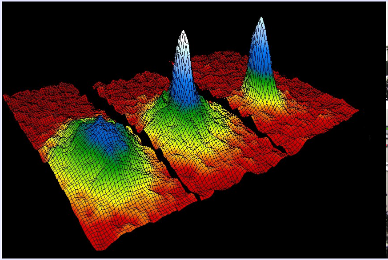
Ground states of spinor Bose-Einstein condensate

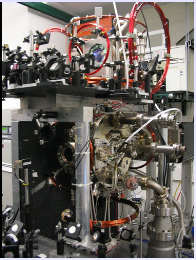
Yongyong Cai
Beijing Computational Science Research Center
joint with Weizhu Bao, W. Liu, Z. Wen, X. Wu, H. Tian
L. Wen, W. M. Liu, J. M. Zhang, and J. Hu

IMS, NUS, Oct. 4, 2019

Bose-Einstein Condensation

- Bose-Einstein condensation (BEC) is a state where the bosons collapse into the lowest quantum state near temperature absolute zero.
- Predicted by Satyendra Nath Bose and Albert Einstein in 1924-1925
- First experiments in 1995, *Science 269 (E. Cornell and C. Wieman et al., ^{87}Rb JILA), PRL 75 (Ketterle et al., ^{23}Na MIT) and PRL 75 (Hulet et al., ^{7}Li Rice).*



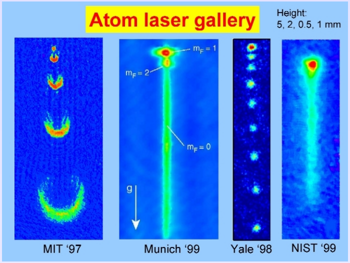


Spinor condensates

- Magnetic trap:
  - internal degree of freedom frozen
  - scalar order parameter
- Optical trap:
  - internal degree of freedom released
  - allow different angular momentum
  - magnetism and superfluidity
  - spin-F BEC, $2F+1$ hyperfine states, vector order parameter

Pseudo spin-1/2 BEC

- Binary BEC can be used as a model producing coherent atomic beams (*J. Schneider, Appl. Phys. B, 69 (1999)*)
- First experiment concerning with the binary BEC was performed in JILA with with $|F=2, m_f=2\rangle$ and $|1,-1\rangle$ spin states of ^{87}Rb. (*C. J. Myatt et al.,Phys. Rev. Lett., 78 (1997)*)



Spin-orbit coupling in spin-1/2

- Interaction of a particle's spin with its motion
- fine structure of Hydrogen
- Electron: orbital angular momentum (generates magnetic field), interacts with the electron spin magnetic moment (internal Zeeman effect)
- Crucial for quantum-Hall effects, topological insulators
- Major experimental breakthrough in 2011, Lin et al. have created a SO coupled BEC, ^{85}Rb: $|\uparrow\rangle = |F = 1, m_f = 0\rangle$ and $|\downarrow\rangle = |F = 1, m_f = -1\rangle$.
- SO coupling in cold atoms have been hot topics in recent years

spin-1/2 BEC

- Coupled Gross-Pitaevskii equations (re-scaled):

$\Psi := (\psi_1(\mathbf{x}, t), \psi_2(\mathbf{x}, t))^T$, $\mathbf{x} \in \mathbb{R}^d$ in d dimensional spaces

$$i\partial_t\psi_1 = \left[-\frac{1}{2}\nabla^2 + V_1 + \frac{\delta}{2} + (\beta_{11}|\psi_1|^2 + \beta_{12}|\psi_2|^2)\right]\psi_1 + \frac{\Omega}{2}\psi_2,$$
$$i\partial_t\psi_2 = \left[-\frac{1}{2}\nabla^2 + V_2 - \frac{\delta}{2} + (\beta_{21}|\psi_1|^2 + \beta_{22}|\psi_2|^2)\right]\psi_2 + \frac{\Omega}{2}\psi_1,$$

- Trapping potential: $V_j(\mathbf{x}) = \frac{1}{2}(\gamma_x^2x^2 + \gamma_y^2y^2 + \gamma_z^2z^2)$ $(j = 1, 2)$ for 3D case
- Interaction constants: β_{jl} between j-th and l-th component (positive for repulsive and negative for attractive)
- Ω: Rabi frequency (internal Josephson junction)
- δ: detuning constant for Raman transition

Conserved quantities

- Mass:

$$N(t) := \|\Psi(\cdot,t)\|^2 = \int_{\mathbb{R}^d} [|\psi_1(\mathbf{x},t)|^2 + |\psi_2(\mathbf{x},t)|^2] d\mathbf{x} \equiv N(0) = 1,$$

