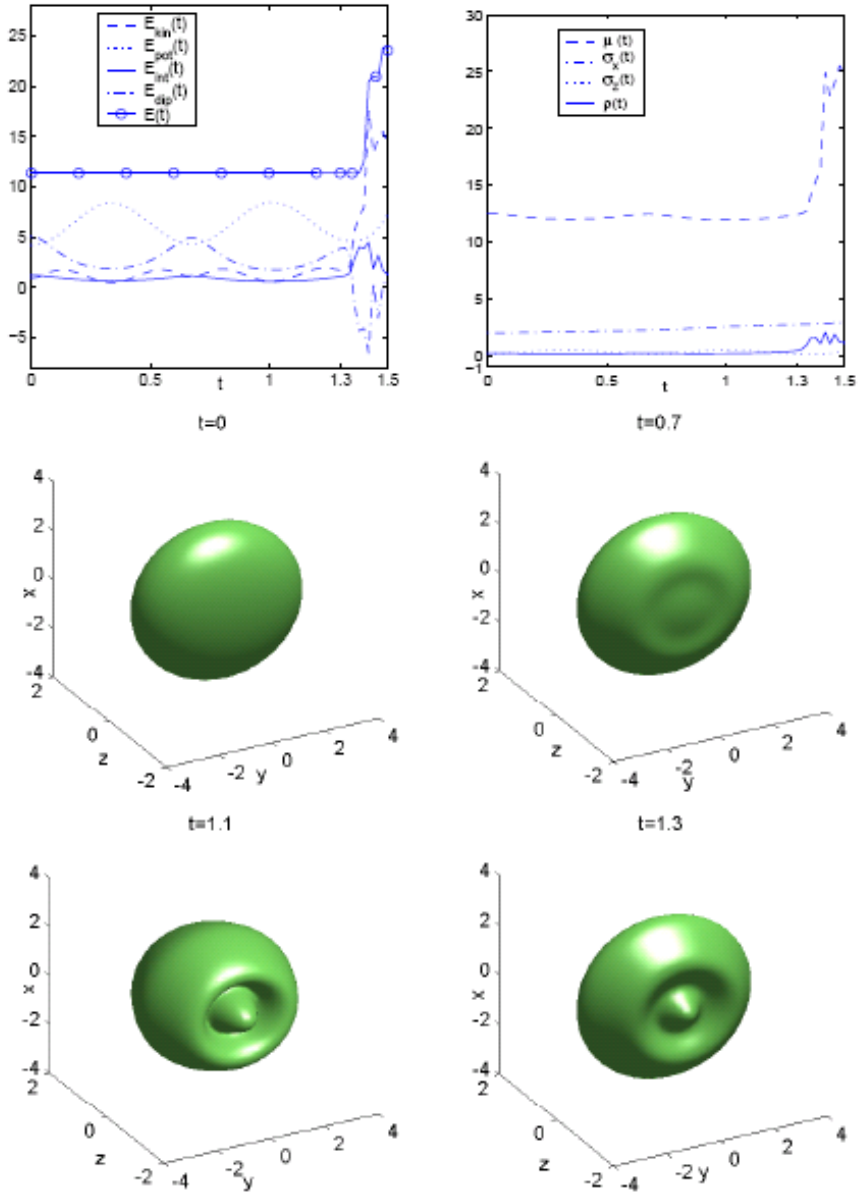


Figure 5: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar interaction constant is suddenly changed from $\lambda = 0.8\beta = 82.864$ to $\lambda = 4\beta = 414.32$ at time $t = 0$.

