Collaborators

- **Analysis**¹ ²
  - Liren Lin (Academia Sinica)

- **Numerics**³ ⁴
  - Jen-Hao Chen (National Hsin Chu Normal University)
  - Weichung Wang (National Taiwan University)

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¹ Characterization of the ground states of spin-1 Bose-Einstein condensates, ArXiv 1102.0832v2, Feb. 2011
² Bifurcation between 2-component and 3-component ground states of spin-1 Bose-Einstein condensates in uniform magnetic fields, ArXiv 1302.0279v1, Feb. 2013
Outline

1 Part 1: Background BECs and spinor BECs
   - What are BECs?
   - Mean field model: Gross-Pitaevskii equation

2 Part 2: Numerics for Ground States of Spin-1 BECs
   - Numerical investigation: no external magnetic field
   - Numerical investigation: in uniform magnetic field

3 Part 3: Analysis for Ground States of Spin-1 BECs
   - Existence and Uniqueness
   - Characterization of the ground states
   - Phase transition diagram

4 Conclusion
What are BECs? Theory

- Boson particles are those particles whose total spin are integers. Alkali atoms are bosons.
- Two identical bosons can occupy the same state.
- Bosons are confined at very low temperature, their de Broglie wave length are long enough. They are coherent and the lowest quantum state become apparent, called BEC.
What are BECs? Experiment

BECs were realized in lab by E. Cornell, W. Ketterle and C. Wieman (1995).
Mean field model for BECs

- $N$ particle system: wave function $\Psi_N(x_1, \cdots, x_N, t)$,

  Hamiltonian:

  $$\mathcal{H}_N = \sum_{j=1}^{N} \left( -\frac{\hbar^2}{2M_a} \nabla^2_j + V(x_j) \right) + \sum_{1\leq j<k\leq N} V_{\text{int}}(x_j - x_k)$$

- Ultracold and dilute gases, the mean field approximation:

  $$V_{\text{int}}(x_j - x_k) \approx g\delta(x_j - x_k)$$

- Hartree ansatz: all boson particles are in the same quantum state

  $$\Psi_N(x_1, \cdots, x_N, t) = \prod_{j=1}^{N} \psi(x_j, t)$$
Gross-Pitaevskii equation

- Hamiltonian:
  \[
  H = \frac{\hbar^2}{2M_a} |\nabla \psi|^2 + V(x)|\psi|^2 + \frac{\beta}{2}|\psi|^4,
  \beta = gN
  \]

- Energy \( \mathbb{E}[\psi] = \int H \, dx \).
- Gross-Pitaevskii equation: \( i\hbar \partial_t \psi = \delta \mathbb{E}/\delta \psi^* \).
  \[
  i\hbar \partial_t \psi = -\frac{\hbar^2}{2M_a} \nabla^2 \psi + V(x)\psi + \beta|\psi|^2\psi
  \]

- \( \psi \) wave function
- \( V(x) \) trap potential: \( V(x) = \frac{1}{2} \sum_{i=1}^{3} \omega_i^2 x_i^2 \).
- Interaction: repulsive if \( \beta > 0 \), attractive if \( \beta < 0 \).
Rigorous Justification of G-P equation

- E. Lieb, R. Seiringer and J. Yngvason (2001) for ground states
- L. Erdös, B. Schlein and H. T. Yau (2010) for dynamics

**A Rigorous Derivation of the Gross–Pitaevskii Energy Functional for a Two-dimensional Bose Gas**

Elliott H. Lieb\(^1\), Robert Seiringer\(^2\), Jakob Yngvason\(^2\)

\(^1\) Departments of Physics and Mathematics, Jadwin Hall, Princeton University, P. O. Box 708, Princeton, NJ 08544, USA
\(^2\) Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria

**Derivation of the Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensate**

By László Erdős, Benjamin Schlein, and Horng-Tzer Yau
One-, multi-component and spinor BECs

- **One-component BECs**: atoms with a single quantum state are trapped. E.g. Using magnetic trap
- **Two-component BECs**: mixture of two different species of bosons. E.g. two isotopes of the same elements, or two different elements
- **Spinor BECs**: mixture of different hyperfine states of the same isotopes. E.g. Spin-1 atoms using optical trap. There are 3 hyperfine states $m_F = 1, 0, -1$
Two-component BECs

- Vector order parameter \((\psi_1, \psi_2)\)

