Dimension reduction for dipolar Gross-Pitaevskii equations

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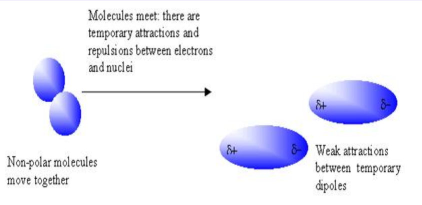
May 2013, CSCAMM

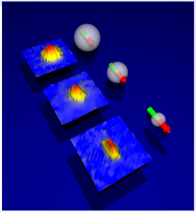
Dipolar Bose-Einstein Condensate

Experimental setup

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

2005@Univ. Stuttgart, Germany with Chroimum (Cr52)
2011@ Stanford with Dysprosium (Dy164)
2012@ Innsbruck, Austria with Erbium (Er168)





Mathematical model

- N-particle system: N-Hamiltonian system (dimensions $3N$)
- Mean-field approximation: particles described by a single wave function.
- Gross-Pitaevskii equation (GPE) for weakly interacting dilute boson gas at zero temperature

$$i\partial_t \psi = -\frac{1}{2}\Delta\psi + V(\mathbf{x})\psi + \beta|\psi|^2\psi, \quad \mathbf{x} \in \mathbb{R}^3$$

- ψ complex wave-function describing the condensates
- $V(\mathbf{x})$ real trap potential
- $\beta > 0$-defocusing (repulsive interaction); $\beta < 0$-focusing (attractive interaction)

Validity of GPE for BEC without dipole-dipole interaction

- from N-body theory for system of trapped particles to GPE theory
- time-independent GPE (R.Seiringer, E.H. Lieb and J. Yngvason PRA,2000)
- time-dependent GPE (H.T. Yau et al., Ann. Math, 2010; Xuwen Chen, ARMA 2013)

Mathematical Model for dipolar BEC

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

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

- Trapping potential: $V(\mathbf{x}) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2)$
- Interaction constants: β (short range), λ (long range)
- Dipole-dipole interaction (DDI) kernel:

$$U_{\rm dip}(\mathbf{x}) = \frac{3}{4\pi} \frac{1 - 3\frac{(\mathbf{x}\cdot\mathbf{n})^2}{|\mathbf{x}|^2}}{|\mathbf{x}|^3} = \frac{3}{4\pi} \frac{1 - 3\cos^2(\theta)}{|\mathbf{x}|^3}, \quad \mathbf{n} \text{ fixed } \& |\mathbf{n}| = 1$$

Mathematical Model

Dipolar kernel:

$$U_{\mathrm{dip}} = \frac{3}{4\pi|\mathbf{x}|^3}\left(1 - 3(\mathbf{x}\cdot\mathbf{n})^2/|\mathbf{x}|^2\right), \quad \mathbf{x} \in \mathbb{R}^3 \tag{2.1}$$

- Highly singular near **0**, $U_{\mathrm{dip}}(\mathbf{x}) = O(\frac{1}{|\mathbf{x}|^3})$
- Fourier transform: $\widehat{(U_{\mathrm{dip}})}(\xi) = -1 + \frac{3(\mathbf{n}\cdot\xi)^2}{|\xi|^2}, \quad \xi \in \mathbb{R}^3$
  - No limit at $\xi = \mathbf{0}$
  - No limit as $|\xi| \to \infty$
  - Omit the singularity at $\xi = 0$, when simulating
  - Locking phenomena in computation

Our formulation

- Identity[1]: $r = |\mathbf{x}|$, $\partial_{\mathbf{n}} = \mathbf{n} \cdot \nabla$, $\partial_{\mathbf{nn}} = \partial_{\mathbf{n}}(\partial_{\mathbf{n}})$

$$U_{\rm dip}(\mathbf{x}) = \frac{3}{4\pi r^3}\left(1 - \frac{3(\mathbf{n}\cdot\mathbf{x})^2}{r^2}\right) = -\delta(\mathbf{x}) - \partial_{\mathbf{nn}}\left(\frac{1}{4\pi r}\right) \qquad (2.2)$$

- Dipole-dipole interaction:

$$U_{\rm dip} * |\psi|^2 = -|\psi|^2 - \partial_{\mathbf{nn}}\varphi, \quad \varphi = \frac{1}{4\pi r} * |\psi|^2, \qquad (2.3)$$

$$\varphi = \frac{1}{4\pi r} * |\psi|^2 \iff -\Delta\varphi = |\psi|^2 \qquad (2.4)$$

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[1] O'Dell et al., PRL 92 (2004), 250401, Parker et al., PRA 79 (2009), 013617

Reformulation

- Gross-Pitaevskii-Poisson type equations:

$$i\partial_t\psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)|\psi|^2 - 3\lambda\partial_{\mathbf{nn}}\varphi\right]\psi,$$
$$\nabla^2\varphi(\mathbf{x},t) = -|\psi(\mathbf{x},t)|^2, \quad \lim_{|\mathbf{x}|\to\infty}\varphi(\mathbf{x},t) = 0,$$