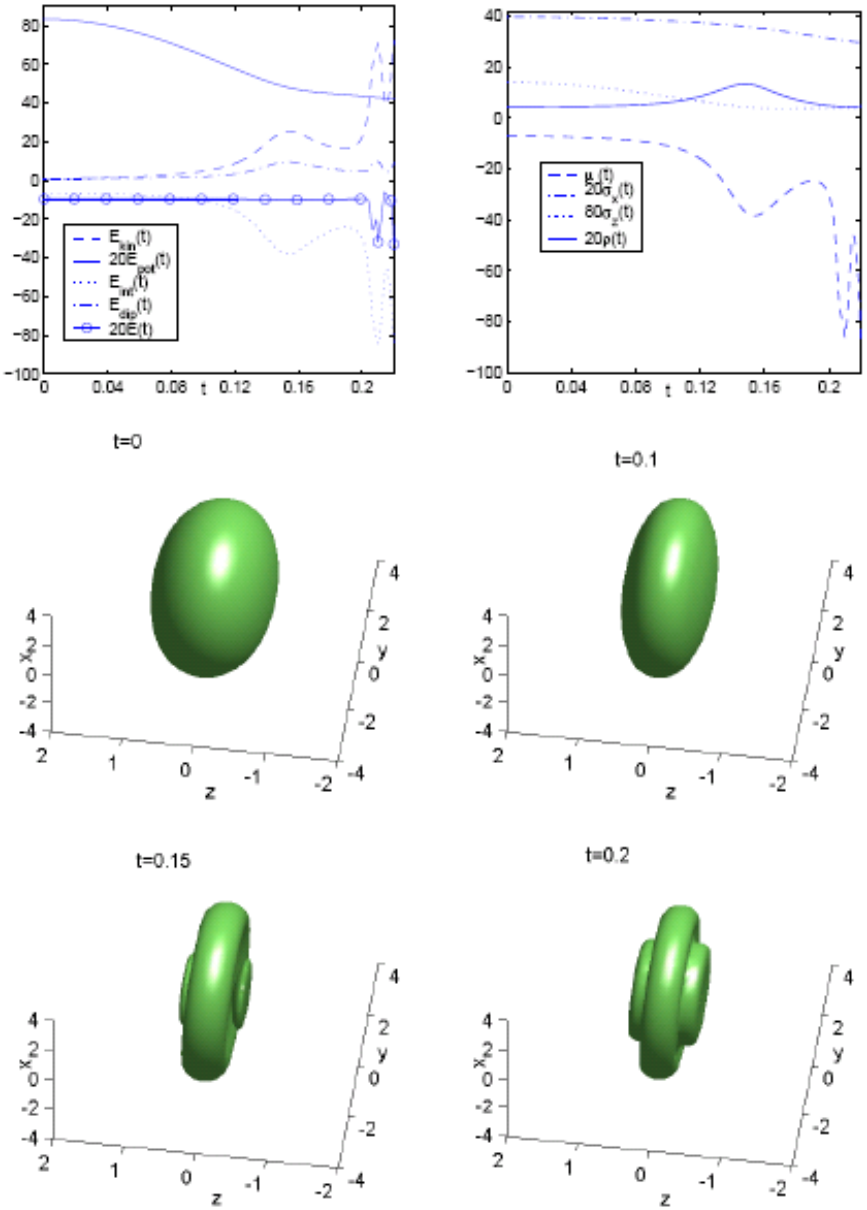
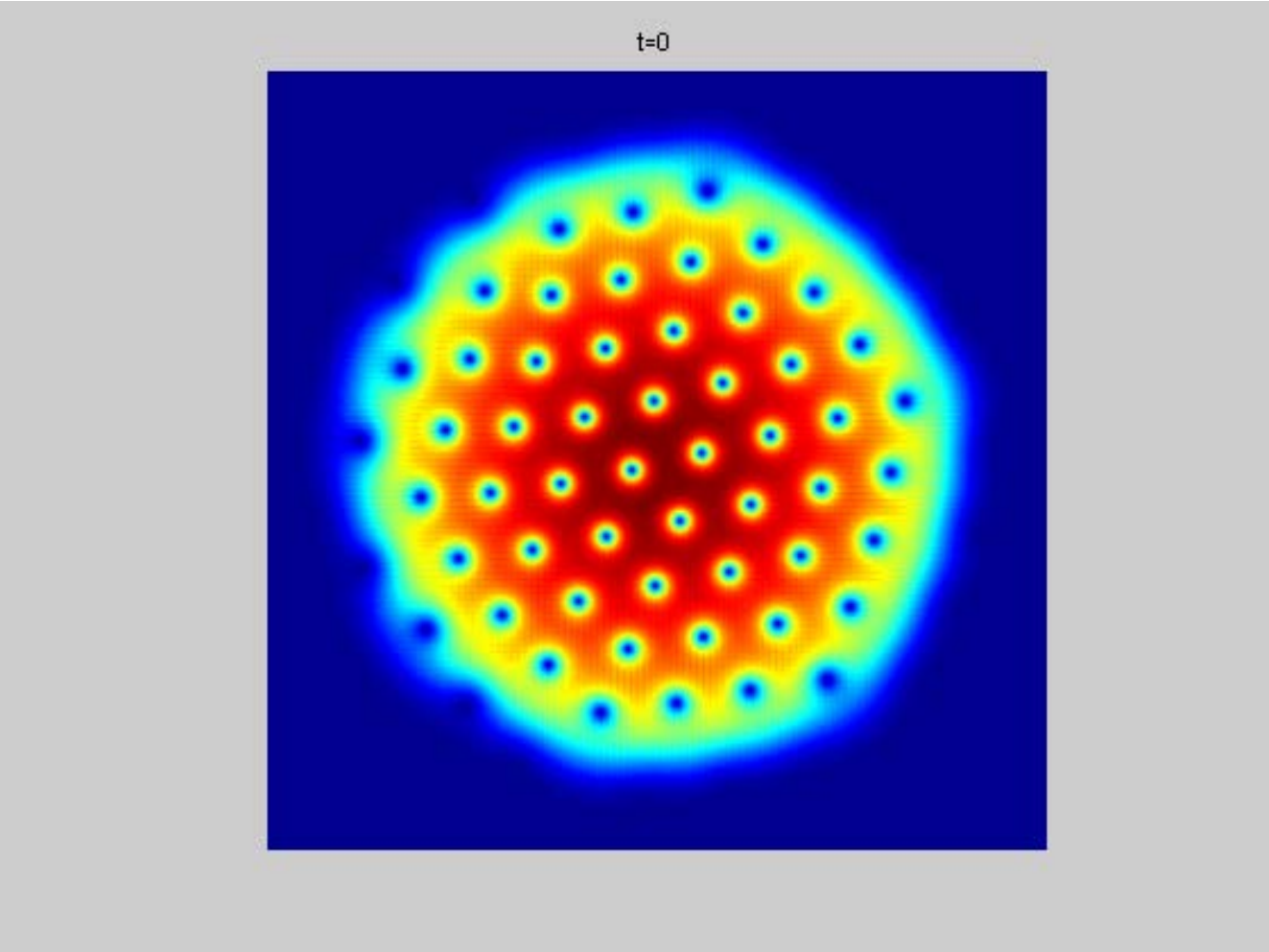


