

# Modeling, Analysis and Simulation for Degenerate Dipolar Quantum Gas

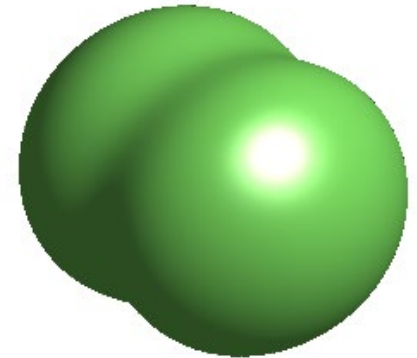


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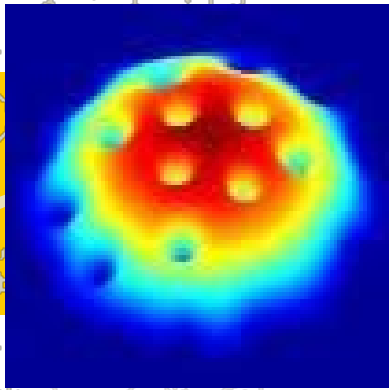
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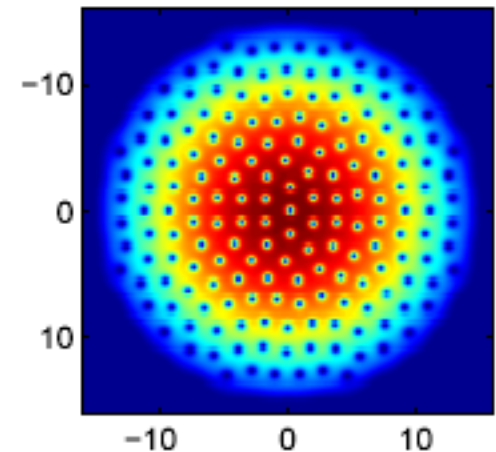
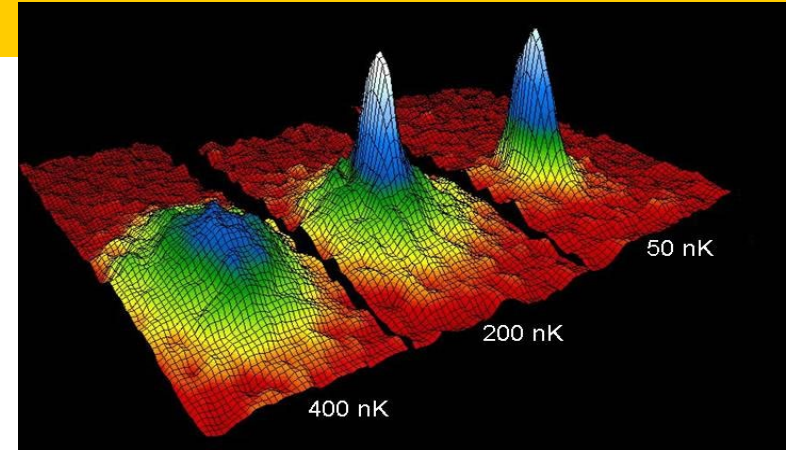


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# Outline



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



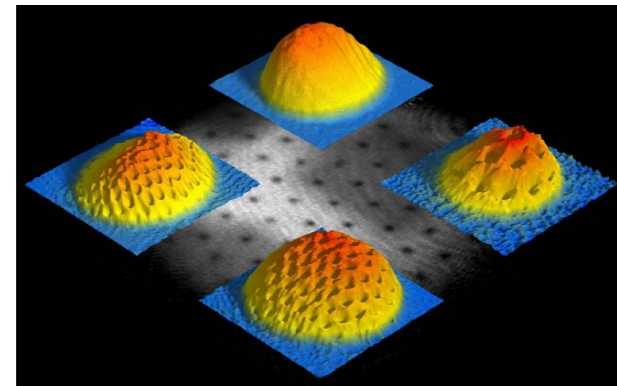
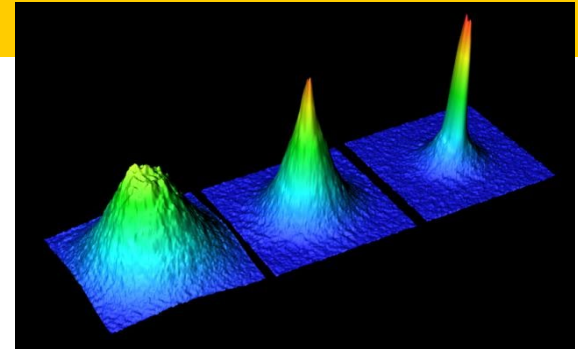
# Degenerate Quantum Gas

## 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
- Contact (Fermi or local) or Coulomb (nonlocal & isotropic) interaction



