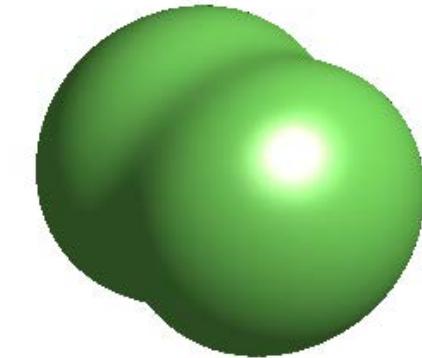


Modeling, Analysis and Simulation for Degenerate Dipolar Quantum Gas



Weizhu Bao

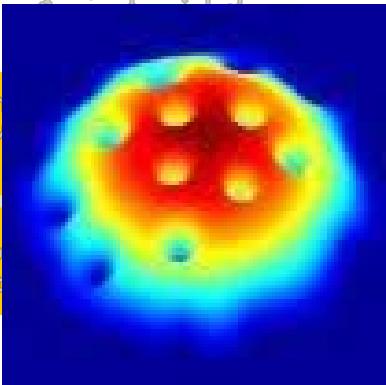


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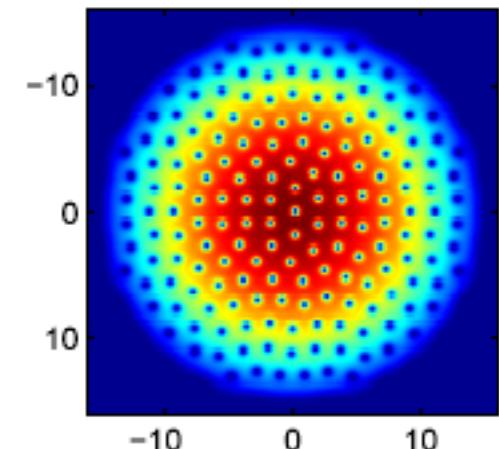
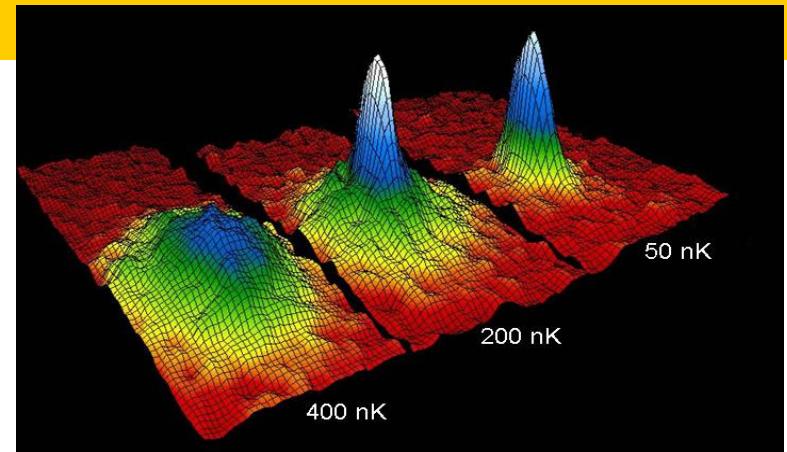
Collaborators: Y. Cai (CSRC), M. Rosenkranz (Postdoc, NUS), N. Ben Abdallah (UPS, France), Z. Lei (Fudan),
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Outline



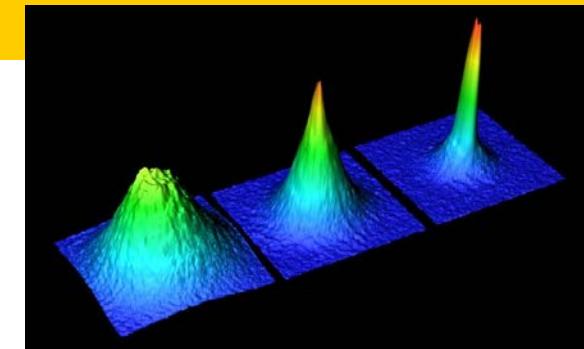
- Motivation--dipolar BEC
- Mathematical models
- Ground state and its theory
- Dynamics and its efficient computation
- Dimension reduction
- Rotating dipolar BEC
- Conclusion & future challenges



Degenerate Quantum Gas

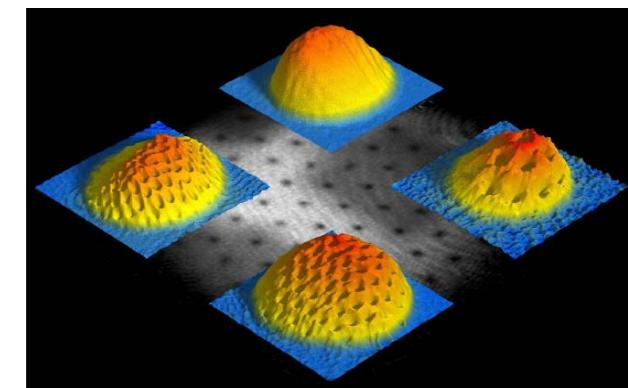
Typical degenerate quantum **gas**

- 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



Dipolar Quantum Gas

Experimental setup

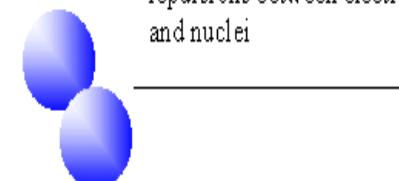
- Molecules meet to form dipoles
- Cool down dipoles to ultracold
- Hold in a magnetic trap
- Dipolar condensation
- Degenerate dipolar quantum gas

Experimental realization

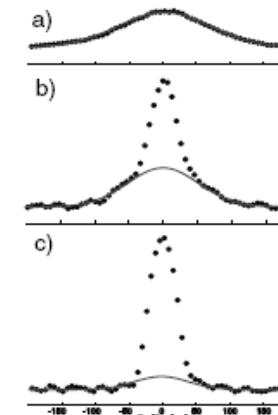
- Chromium (Cr52)
- 2005@Univ. Stuttgart, Germany
- PRL, 94 (2005) 160401

Big-wave in theoretical study

Molecules meet: there are temporary attractions and repulsions between electrons and nuclei



Non-polar molecules move together



Weak attractions between temporary dipoles

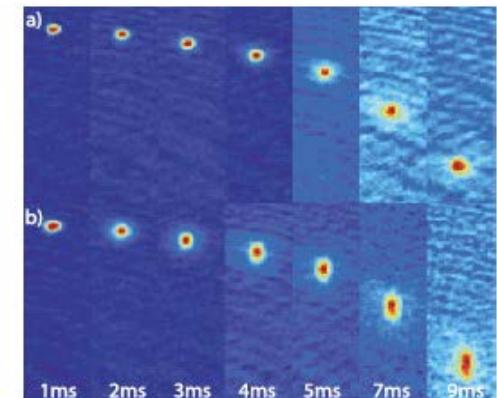


FIG. 3 (color). Time of flight series of absorption images with expansion times from 1 to 9 ms. (a) BEC released from an almost isotropic trap; (b) BEC released from an anisotropic trap.