- Energy

$$E(\psi) = \int_{\mathbb{R}^3}\left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + \frac{\beta-\lambda}{2}|\psi|^4 + \frac{3\lambda}{2}|\partial_{\mathbf{n}}\nabla\varphi|^2\right]d\mathbf{x}$$

Ground States

- Nonconvex minimization problem

$$E(\phi_g) = \min_{\phi \in S} E(\phi), \quad S = \left\{ \phi \big| \|\phi\|_2 = 1,\ E(\phi) < \infty \right\}$$

- Nonlinear Eigenvalue problem (Euler-Lagrange eq.)

$$\mu\phi = \left[-\frac{1}{2}\Delta + V(\mathbf{x}) + (\beta - \lambda)|\phi|^2 - 3\lambda\partial_{\mathbf{nn}}\varphi \right] \phi$$

$$-\Delta\varphi = |\phi|^2, \qquad \lim_{|\mathbf{x}|\to\infty} \varphi(\mathbf{x}) = 0, \qquad \|\phi\|_2 = 1$$

- Chemical potential μ:

$$\mu = \int_{\mathbb{R}^3} \left[\frac{1}{2}|\nabla\psi|^2 + V(\mathbf{x})|\psi|^2 + (\beta - \lambda)|\psi|^4 + 3\lambda|\partial_{\mathbf{n}}\nabla\varphi|^2 \right] d\mathbf{x}$$

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

Ground state results

Theorem

(Bao, Cai & Wang, JCP, 10') Assume

$$V(\mathbf{x}) \geq 0, \quad \mathbf{x} \in \mathbb{R}^3, \text{ and } \lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = \infty (\text{confining potential})$$

- *Results*
  - *Existence of ground state* $\phi_g \in S$ *if* $\beta \geq 0$, $\frac{-\beta}{2} \leq \lambda \leq \beta$
  - *Positive ground state is unique,* $\phi_g = e^{i\theta_0}|\phi_g|$, $\theta_0 \in \mathbb{R}$
  - *Nonexistence of ground states, i.e.* $\liminf_{\phi \in S} E(\phi) = -\infty$
    - $\beta < 0$
    - $\beta \geq 0$ *and* $\lambda < -\frac{\beta}{2}$ *or* $\lambda > \beta$

Numerical method for ground state

- Gradient flow with discrete normalization (imaginary time):

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

$$\nabla^2\varphi(\mathbf{x},t) = -|\phi(\mathbf{x},t)|^2, \qquad \mathbf{x}\in\Omega, \quad t_n \le t < t_{n+1},$$

$$\phi(\mathbf{x},t_{n+1}) := \phi(\mathbf{x},t_{n+1}^+) = \frac{\phi(\mathbf{x},t_{n+1}^-)}{\|\phi(\cdot,t_{n+1}^-)\|_2}, \qquad \mathbf{x}\in\Omega, \quad n\ge 0,$$

$$\phi(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = \varphi(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = 0,\ t\ge 0; \phi(\mathbf{x},0) = \phi_0(\mathbf{x}), \text{with } \|\phi_0\|_2 = 1$$

- Full discretization
  - Backward Euler sine pseudospectral (BESP) method
  - Avoid zero-mode in phase space by using DST

DST vs FFT

- Evaluate $E_{\rm dip}(\phi) = \frac{\lambda}{2}\int_{\mathbb{R}^3}\left(U_{\rm dip} * |\phi|^2\right)|\phi|^2\, d\mathbf{x}$ via DST and FFT for $\phi := \phi(\mathbf{x}) = \pi^{-3/4}\gamma_x^{1/2}\gamma_z^{1/4}e^{-\frac{1}{2}\left(\gamma_x(x^2+y^2)+\gamma_z z^2\right)}$, $\mathbf{x}\in\mathbb{R}^3$
  - Case I: $\gamma_x = 0.25$, $\gamma_z = 1$
  - Case II:$\gamma_x = \gamma_z = 1$
  - Case III: $\gamma_x = 2$, $\gamma_z = 1$

Case I		Case II		Case III	
DST	DFT	DST	DFT	DST	DFT
2.756E-2	2.756E-2	3.555E-18	1.279E-4	0.1018	0.1020
1.629E-3	1.614E-3	9.154E-18	1.278E-4	9.788E-5	2.269E-4
1.243E-7	1.588E-5	7.454E-17	1.278E-4	6.406E-7	1.284E-4