- Hamilton:

  \[
  H = \sum_{i=1}^{2} \left[ \frac{\hbar^2}{2M_i} |\nabla \psi_i|^2 + V_i(x)|\psi_i|^2 + \frac{1}{2} \sum_{j=1}^{2} \beta_{ij} |\psi_j|^2 |\psi_i|^2 \right]
  \]

- Vector G-P equations

  \[
  i\hbar \partial_t \psi_1 = \left[ -\frac{\hbar^2}{2M_1} \nabla^2 + V_1(x) + \beta_{11} |\psi_1|^2 + \beta_{12} |\psi_2|^2 \right] \psi_1
  \]

  \[
  i\hbar \partial_t \psi_2 = \left[ -\frac{\hbar^2}{2M_2} \nabla^2 + V_2(x) + \beta_{12} |\psi_1|^2 + \beta_{22} |\psi_2|^2 \right] \psi_2
  \]
Spinor BECs

- Spin-1 atom has 3 hyperfine states: \( m_F = 1, 0, -1 \).
- Vector order parameter \( \Psi = (\psi_1, \psi_0, \psi_{-1}) \).
- Associate with a spinor \( \Psi \), the spin vector \( F = \Psi^\dagger F \Psi \in \mathbb{R}^3 \), which is just like a magnetic dipole moment.
- \( F = (F_x, F_y, F_z) \) is the spin-1 Pauli operator:

\[
F_x = \frac{1}{\sqrt{2}} \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 0
\end{pmatrix},
F_y = \frac{i}{\sqrt{2}} \begin{pmatrix}
0 & -1 & 0 \\
1 & 0 & -1 \\
0 & 1 & 0
\end{pmatrix},
F_z = \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -1
\end{pmatrix}.
\]
G-P equation for spin-1 BECs

- Hamiltonian:

\[
H = \frac{\hbar^2}{2M_a} |\nabla \Psi|^2 + V(x)|\Psi|^2 + \frac{c_n}{2} |\Psi|^4 + \frac{c_s}{2} |\Psi^\dagger F \Psi|^2
\]

- \(|\Psi|^2 \cdot |\Psi|^2\): spin-independent interaction
- \(|\Psi^\dagger F \Psi|^2\): spin-spin interaction (spin-exchange).

The total energy \( E[\Psi] = \int H \, dx \).

The G-P equation

\[
i\hbar \partial_t \Psi = \frac{\delta E}{\delta \Psi^\dagger}
\]
**Physical parameters**

\[ H = \frac{\hbar^2}{2M_a} |\nabla \Psi|^2 + V(x)|\Psi|^2 + \frac{c_n}{2} |\Psi|^4 + \frac{c_s}{2} |\Psi^\dagger F \Psi|^2 \]

<table>
<thead>
<tr>
<th>Interaction</th>
<th>(c_n)</th>
<th>(c_s)</th>
</tr>
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<tbody>
<tr>
<td>Spin-independent</td>
<td>(4\pi\hbar^2 (a_0 + 2a_2))</td>
<td>(3M_a)</td>
</tr>
<tr>
<td>Repulsive</td>
<td>(c_n) &gt; 0</td>
<td></td>
</tr>
<tr>
<td>Attractive</td>
<td>(c_n) &lt; 0</td>
<td></td>
</tr>
<tr>
<td>Spin-exchange</td>
<td>(4\pi\hbar^2 (a_2 - a_0))</td>
<td>(3M_a)</td>
</tr>
<tr>
<td>Antiferromagnetic</td>
<td>(c_s) antiferromagnetic</td>
<td></td>
</tr>
<tr>
<td>Ferromagnetic</td>
<td>(c_s) ferromagnetic</td>
<td></td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>(c_n)</th>
<th>(c_s)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{87}\text{Rb}) 7.793</td>
<td>-0.0361</td>
<td>ferromagnetic</td>
</tr>
<tr>
<td>(^{23}\text{Na}) 15.587</td>
<td>0.4871</td>
<td>anti-ferromagnetic</td>
</tr>
</tbody>
</table>
Spinor BEC in uniform magnetic field

- Hamilton $H = H_{\text{kin}} + H_{\text{pot}} + H_n + H_s + H_{Zee}$

- Zeeman energy: suppose magnetic field $B \hat{z}$,

$$H_{Zee} = \sum_{j=-1}^{1} E_j(B)n_j$$

where $n_j = |\psi_j|^2$. 
Gauge invariants and conservation laws

- **Energy**
  \[ \mathbb{E}[\Psi] = \int (H_{\text{kin}} + H_{\text{pot}} + H_n + H_s + H_{\text{Zee}}) \, dx \]