- Energy per particle

$$E(\Psi) = \int_{\mathbb{R}^d} \Bigg[\sum_{j=1}^{2} \left(\frac{1}{2}|\nabla\psi_j|^2 + V_j(\mathbf{x})|\psi_j|^2 \right) + \frac{\delta}{2}\left(|\psi_1|^2 - |\psi_2|^2\right)$$
$$+ \Omega \,\mathrm{Re}(\psi_1\overline{\psi}_2) + \frac{\beta_{11}}{2}|\psi_1|^4 + \frac{\beta_{22}}{2}|\psi_2|^4 + \beta_{12}|\psi_1|^2|\psi_2|^2 \Bigg] d\mathbf{x}$$

- Ground state patterns

Ground States

- Nonconvex minimization problem

$$E_g := E\left(\Phi_g\right) = \min_{\Phi \in S} E\left(\Phi\right),$$

and

$$S := \left\{ \Phi = (\phi_1, \phi_2)^T \in H^1(\mathbb{R}^d)^2 \mid \|\Phi\|^2 = 1, E(\Phi) < \infty \right\}$$

- Nonlinear Eigenvalue problem (Euler-Lagrange eq.)

$$\mu\phi_1 = \left[-\frac{1}{2}\nabla^2 + V_1(\mathbf{x}) + \frac{\delta}{2} + (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2) \right] \phi_1 + \frac{\Omega}{2}\phi_2,$$
$$\mu\phi_2 = \left[-\frac{1}{2}\nabla^2 + V_2(\mathbf{x}) - \frac{\delta}{2} + (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2) \right] \phi_2 + \frac{\Omega}{2}\phi_1,$$

- Chemical potential μ:

$$\mu = \mu = E(\Phi) + \int_{\mathbb{R}^d} \left(\frac{\beta_{11}}{2}|\phi_1|^4 + \frac{\beta_{22}}{2}|\phi_2|^4 + \beta_{12}|\phi_1|^2|\phi_2|^2 \right) d\mathbf{x}.$$

Theorem

Under condition $\lim_{|x|\to\infty} V(x) = \infty$, $\begin{pmatrix} \beta_{11} & \beta_{12} \\ \beta_{12} & \beta_{22} \end{pmatrix}$ *is positive definite.* *There exists minimizers, i.e., the ground state* (ψ_1^g, ψ_2^g) *exists, and* $(|\psi_1^g|, |\psi_2^g|)$ *is unique. Moreover,* $(\psi_1^g, \psi_2^g) = (e^{i\theta_1}|\psi_1^g|, e^{i\theta_2|}\psi_2^g|)$, *where*

- *if* $\Omega > 0$, $\theta_1 - \theta_2 = \pm\pi$
- *if* $\Omega < 0$, $\theta_1 - \theta_2 = 0$

Limiting behavior

Theorem

Let (ϕ_1^g, ϕ_2^g) *be the ground state of CGPEs. As* $\Omega \to -\infty$*, we have*

$$\phi_1^g - \phi_2^g \to 0, \quad j = 1, 2.$$

Theorem

Let (ϕ_1^g, ϕ_2^g) *be the ground state of CGPEs. As* $\delta \to -\infty$*, we have*

$$\phi_2^g \to 0.$$

Gradient Flow Discrete Normalized (GFDN)

• Numerical methods for computing the ground state (W. Bao& Q. Du 2004; W. Bao, Z. Wen & X. Wu 2017; I. Danaila& P. Kazemi 2010; X. Antoine, A. Levitt& Q. Tang 2016)

$$\begin{cases} \frac{\partial \phi_1}{\partial t} = \frac{1}{2}\Delta\phi_1 - V(x)\phi_1 - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\phi_1 - \lambda\phi_2 \\ \qquad - \delta\phi_1, \quad t_n < t < t_{n+1}, \\ \frac{\partial \phi_2}{\partial t} = \frac{1}{2}\Delta\phi_2 - V(x)\phi_2 - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\phi_2 - \lambda\phi_1, \\ \qquad\qquad t_n < t < t_{n+1}, \\ \phi_1(x, t_{n+1}) \triangleq \phi_1(x, t_{n+1}^+) = \frac{\phi_1(x, t_{n+1}^-)}{(\|\phi_1(\cdot, t_{n+1}^-)\|_2^2 + \|\phi_2(\cdot, t_{n+1}^-)\|_2^2)^{1/2}}, \\ \phi_2(x, t_{n+1}) \triangleq \phi_2(x, t_{n+1}^+) = \frac{\phi_2(x, t_{n+1}^-)}{(\|\phi_1(\cdot, t_{n+1}^-)\|_2^2 + \|\phi_2(\cdot, t_{n+1}^-)\|_2^2)^{1/2}} \\ \phi_1(x, 0) = \phi_1^0(x), \quad \phi_2(x, 0) = \phi_2^0(x). \end{cases}$$

$$\phi_{1,2}(x, t_n^\pm) = \lim_{t \to t_n^\pm} \phi_{1,2}(x, t) \ \|\phi_1^0\|_2^2 + \|\phi_2^0\|_2^2 = 1$$

DNGF Continued

- Step 1: Apply steepest descent method to unconstrained problem
- Step 2: Project back to satisfy the constraint

Remark: On the projection step, how to determine the projection parameter.