¹⁶⁴Dy

BEC with strong DDI

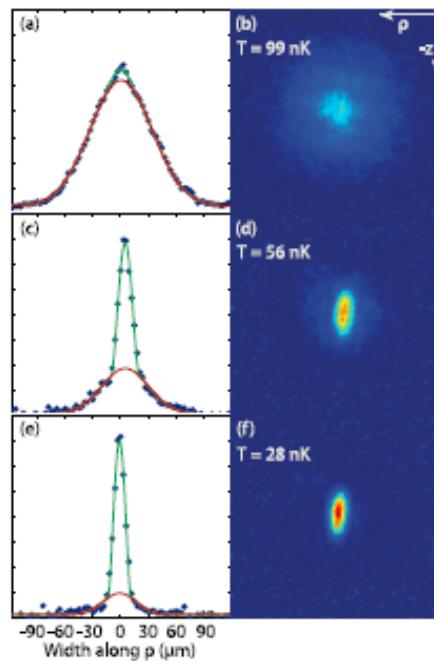


FIG. 2 (color online). TOF profiles of the spin-purified Dy gas for three evaporation time constants, with $\tau = 15$ s in (e) and (f). (a),(c),(e) Data at centers are fit to a parabolic profile (upper curve), which underestimates the condensate fraction, whereas the distributions' wings are fit to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

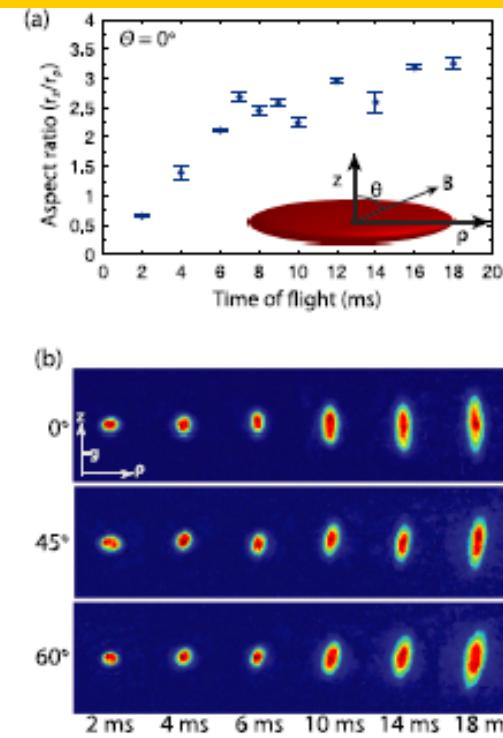


FIG. 3 (color online). Anisotropic expansion profile versus time after trap release. (a) r_z and r_p are the dimensions of the parabolic profile fit to the BEC for $\theta = 0^\circ$. Inset: Schematic of the oblate trap and magnetic-field orientation. (b) Images of the expanding condensate after trap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

Mathematical Model

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

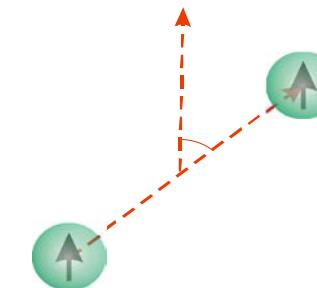
$$i \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[-\frac{1}{2} \Delta + V_{\text{ext}}(\vec{x}) + \beta |\psi|^2 + \lambda (U_{\text{dip}} * |\psi|^2) \right] \psi(\vec{x}, t)$$

- Trap potential $V_{\text{ext}}(z) = \frac{1}{2} (\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2)$
- 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

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

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

$$\begin{aligned} U_{\text{dip}}(\vec{x}) &= \frac{3}{4\pi r^3} \left(1 - \frac{3(\vec{n} \cdot \vec{x})^2}{r^2} \right) = -\delta(\vec{x}) - 3\partial_{\vec{n}\vec{n}} \left(\frac{1}{4\pi r} \right) \\ \Rightarrow \quad U_{\text{dip}}(\xi) &= -1 + \frac{3(\vec{n} \cdot \xi)^2}{|\xi|^2} \end{aligned}$$

Dipole-dipole interaction becomes

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

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



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

A New Formulation

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

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

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

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

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

• Nonlinear Eigenvalue problem (Euler-Langrange eq.)

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

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

• Chemical potential

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

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

Ground State Results

 **Theorem** (Existence, uniqueness & nonexistence) ([Carles, Markowich& Sparber, 09'](#); [Bao, Cai & Wang, JCP, 10'](#))

– Assumptions

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

– Results

- There **exists** a ground state $\phi_g \in S$ if $\beta \geq 0$ & $-\frac{\beta}{2} \leq \lambda \leq \beta$
- Positive ground state is **unique** $\phi_g = e^{i\theta_0} |\phi_g|$ with $\theta_0 \in \mathbb{R}$
- Nonexistence of ground state, i.e. $\lim_{\phi \in S} E(\phi) = -\infty$
 - Case I: $\beta < 0$
 - Case II: $\beta \geq 0$ & $\lambda > \beta$ or $\lambda < -\frac{\beta}{2}$