# Dipolar Quantum Gas

anisotropic & nonlocal interaction

## 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

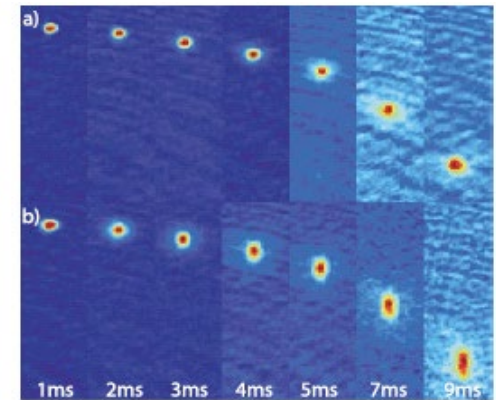
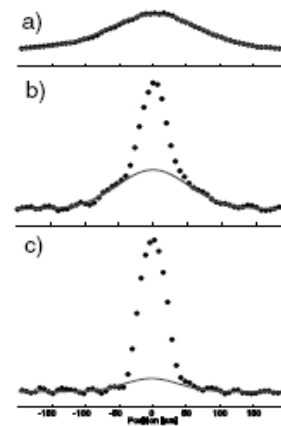
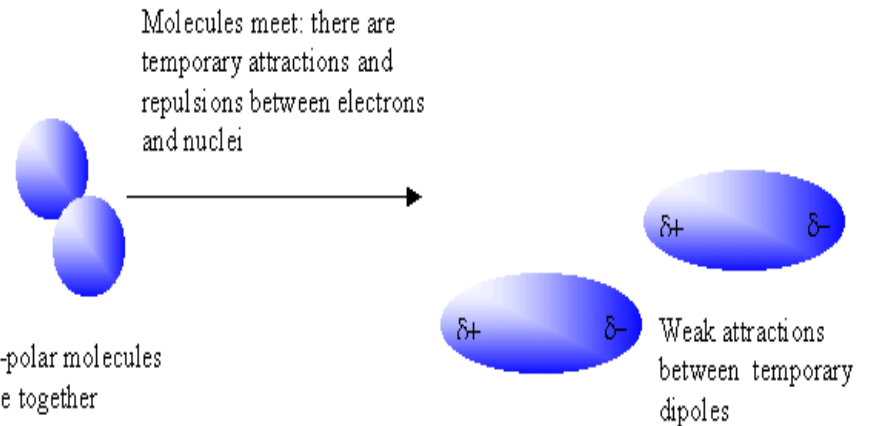


FIG. 3 (color). Time of flight series of absorption images with expansion times from 1 to 9 ms. (a) BEC released from an almost isotropic trap; (b) BEC released from an anisotropic trap.

# BEC with strong dipole-dipole interaction (DDI)

<sup>164</sup>Dy

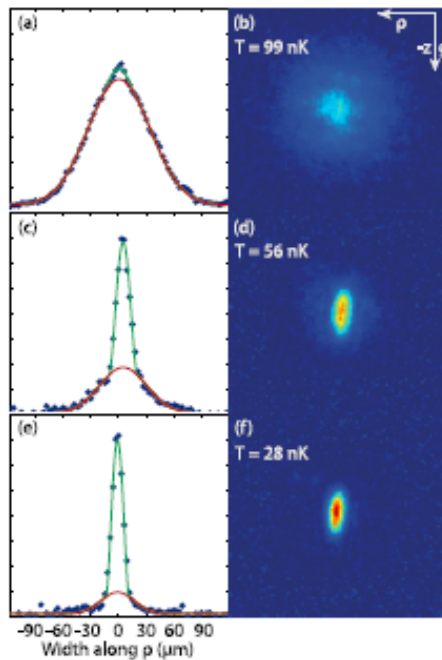


FIG. 2 (color online). TOF profiles of the spin-purified Dy gas for three evaporation time constants, with  $\tau = 15$  s in (e) and (f). (a),(c),(e) Data at centers are fit to a parabolic profile (upper curve), which underestimates the condensate fraction, whereas the distributions' wings are fit to 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  $1.5(2) \times 10^7$  atoms forms at 28(2) nK with density  $10^{14} \text{ cm}^{-3}$ .

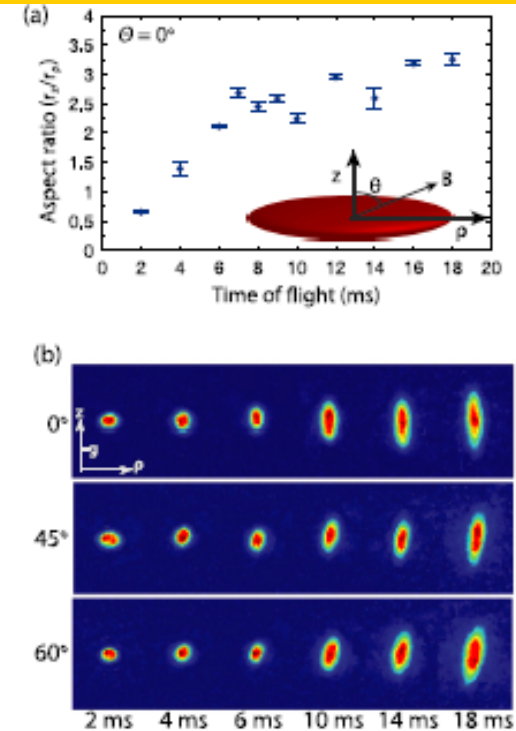


FIG. 3 (color online). Anisotropic expansion profile versus time after trap release. (a)  $r_z$  and  $r_\rho$  are the dimensions of the parabolic profile fit to the BEC for  $\theta = 0^\circ$ . Inset: Schematic of the oblate trap and magnetic-field orientation. (b) The condensate rotates after trap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

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

# 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)

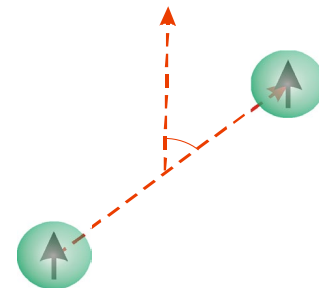
– Long-range **dipole-dipole** interaction kernel

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

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

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

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

✦ **Dipole-dipole** interaction becomes

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

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



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



# A New Formulation

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

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

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

↓ Energy

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

# 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-Lagrange eq.)

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

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

- ✦ **Chemical potential**

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

# 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

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

✦ **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  $\rho$  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