- **Gauge invariant**: energy is invariant under transform
  \[ \Psi \rightarrow e^{i\phi} R_z(\alpha) \Psi \]

- This leads to two conservation laws:
  - **Total number of atoms**
    \[ \int (|\psi_1|^2 + |\psi_0|^2 + |\psi_{-1}|^2) \, dx = N \]
  - **Total magnetization**
    \[ \int (|\psi_1|^2 - |\psi_{-1}|^2) \, dx = M \]
The ground state problem

Ground state problem

\[
\min \mathbb{E}[\Psi] \quad \text{subject to} \quad \int n(x) \, dx = N, \quad \int m(x) \, dx = M.
\]

where

- \( \mathbb{E}[\Psi] = \int H \, dx \)
- \( H = H_{\text{kin}} + H_{\text{pot}} + H_n + H_s + H_{\text{Zee}} \)
- \( n_j = |\psi_j|^2 \),
- \( n = n_1 + n_0 + n_{-1} \)
- \( m = n_1 - n_{-1} \)
A closer look at Hamiltonian

- Express $\psi_j = \sqrt{n_j}e^{i\theta_j}$

- $H_{kin}: |\nabla \Psi|^2 = \sum_j (|\nabla \sqrt{n_j}|^2 + n_j|\nabla \theta_j|^2)$

- Constant phase has least kinetic energy

- $H_s = \frac{c_s}{2} |\Psi^\dagger F \Psi|^2$:

\[
|\Psi^\dagger F \Psi|^2 = (n_1 - n_{-1})^2 + 2n_0(n_1 + n_{-1} + 2\sqrt{n_1n_{-1}} \cos(\Delta \theta))
\]

\[
\Delta \theta = \theta_1 + \theta_{-1} - 2\theta_0
\]

- To minimize $H_s$, we should choose

\[
\Delta \theta = \begin{cases} 
0 & \text{if } c_s < 0 \\
\pi & \text{if } c_s > 0
\end{cases}
\]
Spin-exchange Hamiltonian:

\[
H_s = \frac{c_s}{2} \left[ (n_1 - n_{-1})^2 + 2n_0 (\sqrt{n_1} - s \sqrt{n_{-1}})^2 \right], \ s = \text{sign} c_s
\]

Spin-exchange interaction

<table>
<thead>
<tr>
<th>Interaction</th>
<th>(c_s) &lt; 0 (ferro)</th>
<th>(c_s) &gt; 0 (antiferro)</th>
</tr>
</thead>
<tbody>
<tr>
<td>((n_1, n_{-1}))</td>
<td>(-c_s n_1 n_{-1})</td>
<td>repulsive</td>
</tr>
<tr>
<td>((n_0, n_1))</td>
<td>(c_s n_0 n_1)</td>
<td>attractive</td>
</tr>
<tr>
<td>((n_0, n_{-1}))</td>
<td>(c_s n_0 n_{-1})</td>
<td>attractive</td>
</tr>
</tbody>
</table>
Spinor Bose Condensates in Optical Traps

Tin-Lun Ho
Department of Physics, The Ohio State University, Columbus, Ohio 43210
(Received 18 March 1998)

We show that in an optical trap the ground states of spin-1 bosons such as $^{23}\text{Na}$, $^{39}\text{K}$, and $^{87}\text{Rb}$ can be either ferromagnetic or “polar” states, depending on the scattering lengths in different angular momentum channels. The collective modes of these states have very different spin character and spatial distributions. While ordinary vortices are stable in the polar state, only those with unit circulation are stable in the ferromagnetic state. The ferromagnetic state also has coreless (or Skyrmion) vortices like those of $^3\text{He-A}$. [S0031-9007(98)06714-3]

PACS numbers: 03.75.Fi, 05.30.Jp

Figure: University of Hamburg 2006: First 1D-lattice at the spinor experiment. As a first step towards the exploration of magnetism of spinor quantum gases in periodic potential we have successfully loaded a BEC into a standing wave potential using a Ti:Sa laser at 830nm. The figure shows an absorption image after 21ms time-of-flight demonstrating the interference of matter waves from different lattice sites.
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   - Phase transition diagram

4. Conclusion
Some numerical works

- Weizhu Bao
- Qiang Du
- Wenwei Lin et al.
- Jie Shen
- Chen-Shen Chien et al.
- Chen, Chern, Wang: Pseudo-arclength Continuation method
Pseudo arclength continuation method-1