Table: Errors, mesh size $h = 1, 0.5, 0.25$ from top to bottom

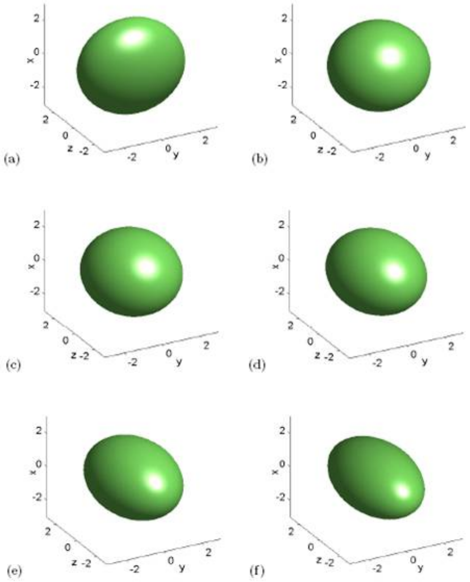


Figure 2: Isosurface plots of the ground state $|\phi_g(\mathbf{x})| = 0.08$ of a dipolar BEC with the harmonic potential $V(\mathbf{x}) = \frac{1}{2}(x^2 + y^2 + z^2)$ and $\beta = 207.16$ for different values of $\frac{\lambda}{\beta}$: (a) $\frac{\lambda}{\beta} = -0.5$; (b) $\frac{\lambda}{\beta}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

Dynamics

- The problem

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

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

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

- Mathematical question: Existence and uniqueness
- Existing results
  - Carles, Markowich & Sparber, Nonlinearity, 21 (2008)
  - Antonelli & Sparber, Physica D (2010)

Well-posedness Results

Theorem

- *Energy space:*
  - $\psi_0 \in X = \left\{ u \in H^1(\mathbb{R}^3) \middle| \|u\|_X^2 = \|\nabla u\|_2^2 + \|u\|_2^2 + \int_{\mathbb{R}^d} V(\mathbf{x})|u|^2 \, d\mathbf{x} < \infty \right\}$
- *Results:*
  - *Local existence,* $\exists T \in (0, \infty]$ *such that problem has a unique solution* $\psi \in C((0, T], X)$
  - *If* $\beta \geq 0$ *and* $-\frac{\beta}{2} \leq \lambda \leq \beta$, *global existence,* $T = \infty$

Dipolar GPE in reduced dimensions

Dimension reduction

• Dimension reduction, i.e. 3D $\longrightarrow$ 2D or 1D (Cai, Rosenkranz, Bao, Lei, PRA, 10')

$$V(\mathbf{x}) = \frac{1}{2}\left(\gamma_r^2(x^2+y^2)+\gamma_z^2 z^2\right), \quad \mathbf{x}=(x,y,z)\in\mathbb{R}^3$$

- $\gamma = \gamma_r/\gamma_z \ll 1$, Disk-shaped BEC, 3D to 2D
- $\gamma = \gamma_r/\gamma_z \gg 1$, Cigar-shaped BEC, 3D to 1D

Quasi-2D dipolar GPE

- Assumption: $V(x,y,z) = V_r(x,y) + \frac{\gamma_z^2}{2} z^2$ ($\gamma = \gamma_r/\gamma_z \ll 1$, $\gamma_r = 1$)
- Ansatz: $\psi(\cdot, t) \approx e^{-\frac{it}{2\gamma}} \phi(x,y,t) w_\gamma(z)$, $w_\gamma(z) = \frac{1}{(\gamma\pi)^{1/4}} e^{-\frac{z^2}{2\gamma}}$
- Substitute the ansatz into dipolar GPE, multiplying both sides by $w_\gamma(z)$ and integrating over z

Quasi-2D dipolar GPE

- Quasi-2D equation:

$$i\partial_t\phi = \left[-\frac{1}{2}\Delta + V_r + \beta_{2D}|\phi|^2 - \frac{3\lambda}{2}(\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} - n_z^2\Delta)\varphi^{2D}\right]\phi,$$

where $\beta_{2D} = \frac{\beta-\lambda+3\lambda n_z^2}{\sqrt{2\gamma\pi}}$, $\mathbf{x} = (x,y)^T$, $\mathbf{n}_\perp = (n_x, n_y)^T$, $\partial_{\mathbf{n}_\perp} = \mathbf{n}_\perp \cdot \nabla$, $\partial_{\mathbf{n}_\perp\mathbf{n}_\perp} = \partial_{\mathbf{n}_\perp}(\partial_{\mathbf{n}_\perp})$, $\Delta = \partial_{xx} + \partial_{yy}$ and

$$\varphi^{2D}(\mathbf{x},t) = U_\gamma^{2D} * |\phi|^2, \quad U_\gamma^{2D}(\mathbf{x}) = \frac{1}{2\sqrt{2}\pi^{3/2}}\int_{\mathbb{R}} \frac{e^{-s^2/2}}{\sqrt{|\mathbf{x}|^2 + \gamma s^2}}\,ds.$$

- As $\gamma \to 0^+$, $\varphi^{2D} \approx (-\Delta)^{-1/2}|\phi|^2$

Properties of $U_\gamma^{2D}(\mathbf{x})$

- $r = |\mathbf{x}|$

$$U_\gamma^{2D}(r) \approx \frac{1}{\sqrt{2\gamma}\pi^{3/2}}\left[-\ln r + \ln 2\sqrt{\gamma} + C\right], \text{ near } r = 0,$$
$$U_\gamma^{2D}(r) \approx \frac{1}{2\pi r}, \quad \text{as } r \to \infty$$