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

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

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

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

## ✦ Full discretization

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

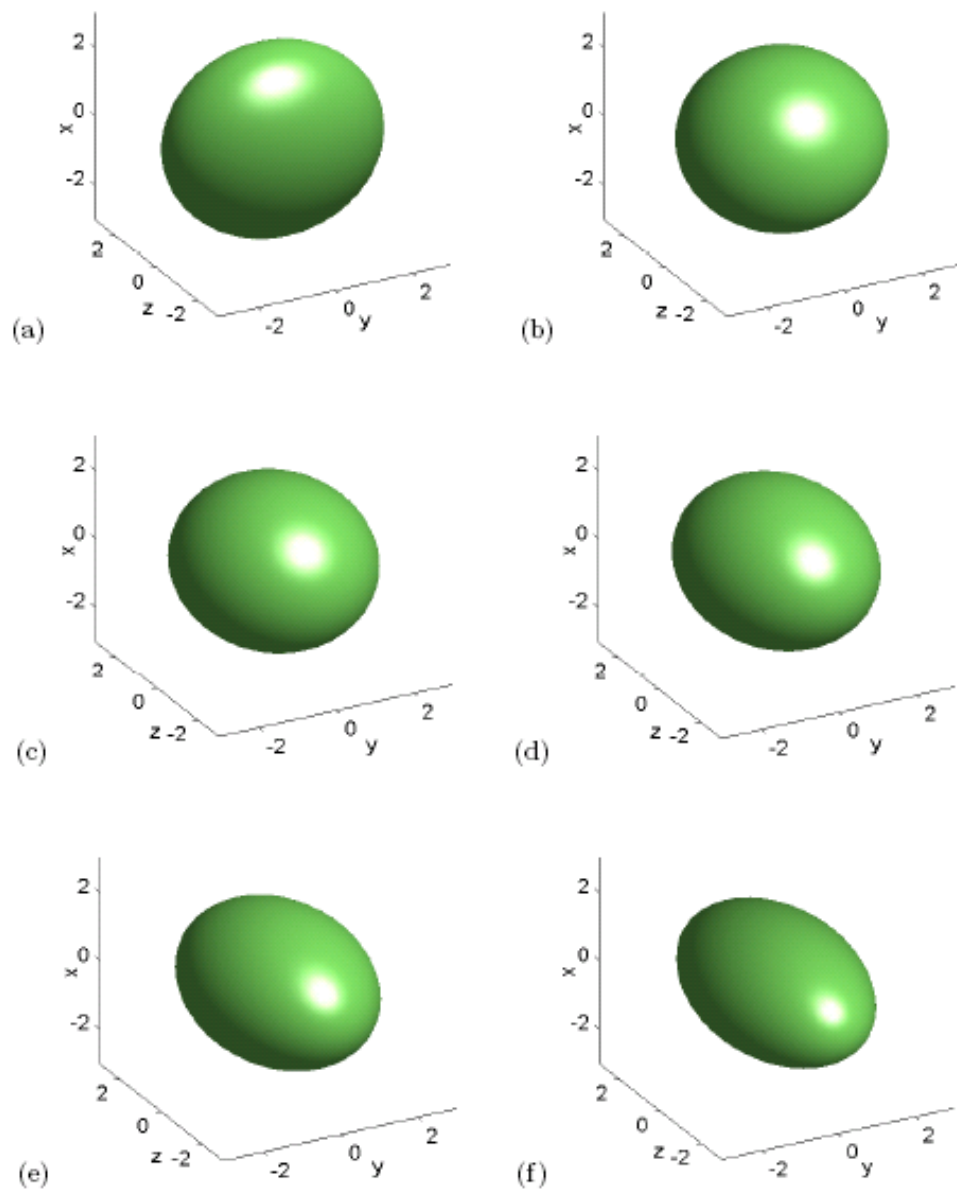


Figure 2: Isosurface plots of the ground state  $|\phi_g(\mathbf{x})| = 0.08$  of a dipolar BEC with the harmonic potential  $V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2 + z^2)$  and  $\beta = 207.16$  for different values of  $\frac{\lambda}{\beta}$ : (a)  $\frac{\lambda}{\beta} = -0.5$ ; (b)  $\frac{\lambda}{\beta}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

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

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



# Finite Time Blowup Results

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

– **Assumptions** (i)  $\beta < 0$       or       $\beta \geq 0$  &  $\lambda < -\frac{\beta}{2}$  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.  $T_{\text{max}} < +\infty$
- If one of the following conditions holds

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

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

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

# 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**

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

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

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

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

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

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

# New numerical methods for DDI

## How to compute nonlocal DDI

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

– FFT (fast Fourier transform)

– DST (discrete sine transform)

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

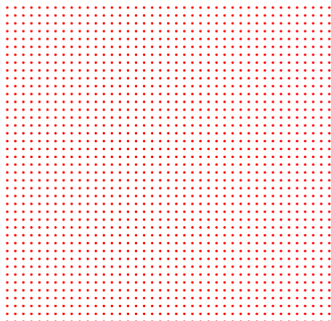
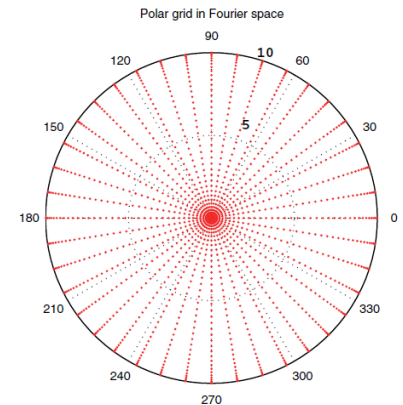
$$\phi = -|\psi|^2 - 3\partial_{nn}\phi \quad \& \quad -\Delta\phi(\vec{x}, t) = |\psi(\vec{x}, t)|^2$$