Continuous Normalized Gradient Flow

DNGF is a splitting scheme for

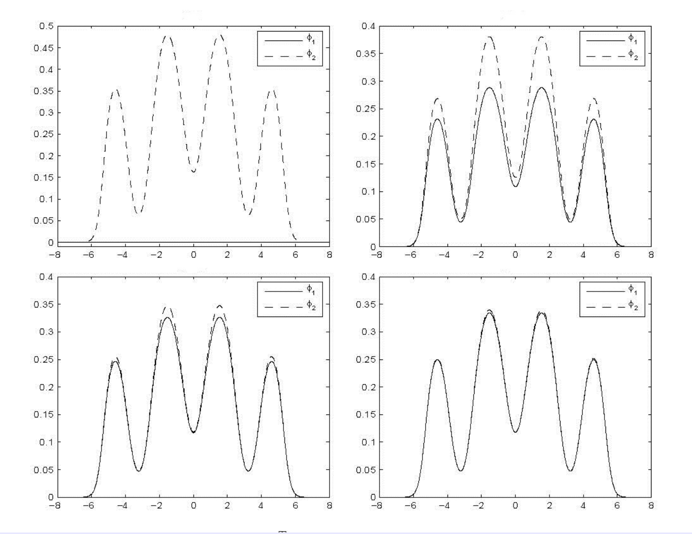
$$\begin{cases} \frac{\partial \phi_1}{\partial t} = \frac{1}{2}\Delta\phi_1 - V(x)\phi_1 - (\beta_{11}|\phi_1|^2 + \beta_{12}|\phi_2|^2)\phi_1 \\ \qquad - \lambda\phi_2 - \delta\phi_1 + \mu(\phi_1, \phi_2, t)\phi_1, \\ \frac{\partial \phi_2}{\partial t} = \frac{1}{2}\Delta\phi_2 - V(x)\phi_2 - (\beta_{12}|\phi_1|^2 + \beta_{22}|\phi_2|^2)\phi_2 \\ \qquad - \lambda\phi_1 + \mu(\phi_1, \phi_2, t)\phi_2, \end{cases}$$

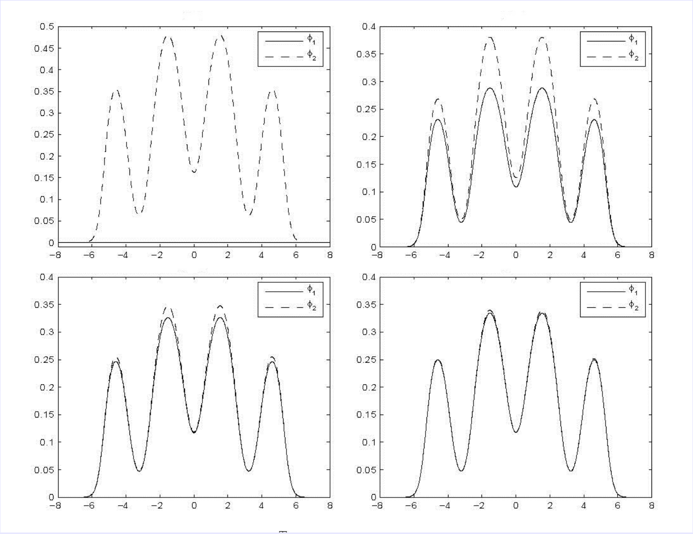
by choosing $\mu(\phi_1, \phi_2, t)$ properly

- $$\int |\Phi(x,t)|^2 \, dx = \int |\Phi(x,0)|^2 \, dx$$
- $$E(\Phi(\cdot, t_2)) \leq E(\Phi(\cdot, t_1)), \quad t_1 < t_2,$$

projection step is equivalent to solve

$$\partial_t \phi_j = \mu(\phi_1, \phi_2, t)\phi_j, \quad j = 1, 2$$


ϕ_1
ϕ_2


0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
−8 −6 −4 −2 0 2 4 6 8
ϕ_1
ϕ_2

Phase separation

Property Let $\beta_{12} \to +\infty$, the phase of two components of the ground state $\Phi_g = (\phi_1^g, \phi_2^g)^T$ will be segregated, i.e. Φ_g will converge to a state such that $\phi_1^g \cdot \phi_2^g = 0$.