Figure 6: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the interaction constant β is suddenly changed from $\beta = 103.58$ to $\beta = -569.69$ at time $t = 0$.

Dynamics of a vortex lattice



Dimension Reduction (3D→ 2D)

- Assumptions

$$\gamma_z \gg \gamma_x \;\&\; \gamma_y = O(1) \quad \& \quad V_{\text{ext}}(\vec{x}) = V_{2D}(x,y) + \frac{z^2}{2\varepsilon^4}, \quad \varepsilon := \frac{1}{\sqrt{\gamma_z}}$$

- Decomposition of the linear operator

$$L := -\frac{1}{2}\Delta + V_{\text{ext}}(\vec{x}) = -\frac{1}{2}\Delta_\perp + V_{2D}(x,y) + L_z$$

$$L_z = -\frac{1}{2}\partial_{zz} + \frac{z^2}{2\varepsilon^4} = \frac{1}{\varepsilon^2}\left(-\frac{1}{2}\partial_{\tilde{z}\tilde{z}} + \frac{\tilde{z}^2}{2}\right)$$

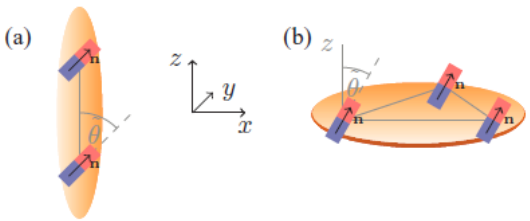


FIG. 1. (Color online) In the quasi-1D setup in (a) the dipolar BEC is confined to the z direction. In the quasi-2D setup in (b) the atoms are confined to the x-y plane. The dipoles are polarized along the axis $\mathbf{n} = (n_x, n_y, n_z)$ with polar angle $\tilde{\theta}$ (i.e., $n_z = \cos\tilde{\theta}$).

- Ansatz

$$\psi(x,y,z,t) \approx e^{-\frac{it}{2\varepsilon^2}}\psi(x,y,t)\,\omega_\varepsilon(z) \quad \& \quad \omega_\varepsilon(z) = \frac{1}{(\varepsilon^2\pi)^{1/4}}\exp\left(-\frac{z^2}{2\varepsilon^2}\right)$$

Dimension Reduction (3D→ 2D)

- 2D equations when $\varepsilon \to 0$ (Bao, Cai, Lei, Rosenkranz, PRA, 10')

$$i\frac{\partial}{\partial t}\psi(x,y,t) = [-\frac{1}{2}\Delta_\perp + V_{2D}(x,y) + \frac{\beta - \lambda + 3\lambda n_3^2}{\varepsilon\sqrt{2\pi}}|\psi|^2$$

$$-\frac{3\lambda}{2}(\partial_{\vec{n}_\perp \vec{n}_\perp} - n_3^2\Delta_\perp)\varphi\,]\psi(x,y,t)$$

$$(-\Delta_\perp)^{1/2}\varphi(x,y,t) = |\psi(x,y,t)|^2, \qquad \lim_{|(x,y)|\to\infty}\varphi(x,y,t) = 0$$

- Energy

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^3}\{\frac{1}{2}|\nabla_\perp\psi|^2 + V_{2D}(\vec{x})|\psi|^2 + \frac{1}{2\varepsilon\sqrt{2\pi}}(\beta - \lambda + 3\lambda n_3^2)|\psi|^4$$

$$+\frac{3\lambda}{4}[\left|\partial_{n_\perp}(-\Delta_\perp)^{1/4}\varphi\right|^2 - n_3^2\left|\nabla_\perp(-\Delta_\perp)^{1/4}\varphi\right|^2]\}d\vec{x}$$

Two-component BEC

- The 3D coupled Gross-Pitaevskii equations

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

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

- Normalization conditions

$$N(t)=\sum_{j=1}^{2}\int_{\mathbb{R}^3}|\psi_j(\vec{x},t)|^2\,d\vec{x}=N_1^0+N_2^0:=N \quad \text{with} \quad N_j^0=\int_{\mathbb{R}^3}|\psi_j(\vec{x},0)|^2\,d\vec{x},$$