Key Techniques in Proof

• Estimate on the Poisson equation

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

• Positivity & semi-lower continuous

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

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

$$\beta \geq 0 \quad \& \quad -\frac{\beta}{2} \leq \lambda \leq \beta$$

• 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

$$\frac{\partial}{\partial t} \phi(\vec{x}, t) = \left[\frac{1}{2} \Delta - V_{\text{ext}}(\vec{x}) - (\beta - \lambda) |\phi|^2 + 3\lambda \partial_{\vec{n}\vec{n}} \varphi \right] \phi(\vec{x}, t),$$
$$-\Delta \phi(\vec{x}, t) = |\phi(\vec{x}, t)|^2, \quad \lim_{|\vec{x}| \rightarrow \infty} \phi(\vec{x}, t) = 0, \quad \vec{x} \in \Omega \text{ & } t_n \leq t < t_{n+1},$$

$$\phi(\vec{x}, t_{n+1}) := \phi(\vec{x}, t_{n+1}^+) = \frac{\phi(\vec{x}, t_{n+1}^-)}{\|\phi(\vec{x}, t_{n+1}^-)\|}, \quad \vec{x} \in \Omega \text{ & } n \geq 0,$$

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

Full discretization

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

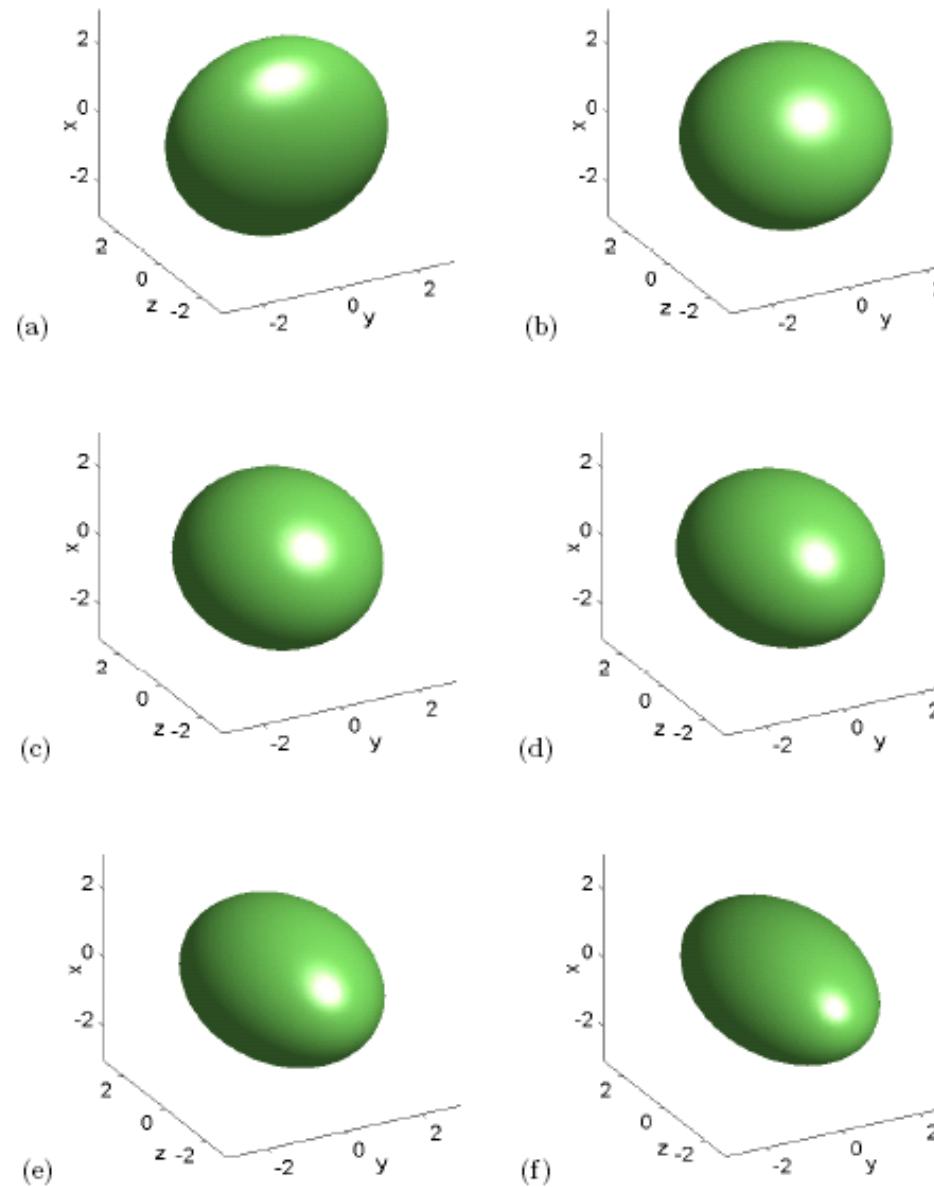


Figure 2: Isosurface plots of the ground state $|\phi_g(\mathbf{x})| = 0.08$ of a dipolar BEC with the harmonic potential $V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2 + z^2)$ and $\beta = 207.16$ for different values of $\frac{\lambda}{\beta}$: (a) $\frac{\lambda}{\beta} = -0.5$; (b) $\frac{\lambda}{\beta}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

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

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

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

• Mathematical questions

- Existence & uniqueness & finite time blow-up???

• Existing results

- Carles, Markowich & Sparber, Nonlinearity, 21 (2008), 2569-2590
- Antonelli & Sparber, 09, Physica D --- existence of solitary waves.

Well-posedness Results

Theorem (well-posedness) (Carles, Markowich & Sparber, 09'; Bao, Cai & Wang, JCP, 10')

- Assumptions

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

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

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

Finite Time Blowup Results

Theorem (finite time blowup) (Carles, Markowich & Sparber, 09'; Bao, Cai & Wang, JCP, 10')

– Assumptions (i) $\beta < 0$ or $\beta \geq 0 \text{ & } \lambda < -\frac{\beta}{2}$ or $\lambda > \beta$

– Results: (ii) $3V_{\text{ext}}(\vec{x}) + \vec{x} \cdot \nabla V_{\text{ext}}(\vec{x}) \geq 0, \quad \forall \vec{x} \in \mathbb{R}^3$

- 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) $E(\psi_0) = 0 \quad \& \quad \text{Im} \int_{\mathbb{R}^3} \bar{\psi}_0(x) (\vec{x} \cdot \nabla \psi_0(\vec{x})) d\vec{x} < 0$