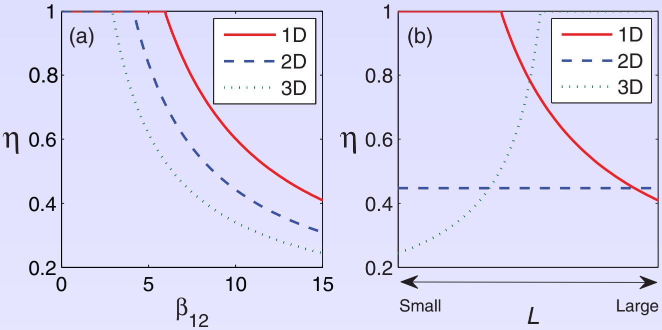
Phase separation

- Repulsive interactions only:

$$E(\phi_1, \phi_2) = \int \frac{1}{2}|\nabla \phi_1|^2 + \frac{1}{2}|\nabla \phi_2|^2 + \frac{\beta_{11}}{2}|\phi_1|^4 + \frac{\beta_{22}}{2}|\phi_2|^4 + \beta_{12}|\phi_1|^2|\phi_2|^2$$

- Homogeneous case: $\beta_{11}\beta_{22} \geq \beta_{12}^2$ mixed; otherwise separated
- Nonhomogeneous case?

- $\beta_{11} = \beta_{22}$, box potential (width L)
- mixing factor: $\eta = 2\int \phi_1\phi_2$



- Exist $\beta_c > \beta$, when $\beta_{12} \leq \beta_c$, $\eta = 1$
- proof by Fundamental gap+elliptic estimates

Fundamental gap

- consider linear case $-\Delta + V(\mathbf{x})$, $\mathbf{x} \in U \subset \mathbb{R}^d$ (U compact convex)[1] with Dirichlet boundary conditions
- eigenvalues $\lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots$, eigenfunctions $\{\phi_k\}_{k=0}^{\infty}$

$$\Delta\phi_k - V(\mathbf{x})\phi_k + \lambda_k\phi_k = 0, \quad \phi_k|_{\partial U} = 0$$

- fundamental gap $:= \lambda_1 - \lambda_0$
- Gap conjecture: Let U be a bounded convex domain with diameter D, $V(\mathbf{x})$ be convex, then the fundamental gap

$$\lambda_1 - \lambda_0 \geq \frac{3\pi^2}{D^2}$$

[1] B. Andrews AND J. Clutterbuck, JAMS, 2011

Spin-1 BEC

- Order parameter $\Psi = (\psi_1, \psi_0, \psi_{-1})$
- Spin-1 GPE

$$i\partial_t \Psi = [H + \beta_0 \rho - p\mathrm{f}_z + q\mathrm{f}_z^2 + \beta_1 \mathbf{F}\cdot\mathbf{f}]\Psi,$$

- $\mathbf{F} = (F_x, F_y, F_z)^T = (\Psi^* \mathrm{f}_x \Psi, \Psi^* \mathrm{f}_y \Psi, \Psi^* \mathrm{f}_z \Psi)^T$
- spin-1 matrices $\mathbf{f} = (\mathrm{f}_x, \mathrm{f}_y, \mathrm{f}_z)^T$ as

$$\mathrm{f}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{f}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{f}_z = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

- $H = -\frac{1}{2}\nabla^2 + V(\mathbf{x})$, $\rho = |\Psi|^2 = \sum_{l=-1}^{1} |\psi_l|^2$
- p and $q = \frac{q_0}{\hbar\omega_s}$ are the linear and quadratic Zeeman terms.
- $\beta_0 = \frac{Nc_0}{x_s^3 \hbar\omega_s} = \frac{4\pi N(a_0+2a_2)}{3x_s}$ and $\beta_1 = \frac{Nc_2}{x_s^3 \hbar\omega_s} = \frac{4\pi N(a_2-a_0)}{3x_s}$

Energy and ground states

- $F_x = \frac{1}{\sqrt{2}}\left[\overline{\psi}_1\psi_0 + \overline{\psi}_0(\psi_1 + \psi_{-1}) + \overline{\psi}_{-1}\psi_0\right]$, $F_y = \frac{i}{\sqrt{2}}\left[-\overline{\psi}_1\psi_0 + \overline{\psi}_0(\psi_1 - \psi_{-1}) + \overline{\psi}_{-1}\psi_0\right]$,
  $F_z = |\psi_1|^2 - |\psi_{-1}|^2$
- Energy:

$$E(\Psi(\cdot,t)) = \int_{\mathbb{R}^d}\left\{\sum_{l=-1}^{1}\left(\frac{1}{2}|\nabla\psi_l|^2 + (V(\mathbf{x}) - pl + ql^2)|\psi_l|^2\right) + \frac{\beta_0}{2}|\Psi|^4 + \frac{\beta_1}{2}|\mathbf{F}|^2\right\}\, d\mathbf{x}$$