- $\widehat{U_\gamma^{2D}}(|\xi|) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{e^{-\frac{\gamma\xi_3^2}{2}}}{|\xi|^2+\xi_3^2} d\xi_3$

$$\widehat{U_\gamma^{2D}}(|\xi|) \approx \frac{1}{|\xi|}, \text{ near } \xi = 0;$$
$$\widehat{U_\gamma^{2D}}(|\xi|) \approx \sqrt{\frac{2\gamma}{\pi}} \cdot \frac{1}{|\xi|^2}, \quad \text{as } |\xi| \to \infty.$$

Cauchy problem for 2D dipolar GPE

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

Theorem

(Bao, Ben Abdallah & Cai, SIMA, 12') Energy space

$$X = \left\{\phi \in H^1(\mathbb{R}^2) \Big| \int_{\mathbb{R}^2} |\mathbf{x}|^2|\phi(\mathbf{x})|^2\, d\mathbf{x} < \infty\right\}$$

- *local well-posedness:* $\exists$ *a unique solution* $\phi(\mathbf{x},t) \in C\left([0,T), X\right)$
- *global well-posedness*
  - $\lambda \geq 0$ *and* $\beta - \lambda > -\sqrt{2\pi}C_b\sqrt{\gamma}$;
  - $\lambda < 0$ *and* $\beta + \frac{1}{2}(1+3|2n_z^2-1|)\lambda > -\sqrt{2\pi}C_b\sqrt{\gamma}$.

Ground state of the 2D equation

- $$E_{2D}(\Phi) = \int_{\mathbb{R}^2} \left[\frac{1}{2}|\nabla\Phi|^2 + V_r(\mathbf{x})|\Phi|^2 + \beta_{2D}|\Phi|^4 - \frac{3\lambda}{4}|\Phi|^2 \widetilde{\varphi^{2D}} \right] d\mathbf{x}$$

  where $\beta_{2D} = \frac{\beta - \lambda + 3n_z^2\lambda}{2\sqrt{2\pi\gamma}}$

  $$\widetilde{\varphi^{2D}} = \left(\partial_{\mathbf{n}_\perp \mathbf{n}_\perp} - n_z^2 \Delta\right) \varphi^{2D}, \qquad \varphi^{2D} = U_\gamma^{2D} * |\Phi|^2.$$

- Ground state

  $$\min E_{2D}(\Phi) \textit{ subject to } \|\Phi\|_{L^2} = 1 \textit{ and } E_{2D}(\Phi) < \infty.$$

continued

Theorem

$V_r(x,y) = \frac{1}{2}(x^2+y^2)$, then

(i) $\exists$ a ground state $\Phi_g \in X$ if

- $\lambda \geq 0$ *and* $\beta - \lambda > -\sqrt{2\pi} C_b \sqrt{\gamma}$;
- $\lambda < 0$ *and* $\beta + \frac{1}{2}(1+3|2n_z^2-1|)\lambda > -\sqrt{2\pi} C_b \sqrt{\gamma}$.

(ii) $\Phi_g = e^{i\theta}|\Phi_g|$ ($\theta \in \mathbb{R}$). the positive ground state $|\Phi_g|$ is unique if :

- $\lambda \geq 0$ *and* $\beta - \lambda \geq 0$;
- $\lambda < 0$ *and* $\beta + \frac{1}{2}(1+3|2n_z^2-1|)\lambda \geq 0$.

(iii) If $\beta + \frac{1}{2}\lambda(1-3n_z^2) < -\sqrt{2\pi} C_b \sqrt{\gamma}$, there exists no ground state of the equation

Numerical method for ground state

- Gradient flow with discrete normalization

$$\partial_t \phi(\mathbf{x}, t) = -\frac{\delta E_{2D}(\phi)}{\delta \phi}, \quad t_n \le t < t_{n+1},$$

$$\phi(\mathbf{x}, t_{n+1}) := \phi(\mathbf{x}, t_{n+1}^{+}) = \frac{\phi(\mathbf{x}, t_{n+1}^{-})}{\|\phi(\cdot, t_{n+1}^{-})\|_2}, \qquad \mathbf{x} \in \Omega, \quad n \ge 0,$$

$$\phi(\mathbf{x}, t)|_{\mathbf{x}\in\partial\Omega} = \varphi(\mathbf{x}, t)|_{\mathbf{x}\in\partial\Omega} = 0,\ t \ge 0; \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \text{with } \|\phi_0\|_2 = 1$$

- Full discretization
  - Backward Euler Fourier pseudospectral (BEFP) method
  - no singularity for zero mode

$$\left|\widehat{U_\gamma^{2D}}(\xi)\right| = \frac{1}{\pi}\left|\int_{\mathbb{R}} \frac{e^{-\gamma s^2/2}}{|\xi|^2 + s^2} ds\right| \le \frac{1}{|\xi|}, \quad \xi \in \mathbb{R}^2,$$

$$\left|\mathcal{F}\left((\partial_{\mathbf{n}_\perp \mathbf{n}_\perp} - n_z^2 \Delta) U_\gamma^{2D}\right)(\xi)\right| \to 0, \text{ as } |\xi| \to 0.$$

