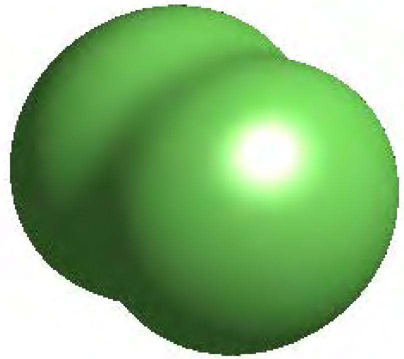
Modeling, Analysis and Simulation for Degenerate Dipolar Quantum Gas



Weizhu Bao

Department of Mathematics

& Center for Computational Science and Engineerir

National University of Singapore

Email: bao@math.nus.edu.sg

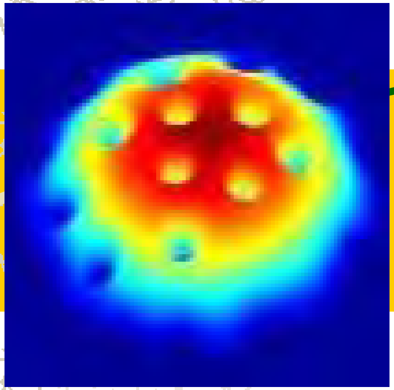
URL: http://www.math.nus.edu.sg/~bao

&

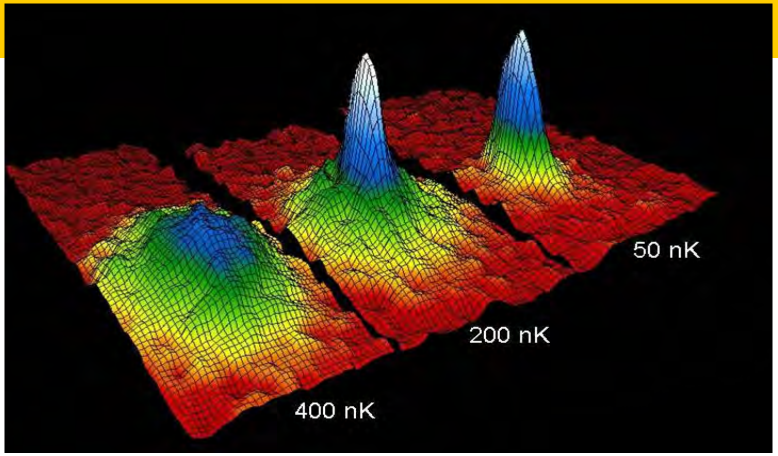
Beijing Computational Science Research Center

URL: http://www.csrc.ac.cn/

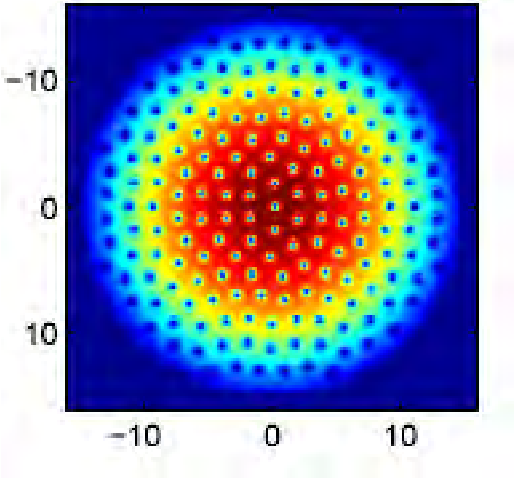
Collaborators: Y. Cai (Postdoc, NUS), M. Rosenkranz (Postdoc, NUS),
N. Ben Abdallah (UPS, France), Z. Lei (Fudan University, China),
H. Wang (Yunan Univ. Economics and Finance, China & NUS)



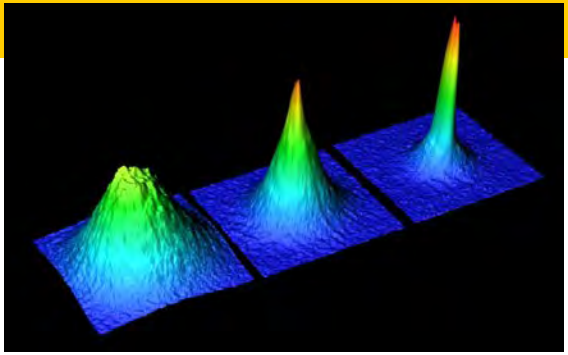
Outline



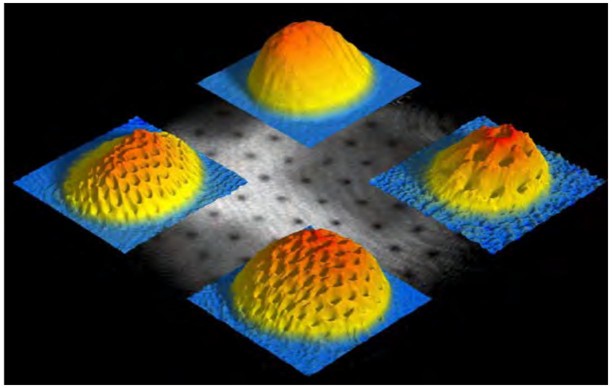
- Motivation---dipolar BEC
- Mathematical models
- Ground state and its theory
- Dynamics and its efficient computation
- Dimension reduction
- Conclusion & future challenges



Degenerate Quantum Gas

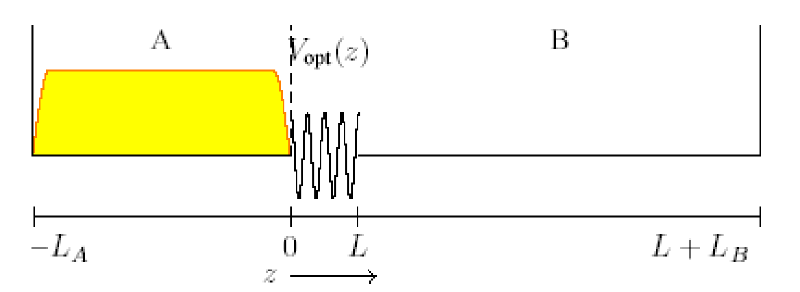


- Typical degenerate quantum gas
  - Liquid Helium 3 & 4
  - Bose-Einstein condensation (BEC)
    - Boson vs Fermion condensation
    - One component, two-component & spin-1
    - Boson-fermion mixture

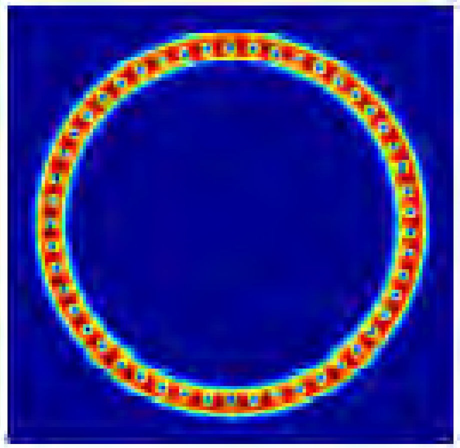


- Typical properties
  - Low (mK) or ultracold (nK) temperature
  - Quantum phase transition & closely related to nonlinear wave
  - Superfluids – flow without friction & quantized vortices

Recent Developments



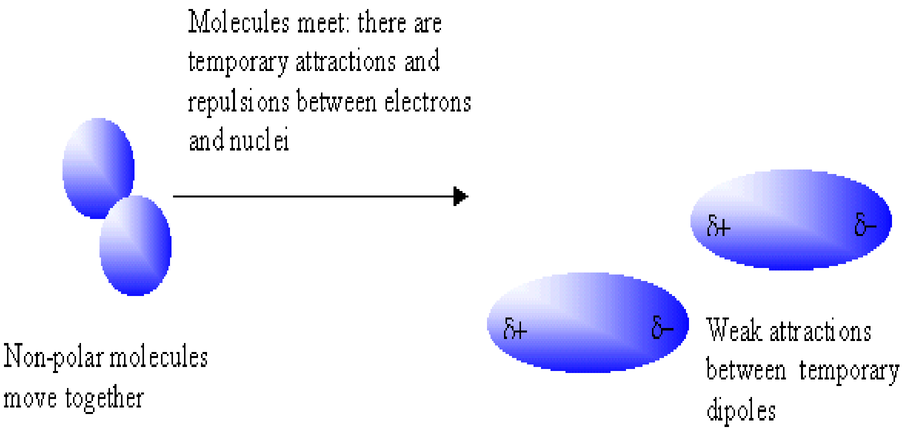
- Quantum transport
  - Move a BEC in an optical lattice
  - Atomic circuit, Quantum computing
- Interaction of BEC and particles
- Quantized vortices for superfluidity
  - Vortex states
  - Vortex lattice patterns
  - Interaction between vortices