- Mass constraint $N(\Psi(\cdot,t)) := \|\Psi(\cdot,t)\|^2 = \int_{\mathbb{R}^d}\sum_{l=-1,0,1}|\psi_l(\mathbf{x},t)|^2\, d\mathbf{x} = N(\Psi(\cdot,0)) = 1$
- Magnetization ($M \in [-1,1]$) $M(\Psi(\cdot,t)) := \int_{\mathbb{R}^d}\sum_{l=-1,0,1} l|\psi_l(\mathbf{x},t)|^2\, d\mathbf{x} = M(\Psi(\cdot,0)) = M$
- Ground state- Find $\left(\Phi_g \in S_M\right)$ such that $E_g := E\left(\Phi_g\right) = \min_{\Phi\in S_M} E\left(\Phi\right)$

$$S_M = \left\{\Phi = (\phi_1,\phi_0,\phi_{-1})^T \mid \|\Phi\| = 1,\ \int_{\mathbb{R}^d}\left[|\phi_1(\mathbf{x})|^2 - |\phi_{-1}(\mathbf{x})|^2\right]\, d\mathbf{x} = M,\ E(\Phi) < \infty\right\}.$$

Properties

Quadratic Zeeman $q = 0$

- Ferromagnetic system-spin-dependent interacton $\beta_1 < 0$
  - Single mode approximation.
    ϕ_j identical up to a constant factor
- Anti-ferromagnetic system-spin-dependent interacton $\beta_1 > 0$
  - $\phi_0 = 0$
- $$|\mathbf{F}|^2 = (|\phi_1|^2 - |\phi_{-1}|^2)^2 + 2|\phi_0|^2(|\phi_1|^2 + |\phi_{-1}|^2) - 4\mathrm{Re}(\phi_0^2\overline{\phi_1\phi_{-1}})$$
- $F_x = F_y \neq 0$: ferromagnetic; $F_x = F_y = 0$: anti-ferromagnetic

Mathematical results

Theorem

Existence: $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = +\infty$, $M \in (-1,1)$, $\beta_0 \geq 0$ *and* $\beta_0 + \beta_1 \geq 0$, *there exists ground state* $\Phi_g = (\phi_1^g, \phi_0^g, \phi_{-1}^g) \in S_M$

- $q = 0$ *and* $\beta_1 < 0$, *ferromagnetic:* $\phi_l^g = e^{i\theta_l}\alpha_l\phi_g$
  $(\theta_1 + \theta_{-1} - 2\theta_0 = (2k+1)\pi$, $\alpha_1 = \frac{1+M}{2}$, $\alpha_{-1} = \frac{1-M}{2}$, $\alpha_0 = \sqrt{\frac{1-M^2}{2}}$
- $q < 0$ *and* $\beta_1 > 0$, *anti-ferromagnetic:* $\phi_0^g = 0$, *and* $\tilde{\Phi}_g = (\phi_1^g, \phi_{-1}^g)^T$ *is a minimizer of the pseudo spin-1/2 system*

Numerical methods

Normalized Gradient Flow:

$$\partial_t \phi_1 = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_0+\beta_1)(|\phi_1|^2+|\phi_0|^2) - (\beta_0-\beta_1)|\phi_{-1}|^2\right]\phi_1 - \beta_1\bar{\phi}_{-1}\phi_0^2 + [\mu_\Phi(t)+\lambda_\Phi(t)]\,\phi_1$$

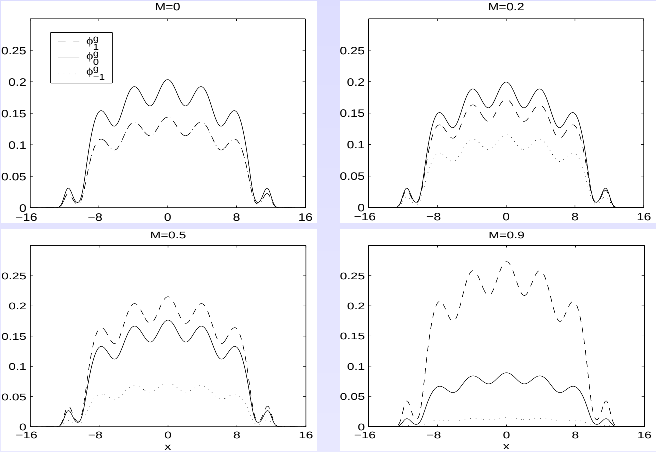
$$\partial_t \phi_0 = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x}) - (\beta_0+\beta_1)(|\phi_1|^2+|\phi_{-1}|^2) - \beta_0|\phi_0|^2\right]\phi_0 - 2\beta_1\phi_{-1}\,\bar{\phi}_0\phi_1 + \mu_\Phi(t)\,\phi_0$$

$$\partial_t \phi_{-1} = \left[\frac{1}{2}\nabla^2 - V(\mathbf{x})(\beta_0+\beta_1)(|\phi_{-1}|^2+|\phi_0|^2) - (\beta_0-\beta_1)|\phi_1|^2\right]\phi_{-1} - \beta_1\phi_0^2\,\bar{\phi}_1 + [\mu_\Phi(t)-\lambda_\Phi(t)]\,\phi_{-1}$$