- Euler-Lagrange equation

\[
(\mu + \lambda)\psi_1 = \tilde{H}_n\psi_1 + c_s(n_1 + n_0 - n_{-1})\psi_1 + c_s\psi_{-1}\psi_0^2
\]

\[
\mu\psi_0 = \tilde{H}_n\psi_0 + c_s(n_1 + n_{-1})\psi_0 + 2c_s\psi_{-1}\psi_0\psi_1
\]

\[
(\mu - \lambda)\psi_{-1} = \tilde{H}_n\psi_{-1} + c_s(n_0 + n_{-1} - n_1)\psi_{-1} + c_s\psi_1\psi_0^2
\]

- Two constraints: \( \int n \, dx = N, \int m \, dx = M. \)
- Solve the nonlinear eigenvalue problem + 2 constraints:

\[
F(\mathbf{x}, \tau) = 0
\]

with \( \mathbf{x} = (\psi_1, \psi_0, \psi_{-1}, \mu, \lambda) \) and \( c_n(\tau), c_s(\tau) \) chosen.

- The solution is a curve \( \mathbf{x}(\tau), \) or \( \mathbf{u}(\tau) := [\mathbf{x}(\tau), \tau]. \)
Pseudo arclength continuation method-2

- PACM: Continuation method to find $u(\cdot)$ by iteration from $u_i$ to $u_{i+1}$ with $F(u_i) = 0$ and $F(u_{i+1}) = 0$:
  - Prediction:
    - Find tangent: $\dot{u}_i = [\dot{x}_i, \dot{\tau}_i]$ by solving
      $$\mathcal{D}F(u_i(s))\dot{u}_i = 0, \quad \mathcal{D}F(u_i(s)) = [F_x(u_i(s)), F_\tau(u_i(s))] .$$
    - Euler predictor: $u_{i+1}^{(1)} = u_i + \delta_i \dot{u}_i$
  - Correction:
    - Orthogonal projection
      $$\begin{cases}
        F(u_{i+1}) = 0, \\
        (u_{i+1} - u_{i+1}^{(1)}) \cdot \dot{u}_i = 0,
      \end{cases}$$
    - Solved by Newton’s method
Pseudo arclength continuation method-3

Initialization

Starting from \((c_n, c_s) = (0, 0)\): the linear eigenvalue problem:

\[
\left( -\frac{\hbar^2}{2M_a} \nabla^2 + V \right) \tilde{\psi} = \tilde{\mu} \tilde{\psi}.
\]

Define a single mode approximation solution by

\[
\tilde{\Psi} = (\gamma_1, \gamma_0, \gamma_{-1}) \tilde{\psi}
\]

where

\[
\gamma = \left(1 + M, \sqrt{2(1 - M^2)}, 1 - M \right)/2 \tag{3C}
\]

\[
\gamma = \left(\sqrt{1 + M}, 0, \sqrt{1 - M} \right)/\sqrt{2} \tag{2C}
\]

Find the initial state \(x_0\) by solving \(F(x, 0) = 0\) by Newton’s method with initial \((\tilde{\Psi}, \tilde{\mu}, 0, 0)\).
Numerical investigation: no external magnetic field

Goal: Study the structures of ground state and excited states as $c_s$ varies.

- **Experiment 1 ($^{87}\text{Rb: Ferromagnetic}$)**
  - $V = 0$, $M = 0.2$
  - $c_s \in (-0.5, -0.2)$

- **Experiment 2 ($^{23}\text{Na: Anti-ferromagnetic}$)**
  - $V = x^2/20$, $M = 0.2$
  - $c_s \in (0.2, 5)$
Characterization of ground states ($B = 0$)

- Ferromagnetic systems: SMA
- Antiferromagnetic systems:
  - $2C$ if $M \neq 0$
  - SMA if $M = 0$
- SMA: $A_1 = \{ u \in \mathcal{A} | u = (\gamma_1, \gamma_0, \gamma_{-1}) \rho \}$
- $2C$: $A_2 = \{ u \in \mathcal{A} | u_0 \equiv 0 \}$
Numerical investigation: uniform magnetic field