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

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

sphere coordinate

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



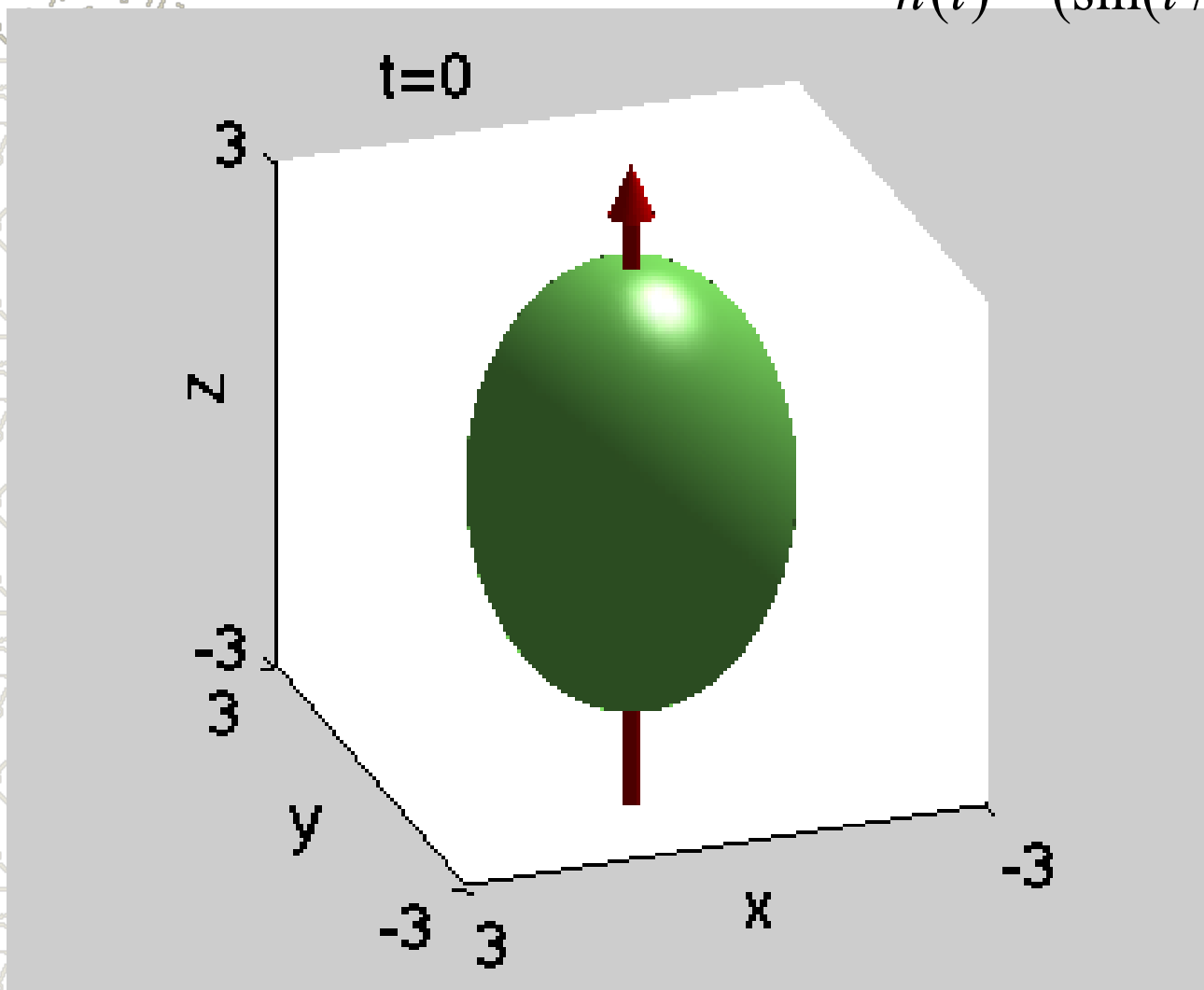
# Numerical results (Bao, Tang & Zhang, CiCP, 16')

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

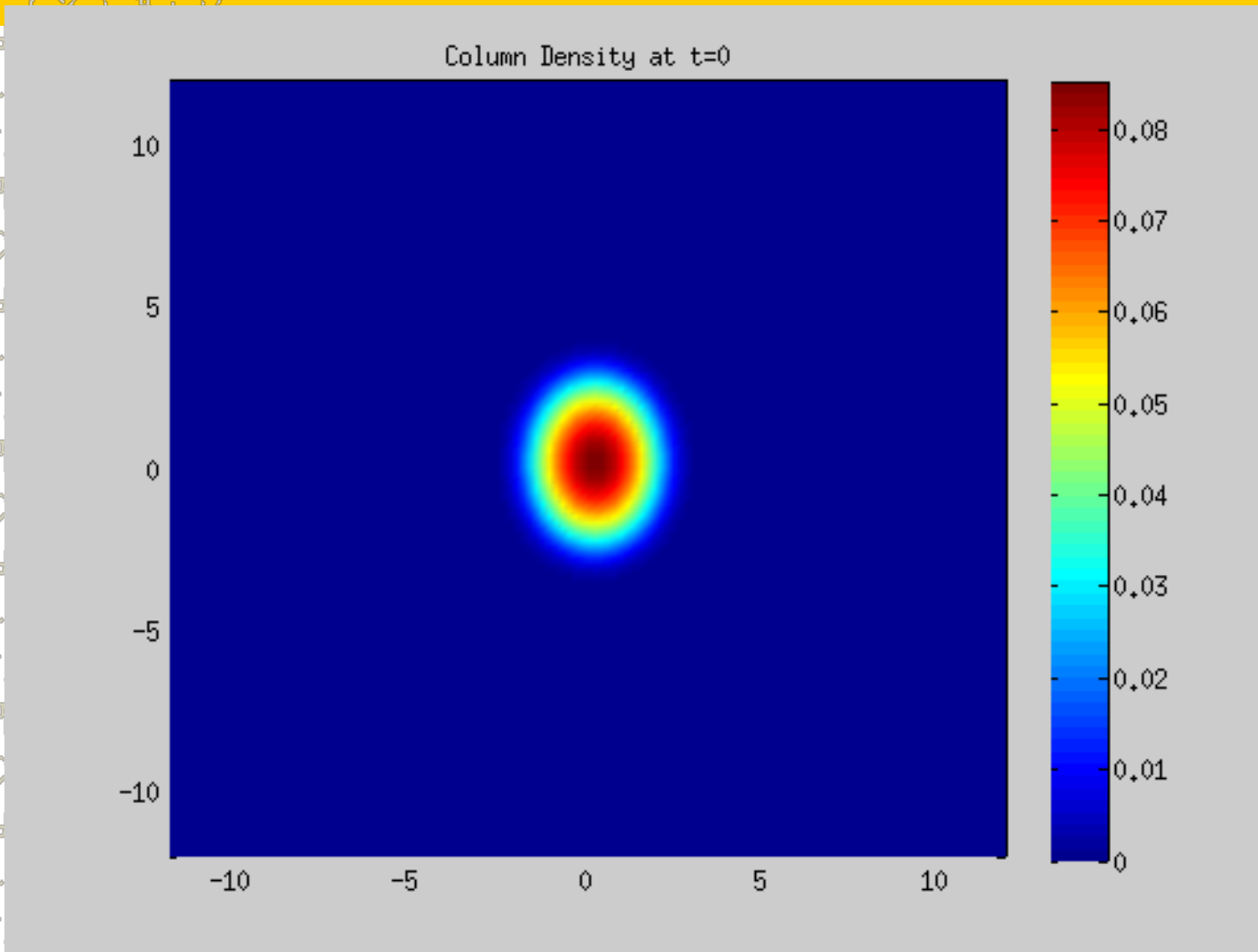
<i>NUFFT</i>	$h=2$	$h=1$	$h=1/2$	$h=1/4$
$L=4$	1.118E-01	3.454E-04	1.335E-04	1.029E-04
$L=8$	5.281E-02	3.428E-04	9.834E-12	1.601E-14
$L=16$	5.202E-02	3.551E-04	1.143E-11	8.089E-15
<i>DST</i>	$h=1$	$h=1/2$	$h=1/4$	$h=1/8$
$L=8$	6.919E-02	7.720E-02	8.124E-02	8.327E-02
$L=16$	2.709E-02	2.853E-02	2.925E-02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