- Intro- & inter-atom Interactions

$$U_{jl}=\frac{4\pi\hbar^2 a_{jl}}{m} \qquad \text{with} \qquad a_{12}=a_{21}$$

Two-component BEC

- Nondimensionalization

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

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

- Normalization conditions
  - There is external driven field $\lambda \neq 0$

$$N(t)=\int_{\mathbb{R}^3}|\psi_1(\vec{x},t)|^2\,d\vec{x}+\int_{\mathbb{R}^3}|\psi_2(\vec{x},t)|^2\,d\vec{x}=1$$

  - No external driven field $\lambda = 0$

$$\int_{\mathbb{R}^3}|\psi_1(\vec{x},t)|^2\,d\vec{x}=\frac{N_1^0}{N},\qquad \int_{\mathbb{R}^3}|\psi_2(\vec{x},t)|^2\,d\vec{x}=\frac{N_2^0}{N}$$

Two-component BEC

- Energy

$$E(\Psi)=\int_{\mathrm{R}^d}[\sum_{j=1}^{2}(\frac{1}{2}|\nabla\psi_j|^2+V(\vec{x})|\psi_j|^2-\Omega\psi_j * L_z\psi_j+\sum_{l=1}^{2}\frac{\beta_{jl}}{2}|\psi_j|^2|\psi_l|^2)-2\lambda\,\mathrm{Re}(\psi_1^*\psi_2)]d\vec{x}$$

- Reduction to one-component: $\lambda=0,\ N_1^0\gg N_2^0,\ N_1^0=O(N)$

$$N_2(t)=\int_{\mathbb{R}^3}|\psi_2(\vec{x},t)|^2\,d\vec{x}=\frac{N_2^0}{N}:=\varepsilon\ll 1,\quad N_1(t)=\int_{\mathbb{R}^3}|\psi_1(\vec{x},t)|^2\,d\vec{x}=\frac{N_1^0}{N}:=1-\varepsilon\approx 1$$

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

$$\psi(\vec{x},t)=\sqrt{N/N_1^0}\,\psi_1(\vec{x},t)\quad\&\quad\beta=N_1^0\beta_{11}/N\qquad\frac{|E(\Psi)-E_s(\psi)|}{E_s(\psi)}=O(\varepsilon)$$

Ground state

- No external field: $\lambda = 0$

$$\min_{\|\phi_1\|=\alpha, \|\phi_2\|=\beta} E(\phi_1, \phi_2) \quad \text{with} \quad \alpha + \beta = 1$$

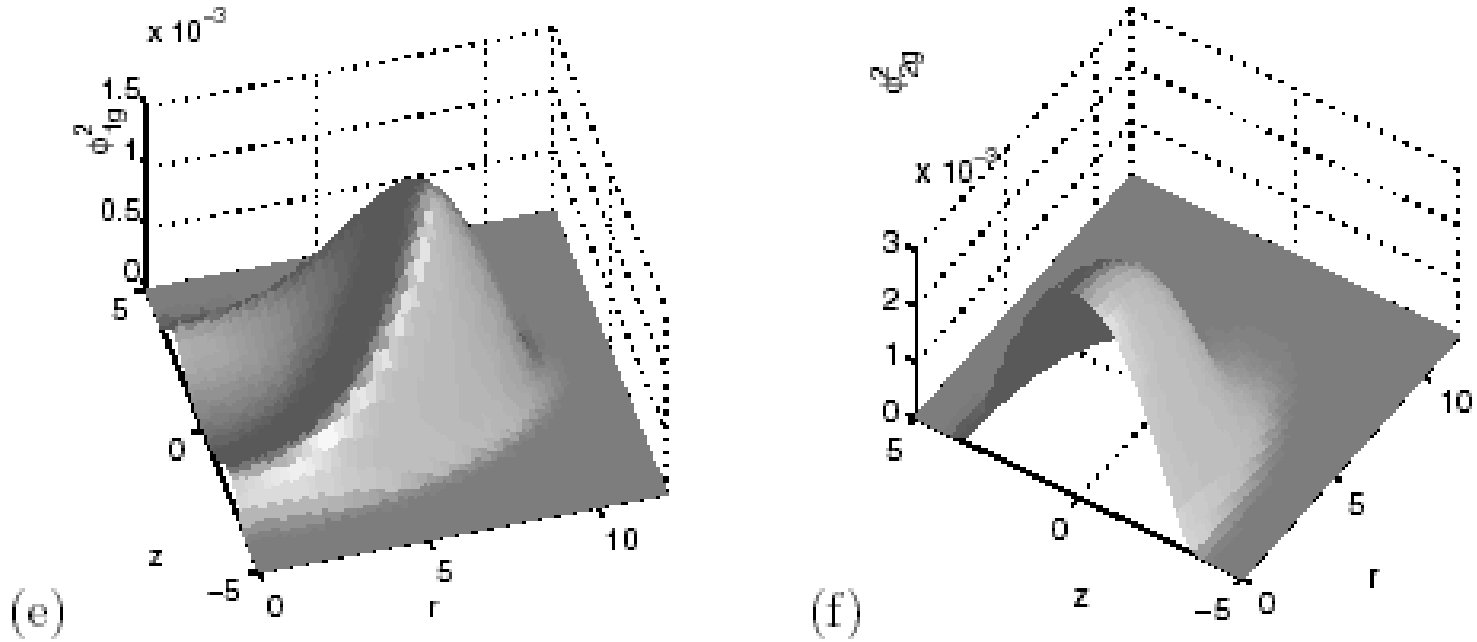
- Nonlinear eigenvalue problem

$$\mu_1 \phi_1(\vec{x}) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2]\phi_1$$

$$\mu_2 \phi_2(\vec{x}) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{21}|\phi_1|^2 + \beta_{22}|\phi_2|^2]\phi_2$$