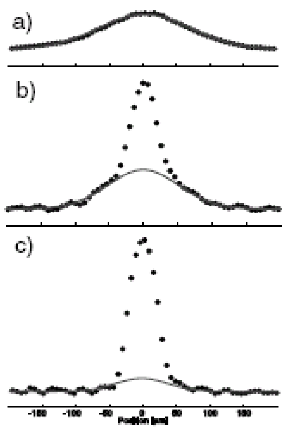


- Fermion condensate, Boson-fermion, atom-molecule, …

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





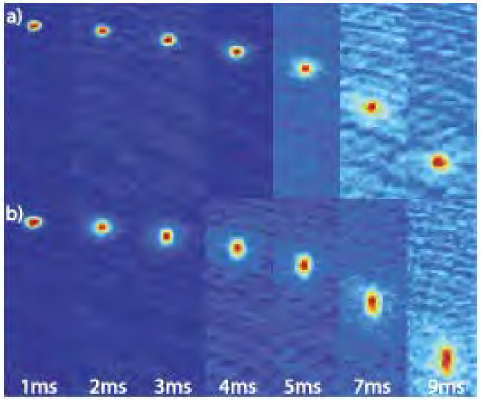


FIG. 3 (color). Time of flight series of absorption images with expansion times from 1 to 9 ms. (a) BEC released from an almost isotropic trap; (b) BEC released from an anisotropic trap.

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

BEC with strong DDI

^{164}Dy

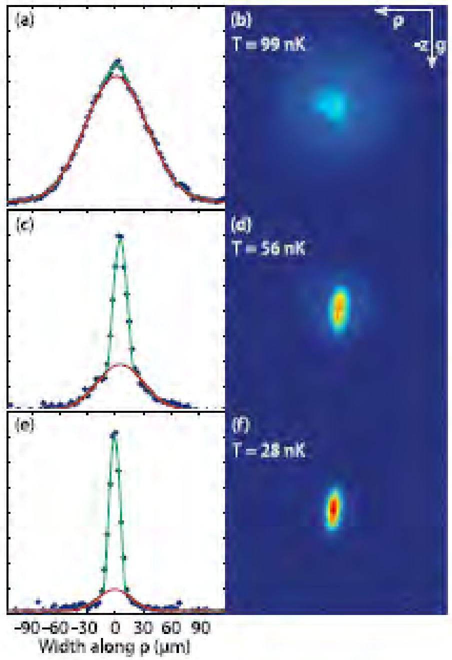


FIG. 2 (color online). TOF profiles of the spin-purified Dy gas for three evaporation time constants, with $\tau = 15$ s in (e) and (f). (a),(c),(e) Data at centers are fit to a parabolic profile (upper curve), which underestimates the condensate fraction, whereas the distributions' wings are fit to 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}.

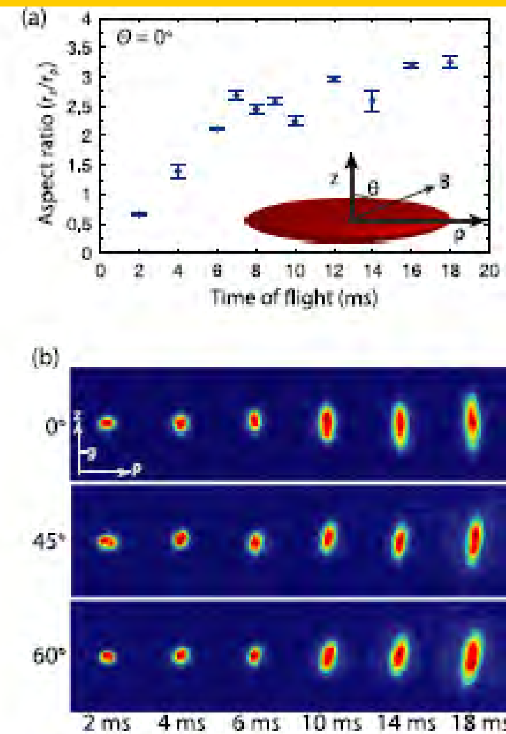


FIG. 3 (color online). Anisotropic expansion profile versus time after trap release. (a) r_z and r_ρ are the dimensions of the parabolic profile fit to the BEC for $\theta = 0°$. Inset: Schematic of the oblate trap and magnetic-field orientation. (b) Images of the expanding condensate after trap release. 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 !! $\widehat{U}_{\text{dip}}(\xi) = -1 + \frac{3(\vec{n}\cdot\xi)^2}{|\xi|^2} \qquad \xi \in \mathbb{R}^3$
    - 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)

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

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

- Dipole-dipole interaction becomes

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

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

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

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

- 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 $\qquad \phi_g = e^{i\theta_0} |\phi_g| \quad \text{with} \quad \theta_0 \in \mathbb{R}$
    - 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

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

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

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

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

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

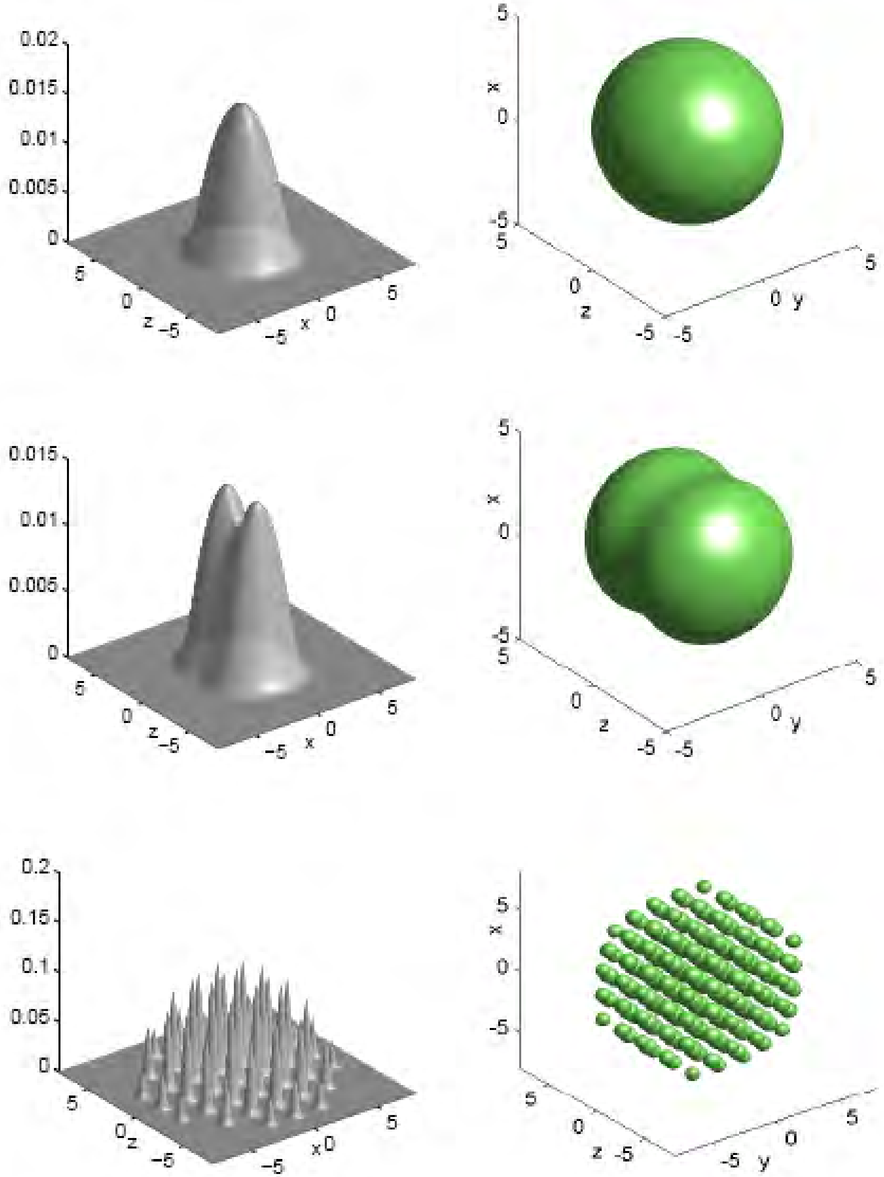


Figure 1: Surface plots of $|\phi_g(x, 0, z)|^2$ (left column) and isosurface plots of $|\phi_g(x, y, z)| = 0.01$ (right column) for the ground state of a dipolar BEC with $\beta = 401.432$ and $\lambda = 0.16\beta$ for harmonic potential (top row), double-well potential (middle row) and optical lattice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