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

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**

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

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

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

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

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

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

New numerical methods for DDI

How to compute nonlocal DDI

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

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

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

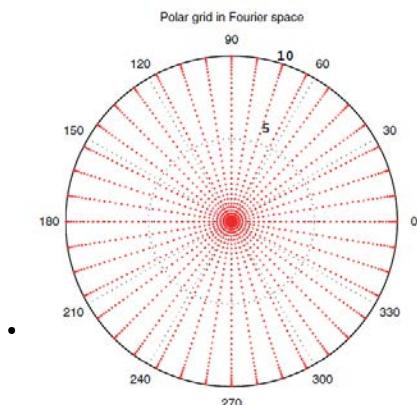
$$\phi = -|\psi|^2 - 3\partial_{nn}\varphi \quad \& \quad -\Delta\varphi(\vec{x}, t) = |\psi(\vec{x}, t)|^2$$

- Nonuniform FFT (Bao, Jiang, Greengard, SISC, 14')

$$\phi = \int_{\mathbb{R}^3} \hat{U}_{\text{dip}}(\xi) \hat{\rho}(\xi, t) e^{i\xi \cdot x} d\xi \quad \rho = |\psi|^2$$

sphere coordinate

$$= \int_{S^2 \times \mathbb{R}^+} \hat{U}_{\text{dip}}(\xi) |\xi|^2 \hat{\rho}(\xi, t) e^{i\xi \cdot x} \dots$$



Numerical results

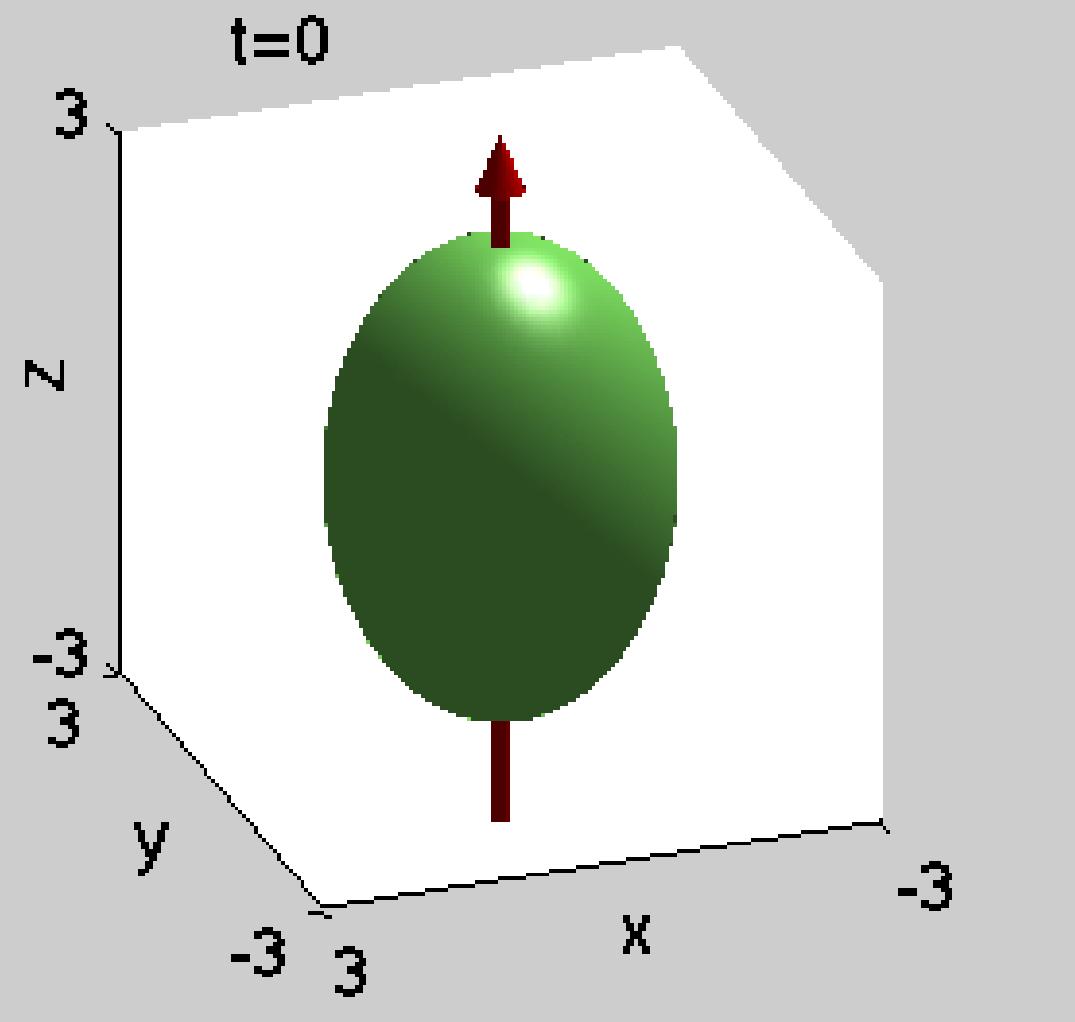
(Bao, Tang & Zhang, CiCP, 16')

$$\Phi(\mathbf{x}, t) = \int_{\mathbb{R}^d} U_{\text{dip}}(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}, t) d\mathbf{y}; \quad e_h := \|\Phi - \Phi_h\|_{L^2} / \|\Phi\|_{L^2},$$

NUFFT	$h=2$	$h=1$	$h=1/2$	$h=1/4$
$L=4$	1.118E-01	3.454E-04	1.335E-04	1.029E-04
$L=8$	5.281E-02	3.428E-04	9.834E-12	1.601E-14
$L=16$	5.202E-02	3.551E-04	1.143E-11	8.089E-15
DST	$h=1$	$h=1/2$	$h=1/4$	$h=1/8$
$L=8$	6.919E-02	7.720E-02	8.124E-02	8.327E-02
$L=16$	2.709E-02	2.853E-02	2.925E-02	2.961E-02
$L=32$	1.008E-02	1.033E-02	1.046E-02	1.052E-02