Convergence of the 3D GPE to 2D GPE

Theorem

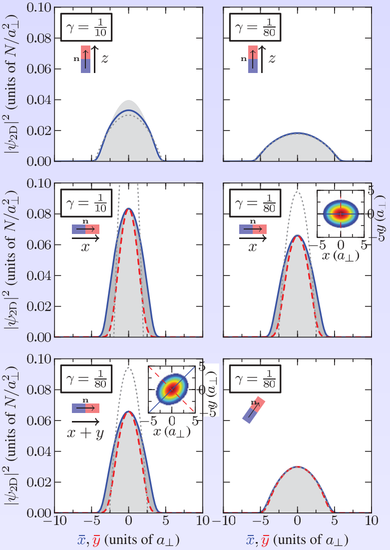
Suppose $\beta = \sqrt{\gamma}\beta_0$, $\lambda = \sqrt{\gamma}\lambda_0$, $-\frac{\beta_0}{2} \le \lambda_0 \le \beta_0$ *and* $\beta_0 \ge 0$, *let* $\psi^\gamma \in C([0,\infty); X_3)$ *and* $\phi \in C([0,\infty); X_2)$ *be the unique solutions of the 3D and 2D equations, respectively, satisfying*

$$\psi^\gamma(t=0) = \phi(t=0) w_\gamma(z),$$

then for any $T > 0$, *there exists* $C_T > 0$ *such that*

$$\left\| \psi^\gamma(x,y,z,t) - e^{-i\frac{t}{2\gamma}} \phi(x,y,t) w_\gamma(z) \right\|_{L^2(\mathbb{R}^3)} \le C_T \sqrt{\gamma}, \ \forall t \in [0, T].$$

Comparison of the ground states

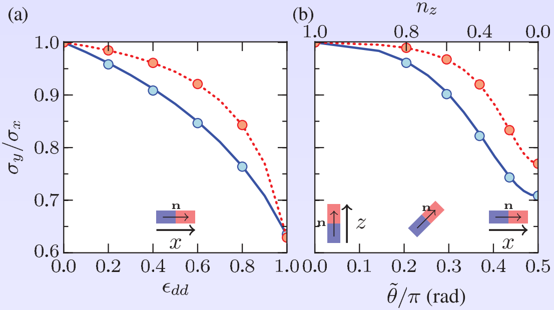


Comparison of the ground states

- Aspect ration: σ_x/σ_y

$$\sigma_\alpha = \sqrt{\int_{\mathbb{R}^d} \alpha^2 |\psi_d(\mathbf{x})|^2 \, d\mathbf{x}}, \quad \alpha = x, y$$

- $\varepsilon_{dd} = \lambda/\beta$



Dipolar GPE in 1D

- Assumption: $V(x,y,z) = \frac{z^2}{2} + \frac{\gamma^2(x^2+y^2)}{2}$ $(\gamma \gg 1)$
- Ansatz: $\psi(\cdot,t) \approx e^{-i\gamma t}\phi(z,t)w_\gamma(x,y)$,
  $w_\gamma(x,y) = \gamma^{1/2}\pi^{-1/2}e^{-\frac{x^2+y^2}{2}\gamma}$
- 1D dipolar GPE:

$$i\partial_t\phi = \left[-\frac{1}{2}\partial_{zz} + \frac{z^2}{2} + \beta_{1D}|\phi|^2 - \frac{3\lambda\sqrt{\gamma}(3n_z^2-1)}{8\sqrt{2\pi}}\partial_{zz}\varphi^{1D}\right]\phi,$$

where $\beta_{1D} = \gamma\frac{\beta+\frac{1}{2}\lambda(1-3n_z^2)}{2\pi}$,

$$\varphi^{1D}(z,t) = U_\gamma^{1D} * |\phi|^2,\ U_\gamma^{1D}(z) = \frac{\sqrt{2\gamma}e^{\gamma z^2/2}}{\sqrt{\pi}}\int_{|z|}^{\infty} e^{-\gamma s^2/2}\,ds,\ z \in \mathbb{R}.$$

Properties of $U_\gamma^{1D}(z)$

- $$U_\gamma^{1D}(z) = 1 - \sqrt{\frac{2\gamma}{\pi}}|z| + O(z^2), \quad z \text{ near } 0$$
$$U_\gamma^{1D}(z) \approx \frac{1}{\sqrt{\pi}|z|},$$