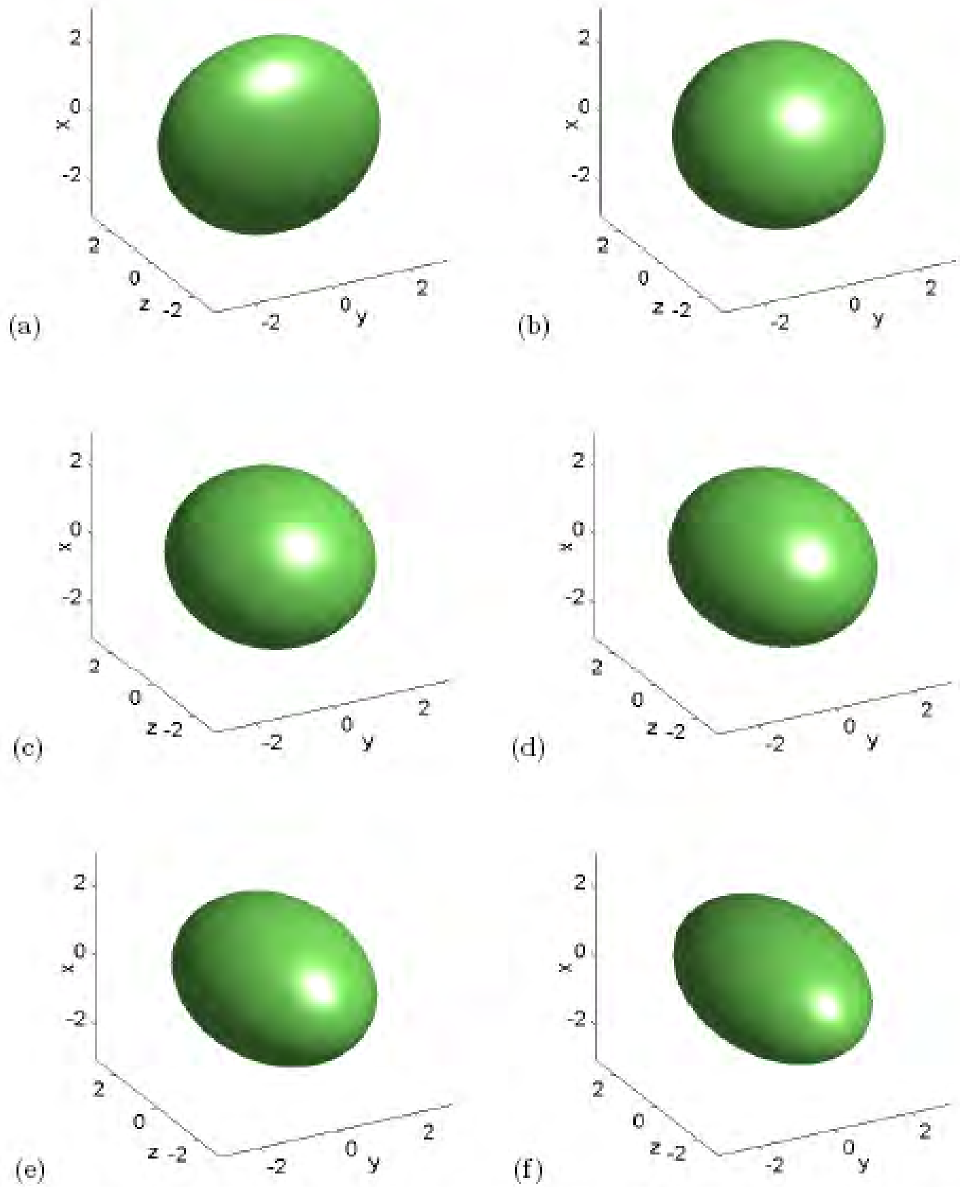


Figure 2: Isosurface plots of the ground state $|\phi_g(\mathbf{x})| = 0.08$ of a dipolar BEC with the harmonic potential $V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2 + z^2)$ and $\beta = 207.16$ for different values of $\frac{\lambda}{\beta}$: (a) $\frac{\lambda}{\beta} = -0.5$; (b) $\frac{\lambda}{\beta}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

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

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

  - Results
    - Local existence, i.e.

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

- 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 $\beta\geq 0\ \&\ \lambda<-\frac{\beta}{2}$ 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) $E(\psi_0)=0 \quad \& \quad \mathrm{Im}\int_{\mathbb{R}^3}\bar{\psi}_0(x)\,(\vec{x}\cdot\nabla\psi_0(\vec{x}))\,d\vec{x}<0$

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

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

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

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

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

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

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

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

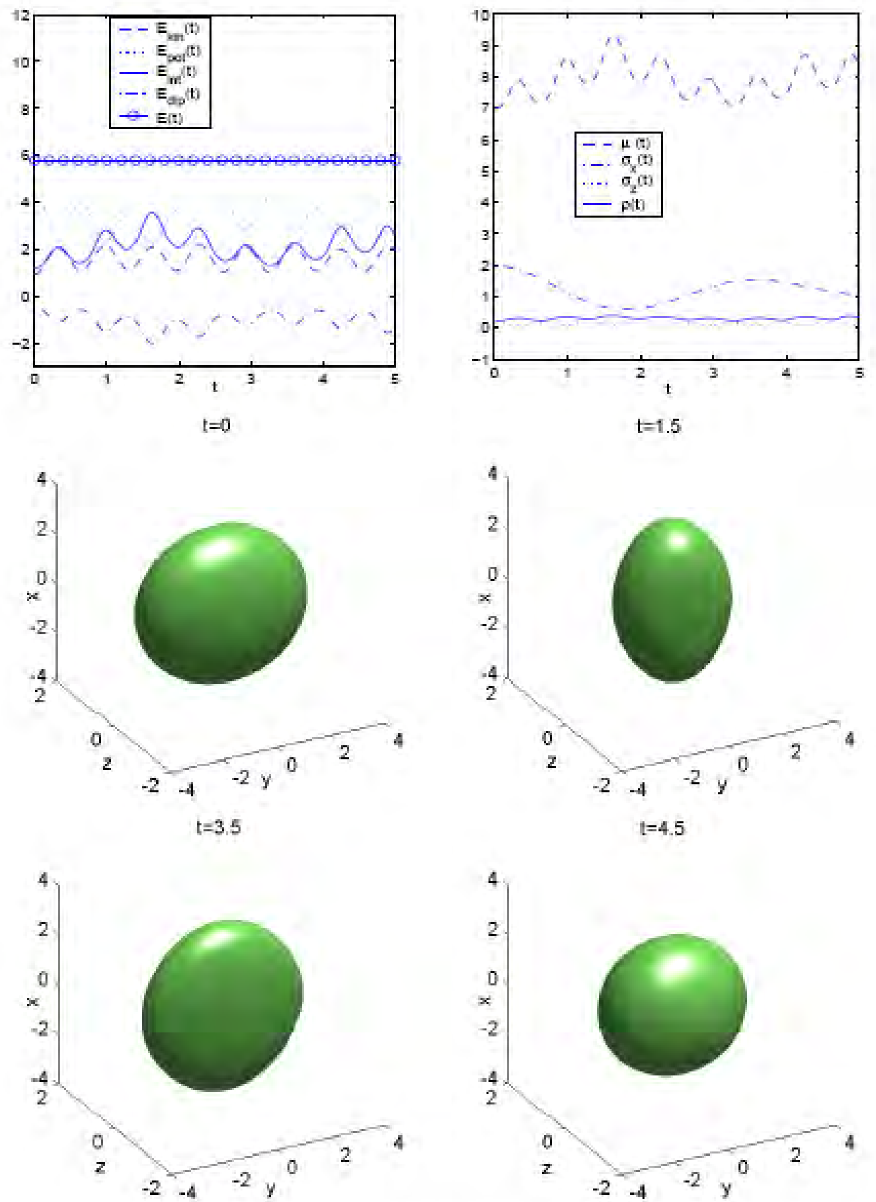


Figure 3: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar direction is suddenly changed from $\mathbf{n} = (0,0,1)^T$ to $(1,0,0)^T$ at time $t = 0$.