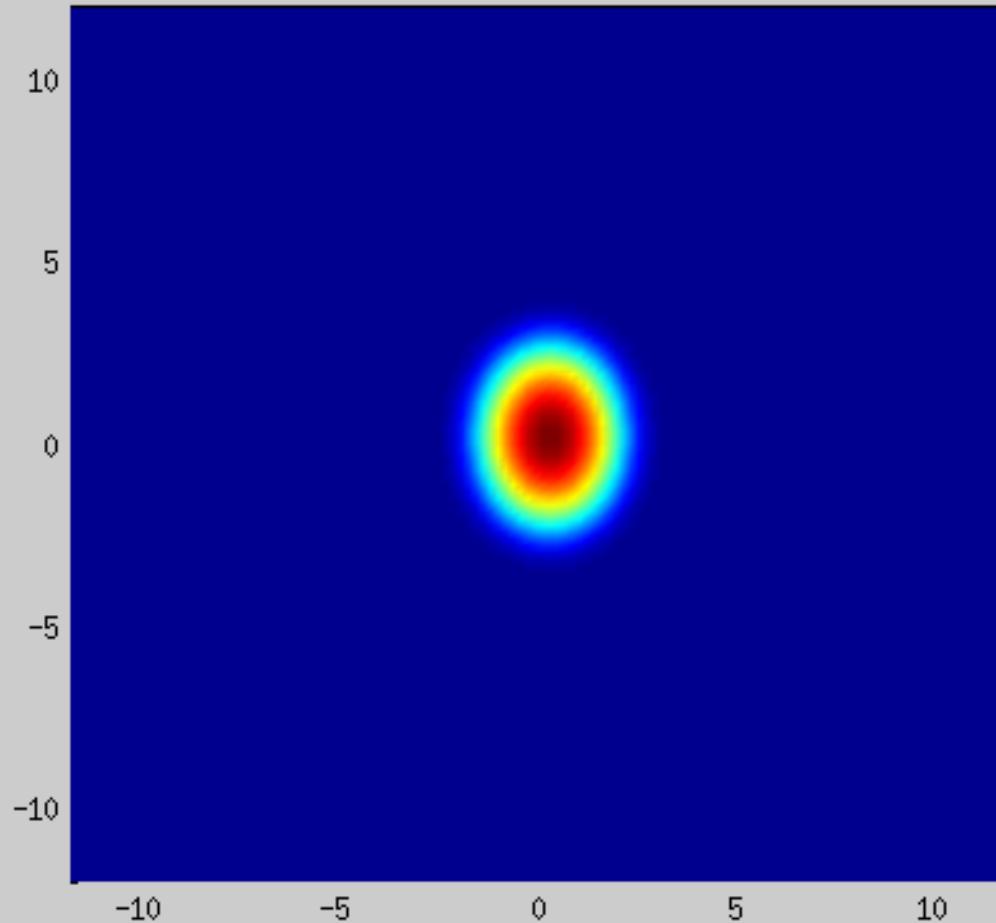
Dynamics of a BEC with DDI

$$\vec{n}(t) = (\sin(t/5), 0, \cos(t/5))^T$$



Collapse of a BEC with DDI

Column Density at $t=0$



$$\vec{n} = (0, 0, 1)^T$$

``Clover''

Dimension Reduction

• Gross-Pitaevskii-Poisson equations

$$i \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[-\frac{1}{2} \Delta + V_{\text{ext}}(\vec{x}) + (\beta - \lambda) |\psi|^2 - 3\lambda \partial_{\vec{n}\vec{n}} \varphi \right] \psi(\vec{x}, t)$$
$$-\Delta \varphi(\vec{x}, t) = |\psi(\vec{x}, t)|^2, \quad \lim_{|\vec{x}| \rightarrow \infty} \varphi(\vec{x}, t) = 0, \quad \vec{x} \in \mathbb{R}^3, \quad t > 0$$

• Strongly anisotropic potential

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

– Case I: 3D \rightarrow 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 \rightarrow 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 & Weishaupt, 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'](#)) – use the convolution formulation

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

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

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

Ansatz

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

Dimension Reduction (3D → 2D)

2D equations (Bao, Cai, Lei, Rosenkranz, PRA, 10')