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

“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

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

– 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 & 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') – use the convolution formulation



# Dimension Reduction (3D $\rightarrow$ 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

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

# Dimension Reduction (3D $\rightarrow$ 2D)

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

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

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

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

# Ground State Results for quasis-2D

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

**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

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

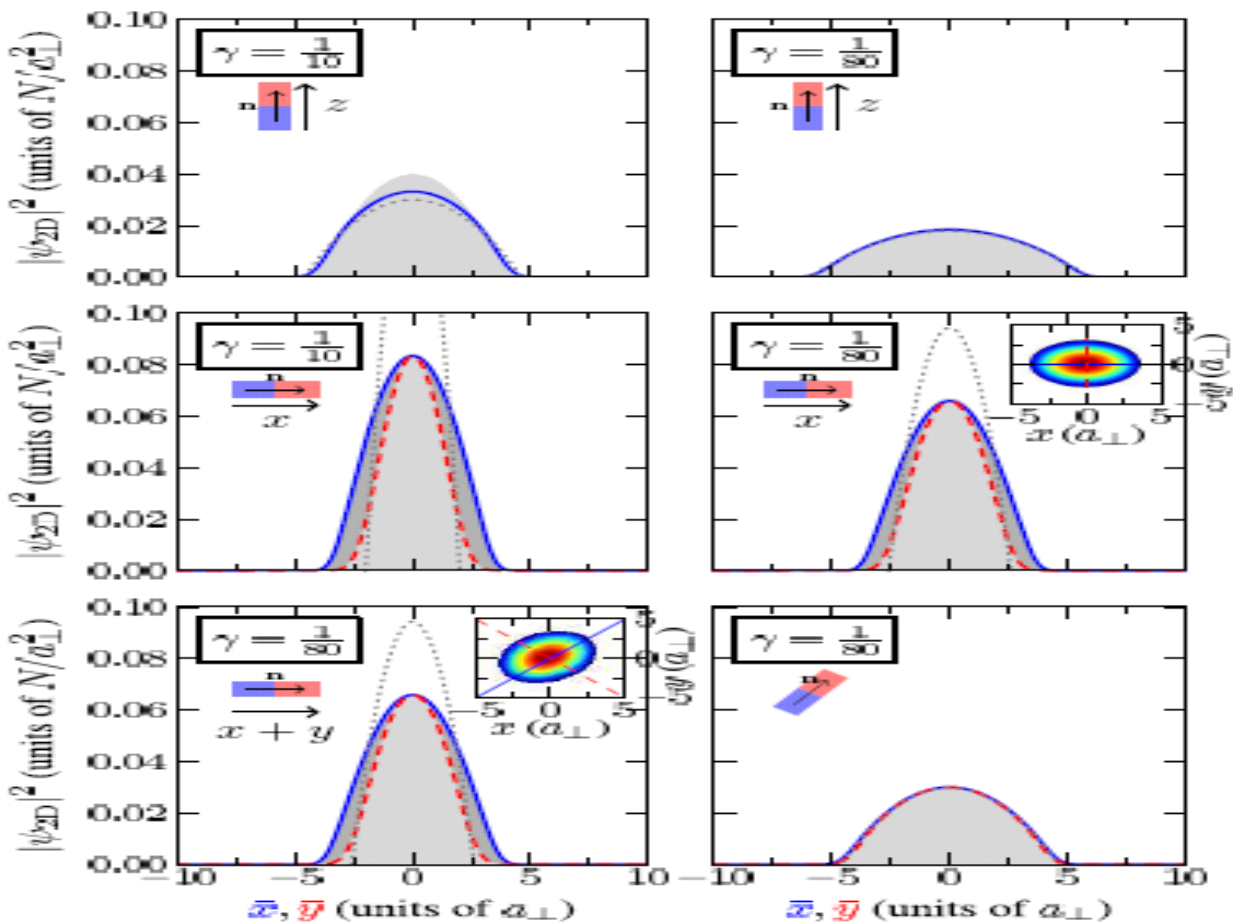


FIG. 4. (Color online) Cuts through the radial density profiles of the quasi-2D dipolar BEC given by Eq. (16) for various polarizations and trap anisotropies. The cuts are taken along the axes with largest ( $\bar{x}$  axis, solid blue lines) and smallest extend of the BEC ( $\bar{y}$  axis, dashed red). 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).