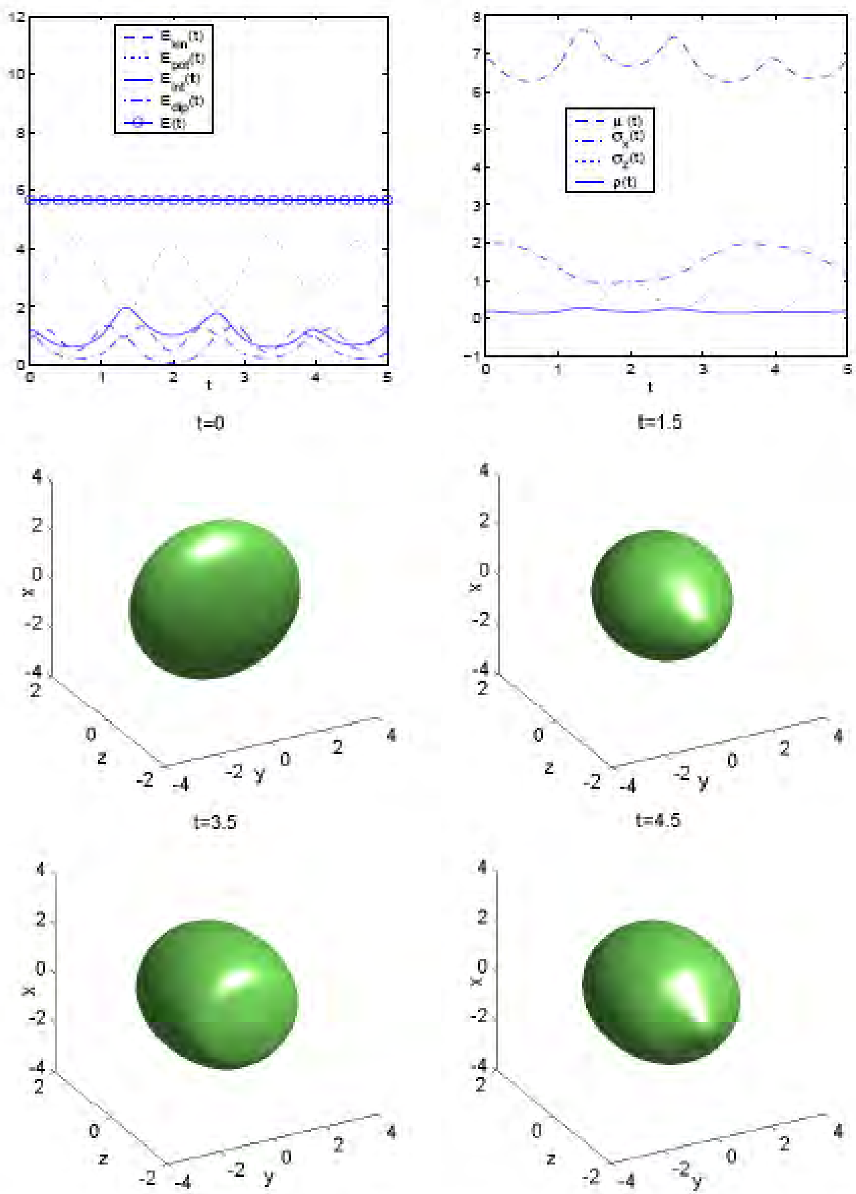


Figure 4: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the trap potential is suddenly changed from from $\frac{1}{2}(x^2 + y^2 + 25z^2)$ to $\frac{1}{2}(x^2 + y^2 +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

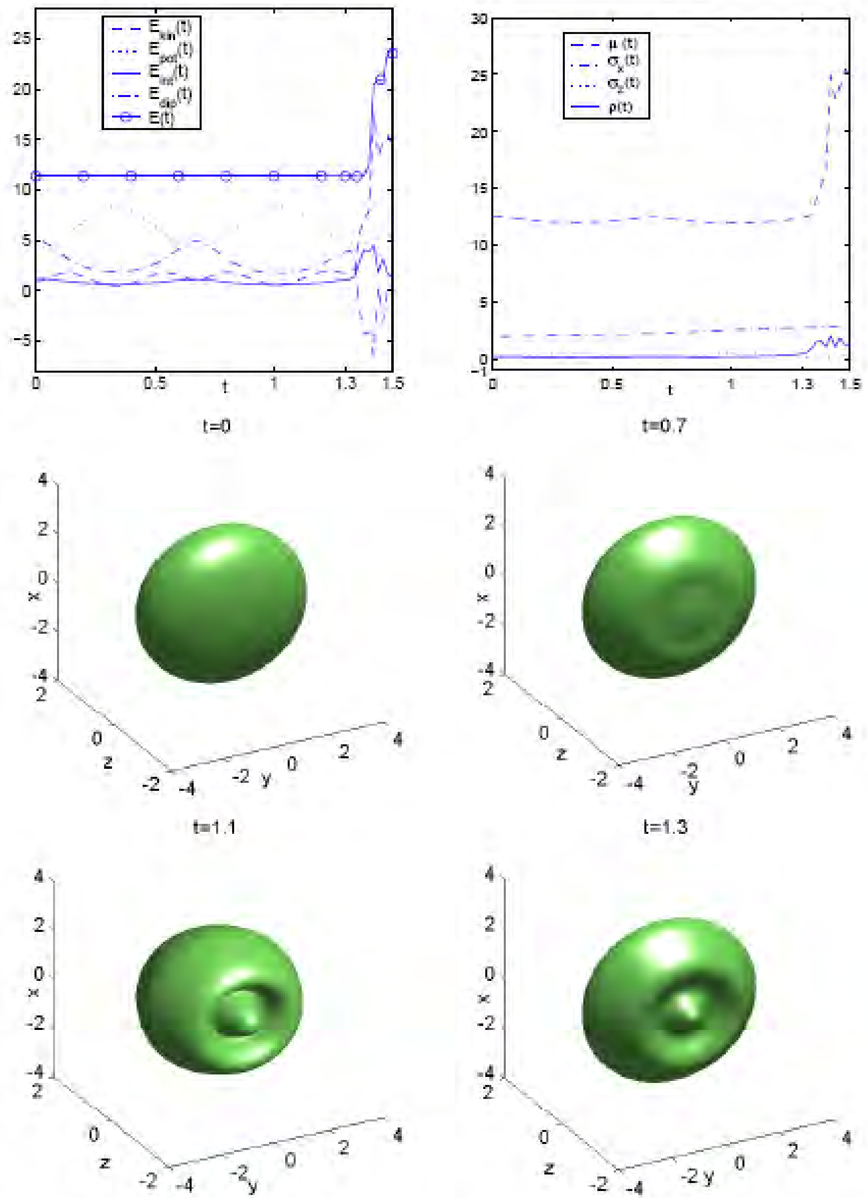


Figure 5: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x},t) := |\psi(\mathbf{x},t)|^2 = 0.01$ at different times for a dipolar BEC when the dipolar interaction constant is suddenly changed from $\lambda = 0.8\beta = 82.864$ to $\lambda = 4\beta =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