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

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

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

Ground State Results for quais-2D

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

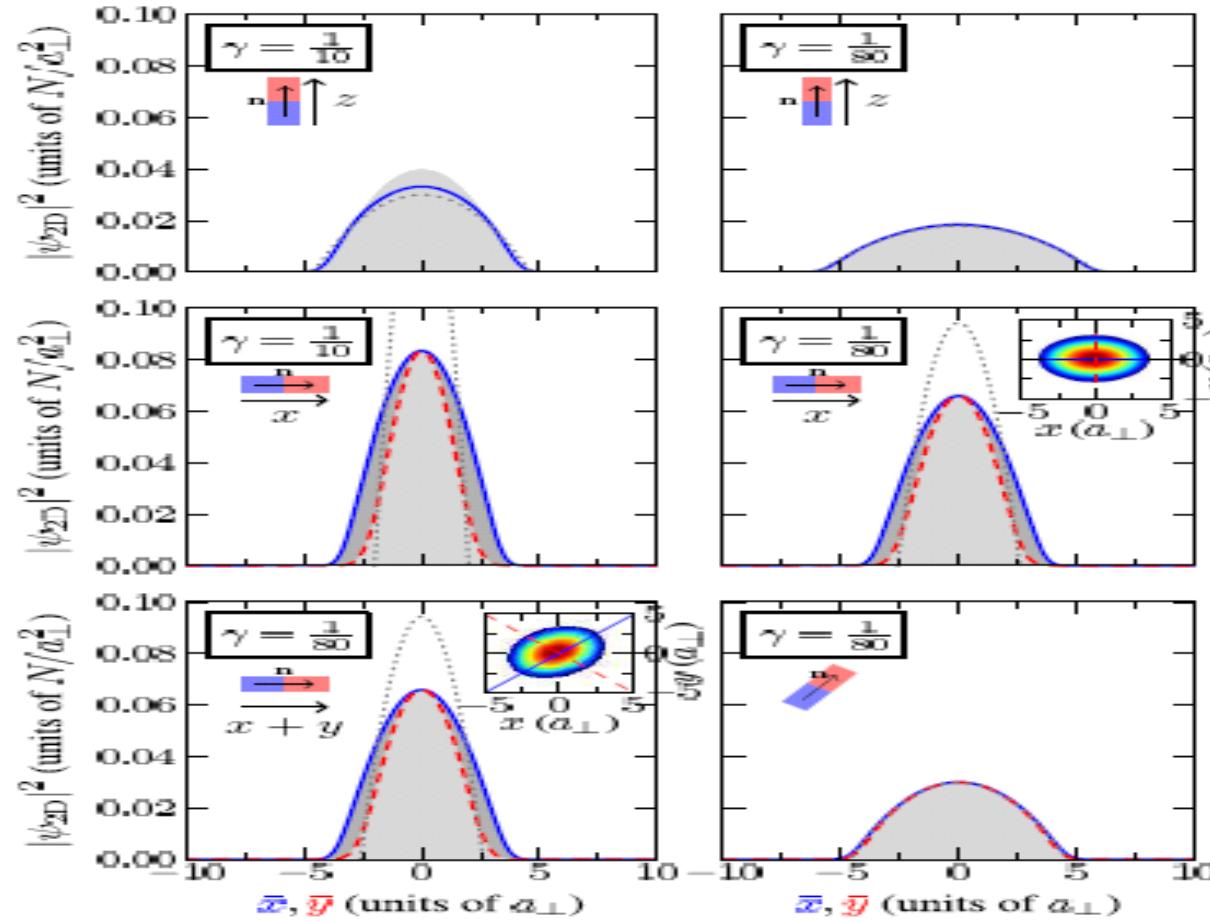


Theorem (Existence & uniqueness) ([Bao, Ben Abdallah, Cai, SIMA, 12'](#))

– **Results** $V_{2D}(\vec{x}) \geq 0, \forall \vec{x} \in \mathbb{R}^2$ & $\lim_{|\vec{x}| \rightarrow \infty} V_{2D}(\vec{x}) = +\infty$ (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 $\lambda < 0$ & $\beta + \frac{\lambda}{2} (1 + 3 |2n_3^2 - 1|) > -\varepsilon \sqrt{2\pi} C_b$
- Positive ground state is unique $\phi_g = e^{i\theta_0} |\phi_g|$ with $\theta_0 \in \mathbb{R}$
 - Case I: $\lambda \geq 0$ & $\beta - \lambda \geq 0$
 - Or case II $\lambda < 0$ & $\beta + \frac{\lambda}{2} (1 + 3 |2n_3^2 - 1|) \geq 0$
- No ground state if

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



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

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).

Dimension Reduction (3D → 2D)

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

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

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

Energy

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

Ground State Results for quais-2D

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



Theorem (Existence & uniqueness) ([Bao, Ben Abdallah, Cai, SIMA, 12'](#))

- There exists a ground state $\phi_g \in S$ if
 - Case I: $\lambda = 0 \text{ & } \beta > -\varepsilon\sqrt{2\pi}C_b$
 - Or case II $\lambda > 0, n_3 = 0 \text{ & } \beta - \lambda > -\varepsilon\sqrt{2\pi}C_b$
 - Or case III $\lambda < 0, n_3^2 \geq 1/2 \text{ & } \beta - \lambda(1 - 3n_3^2) > -\varepsilon\sqrt{2\pi}C_b$
- Positive ground state is unique $\phi_g = e^{i\theta_0} |\phi_g|$ with $\theta_0 \in \mathbb{R}$
 - Case I: $\lambda = 0 \text{ & } \beta \geq 0$
 - Or case II $\lambda > 0, n_3 = 0 \text{ & } \beta \geq \lambda$
 - Or case III $\lambda < 0, n_3^2 \geq 1/2 \text{ & } \beta - \lambda(1 - 3n_3^2) \geq 0$
- No ground state
 $\lambda > 0 \text{ & } n_3 \neq 0$ or $\lambda < 0 \text{ & } 2n_3^2 < 1$ or $\lambda = 0 \text{ & } \beta < -\varepsilon\sqrt{2\pi}C_b$

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

Then we have

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

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

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

Dimension Reduction (3D → 1D)

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

$$i \frac{\partial}{\partial t} \psi(z, t) = [-\frac{1}{2} \partial_{zz} + V_{1D}(z) + \frac{2\beta + \lambda(1 - 3n_3^2)}{4\pi\varepsilon^2} |\psi|^2 + \frac{3\lambda(1 - 3n_3^2)}{8\varepsilon\sqrt{2\pi}} \partial_{zz} \varphi] \psi(z, t)$$
$$\varphi(z, t) = U_\varepsilon^{1D} * |\psi|^2, \quad U_\varepsilon^{1D}(z) = \frac{2e^{z^2/2\varepsilon^2}}{\sqrt{\pi}} \int_{|z|}^\infty e^{-s^2/2\varepsilon^2} ds,$$

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

Ground State Results for quais-1D

$V_{1D}(z) \geq 0, \forall z \in \mathbb{R} \text{ & } \lim_{|z| \rightarrow \infty} V_{1D}(z) = +\infty$ (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: $\lambda(1 - 3n_3^2) \geq 0$ & $\beta - \lambda(1 - 3n_3^2) \geq 0$
 - Or case II $\lambda(1 - 3n_3^2) < 0$ & $\beta + \lambda(1 - 3n_3^2)/2 \geq 0$



Dynamics results – global well-posedness of the Cauchy problem



Convergence rate if $\beta = O(\varepsilon^2)$ & $\lambda = O(\varepsilon^2)$

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

Rotating Dipolar BEC

Mathematical model

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

- Where $L_z = i(y\partial_x - x\partial_y)$

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

Ground states

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

$$E(\phi) := \int_{\mathbb{R}^3} \left[\frac{1}{2} |\nabla \phi|^2 + V_{\text{ext}}(x) |\phi|^2 - \Omega \bar{\phi} L_z \phi + \frac{\beta}{2} |\phi|^4 + \frac{\lambda}{2} (U_{\text{dip}} * |\phi|^2) |\phi|^2 \right] d\vec{x}$$