- Hamiltonian $H = H_{kin} + H_{pot} + H_n + H_s + H_{Zee}$
- Zeeman shift energy: Suppose magnetic field $B\hat{z}$,

$$H_{Zee} = \sum_{j=-1}^{1} E_j(B)n_j$$

$$= q(n_1 + n_{-1}) + p(n_1 - n_{-1}) + E_0n$$

where $n_j = |\psi_j|^2$ and

$$p = \frac{1}{2}(E_{-1} - E_1) \approx -\frac{\mu_B B}{2}$$

$$q = \frac{1}{2}(E_{-1} + E_1 - 2E_0) \approx \frac{\mu_B^2 B^2}{4E_{\text{hfs}}}$$
- The energy

\[ E[\Psi] = \int (H + q(n_1 + n_{-1})) \, dx + E_0N + pM \]

\[ H = H_{kin} + H_{pot} + H_n + H_s \]

- Ground state problem

\[ \min E[\Psi] \text{ subject to } \int n(x) \, dx = N, \int m(x) \, dx = M. \]

- Important observation: \( q \uparrow \implies n_{\pm1} \downarrow \)
Numerical Investigation (Antiferromagnetic $c_s > 0$)

Goal: Study phase transition diagram on $q$-$M$ plane for spinor BECs as the external field $B$ (or $q$) varies.

- Tests for $\epsilon = 0.1, 0.5, 1.0$, where $\epsilon^2 = \hbar^2 / 2M_a$.
- Varying $M$: ranging from $0.05 - 0.9$.
- For each fixed $\epsilon, M$, perform Pseudo Arclength Continuity Method with continuation parameter: $q$ ranging from 0 to 0.5.
Antiferromagnetic systems: $\epsilon = 0.5$

Figure: $\epsilon = 0.5$. Blue line is the transition: $2C \rightarrow 3C$ (symmetric). Red line is the transition: $3C$ (symmetric) $\rightarrow$ NS$+2C$. 
**Table**: (Case 1) Ground state patterns of antiferromagnetic BEC \(^{23}\text{Na}\) with \(M = 0.3\) in the constant potential.

<table>
<thead>
<tr>
<th>State</th>
<th>Profile</th>
<th>State</th>
<th>Profile</th>
<th>State</th>
<th>Profile</th>
</tr>
</thead>
<tbody>
<tr>
<td>(q = -1)</td>
<td><img src="profile1.png" alt="2C profile" /></td>
<td>(q = 0)</td>
<td><img src="profile2.png" alt="2C profile" /></td>
<td>(q = 0.02582)</td>
<td><img src="profile3.png" alt="3C profile" /></td>
</tr>
<tr>
<td>(q = 0.1115)</td>
<td><img src="profile4.png" alt="2C+NS profile" /></td>
<td>(q = 1)</td>
<td><img src="profile5.png" alt="2C+NS profile" /></td>
<td>(q = 3)</td>
<td><img src="profile6.png" alt="MS+NS profile" /></td>
</tr>
</tbody>
</table>
Numerical Investigation (ferromagnetic $c_s < 0$)

Goal: Study phase transition diagram on $q$-$M$ plane for spinor BECs as the external field $B$ (or $q$) varies.

- Tests for $\epsilon = 0.1, 0.5, 1.0$, where $\epsilon^2 = \hbar^2/2M_a$.
- Varying $M$: ranging from 0.05 – 0.9.
- For each fixed $\epsilon, M$, perform Pseudo Arclength Continuity Method with continuation parameter: $q$ ranging from 0 to $-0.5$. 
Ferromagnetic systems: $\epsilon = 0.5$

Figure: $\epsilon = 0.5$. Blue line is the transition: 3C (symmetric) $\rightarrow$ NS+2C.
Table: (Case 3) Ground state patterns of ferromagnetic BEC ($^{87}$Rb) with $M = 0.3$ in the constant potential.

<table>
<thead>
<tr>
<th>State</th>
<th>Profile</th>
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<tbody>
<tr>
<td>MS+MS</td>
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<tr>
<td>MS+MS+NS</td>
<td><img src="image2.png" alt="Graph" /></td>
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<tr>
<td>2C+NS</td>
<td><img src="image3.png" alt="Graph" /></td>
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<tr>
<td>State</td>
<td>Profile</td>
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<tr>
<td>3C</td>
<td><img src="image4.png" alt="Graph" /></td>
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<td>3C</td>
<td><img src="image5.png" alt="Graph" /></td>
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<tr>
<td>2C$^{1,0}$</td>
<td><img src="image6.png" alt="Graph" /></td>
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</tbody>
</table>
Experimental Results: Phase transition $2C \rightarrow 3C$

PHYSICAL REVIEW A 86, 061601(R) (2012)