- $\widehat{U_\gamma^{1D}}(\xi) = \frac{\sqrt{2}}{\sqrt{\gamma\pi}} \int_0^\infty \frac{e^{-\frac{s}{2\gamma}}}{\xi^2+s} ds$
$$\widehat{U_\gamma^{1D}}(\xi) \approx \frac{\sqrt{2}}{\sqrt{\gamma\pi}}(-\gamma_e - 2\ln|\xi| + \ln(2\gamma)), \quad \xi \text{ near } 0$$
$$\widehat{U_\gamma^{1D}}(\xi) \approx \frac{2\sqrt{2\gamma}}{\sqrt{\pi}|\xi|^2}, \quad \text{as } \xi \to \infty.$$

- γ_e- Euler-Mascheroni constant

Cauchy problem for 1D dipolar GPE

Theorem

(Well-posedness) Energy space

$$X = \left\{ \phi \in H^1(\mathbb{R}) \middle| \int_{\mathbb{R}} |x|^2 |\phi(x)|^2 \, dx < \infty \right\}$$

- *global well-posed:* $\exists$ *a unique solution* $\phi(x, t) \in C([0, T), X)$

Energy for 1D dipolar GPE

- $$E_{1D}(\Phi) = \int_{\mathbb{R}} [\frac{|\partial_z \Phi|^2}{2} + \frac{z^2}{2}|\Phi|^2 + \frac{1}{2}\beta_{1D}|\Phi|^4 + \frac{3\lambda\sqrt{\gamma}(1-3n_z^2)}{16\sqrt{2\pi}}|\Phi|^2\varphi]dz,$$

  where $\beta_{1D} = \gamma\frac{\beta+\frac{1}{2}\lambda(1-3n_z^2)}{2\pi}$ and

  $$\varphi(z) = \partial_{zz}(U_\gamma^{1D} * |\Phi|^2).$$

- Ground state

  $$\min E_{1D}(\Phi) \text{ subject to } \|\Phi\|_{L^2} = 1 \text{ and } E_{1D}(\Phi) < \infty.$$

Ground state for 1D dipolar GPE

Theorem

For any parameter β, λ and γ, there exists a ground state of the 1D equation and the positive ground state $|\Phi_g|$ is unique under one of the following conditions:

- $\lambda(1-3n_z^2) \geq 0$ *and* $\beta - (1-3n_z^2)\lambda \geq 0$;
- $\lambda(1-3n_z^2) < 0$ *and* $\beta + \frac{\lambda}{2}(1-3n_z^2) \geq 0$.

Moreover, $\Phi_g = e^{i\theta_0}|\Phi_g|$ *for some constant* $\theta_0 \in \mathbb{R}$.

Numerical method for ground state

- Gradient flow with discrete normalization

$$\partial_t \phi(x,t) = -\frac{\delta E_{1D}(\phi)}{\delta \phi}, \quad t_n \le t < t_{n+1},$$

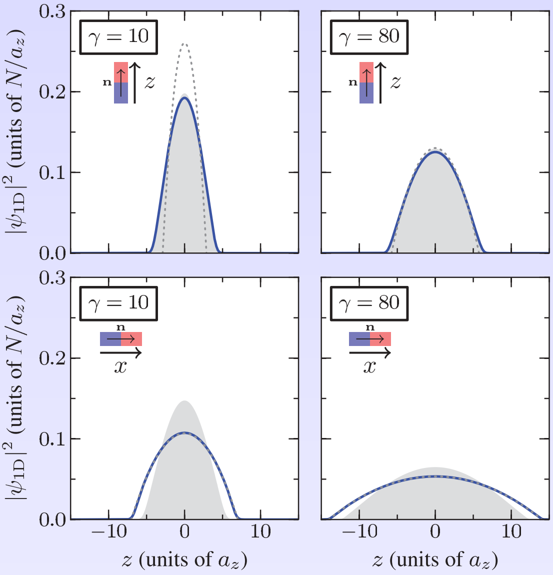
$$\phi(x, t_{n+1}) := \phi(x, t_{n+1}^+) = \frac{\phi(\mathbf{x}, t_{n+1}^-)}{\|\phi(\cdot, t_{n+1}^-)\|_2}, \qquad x \in \Omega, \quad n \ge 0,$$

$$\phi(x,t)|_{x\in\partial\Omega} = \varphi(x,t)|_{x\in\partial\Omega} = 0,\ t \ge 0; \phi(x,0) = \phi_0(x), \text{with } \|\phi_0\|_2 = 1$$

- Full discretization
  - Backward Euler Fourier pseudospectral (BEFP) method
  - no singularity for zero mode

$$\left|\widehat{\partial_{zz} U_\gamma^{1D}}(\xi)\right| \to 0, \quad \text{as } |\xi| \to 0.$$