$$\vec{n} = (\sin \vartheta, 0, \cos \vartheta)^T$$

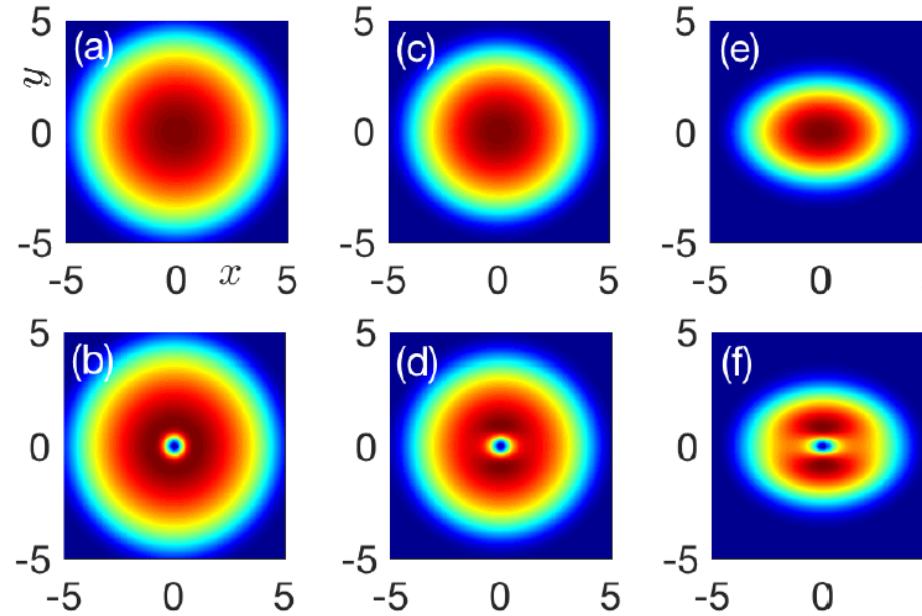
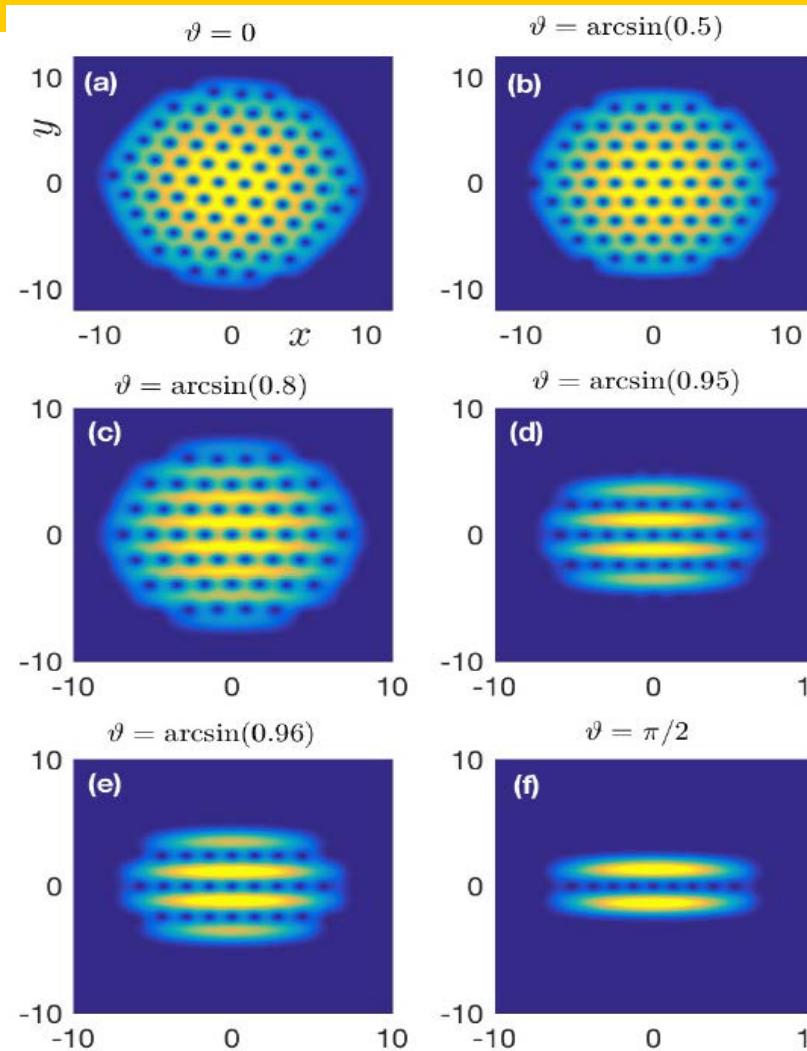
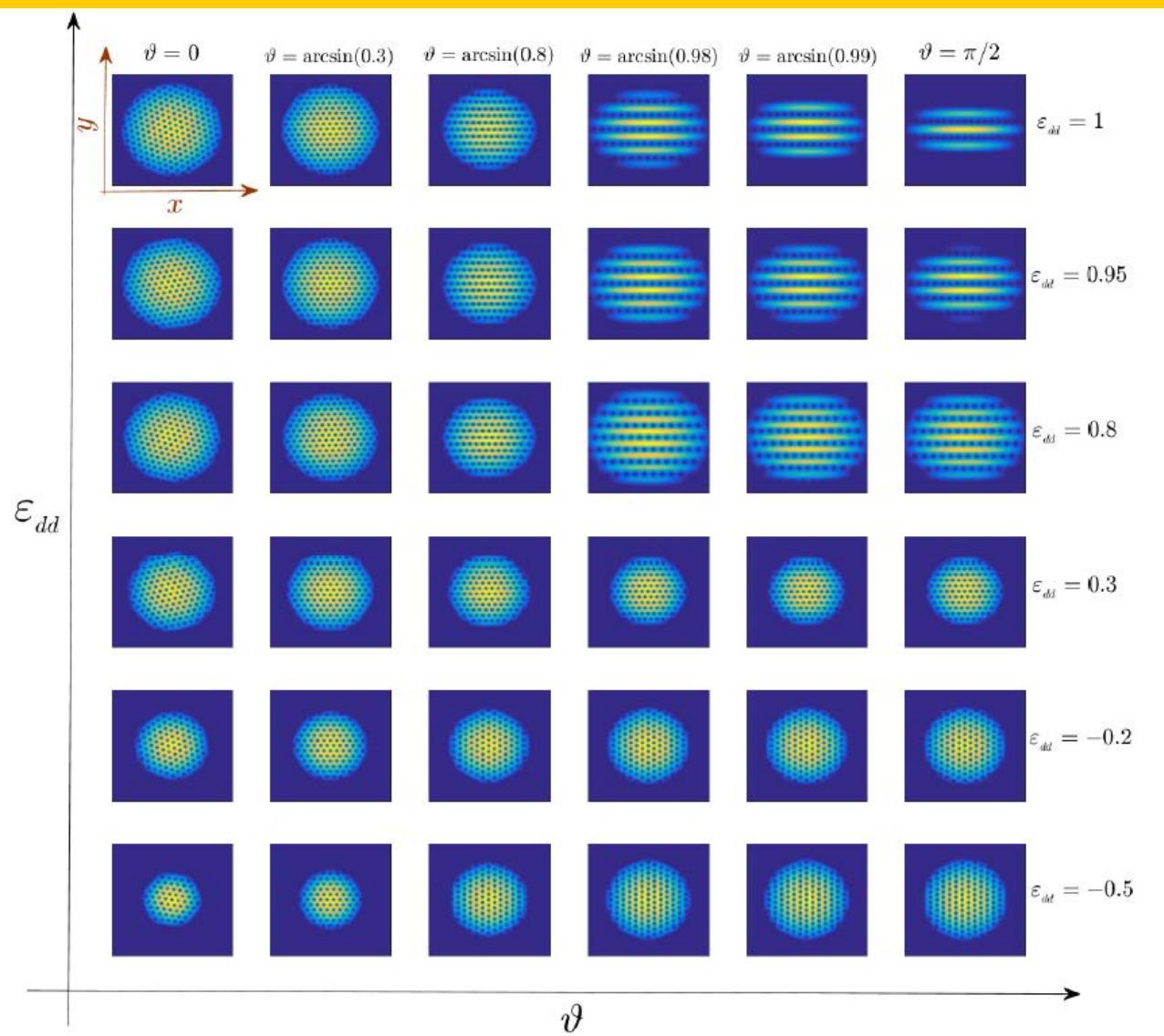