Phase diagram of spin-1 antiferromagnetic Bose-Einstein condensates

David Jacob, Lingxuan Shao, Vincent Corre, Tilman Zibold, Luigi De Sarlo, Emmanuel Mimoun, Jean Dalibard, and Fabrice Gerbier

Laboratoire Kastler Brossel, CNRS, ENS, UPMC, 24 rue Lhomond, 75005 Paris
Collège de France, 11 place Marcelin Berthelot, 75231 Paris, France
(Received 10 September 2012; published 5 December 2012)

FIG. 3. (Color online) (a) Experimental phase diagram showing the population $n_0$ of the $m = 0$ Zeeman state versus magnetization and applied magnetic field $B$. The plot shows a contour interpolation through all data points, with magnetization ranging from 0 to 0.8. The white line is the predicted critical field $B_c$ separating the two phases, deduced from Eq. (4) via $q_c = q_B B_c^2$. (b) Theoretical prediction for $n_0$.
Summary of numerical studies (antiferromagnetic)

- **Ground state patterns** (for $c_s > 0$):
  - $2C$, $3C$ (symmetric), $2C + NS$, $MS + NS$
- As $q \uparrow$, then $n_0 \uparrow$ and $n_{\pm 1} \downarrow$.
- **Phase separation** between $n_0$ and $n_{\pm 1}$ as $q \uparrow$.
- On $q$-$M$ plane, **bifurcation curves**: $q_{2C \rightarrow 3C}$, $q_{3C \rightarrow 2C + NS}$.
- For $q < q_{2C \rightarrow 3C}$, the $2C$ state is independent of $q$.
- For $q > q_{3C \rightarrow 2C + NS}$, there is a **symmetry breaking**.
- As $M \sim 0$, then $n_0 \gg n_1, n_{-1}$ and it takes stronger $q$ to break the symmetry.
- **Existence of 3C (symmetric)** is due to strong homogenization effect of the kinetic operator, which becomes more apparently for large $\epsilon$. 
Summary of numerical studies (ferromagnetic)

- **Ground state patterns** (for $c_s < 0$):
  - 3C (symmetric), 2C + NS, 2C
- As $q \downarrow$, then $n_0 \downarrow$ and $n_{\pm 1} \uparrow$.
- **Phase separation** between $n_1$ and $n_{-1}$ as $q \downarrow$.
- On $q$-$M$ plane, bifurcation curve: $q_{3C \rightarrow 2C + NS}$.
- For $q > q_{3C \rightarrow 2C + NS}$, there is a symmetry breaking.
- It is easier to break the symmetry because $n_1$ and $n_{-1}$ are not small even when $M \sim 0$, and there is a strong repulsion between $n_1$ and $n_{-1}$. 
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   - Phase transition diagram

4. Conclusion
Variational Method for Spinor BECs in $\mathbb{R}^3$

- Existence and Uniqueness
- Characterization of ground states
  - $q = 0$ (no magnetic field)
  - $q \neq 0$ (for antiferromagnetic system)
- Phase transition diagram (antiferromagnetic)
Assumptions and Variational Problem

- **Assumptions**
  - (A1): $V(x) \geq 0$ and $V(x) \to \infty$ as $|x| \to \infty$ in $\mathbb{R}^3$
  - (A2): $c_n > 0$, $|c_s| < c_n$
  - (A3): $q \geq 0$

- **Ground state problem**

$$
\min \mathcal{E}[u] = \int H(u) \, dx \text{ subject to } \mathcal{N}[u] = 1, \mathcal{M}[u] = M.
$$

$$
H(u) = |\nabla u|^2 + V \rho^2 + \frac{c_n}{2} \rho^4 + \frac{c_s}{2} \left[ (u_1^2 - u_{-1}^2)^2 + 2u_0^2(u_1 - su_{-1})^2 \right] + q(u_1^2 + u_{-1}^2)
$$

where $\rho = |u|$.
Admissible class

- Function class

\[ \mathcal{B} = \left\{ (u_1, u_0, u_{-1}) \mid u_j \geq 0, u_j \in H^1 \cap L^2_V \cap L^4(\mathbb{R}^3) \right\}. \]

where \( \|f\|^2_{L^2_V} := \int |f|^2 V. \)

- Admissible class

\[ \mathcal{A} = \left\{ u \in \mathcal{B} \mid \mathcal{N}[u] = 1, \mathcal{M}[u] = M \right\} \]