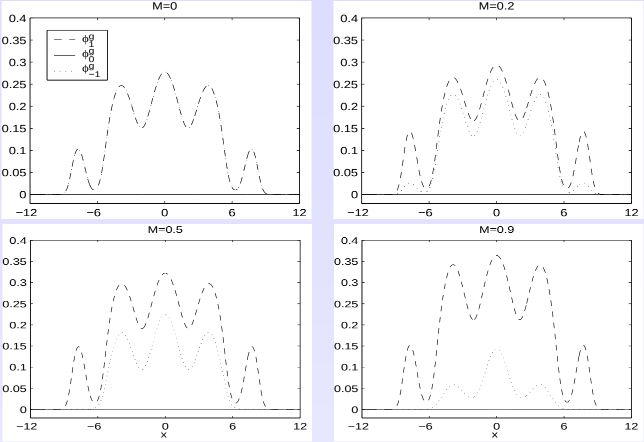
- Gradient flow part (imaginary time spin-1 GPE)+projection (Lagrange multipliers)//Gradient flow part (imaginary time spin-1 GPE+Lagrange multipliers) + projection (Lagrange part)
- For projection constants: $\phi_l(\mathbf{x}, t_{n+1}^+) = \sigma_l\phi_l(\mathbf{x}, t_{n+1}^-)$ $(l = \pm 1, 0)$, two equations from Mass and Magnetization constraints, from $\partial_t\phi_l(\mathbf{x}, t) = [\mu_\Phi(t) + l\lambda_\Phi(t)]\phi_l(\mathbf{x}, t)$, an additional equation $\sigma_1\sigma_{-1} = \sigma_0^2$. (quadrattic equation to be solved for σ_l)

Numerical results

Ferromagnetic interaction



Anti-ferromagnetic interaction



Spin-2 BEC

- Order parameter $\Psi = (\psi_2, \psi_1, \psi_0, \psi_{-1}, \psi_{-2})$
- Spin-2 GPE

$$i\partial_t \Psi = [H + \beta_0 \rho - p\mathrm{f}_z + q\mathrm{f}_z^2 + \beta_1 \mathbf{F}\cdot\mathbf{f}]\Psi + \beta_2 A_{00} \mathbf{A}\overline{\Psi}$$

- $\mathbf{F} = (F_x, F_y, F_z)^T = (\Psi^* \mathrm{f}_x \Psi, \Psi^* \mathrm{f}_y \Psi, \Psi^* \mathrm{f}_z \Psi)^T$
- spin-2 matrices $\mathbf{f} = (\mathrm{f}_x, \mathrm{f}_y, \mathrm{f}_z)^T$ as $\mathrm{f}_z = \mathrm{diag}(2, 1, 0, -1, -2)$

$$\mathrm{f}_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathrm{f}_y = i\begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & -\sqrt{\frac{3}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{3}{2}} & 0 & -\sqrt{\frac{3}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{3}{2}} & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

- $H = -\frac{1}{2}\nabla^2 + V(\mathbf{x})$, $\rho = |\Psi|^2 = \sum_{l=-1}^{1} |\psi_l|^2$
- p and $q = \frac{q_0}{\hbar\omega_s}$ are the linear and quadratic Zeeman terms.
- $\beta_0 = \frac{Nc_0}{x_s^3 \hbar\omega_s} = \frac{4\pi N(a_0+2a_2)}{3x_s}$ (spin-independent contact interaction) and $\beta_1 = \frac{Nc_2}{x_s^3 \hbar\omega_s} = \frac{4\pi N(a_2-a_0)}{3x_s}$ (spin-exchange), β_2 (spin-singleton interaction)

Energy and ground states

- $F_x = \overline{\psi}_2\psi_1 + \overline{\psi}_1\psi_2 + \overline{\psi}_{-2}\psi_{-1} + \overline{\psi}_{-1}\psi_{-2} + \frac{\sqrt{6}}{2}(\overline{\psi}_1\psi_0 + \overline{\psi}_0\psi_1 + \overline{\psi}_0\psi_{-1} + \overline{\psi}_{-1}\psi_0),$
  $F_y = i\left[\overline{\psi}_1\psi_2 - \overline{\psi}_2\psi_1 + \overline{\psi}_{-2}\psi_{-1} - \overline{\psi}_{-1}\psi_{-2} + \frac{\sqrt{6}}{2}(\overline{\psi}_0\psi_1 - \overline{\psi}_1\psi_0 + \overline{\psi}_{-1}\psi_0 - \overline{\psi}_0\psi_{-1})\right],$
  $F_z = 2|\psi_2|^2 + |\psi_1|^2 - |\psi_{-1}|^2 - 2|\psi_{-2}|^2$
- $$\mathbf{A} = \frac{1}{\sqrt{5}}\begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$
  and $A_{00} := A_{00}(\Psi) = \Psi^T\mathbf{A}\Psi$ with $A_{00} = \frac{1}{\sqrt{5}}(2\psi_2\psi_{-2} - 2\psi_1\psi_{-1} + \psi_0^2)$
- Energy:
  $$E(\Psi(\cdot,t)) = \int_{\mathbb{R}^d}\left\{\sum_{l=-2}^{2}\left(\frac{1}{2}|\nabla\psi_l|^2 + (V(\mathbf{x}) - pl + ql^2)|\psi_l|^2\right) + \frac{\beta_0}{2}|\Psi|^4 + \frac{\beta_1}{2}|\mathbf{F}|^2 + \frac{\beta_2}{2}|A_{00}|^2\right\}\,d\mathbf{x}$$
- Mass constraint $N(\Psi(\cdot,t)) := \|\Psi(\cdot,t)\|^2 = \int_{\mathbb{R}^d}\sum_{l=-2}^{2}|\psi_l(\mathbf{x},t)|^2\,d\mathbf{x} = N(\Psi(\cdot,0)) = 1$
- Magnetization $(M \in [-2,2])$ $M(\Psi(\cdot,t)) := \int_{\mathbb{R}^d}\sum_{l=-2}^{2} l|\psi_l(\mathbf{x},t)|^2\,d\mathbf{x} = M(\Psi(\cdot,0)) = M$
- Ground state- Find $(\Phi_g \in S_M)$ such that $E_g := E(\Phi_g) = \min_{\Phi\in S_M} E(\Phi)$