FIG. 2. (Color online) Density of a rotating dipolar BEC around the critical rotation frequency Ω_c for fixed $\gamma = 10$, $g = 250$, $g_d = 200$, different polarization axis $\mathbf{n} = (\sin \vartheta, 0, \cos \vartheta)$ ($\vartheta = 0$ left panel (a),(b); $\vartheta = \pi/4$ middle panel (c), (d); $\vartheta = \pi/2$ right panel, (e),(f)). The rotational critical rotational frequency Ω_c is found to be $0.195 < \Omega_c < 0.196$ (left panel), $0.232 < \Omega_c < 0.233$ (middle panel), $0.357 < \Omega_c < 0.358$, with the corresponding lower bound of rotational frequency for the non-vortex states and the upper bound for the vortex state.

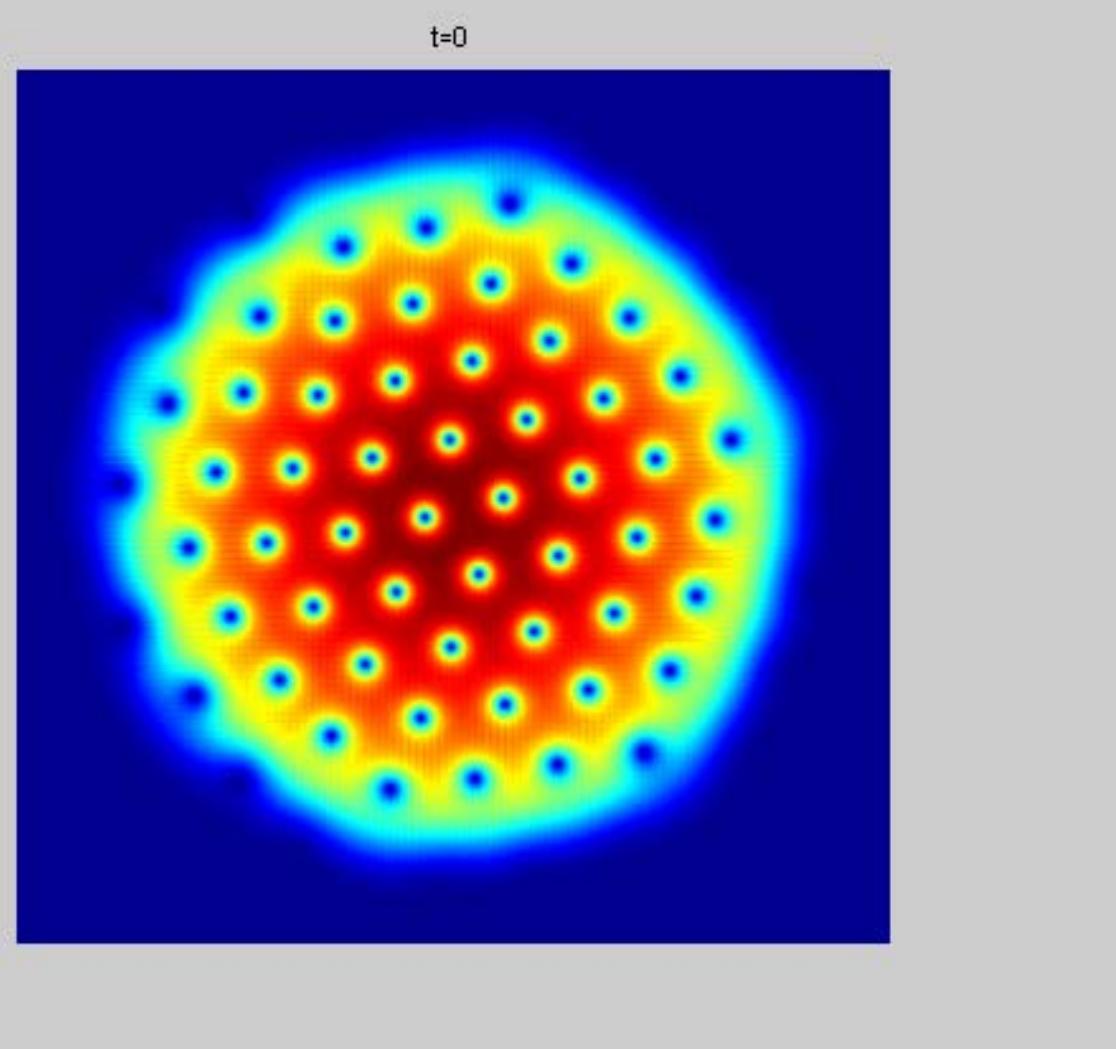
$$\vec{n} = (\sin \vartheta, 0, \cos \vartheta)^T$$



$$\vec{n} = (\sin \vartheta, 0, \cos \vartheta)^T$$



Dynamics of a rotating dipolar BEC



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 --- $3D \rightarrow 2D$ & $3D \rightarrow 1D$
- 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!!