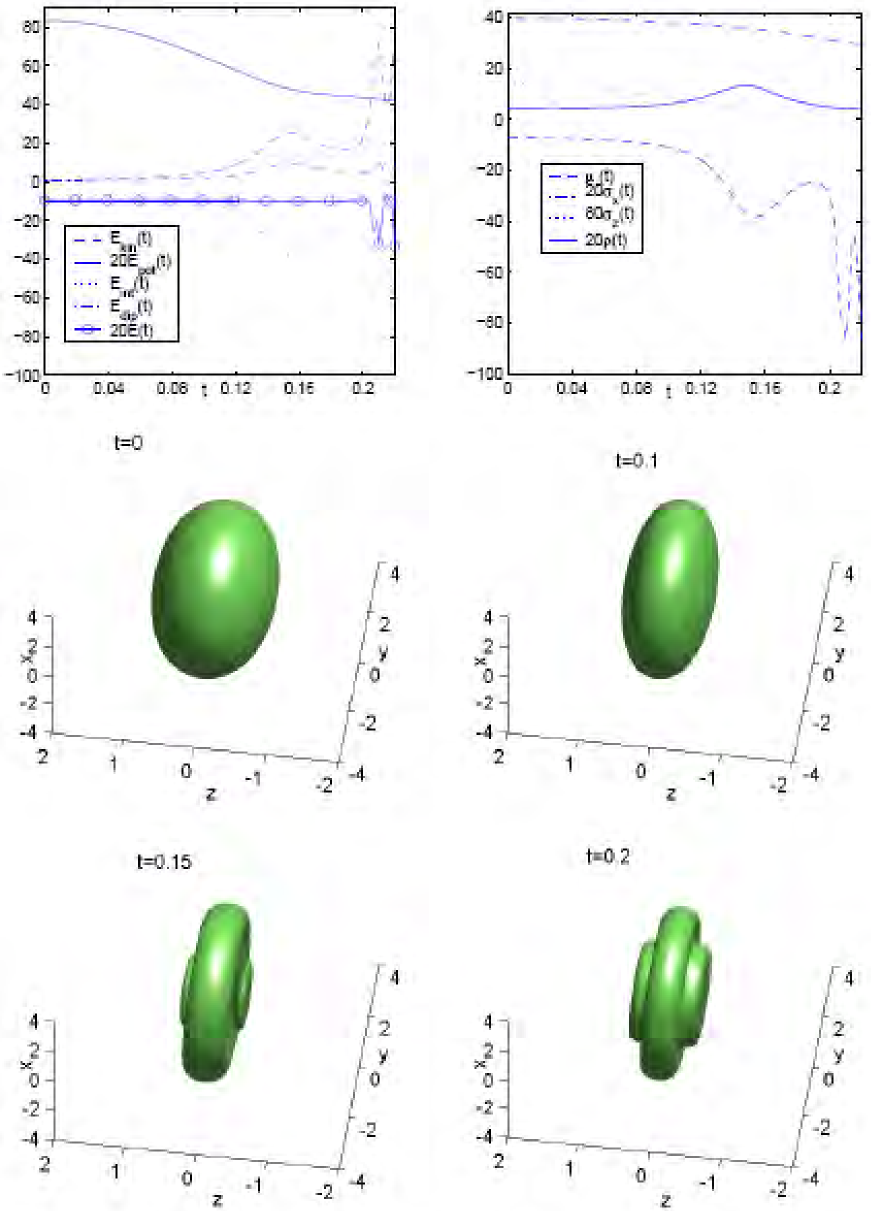


Figure 6: Time evolution of different quantities and isosurface plots of the density function $\rho(\mathbf{x}, t) := |\psi(\mathbf{x}, t)|^2 = 0.01$ at different times for a dipolar BEC when the interaction constant β is suddenly changed from $\beta = 103.58$ to $\beta = -569.69$ at time $t = 0$.

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

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

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

Dimension Reduction

- Gross-Pitaevskii-Poisson equations

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

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

- Strongly anisotropic potential

$$V_{\text{ext}}(\vec{x})=\frac{1}{2}\left(\gamma_x^2x^2+\gamma_y^2y^2+\gamma_z^2z^2\right)$$

  - Case I: 3D → 2D

$$\gamma_z\gg\gamma_x\approx\gamma_y\quad\&\quad \vec{n}=(n_1,n_2,n_3)^T,\quad |\vec{n}|^2=n_1^2+n_2^2+n_3^2=1$$

  - Case II: 3D → 1D $\gamma_z\gg\gamma_x\quad\&\quad\gamma_y\gg\gamma_x$

Dimension Reduction

- Existing results
  - BEC without dipole-dipole interaction: $\lambda = 0$
    - Formal asymptotic (Bao, Markowich, Schmeiser & Weishaupl, M3AS, 05')
    - Numerical results (Bao, Ge, Jaksch, Markowich & Weishaeupl, CPC, 07')
    - Rigorous proof (Ben Abdallah, Mehats et al., SIMA, 05; JDE 08')
    - From N-body to mean field theory (Lieb, Seiringer & Yngvason, CMP, 04'; Erdos, Schlein & Yau, Ann. Math., 10')
  - Dipolar BEC (Carles, Markowich & Sparber, Nonlinearity, 08') – formal result

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

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

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

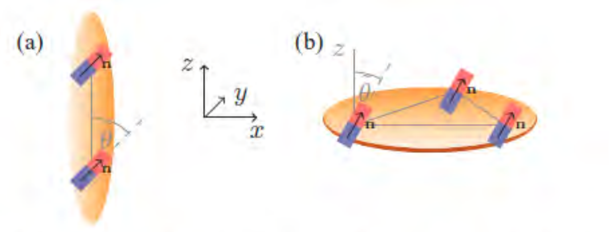


FIG. 1. (Color online) In the quasi-1D setup in (a) the dipolar BEC is confined to the z direction. In the quasi-2D setup in (b) the atoms are confined to the x-y plane. The dipoles are polarized along the axis $\mathbf{n} = (n_x, n_y, n_z)$ with polar angle $\tilde{\theta}$ (i.e., $n_z = \cos\tilde{\theta}$).

- 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 (Bao, Cai, Lei, Rosenkranz, PRA, 10')

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

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

$$\varphi(x,y,t)=U_\varepsilon^{2D}*|\psi|^2,$$

$$U_\varepsilon^{2D}(x,y)=U_\varepsilon^{2D}(r)=\frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}}\frac{\exp\left(-s^2/2\right)}{\sqrt{r^2+\varepsilon^2s^2}}ds,\quad r=\sqrt{x^2+y^2}$$

Asymptotic of 2D Kernel

- For fixed $\varepsilon > 0$

$$U_\varepsilon^{2D}(r) \approx \begin{cases} \dfrac{1}{\pi^{3/2}\varepsilon\sqrt{2}}\left(-\ln r + \ln 2\varepsilon + C\right), & r \to 0 \\ \dfrac{1}{2\pi r}, & r \to \infty \end{cases}$$

- When $\varepsilon \to 0$

$$U_\varepsilon^{2D}(r) \approx \frac{1}{2\pi r}, \qquad r > 0$$

Fourier Transform of 2D Kernel

- Fourier transform

$$\widehat{U}_\varepsilon^{2D}(\xi_1,\xi_2)=\widehat{U}_\varepsilon^{2D}(|\xi|)=\frac{1}{\pi}\int_{\mathbb{R}}\frac{\exp\left(-\varepsilon^2 s^2/2\right)}{|\xi|^2+s^2}ds$$

- Asymptotic
  - For fixed $\varepsilon>0$

$$\widehat{U}_\varepsilon^{2D}(|\xi|)\approx\begin{cases}\dfrac{1}{|\xi|}, & |\xi|\to 0\\ \left(\dfrac{2}{\pi}\right)^{1/2}\dfrac{1}{\varepsilon|\xi|^2}, & |\xi|\to\infty\end{cases}$$

  - When $\varepsilon\to 0$

$$\widehat{U}_\varepsilon^{2D}(|\xi|)\approx\frac{1}{|\xi|},\qquad \xi\in\mathbb{R}^2$$

Ground State Results for quais-2D

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

- Theorem (Existence & uniqueness) (Bao, Ben Abdallah, Cai, SIMA, 12')
  - Results $V_{2D}(\vec{x}) \geq 0, \forall \vec{x} \in \mathbb{R}^2$ & $\lim_{|\vec{x}|\to\infty} V_{2D}(\vec{x}) = +\infty$ (confinement potential)
    - There exists a ground state $\phi_g \in S$ if
      - Case I: $\lambda \geq 0 \;\&\; \beta - \lambda > -\varepsilon\sqrt{2\pi}C_b$
      - Or case II $\lambda < 0 \quad \& \quad \beta + \frac{\lambda}{2}\left(1 + 3|2n_3^2 - 1|\right) > -\varepsilon\sqrt{2\pi}C_b$
    - Positive ground state is unique $\phi_g = e^{i\theta_0}|\phi_g|$ with $\theta_0 \in \mathbb{R}$
      - Case I: $\lambda \geq 0 \quad \& \quad \beta - \lambda \geq 0$
      - Or case II $\lambda < 0 \quad \& \quad \beta + \frac{\lambda}{2}\left(1 + 3|2n_3^2 - 1|\right) \geq 0$
    - No ground state if

$$\beta + \frac{\lambda}{2}\left(1 - 3n_3^2\right) < -\varepsilon\sqrt{2\pi}C_b$$