- Ground states: let \( E_g(M, q) = \inf_{\mathbf{v} \in \mathcal{A}} \mathcal{E}[\mathbf{v}] \) and

\[ \mathbb{G}_{M,q} = \left\{ u \in \mathcal{A} \mid \mathcal{E}[u] = E_g(M, q) \right\} \]
Existence

Theorem (Existence)

\[ \mathbb{G} \neq \emptyset, \text{ i.e. there does exist a ground state. Furthermore, for each } u_j, \text{ either } u_j \equiv 0 \text{ or } u_j > 0 \text{ on all of } \mathbb{R}^3. \]

- Direct method of calculus of variation.
- Coerciveness:
  - Trap potential gives \( H^1 \cap L_V \subset\subset L^2. \)
  - \( c_n > 0, |c_s| < c_n, \) give \( H_n + H_s \leq C|u|^4. \)
- Strong maximum principle: \( u_j > 0 \text{ or } u_j \equiv 0. \)
Uniqueness

**Theorem**

The 2C state \( z = (z_1, 0, z_{-1}) \) is unique and is independent of \( q \):

- The energy functional is convex in \( (z_1^2, 0, z_{-1}^2) \).

\[
H(z) = |\nabla z|^2 + V \rho^2 + \frac{c_n}{2} \rho^4 \\
+ \frac{c_s}{2} \left[ (z_1^2 - z_{-1}^2)^2 \right] + q(z_1^2 + z_{-1}^2)
\]

- \( \int q(z_1^2 + z_{-1}^2) \, dx = qN \).

Remark. The ground states may not be unique in general!

E.g. In 1D, there are two solutions after symmetry breaking.
Characterization of ground states \((q = 0)\)

- Ferromagnetic systems: SMA
- Antiferromagnetic systems:
  - 2C if \(M \neq 0\)
  - SMA if \(M = 0\)

SMA: \(A_1 = \{ \mathbf{u} \in \mathcal{A} | \mathbf{u} = (\gamma_1, \gamma_0, \gamma_{-1})\rho \}\)

2C: \(A_2 = \{ \mathbf{u} \in \mathcal{A} | u_0 \equiv 0 \}\)
Ground states: \( c_s < 0, \; q = 0 \)

The ground states in ferromagnetic systems are SMA.

**Theorem**

*In ferromagnetic systems \((c_s < 0)\),*

(i) *For any \( u \in \mathcal{A} \), define \( \rho = |u| \) and*

\[
\begin{align*}
\gamma_1^* &= \frac{1}{2} \left( 1 + \frac{M}{N} \right) \\
\gamma_0^* &= \sqrt{\frac{1}{2} \left( 1 - \frac{M^2}{N^2} \right)} \\
\gamma_{-1}^* &= \frac{1}{2} \left( 1 - \frac{M}{N} \right).
\end{align*}
\]

*Then \( H(\gamma^* \rho) \leq H(u) \);*

(ii) *if \( u \in \mathcal{G} \cap (C^2(D))^3 \), then \( u = \gamma^* \rho \).*

Here, \( \mathcal{G} \) is the set of ground states,
Ground state $c_s > 0$, $q = 0$, $M \neq 0$

The ground states in antiferromagnetic systems with $M \neq 0$ are 2C.

**Theorem**

*In antiferromagnetic systems $(c_s > 0)$,*

1. **Given any** $u \in A$, **define** $\tilde{u} = (\tilde{u}_1, \tilde{u}_0, \tilde{u}_{-1})$

   \[
   \tilde{u}_0 \equiv 0, \quad \sum \tilde{u}_j^2 = \sum u_j^2, \quad \tilde{u}_1 - \tilde{u}_{-1} = u_1 - u_{-1}
   \]

   *then* $H(\tilde{u}) \leq H(u)$ *for any* $u \in A$;

2. **if** $M \neq 0$ *and* $u \in G \cap (C^2(D))^3$, *then* $u = \tilde{u}$. 


**Ground states:** \( c_s > 0, \ q = 0, \ M = 0 \)

The ground states in antiferromagnetic systems with \( M = 0 \) are SMA.