$$S_M = \left\{\Phi = (\phi_2,\phi_1,\phi_0,\phi_{-1},\phi_{-2})^T \mid \|\Phi\| = 1,\ \int_{\mathbb{R}^d}\sum_{l=-2}^{2}|\psi_l|^2\,d\mathbf{x} = M,\ E(\Phi) < \infty\right\}.$$

Ground state properties

- Uniform gas, $q = 0$ (cf. Ueda 09)
  - Ferromagnetic: $\beta_1 < 0$ and $\beta_1 < \frac{\beta_2}{20}$, $F_x, F_y \neq 0$, $A_{00} = 0$
  - Nematic: $\beta_1 < 0$ and $\beta_1 > \frac{\beta_2}{20}$, $F_x, F_y = 0$, $A_{00} \neq 0$
  - Cylic: $\beta_1 > 0$ and $\beta_2 > 0$, $F_x = F_y = 0$, $A_{00} = 0$

Mathematical results

Theorem

Existence: $\lim_{|\mathbf{x}|\to\infty} V(\mathbf{x}) = +\infty$, $M \in (-2,2)$ $\beta_0 + 4\beta_1 \geq 0$ *with* $\frac{\beta_2}{20} > \beta_1$ *and* $\beta_1 < 0$*; or* $M \in (-2,2)$, $\beta_0 + \frac{\beta_2}{5} \geq 0$ *with* $\beta_2 < 0$ *and* $\frac{\beta_2}{20} \leq \beta_1$*; or* $M \in (-2,2)$, $\beta_0 \geq 0$, $\beta_1 \geq 0$ *and* $\beta_2 \geq 0$*., there exists ground state* $\Phi_g = (\phi_2^g, \phi_1^g, \phi_0^g, \phi_{-1}^g, \phi_{-2}^g) \in S_M$

- $q = 0$ *and* $\beta_1 < 0$, $\beta_1 < \frac{\beta_2}{20}$*, ferromagnetic (SMA):* $\phi_l^g = e^{i\theta_1 + il\theta_2}\alpha_l\phi_g$ *with* $\alpha_2 = \frac{(2+M)^2}{16}$, $\alpha_1 = \frac{(2+M)\sqrt{4-M^2}}{8}$, $\alpha_0 = \frac{\sqrt{6}(4-M^2)}{16}$, $\alpha_{-1} = \frac{(2-M)\sqrt{4-M^2}}{8}$ *and* $\alpha_{-2} = \frac{(2-M)^2}{16}$
- $q < 0$ *and* $\beta_1 < 0$, $\beta_1 \geq \frac{\beta_2}{20}$*, nematic:* $\phi_0^g = \phi_1^g = \phi_{-1}^g = 0$*, and* $\tilde{\Phi}_g = (\phi_2^g, \phi_{-2}^g)^T$ *is a minimizer of the pseudo spin-1/2 system*
- $\beta_1 > 0$, $\beta_2 > 0$*, cylic: more complicated than the uniform gas case*

Numerical methods

- NGF: $\partial_t \Phi = -[H + \beta_0 \rho - p\mathrm{f}_z + q\mathrm{f}_z^2 + \beta_1 \mathbf{F}\cdot\mathbf{f}]\Phi - \beta_2 A_{00}\mathbf{A}\Phi + \mu_\Phi(t)\Phi + \lambda_\Phi(t)\mathrm{f}_z\Phi$
- GFDN:

$$\frac{\Phi^{(1)} - \Phi^n}{\tau} = -[H + \beta_0 \rho^n - p\mathrm{f}_z + q\mathrm{f}_z^2 + \beta_1 \mathbf{F}^n \cdot \mathbf{f}]\Phi^{(1)} - \beta_2 A_{00}^n \mathbf{A}\overline{\Phi^{(1)}} + \mu_{\Phi^n}\Phi^n + \lambda_{\Phi^n}\mathrm{f}_z\Phi^n,$$

projection step for $\Phi^{(1)} = (\phi_2^{(1)}, \phi_1^{(1)}, \phi_0^{(1)}, \phi_{-1}^{(1)}, \phi_{-2}^{(1)})^T$

$$\Phi^{n+1} = \mathrm{diag}(\alpha_2, \alpha_1, \alpha_0, \alpha_{-1}, \alpha_{-2})\Phi^{(1)}$$