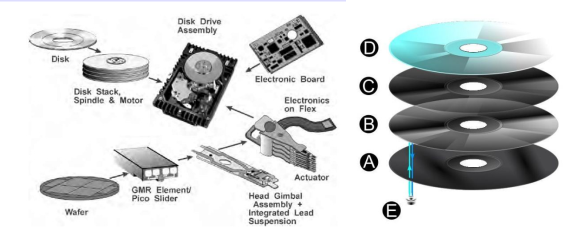
Comparison of the ground states



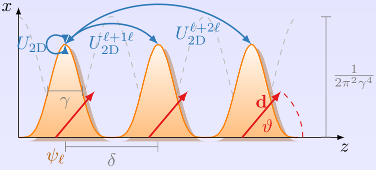
Multi-layered dipolar BEC

Layered structure

- Layered structure in daily life



- Layered dipolar BEC



Dipolar GPE

- Dipolar BEC confined in a 'transverse harmonic potential'+ 'longitude optical lattice'
- $V(x,y,z) = \frac{1}{2}(x^2+y^2) + \frac{V_0\pi^2}{2}\sin^2(\pi z)$, $\mathbf{x} = (\vec{x}, z)$, $\vec{x} = (x,y)$
- Dipolar GPE in 3D:

$$i\partial_t\psi = \left[-\frac{1}{2}\nabla^2 + V(\mathbf{x}) + (\beta-\lambda)|\psi|^2 + \lambda\varphi\right]\psi$$

$$\varphi = \partial_{\mathbf{nn}}\left(\frac{1}{-4\pi r} * |\psi|^2\right), \quad \mathbf{n} = (n_x, n_y, n_z)^T, \ |\mathbf{n}| = 1$$

Quasi-2D regime

- $V_0 \gg 1$, optical lattice approximated by a train of harmonic potentials
- the wave function separates as (Rosenkranz, Cai & Bao, preprint, 11')

$$\psi(\mathbf{x}, t) = e^{-it/2\gamma^2} \sum_{\ell} \psi_\ell(\vec{x}, t) w_\ell(z)$$

$$\gamma = V_0^{-1/4} \pi^{-1/2}$$

$$w_\ell(z) = w(z - z_\ell) = (1/\pi\gamma^2)^{1/4} e^{-(z-z_\ell)^2/2\gamma^2}$$

- the Gaussians $w_\ell(z)$ do not mutually overlap

$$\int_{\mathbb{R}} w_\ell(z) w_j(z) dz \approx 0, \quad \ell \neq j$$

Quasi-2D equation

- The 2D equation for $\psi_\ell = \psi_\ell(\vec{x}, t)$ at ℓth site ($V_{\text{ho}} = \frac{1}{2}|\vec{x}|^2$)

$$i\partial_t \psi_\ell = \left[-\frac{1}{2}\nabla^2 + V_{\text{ho}} + \frac{1}{\sqrt{2\pi}\gamma}\left[\beta - \lambda(1-3n_z^2)\right]|\psi_\ell|^2 + V_{\text{2D}}^\ell\right]\psi_\ell.$$

- potential V_{2D}^ℓ, Fourier transform $\widehat{V_{\text{2D}}^\ell}(\mathbf{k})$, $\mathbf{k} = k(\cos\varphi, \sin\varphi)$

$$\hat{V}_{\text{2D}}^\ell(\mathbf{k}) = 3\lambda \sum_j \Big(\left[(n_x\cos\varphi + n_y\sin\varphi)^2 - n_z^2\right]\widehat{U}_{\text{even}}^{j\ell}(k) + 2in_z(n_x\cos\varphi + n_y\sin\varphi)\widehat{U}_{\text{odd}}^{j\ell}(k)\Big)\widehat{|\psi_j|^2}(\mathbf{k}).$$

- $\delta_{\ell j} = \ell - j$, $\eta(s) = \exp(s^2)\text{erfc}(s)$, $\text{erfc}(s) = 1 - \text{erf}(s)$

$$\hat{U}_{\text{even}}^{j\ell}(k) = \frac{k}{4}e^{-\frac{\delta_{\ell j}^2}{2\gamma^2}}\left[\eta\left(\frac{\gamma^2 k + \delta_{\ell j}}{\sqrt{2}\gamma}\right) + \eta\left(\frac{\gamma^2 k - \delta_{\ell j}}{\sqrt{2}\gamma}\right)\right],$$

$$\hat{U}_{\text{odd}}^{j\ell}(k) = \frac{k}{4}e^{-\frac{\delta_{\ell j}^2}{2\gamma^2}}\left[\eta\left(\frac{\gamma^2 k + \delta_{\ell j}}{\sqrt{2}\gamma}\right) - \eta\left(\frac{\gamma^2 k - \delta_{\ell j}}{\sqrt{2}\gamma}\right)\right],$$

$\widehat{V_{2D}}$ decomposition

- separate $l = j$ (intralayer) and $l \neq j$ (interlayer)

$$\hat{V}_{2\mathrm{D}}^{\ell}(\mathbf{k}) = 3\beta[(n_x\cos\varphi + n_y\sin\varphi)^2 - n_z^2]\widehat{U}_{2\mathrm{D}}(k)\widehat{|\psi_\ell|^2}(\mathbf{k}) + 3\lambda\sum_{j\neq\ell}[n_x\cos\varphi + n_y\sin\varphi - in_z\mathrm{sign}(\delta_{\ell j})]^2 \times \hat{U}_{2\mathrm{D}}^{j\ell}(k)\widehat{|\psi_j|^2}(\mathbf{k}),$$