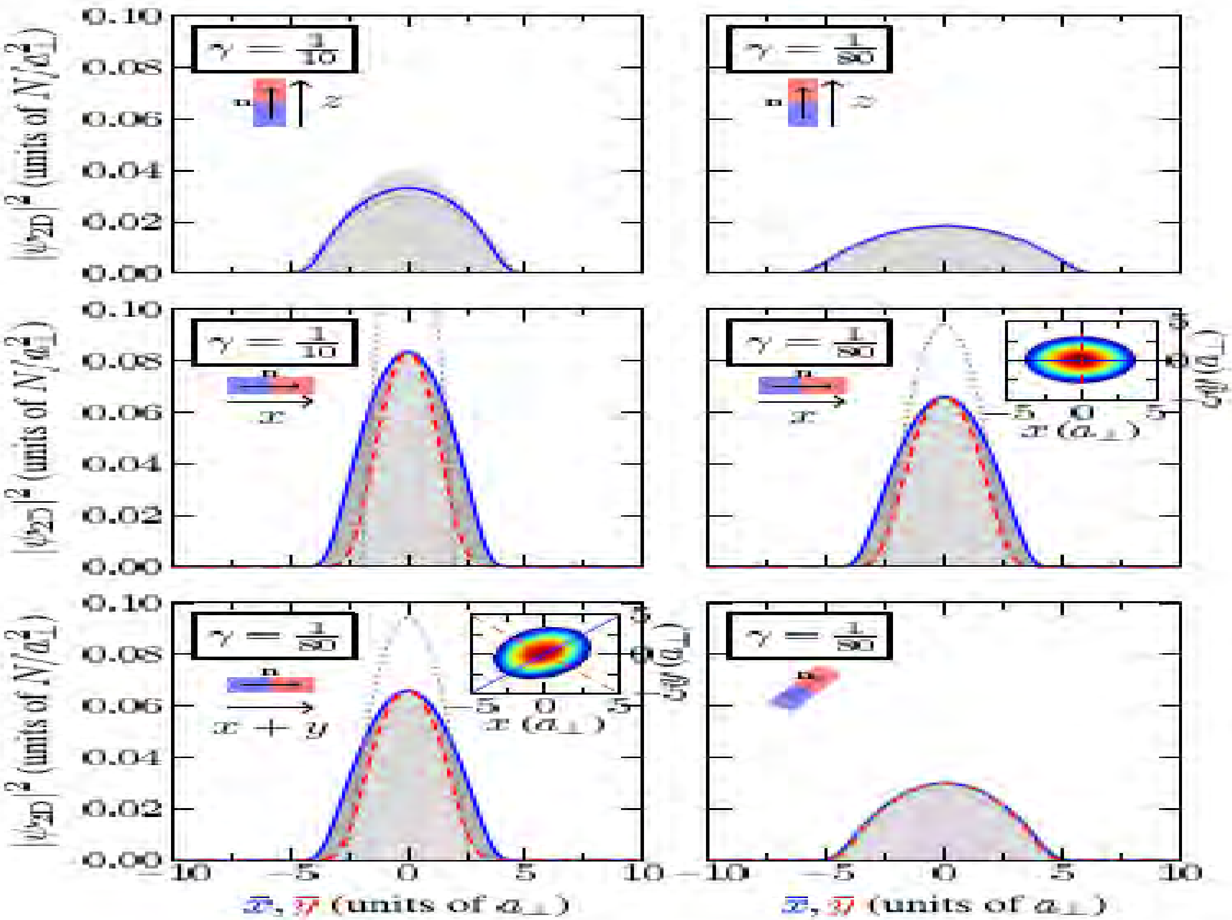


FIG. 4. (Color online) Cuts through the radial density profiles of the quasi-2D dipolar BEC given by Eq. (16) for various polarizations and trap anisotropies. The cuts are taken along the axes with largest ($\bar{x}$ axis, solid blue lines) and smallest extend of the BEC ($\bar{y}$ axis, dashed red). The insets show density plots of the quasi-2D BEC and the lines indicate the position of the cuts ($\bar{x}$ and $\bar{y}$ axes, respectively). The gray dotted lines are the analytical profiles $n_{2D}(r)$ and the shaded areas are the profiles obtained from the 3D GPE, Eq. (1). For sufficiently large confinement the 3D GPE profiles are not distinguishable from our 2D solution. We choose $\beta_{2D} = 100$, $\epsilon_{dd} = 0.9$ and the dipole axis $\mathbf{n} = (0, 0, 1)$ (top panel), $\mathbf{n} = (1, 0, 0)$ (middle panel), $\mathbf{n} = \frac{1}{\sqrt{2}}(1, 1, 0)$ (bottom left panel) and $\mathbf{n} = \frac{1}{\sqrt{3}}(1, 1, 1)$ (bottom right panel).

$$\gamma := \frac{\gamma_x}{\gamma_z} = \varepsilon^2 \to 0$$

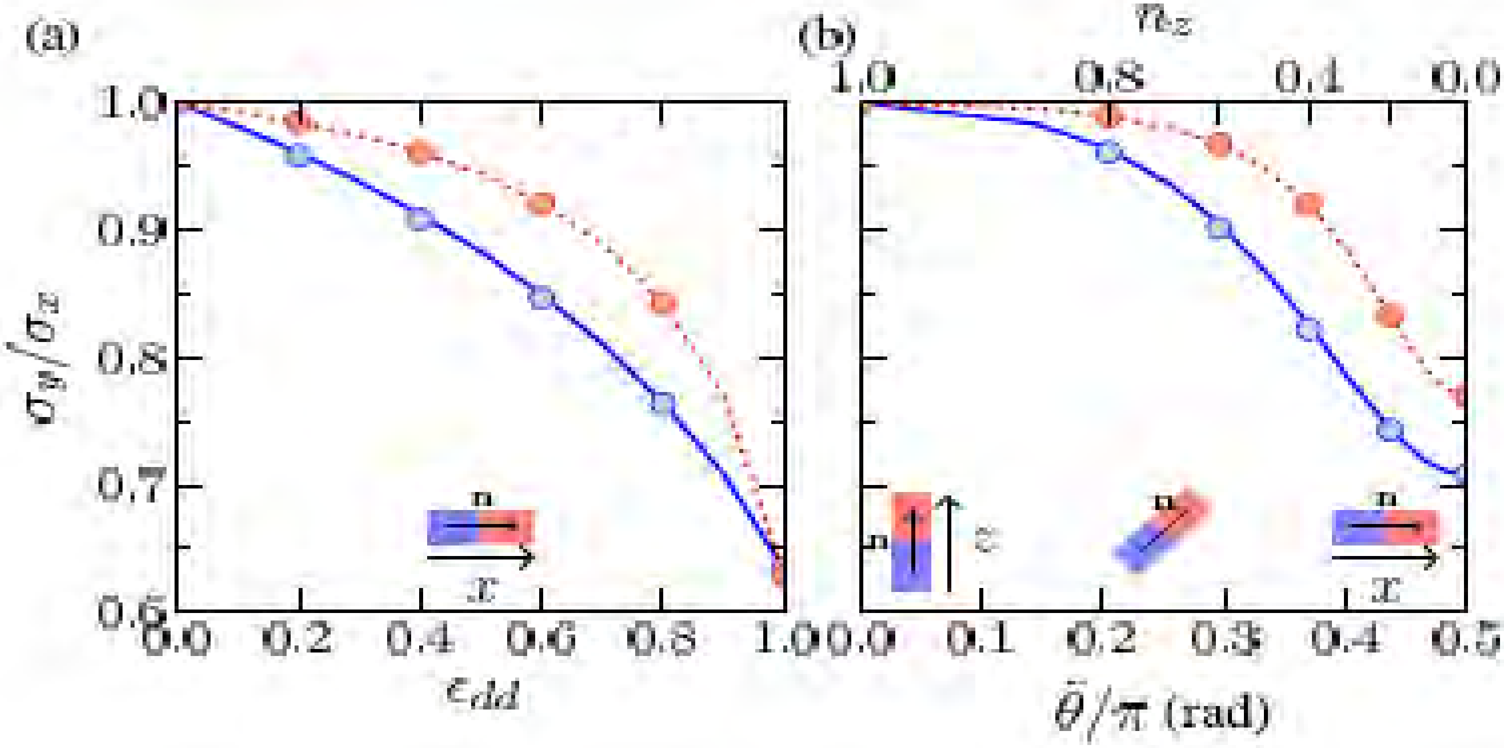


FIG. 5. (Color online) Aspect ratio of the quasi-2D BEC for (a) varying dipole strength ϵ_{dd} with polarization along the x axis and (b) varying polarization angle in the x-z plane [$\mathbf{n} = (\sin\tilde{\theta}, 0, \cos\tilde{\theta})$] with $\epsilon_{dd} = 0.9$. We use the trap aspect ratios $\gamma = 1/10$ (solid lines) and $\gamma = 1/80$ (dotted) with $\beta_{2D} = 100$. The circles indicate the corresponding condensate aspect ratio according to the numerical solution the 3D GPE, Eq. (1). The upper axis in (b) shows $n_z = \cos\tilde{\theta}$.