- Existence & uniqueness of positive solution
- Numerical methods can be extended

Ground states



crater

Ground state

- With external field: $\lambda \neq 0$

$$\min_{\|\phi_1\|^2+\|\phi_2\|^2=1} E(\phi_1,\phi_2)$$

- Nonlinear eigenvalue problem

$$\mu\,\phi_1(\vec{x}) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2]\phi_1 - \lambda\phi_2$$

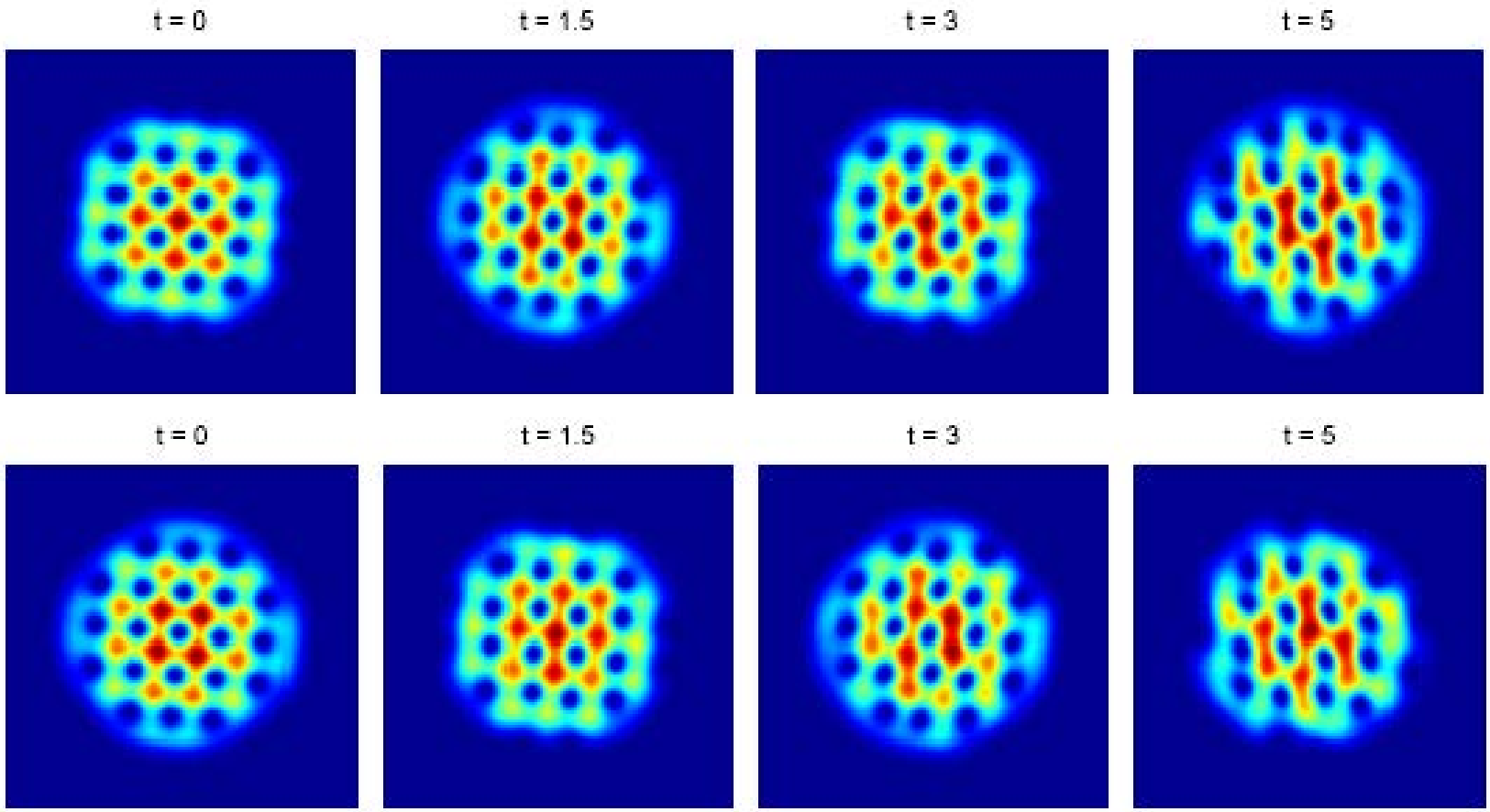
$$\mu\,\phi_2(\vec{x}) = [-\frac{1}{2}\nabla^2 + V(\vec{x}) - \Omega L_z + \beta_{21}|\phi_1|^2 + \beta_{22}|\phi_2|^2]\phi_2 - \lambda\phi_1$$