- $\hat{U}_{2\mathrm{D}} = 2\hat{U}_{2\mathrm{D}}^{00}$ and

$$\hat{U}_{2\mathrm{D}}^{j\ell}(k) = \frac{k}{4}e^{-\frac{\delta_{\ell j}^2}{2\gamma^2}}\eta\left(\frac{\gamma^2 k - |\delta_{\ell j}|}{\sqrt{2}\gamma}\right).$$

- if $\gamma \ll 1$

$$\hat{U}_{2\mathrm{D}}^{j\ell}(k) \simeq \frac{k}{2}e^{-|\delta_{\ell j}|k} \quad (\ell \neq j).$$

Single mode approximation

- If we assume that the the BEC densities in each layer vary little over the central sites, we can simplify the 2D model to a equation for the central site wave function $\psi_0(\vec{x}, t)$
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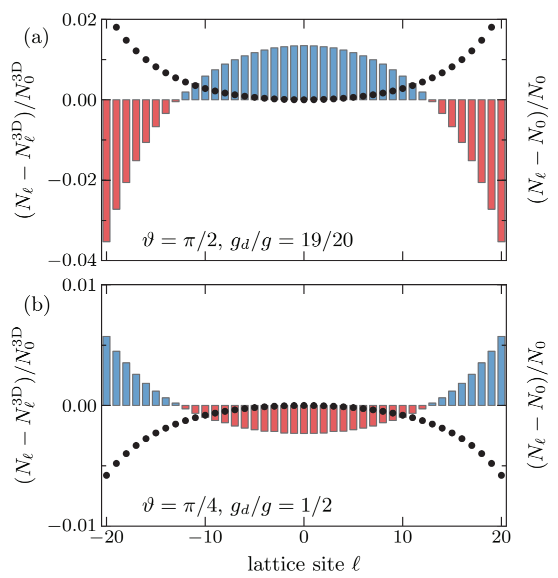
$$i\partial_t\psi_0 = \left[-\frac{1}{2}\nabla^2 + V_{\text{ho}} + \frac{1}{\sqrt{2\pi}\gamma}\left[\beta - \lambda\left(1 - 3n_z^2\right)\right]|\psi_0|^2 + V_{\text{2D}}\right]\psi_0$$

$$\begin{aligned}\hat{V}_{\text{2D}}(\mathbf{k}) = 3\beta\Big(&[(n_x\cos\varphi + n_y\sin\varphi)^2 - n_z^2]\hat{U}_{\text{2D}}(k)\\ &+ \sum_{j\neq 0}[n_x\cos\varphi + n_y\sin\varphi - in_z\text{sign}(\delta_{0j})]^2\,\hat{U}_{\text{2D}}^{j0}(k)\Big)\\ &\times \widehat{|\psi_0|^2}(\mathbf{k}).\end{aligned}$$

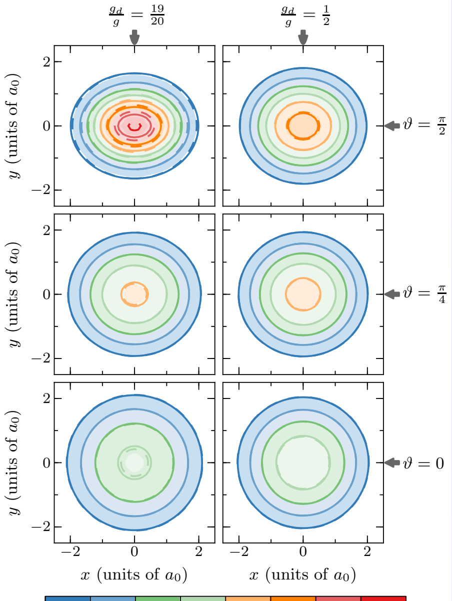
Numerical methods for ground states

- For both 3D and 2D models, using gradient flow with discrete normalization
- For 3D GPE, the wave function vanishes at the boundary, backward Euler Sine pseudospectral
- For 2D model, backward Euler Fourier pseudospectral
- $\mathbf{n} = (\sin\vartheta, 0, \cos\vartheta)^T$

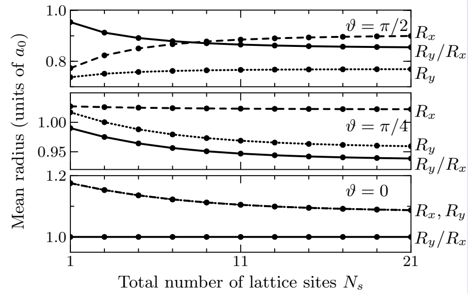
Comparison-particle number difference



Central site density difference



Mean-radius vs site number



Conclusion

- Dipolar Gross-Pitaevskii equations in reduced dimensions (1D, 2D)
- Ground state and Cauchy problem for the 1D and 2D equations
- Model for multi-layered dipolar Bose-Einstein condensate
- Efficient numerical implementation and good agreement

THANK YOU !