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

$$E(\psi(\cdot,t)) := \int_{\mathbb{R}^3}\{\frac{1}{2}|\nabla_\perp\psi|^2 + V_{2D}(\vec{x})|\psi|^2 + \frac{1}{2\varepsilon\sqrt{2\pi}}(\beta-\lambda+3\lambda n_3^2)|\psi|^4 + \frac{3\lambda}{4}[\left|\partial_{n_\perp}(-\Delta_\perp)^{1/4}\varphi\right|^2 - n_3^2\left|\nabla_\perp(-\Delta_\perp)^{1/4}\varphi\right|^2]\}d\vec{x}$$

Ground State Results for quais-2D

$$V_{\rm 2D}(\vec{x}) \ge 0, \forall \vec{x} \in \mathbb{R}^2 \ \& \lim_{|\vec{x}|\to\infty} V_{\rm 2D}(\vec{x}) = +\infty \quad \text{(confinement potential)}$$

- Theorem (Existence & uniqueness) (Bao, Ben Abdallah, Cai, SIMA, 12')
  - There exists a ground state $\phi_g \in S$ if
    - Case I: $\lambda = 0 \ \& \ \beta > -\varepsilon\sqrt{2\pi}C_b$
    - Or case II $\lambda > 0, \quad n_3 = 0 \quad \& \quad \beta - \lambda > -\varepsilon\sqrt{2\pi}C_b$
    - Or case III $\lambda < 0, \quad n_3^2 \ge 1/2 \quad \& \quad \beta - \lambda\left(1 - 3n_3^2\right) > -\varepsilon\sqrt{2\pi}C_b$
  - Positive ground state is unique $\phi_g = e^{i\theta_0}|\phi_g| \quad \text{with} \quad \theta_0 \in \mathbb{R}$
    - Case I: $\lambda = 0 \quad \& \quad \beta \ge 0$
    - Or case II $\lambda > 0, \quad n_3 = 0 \quad \& \quad \beta \ge \lambda$
    - Or case III $\lambda < 0, \quad n_3^2 \ge 1/2 \quad \& \quad \beta - \lambda\left(1 - 3n_3^2\right) \ge 0$
  - No ground state

$$\lambda > 0 \ \& \ n_3 \ne 0 \quad \text{or} \quad \lambda < 0 \ \& \ 2n_3^2 < 1 \quad \text{or} \quad \lambda = 0 \ \& \ \beta < -\varepsilon\sqrt{2\pi}C_b$$

Well-posedness & convergence rate

- Well-posedness of the Cauchy problem related to the 2D equations
- Finite time blow-up may happen!!

- Theorem (convergence rate) (Bao, Ben Abdallah, Cai, SIMA, 12')

  Assume $\beta \geq 0, \quad -\frac{\beta}{2} \leq \lambda \leq \beta, \quad \beta = O(\varepsilon), \quad \lambda = O(\varepsilon)$

  Then we have

$$\left\| \psi(x,y,z,t) - e^{-\frac{i\,t}{2\varepsilon^2}} \psi(x,y,t)\,\omega_\varepsilon(z) \right\|_{L^2} \leq C_T \varepsilon, \quad 0 \leq t \leq T$$

Dimension Reduction (3D→ 1D)

- Assumptions

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

- Decomposition of the linear operator

$$L := -\frac{1}{2}\Delta + V_{\text{ext}}(\vec{x}) = -\frac{1}{2}\partial_{zz} + V_{1D}(z) + L_{xy}$$

$$L_{xy} = -\frac{1}{2}\Delta_{xy} + \frac{x^2+y^2}{2\varepsilon^4} = \frac{1}{\varepsilon^2}\left(-\frac{1}{2}\Delta_{\tilde{x}\tilde{y}} + \frac{\tilde{x}^2+\tilde{y}^2}{2}\right)$$

- Ansatz

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

Dimension Reduction (3D→ 1D)

- 1D equations (Bao, Cai, Lei, Rosenkranz, PRA, 10')

$$i\frac{\partial}{\partial t}\psi(z,t)=[-\frac{1}{2}\partial_{zz}+V_{1D}(z)+\frac{2\beta+\lambda(1-3n_3^2)}{4\pi\varepsilon^2}|\psi|^2$$

$$+\frac{3\lambda(1-3n_3^2)}{8\varepsilon\sqrt{2\pi}}\partial_{zz}\varphi\,]\,\psi(z,t)$$

$$\varphi(z,t)=U_\varepsilon^{1D}*|\psi|^2,\qquad U_\varepsilon^{1D}(z)=\frac{2e^{z^2/2\varepsilon^2}}{\sqrt{\pi}}\int_{|z|}^{\infty}e^{-s^2/2\varepsilon^2}\,ds,$$

– Linear case if $n_3^2=1/3\ \&\ \beta=0\ \&\ \lambda\neq 0$

Asymptotic of 1D Kernel

- For fixed $\varepsilon > 0$

$$U_\varepsilon^{1D}(z) \approx \begin{cases} 1 - \dfrac{\sqrt{2}}{\sqrt{\pi\varepsilon}}|z| + O(z^2), & z \to 0 \\ \dfrac{\sqrt{2\varepsilon}}{\sqrt{\pi}\, z}, & z \to \infty \end{cases}$$

- When $\varepsilon \to 0$

$$U_\varepsilon^{1D}(z) \approx \begin{cases} 1, & z = 0 \\ 0, & z \neq 0 \end{cases}$$

Fourier Transform of 1D Kernel

- Fourier transform

$$\widehat{U}_{\varepsilon}^{1D}(\xi) = \frac{\sqrt{2}\varepsilon}{\sqrt{\pi}} \int_0^\infty \frac{\exp\left(-\varepsilon^2 s/2\right)}{\xi^2 + s} ds,$$

- Asymptotic
  - For fixed $\varepsilon > 0$

$$\widehat{U}_{\varepsilon}^{1D}(\xi) \approx \begin{cases} \frac{\sqrt{2}\varepsilon}{\sqrt{\pi}}\left(-\gamma_e - 2\ln|\xi| - \ln\frac{\varepsilon}{2}\right), & |\xi| \to 0 \\ \frac{2\sqrt{2}}{\varepsilon\sqrt{\pi}|\xi|^2}, & |\xi| \to \infty \end{cases}$$

  - When $\varepsilon \to 0$

$$\widehat{U}_{\varepsilon}^{1D}(|\xi|) \approx ??, \qquad \xi \in \mathbb{R}$$

Ground State Results for quais-1D

$$V_{1D}(z) \geq 0, \forall z \in \mathbb{R} \ \& \lim_{|z|\to\infty} V_{1D}(z) = +\infty \quad \text{(confinement potential)}$$

- Theorem (Existence & uniqueness) (Bao, Ben Abdallah, Cai, SIMA, 12')
  - There exists a ground state $\phi_g \in S$ for any $\beta, \lambda, \varepsilon, n_1$
  - Positive ground state is unique $\phi_g = e^{i\theta_0} |\phi_g|$ with $\theta_0 \in \mathbb{R}$
    - Case I: $\lambda\left(1-3n_3^2\right) \geq 0 \quad \& \quad \beta - \lambda(1-3n_3^2) \geq 0$
    - Or case II $\lambda\left(1-3n_3^2\right) < 0 \quad \& \quad \beta + \lambda\left(1-3n_3^2\right)/2 \geq 0$
- Dynamics results – global well-posedness of the Cauchy problem
- Convergence rate if $\beta = O(\varepsilon^2) \,\&\, \lambda = O(\varepsilon^2)$

$$\left\| \psi(x,y,z,t) - e^{-\frac{it}{\varepsilon^2}} \psi(z,t)\,\omega_\varepsilon(x,y) \right\|_{L^2} \leq C_T \varepsilon, \quad 0 \leq t \leq T$$