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

# Dimension Reduction (3D $\rightarrow$ 2D)

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

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

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

• **Energy**

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

# Ground State Results for quais-2D

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

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

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

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

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 $\rightarrow$ 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 $\rightarrow$ 1D)

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

$$i \frac{\partial}{\partial t} \psi(z, t) = \left[ -\frac{1}{2} \partial_{zz} + V_{1D}(z) + \frac{2\beta + \lambda(1 - 3n_3^2)}{4\pi\epsilon^2} |\psi|^2 + \frac{3\lambda(1 - 3n_3^2)}{8\epsilon\sqrt{2\pi}} \partial_{zz} \varphi \right] \psi(z, t)$$

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

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

# Ground State Results for quasis-1D

$V_{1D}(z) \geq 0, \forall z \in \mathbb{R}$  &  $\lim_{|z| \rightarrow \infty} V_{1D}(z) = +\infty$  (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  $\beta = O(\varepsilon^2)$  &  $\lambda = O(\varepsilon^2)$

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

# 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

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

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

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

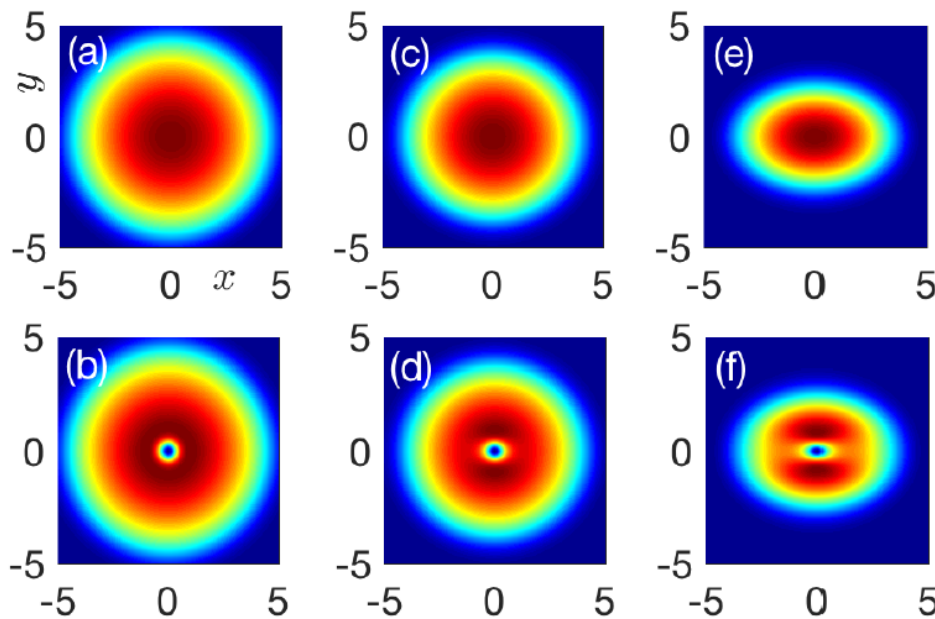
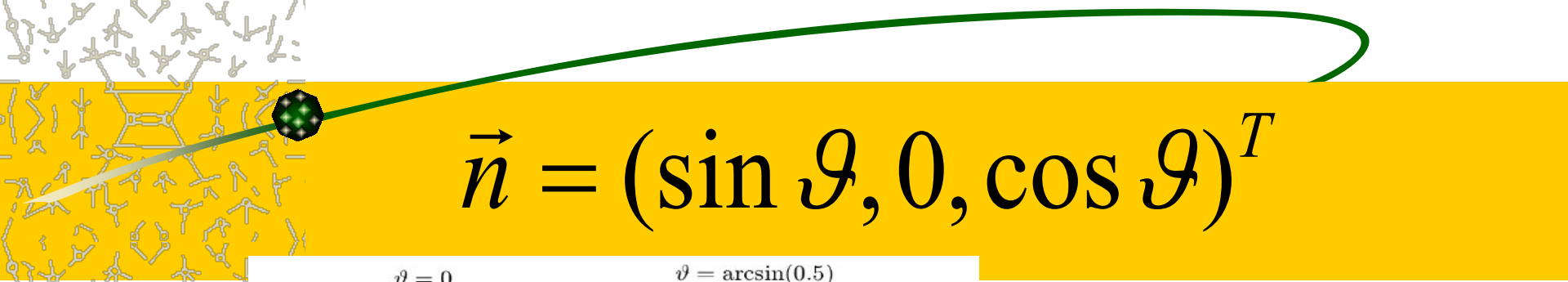
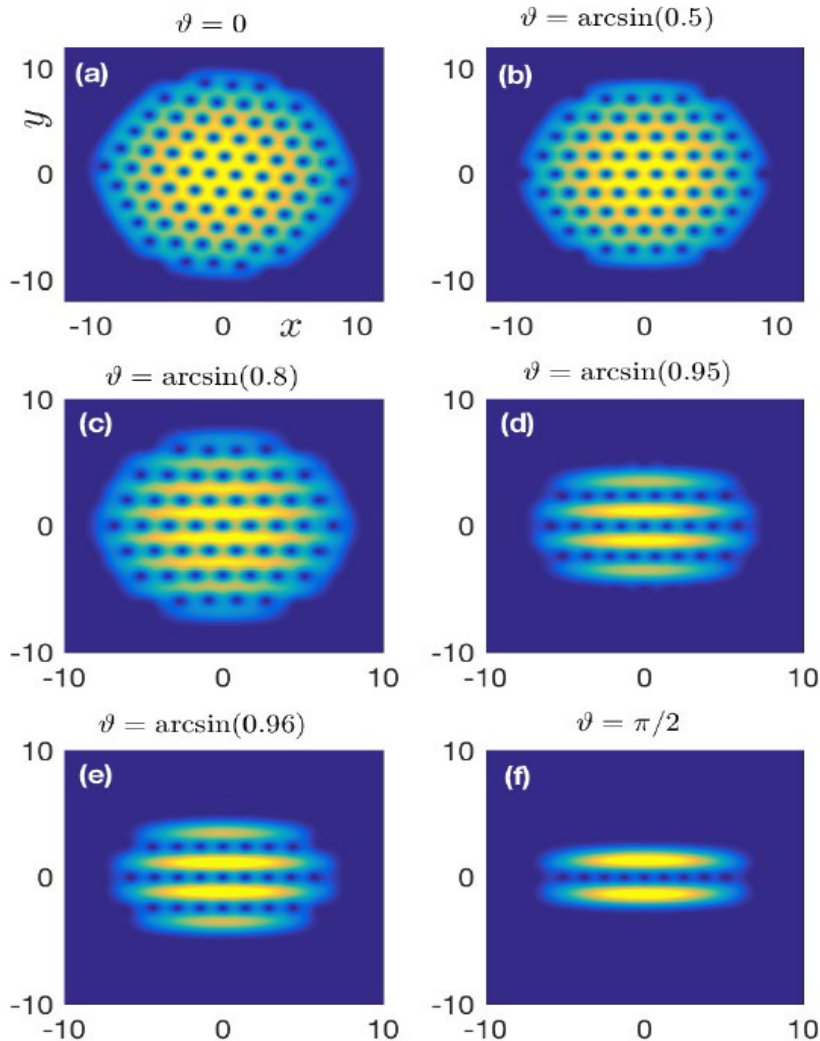