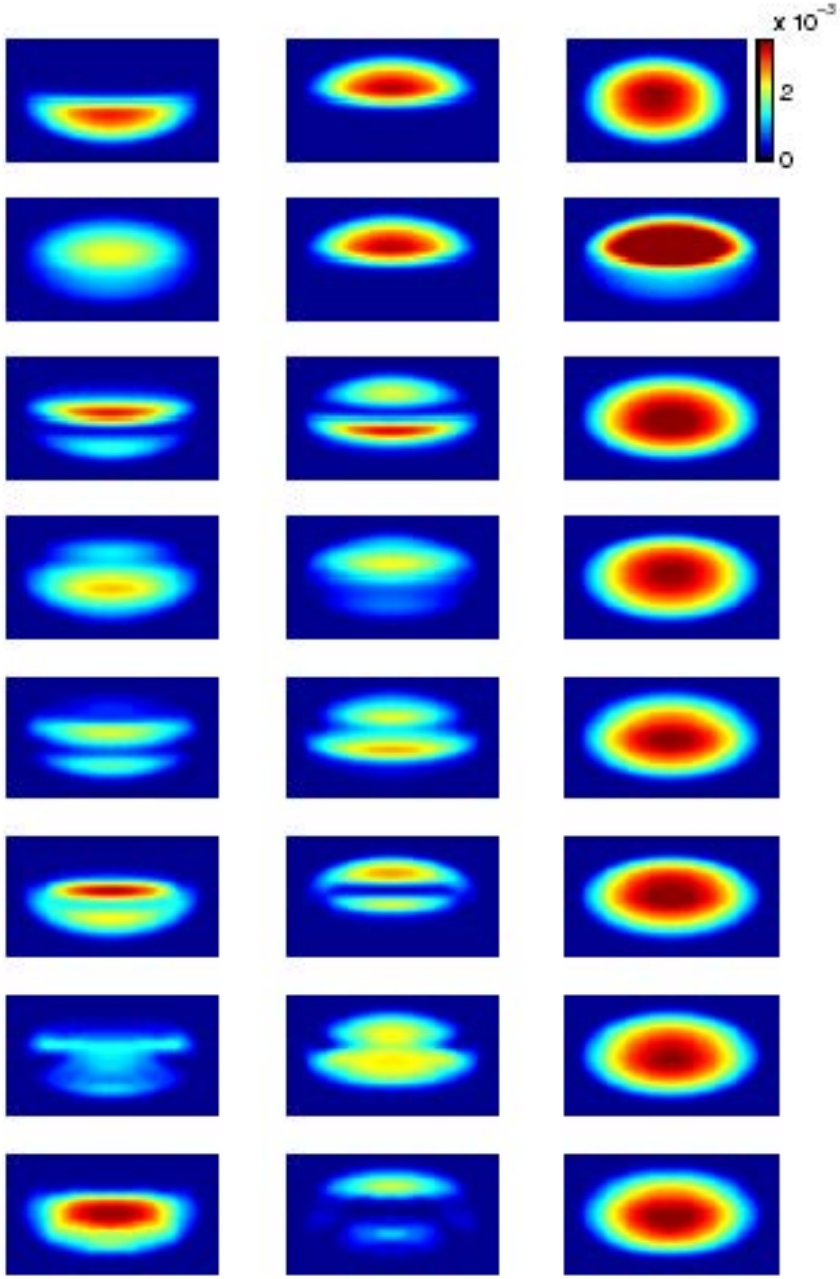
- Existence & uniqueness of positive solution ???
- Numerical methods can be extended????