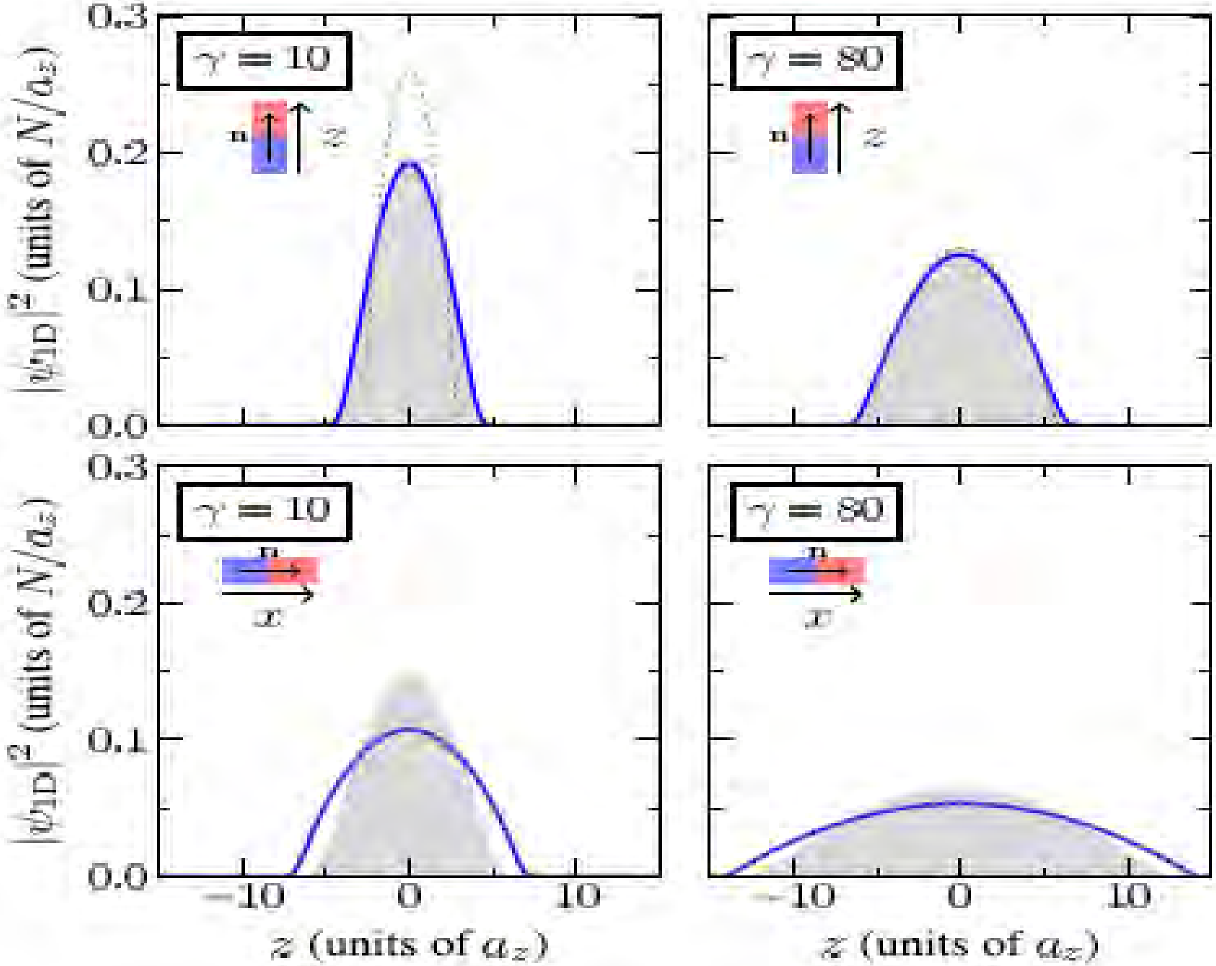


FIG. 3. (Color online) Linear density of the quasi-1D BEC according to the solution of our 2D equation, Eq. (9) (blue solid lines), the corresponding analytical prediction of Eq. (12) (gray dotted), and the full 3D GPE of Eq. (1) (shaded area). In the upper panel dipoles are aligned with the BEC axis, while in the lower panel they are aligned perpendicular to the BEC axis. We choose $\beta_{1D} = 100$, $\epsilon_{dd} = 0.9$ and the γ given in the plots.

$$\gamma := \frac{\gamma_x}{\gamma_z} = \frac{1}{\varepsilon^2} \to \infty$$

Reduction in Multilayered Potential

- With multilayered potential in z-direction

$$V_{\text{ext}}(\vec{x}) = V_{2D}(x, y) + V_0 \sin^2(\pi z) \qquad V_0 \gg \hbar\omega$$

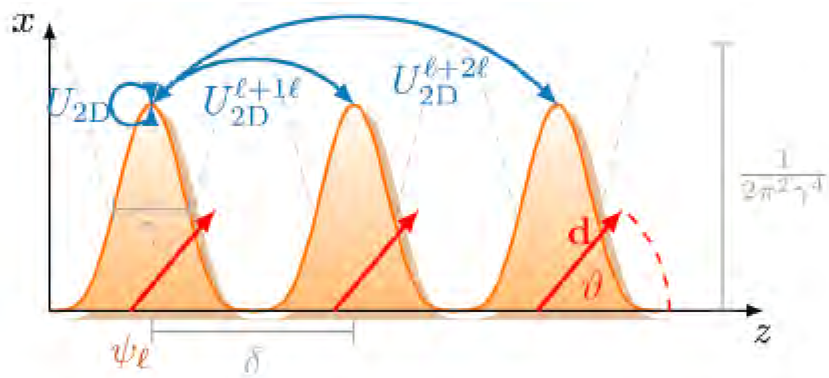
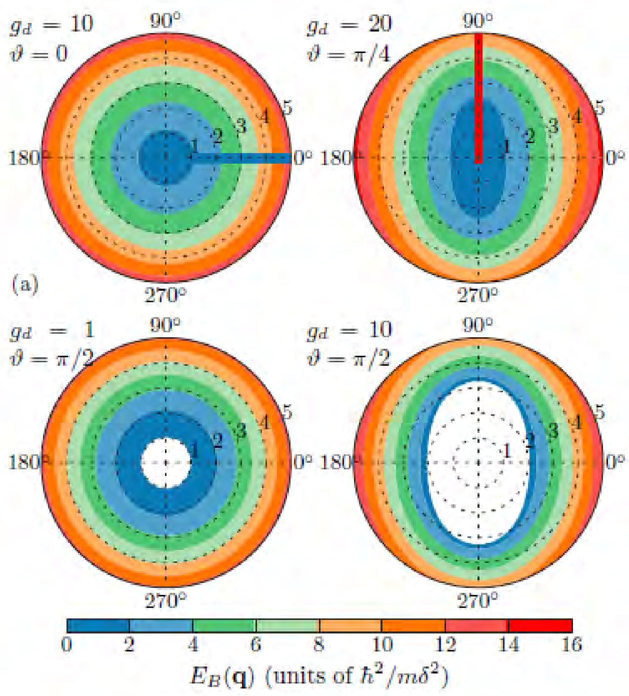


FIG. 1. (Color online) Setup of the multilayered dipolar BEC polarized along **d**. An optical lattice along z separates the dipolar BEC into 2D layers in the x-y plane with distance δ. Apart from the intralayer DDI U_{2D}, each layer interacts with other layers via the interlayer DDI $U_{2D}^{j\ell}$.

Reduction in Multilayered Potential

- GPEs with infinite many equations; Effective single-mode approximation; Bogoliubov enegies (Rosenkranz, Cai &Bao, PRA, 88 (2013) 013616)



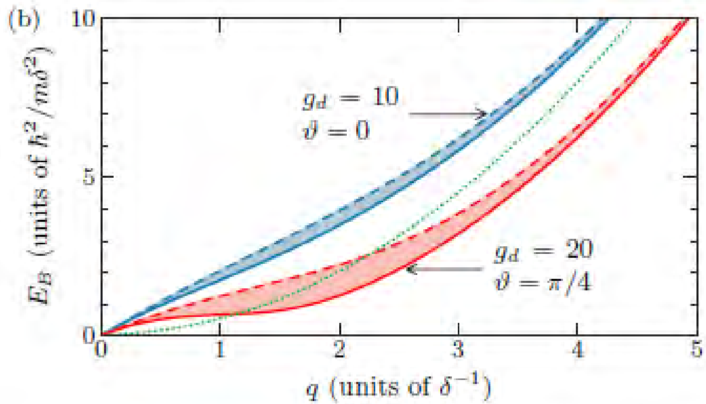


FIG. 6. (Color online) Bogoliubov energies for different polarizations and DDI strengths. (a) Polar plots marked with the magnitude and angle of **q**. White areas mark unstable regions. (b) Cuts through Bogoliubov energies at the polar angles indicated in (a). Solid lines include intra- and interlayer DDIs, whereas dashed lines only include the intralayer DDI. The green dotted line represents ^{52}Cr. The interlayer DDI does not influence high energies where the in-plane excitations become particle-like. Parameters are as in Fig. 3, with $g = 0$ and $\nu = 1/10$.

Conclusion & future challenges

- Conclusion
  - Ground state in 3D – existence, uniqueness & nonexistence
  - Dynamics in 3D – well-posedness & finite time blowup
  - Efficient numerical methods via DST
  - Dimension Reduction --- 3D→ 2D & 3D→1D
  - Ground states and dynamics in quasi-2D & quasi-1D
- Future challenges
  - Convergence rate for reduction in O(1) regime
  - In rotating frame & multi-component & spin-1
  - Dipolar BEC with random potential – disorder!!