FIG. 2. (Color online) Density of a rotating dipolar BEC around the critical rotation frequency  $\Omega_c$  for fixed  $\gamma = 10$ ,  $g = 250$ ,  $g_d = 200$ , different polarization axis  $\mathbf{n} = (\sin \vartheta, 0, \cos \vartheta)$  ( $\vartheta = 0$  left panel (a),(b);  $\vartheta = \pi/4$  middle panel (c), (d);  $\vartheta = \pi/2$  right panel, (e),(f)). The rotational critical rotational frequency  $\Omega_c$  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.

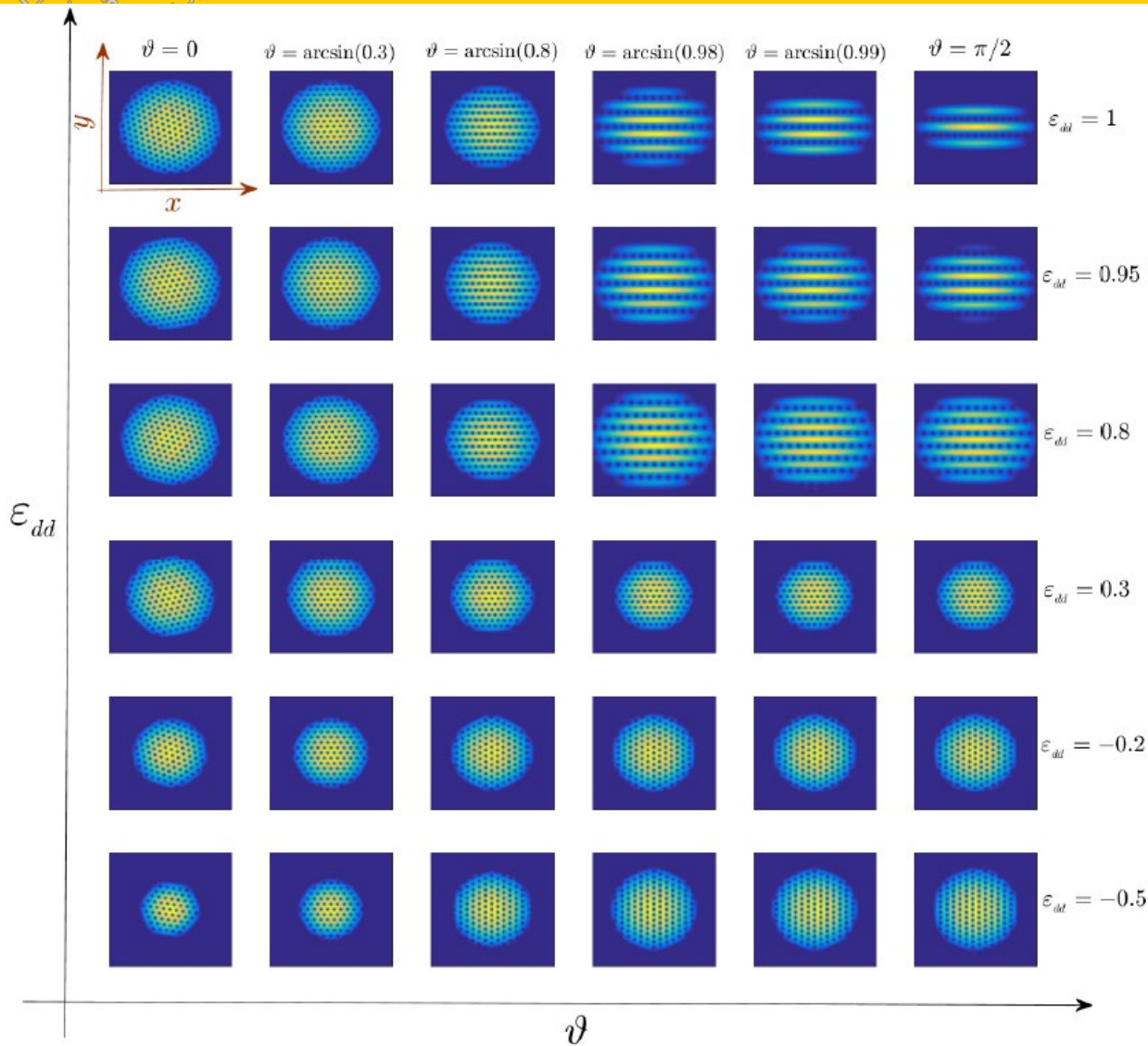
Y. Cai, Y. Yuan, M. Rosenkranz, H. Pu and W. Bao, Vortex patterns and the critical rotational frequency in rotating dipolar Bose-Einstein condensates, Phys. Rev. A, Vol. 98 (2018), article 023610


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



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# Impurities Bound by Vortex lattice

PRL 116, 240402 (2016)