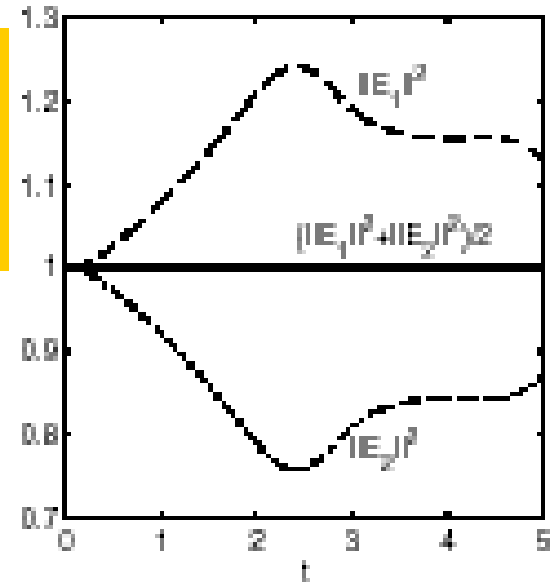
Dynamics

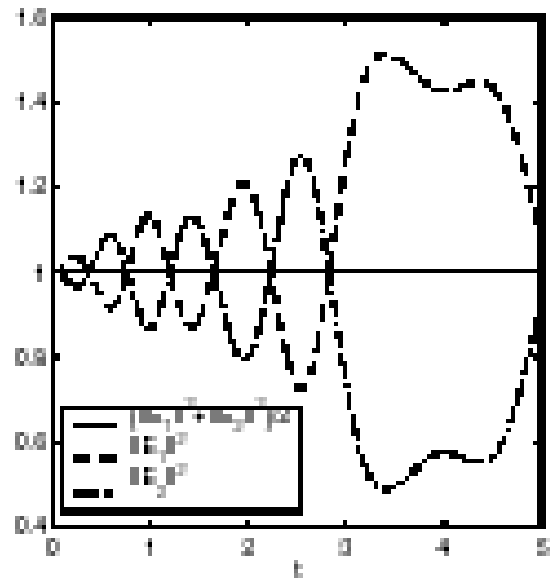
- Dynamical laws:
  - Conservation of Angular momentum expectation
  - Dynamics of condensate width
  - Dynamics of a stationary state with a shift
  - Dynamics of mass of each component, they are periodic function when $\beta_{11} = \beta_{12} = \beta_{22}$
  - Vortex can be interchanged!
- Numerical methods
  - Time-splitting spectral method

Dynamics

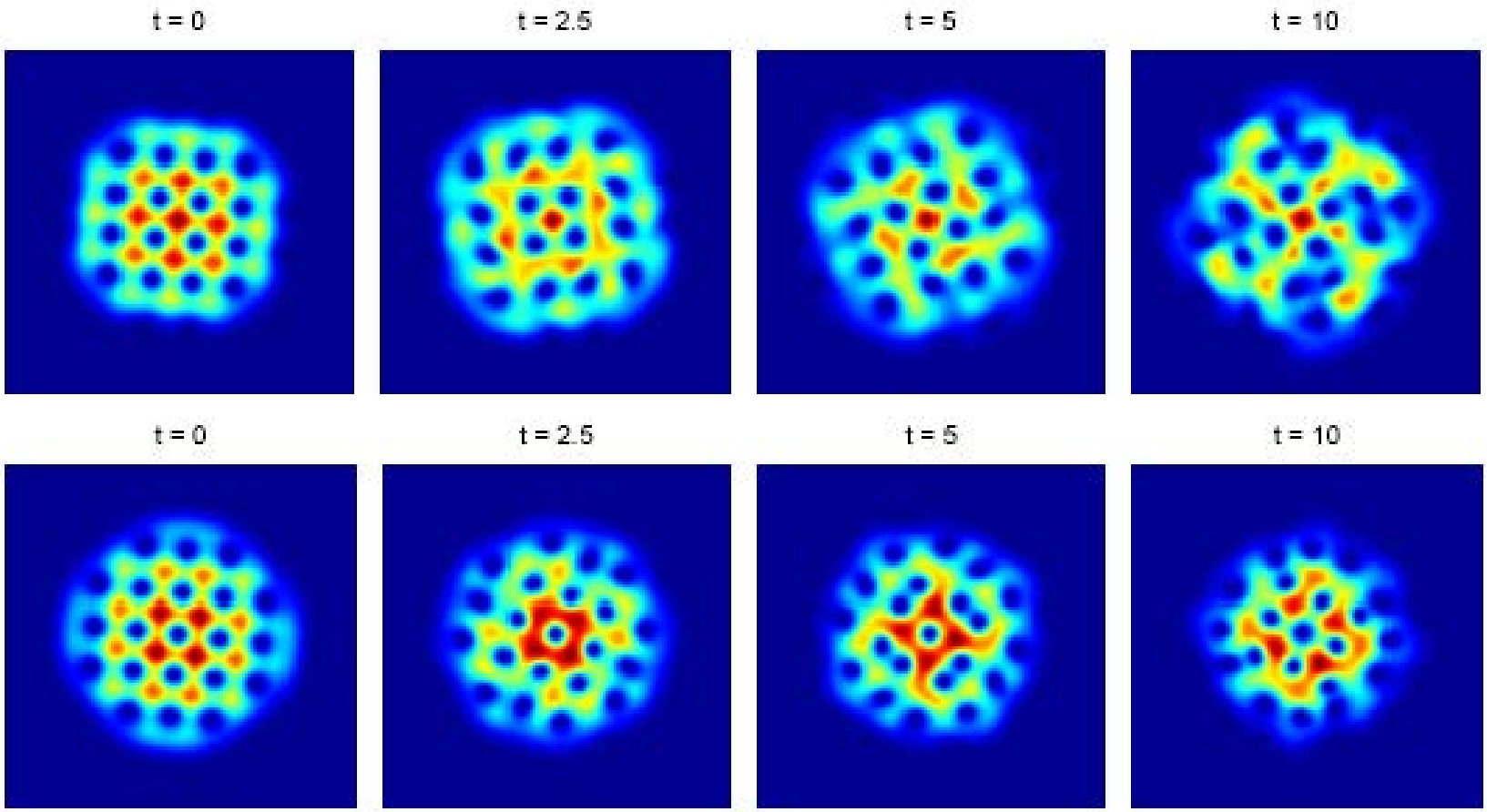



x 10^-3
2
0


|E_1|^2
(|E_1|^2+|E_2|^2)/2
|E_2|^2
t


t

Dynamics



Two-Component BEC

- Semiclassical scaling

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

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

- Semiclassical limit
  - No external field: $\lambda=0$
    - WKB expansion, two-fluid model
  - With external field: $\lambda\neq 0$
    - WKB expansion doesn't work, Winger transform