- Determine the five projection constants with Mass and Magnetization constraints

Different projection strategies

- view projection as the split-step for $\partial_t \phi_l = (\mu + l\lambda)\phi_l$
  - $\alpha_l = e^{\Delta t(\mu + l\lambda)} = c_0 c_1^l$ (two unknowns c_0, c_1)

$$c_0^2 \left(c_1^4 \|\phi_2^{(1)}\|^2 + c_1^2 \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + c_1^{-2} \|\phi_{-1}^{(1)}\|^2 + c_1^{-4} \|\phi_{-2}^{(1)}\|^2 \right) = 1,$$
$$c_0^2 \left(2c_1^4 \|\phi_2^{(1)}\|^2 + c_1^2 \|\phi_1^{(1)}\|^2 - c_1^{-2} \|\phi_{-1}^{(1)}\|^2 - 2c_1^{-4} \|\phi_{-2}^{(1)}\|^2 \right) = M.$$

A quartic equation to be solved, positive root

  - $\alpha_l = e^{\Delta t(\mu + l\lambda)} \approx (1 + \Delta\mu + l\lambda) = c_0(1 + lc_1)$

$$(1+2c_1)^2 \|\phi_2^{(1)}\|^2 + (1+c_1)^2 \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + (1-c_1)^2 \|\phi_{-1}^{(1)}\|^2 + (1-2c_1)^2 \|\phi_{-2}^{(1)}\|^2 = \frac{1}{c_0^2}$$
$$2(1+2c_1)^2 \|\phi_2^{(1)}\|^2 + (1+c_1)^2 \|\phi_1^{(1)}\|^2 - (1-c_1)^2 \|\phi_{-1}^{(1)}\|^2 - 2(1-2c_1)^2 \|\phi_{-2}^{(1)}\|^2 = \frac{M}{c_0^2}$$

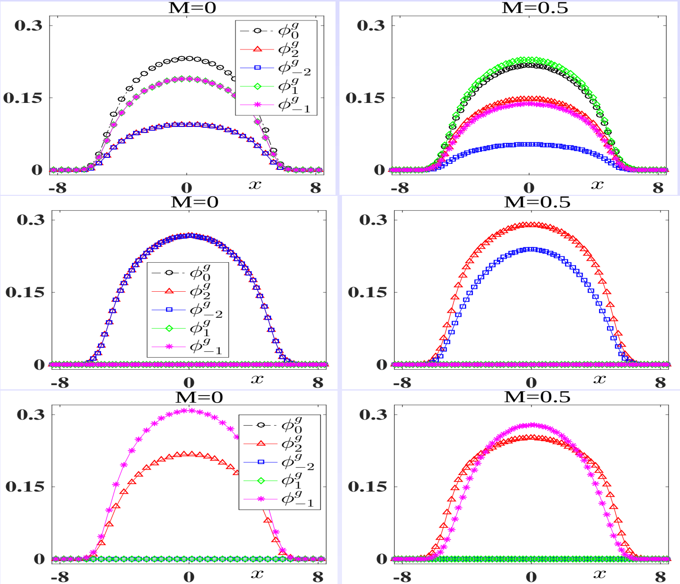
A quadratic equation to be solved, positive root not guaranteed

  - $\alpha_l = 1/e^{-\Delta t(\mu + l\lambda)} \approx 1/(1 - \Delta\mu - l\lambda) = 1/(c_0(1 + lc_1))$

$$(1+2c_1)^{-2} \|\phi_2^{(1)}\|^2 + (1+c_1)^{-2} \|\phi_1^{(1)}\|^2 + \|\phi_0^{(1)}\|^2 + (1-c_1)^{-2} \|\phi_{-1}^{(1)}\|^2 + (1-2c_1)^{-2} \|\phi_{-2}^{(1)}\|^2 = c_0^2$$
$$2(1+2c_1)^{-2} \|\phi_2^{(1)}\|^2 + (1+c_1)^{-2} \|\phi_1^{(1)}\|^2 - (1-c_1)^{-2} \|\phi_{-1}^{(1)}\|^2 - 2(1-2c_1)^{-2} \|\phi_{-2}^{(1)}\|^{-2} = Mc_0^2$$

An octic equation to be solved, positive root (guaranteed)

Numerical example



Summary

- Ground states of spin-1/2, 1, 2 BECs
- Rigorous ground state properties
- Projection methods for computing ground states

THANK YOU!