PHYSICAL REVIEW LETTERS

week ending  
17 JUNE 2016

## Hubbard Model for Atomic Impurities Bound by the Vortex Lattice of a Rotating Bose-Einstein Condensate

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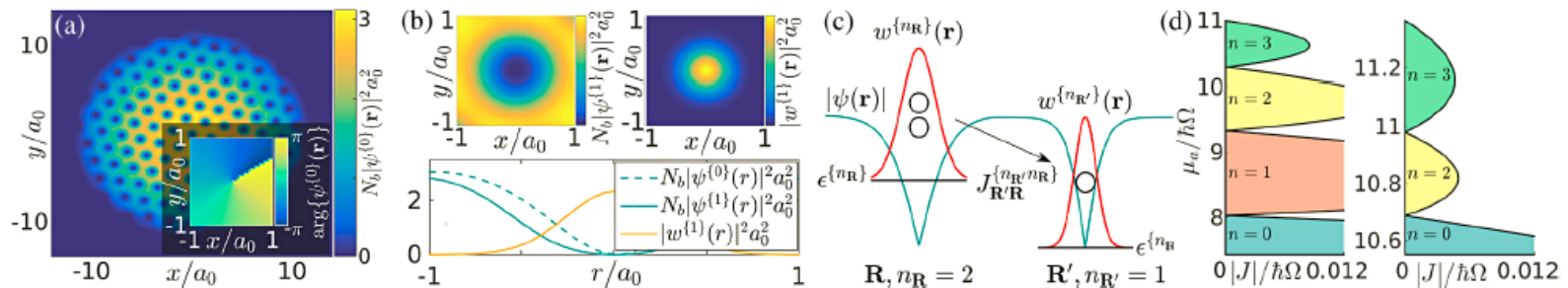
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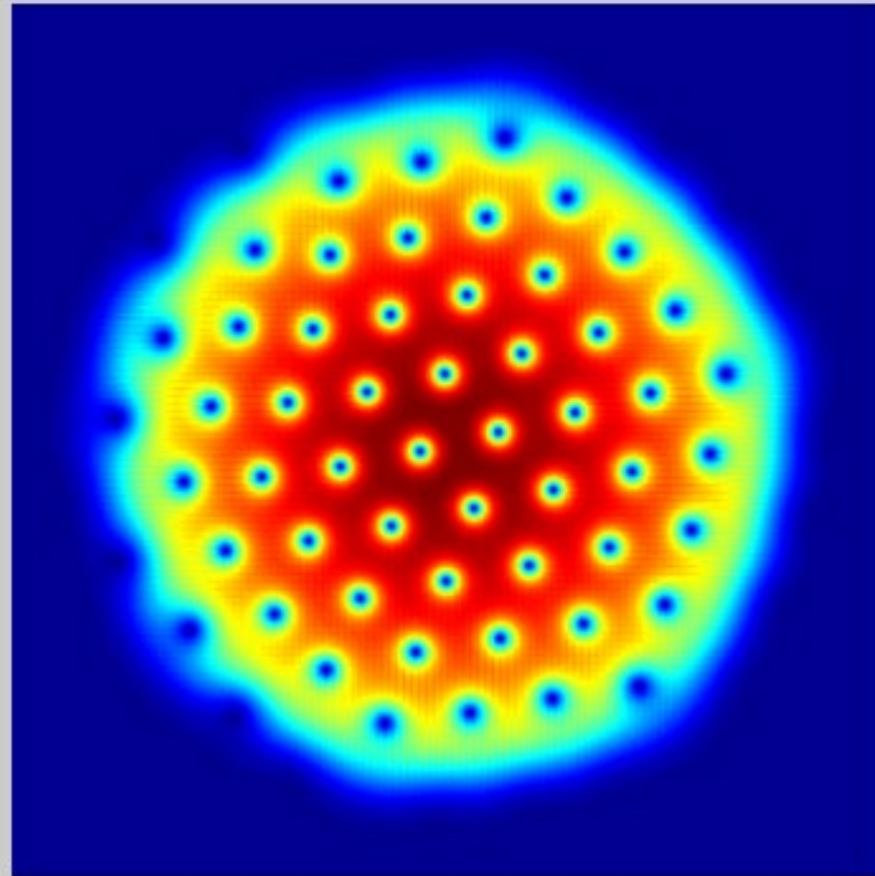
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We investigate cold bosonic impurity atoms trapped in a vortex lattice formed by condensed bosons of another species. We describe the dynamics of the impurities by a bosonic Hubbard model containing occupation-dependent parameters to capture the effects of strong impurity-impurity interactions. These



# Dynamics of a rotating dipolar BEC



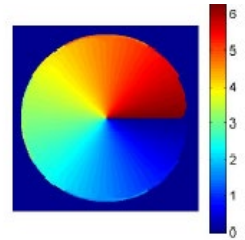
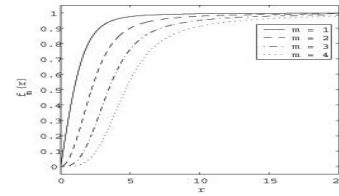


# Reduced Dynamic Laws of Quantized Vortices

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

- With initial condition

$$\psi(\vec{x}, 0) = \psi_0^\varepsilon(\vec{x}) \rightarrow \prod_{j=1}^N \phi_{m_j}(\vec{x} - \vec{x}_j^0) = \prod_{j=1}^N \phi_{m_j}(x - x_j^0, y - y_j^0)$$



- Reduced dynamical laws as  $\varepsilon \rightarrow 0$

$$\frac{d \vec{x}_j(t)}{dt} = 2 \sum_{l=1, l \neq j}^N m_l \frac{J(\vec{x}_j(t) - \vec{x}_l(t))}{|\vec{x}_j(t) - \vec{x}_l(t)|^2}, \quad t \geq 0, \quad \vec{x}_j(0) = \vec{x}_j^0, \quad 1 \leq j \leq N$$

$$J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

- Global well-posedness ??
- Numerical challenges when  $N \gg 1$  & some  $m_l = 1$  and some  $m_l = -1$
- **Mean field model when  $N \rightarrow \infty$  ???**

# 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!!
- Quantized vortex lattice pattern & dynamics --- kinetic models