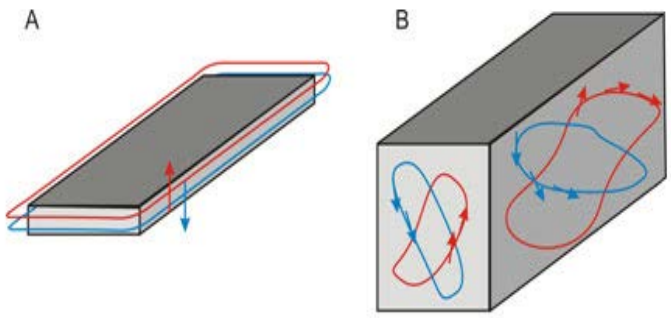
Spin-orbit coupled BEC

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

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

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

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



2D topological insulator 3D topological insulator

Spinor BEC

- Spinor F=1 BEC

$$i\hbar\frac{\partial}{\partial t}\psi_1 = [-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) - \Omega L_z + g_n\rho]\psi_1 + g_s(\rho_1 + \rho_0 - \rho_{-1})\psi_1 + g_s\psi_{-1}^*\psi_0^2$$

$$i\hbar\frac{\partial}{\partial t}\psi_0 = [-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) - \Omega L_z + g_n\rho]\psi_0 + g_s(\rho_1 + \rho_{-1})\psi_1 + 2g_s\psi_1\psi_{-1}\psi_0^*$$

$$i\hbar\frac{\partial}{\partial t}\psi_{-1} = [-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) - \Omega L_z + g_n\rho]\psi_{-1} + g_s(\rho_{-1} + \rho_0 - \rho_1)\psi_1 + g_s\psi_1^*\psi_0^2$$

- With

$$\rho = \rho_{-1} + \rho_0 + \rho_1, \quad \rho_j = |\psi_j|^2, \quad g_n = \frac{4\pi\hbar^2}{m}\frac{a_0 + 2a_2}{3}, \quad g_s = \frac{4\pi\hbar^2}{m}\frac{a_2 - a_0}{3}$$

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

Spinor BEC

- Total mass conservation

$$N(t)=\sum_{j=-1}^{1}\int_{\mathbb{R}^3}|\psi_j(\vec{x},t)|^2\,d\vec{x}\equiv N_{-1}^0+N_0^0+N_1^0:=N \quad \text{with} \quad N_j^0=\int_{\mathbb{R}^3}|\psi_j(\vec{x},0)|^2\,d\vec{x},$$

- Total magnetization conservation

$$M(t)=\int_{\mathbb{R}^3}|\psi_1(\vec{x},t)|^2\,d\vec{x}-\int_{\mathbb{R}^3}|\psi_{-1}(\vec{x},t)|^2\,d\vec{x}\equiv N_1^0-N_1^0:=M$$

- Energy conservation

$$E(\Psi)=\int_{\mathrm{R}^d}[\sum_{\mathrm{j=-1}}^{1}(\frac{\hbar^2}{2\mathrm{m}}|\nabla\psi_j|^2+V(\vec{x})|\psi_j|^2-\Omega\psi_j*L_z\psi_j)+\frac{g_n}{2}\rho^2+$$

$$\frac{g_s}{2}(\rho_1^2+\rho_{-1}^2+2\rho_1\rho_0+2\rho_{-1}\rho_0-2\rho_1\rho_{-1})+g_s(\psi_{-1}^*\psi_0^2\psi_1^*+\psi_{-1}(\psi_0^*)^2\psi_1)]d\vec{x}$$

Spinor BEC

- Dimension reduction
- Ground state
  - Existence & uniqueness of positive solution??
  - Numerical methods ???
- Dynamics
  - Dynamical laws
  - Numerical methods: TSSP
- Semiclassical limit & hydrodynamics equation??

Conclusions

- Review of BEC
- Experiment progress
- Mathematical modeling
- Efficient methods for computing ground & excited states
- Efficient methods for dynamics of GPE
- Comparison with experimental results
- Rotating BEC & dipolar BEC
- Multi-component BEC – two-component, spin-1 BEC, spin-orbit-coupled BEC

Future Challenges

- Multi-component BEC for bright laser
- Applications of BEC in science and engineering
- Precise measurement
- Fermions condensation, BEC in solids & waveguide
- Dynamics in optical lattice, atom tunneling, random potential
- Superfluidity & dissipation, quantized vortex lattice
- Coupling GPE & QBE for BEC at finite temperature
- Mathematical theory for BEC
- Interdisciplinary research: experiment,physics, mathematics, computation, ...

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