**Theorem**

If \( c_s > 0 \) and \( M = 0 \) or \( c_s = 0 \), then the ground states are

\[
(t\rho, \sqrt{1 - 2t^2\rho}, t\rho), \ t \in [0, 1/\sqrt{2}],
\]

where \( \rho \) minimizes

\[
\min_{f \in \mathcal{A}_s} \int_D |\nabla f|^2 + V f^2 + c_n f^4.
\]
Characterization of ground state $c_s > 0, \ q > 0$

**Proposition**

(1) For $M = 0, \ q > 0, \ u \in \mathbb{G}_{0,q}$ satisfies $u_1 = u_{-1} \equiv 0$

(2) For $M = 1, \ q \geq 0, \ u \in \mathbb{G}_{1,q}$ satisfies $u_0 = u_{-1} \equiv 0$

(3) For $0 < M < 1$ and $q \geq 0, \ u \in \mathbb{G}_{M,q}$ satisfies $u_{-1} < u_1$. 
Phase transition from 2C to 3C

**Theorem**

For $0 < M < 1$, there is a $q_c(M) > 0$ such that for $q > q_c(M)$ (resp. $q < q_c(M)$), $u \in G_{M,q}$ implies $u_0 > 0$ (resp. $u = z^M$).
Key: Mass redistribution reduces kinetic energy

- Mass redistribution: \((u_1, \ldots, u_n) \rightarrow (v_1, \ldots, v_m)\) by
  \[
  v_\ell^2 = \sum_k b_{\ell k} u_k^2, \quad b_{\ell k} \geq 0, \sum_\ell b_{\ell k} = 1.
  \]

- Mass redistribution reduces kinetic energy
  \[
  |\nabla v|^2 \leq |\nabla u|^2
  \]
  \[
  |\nabla v|^2 = |\nabla u|^2 \text{ if and only if } u_j \nabla u_k = u_k \nabla u_j \text{ for every } j \neq k \text{ with } b_{\ell j} b_{\ell k} \neq 0 \text{ for at least one } \ell.
  \]

- Key step
  \[
  \sum_k b_{\ell k} |\nabla u_k|^2 - |\nabla v_\ell|^2 = \begin{cases} 
  \frac{1}{v_\ell^2} \sum_{j<k} b_{\ell j} b_{\ell k} |u_j \nabla u_k - u_k \nabla u_j|^2 & \text{on where } v_\ell > 0 \\
  0 & \text{on where } v_\ell = 0,
  \end{cases}
  \]

- For \(m = 1\), see Lieb and Loss.
Recall: Phase transition from 2C to 3C

Proof.

1. **Claim 1**: For $q$ large enough, $u \in G_{M,q}$ we have $u_0 > 0$.

2. **Claim 2**: Assume for some $q$ there exists $u \in G_{M,q}$ with $u_0 > 0$, then for every $q' > q$, $v \in G_{M,q'}$ satisfies $v_0 > 0$.

3. **Claim 3**: There exist a $q > 0$ such that $u \in G_{M,q}$ implies $u = z$ (i.e. $u_0 = 0$).
Claim 1: For $q \gg 1$, $u \in \mathbb{G}_{M,q}$, we have $u_0 > 0$.

Proof.

1. Suppose $z \in \mathbb{G}_{M,q}$, then $z$ is independent of $q$;
2. Consider the redistribution to make $\mathcal{E}_{Zee}$ smaller:

   $$v_1^2 = (1 - r)z_1^2, \quad v_0^2 = rz_1^2 + z_{-1}^2, \quad v_{-1}^2 = 0,$$

   where $r$ is chosen to keep $\mathcal{M}[v] = \mathcal{M}[z]$.
3. This redistribution does not increase $H_{kin}$ and leads to

   $$\mathcal{E}_s[z] + \mathcal{E}_{Zee}[z] \leq \mathcal{E}_s[v] + \mathcal{E}_{Zee}[v]$$

4. $q$ has an upper bound by

   $$\left(1 - M\right)q = \mathcal{E}_{Zee}[z] - \mathcal{E}_{Zee}[v] \leq \mathcal{E}_s[v] - \mathcal{E}_s[z],$$

   RHS is independent of $q$. 
Claim 3: $\exists q > 0$ such that $u \in G_{M,q} \Rightarrow u_0 = 0$.

1. For 3C, $q$ has lower bound:
   Consider the redistribution to make $E_{Zee}$ smaller:
   \[
   \begin{align*}
   v_1^2 &= u_1^2 + \frac{1}{2} u_0^2, \\
   v_0^2 &= 0, \\
   v_{-1}^2 &= u_{-1}^2 + \frac{1}{2} u_0^2.
   \end{align*}
   \]

2. This redistribution does not increase $H_{kin}$ and leads to
   \[
   E_s[u] + E_{Zee}[u] \leq E_s[v] + E_{Zee}[v]
   \]
   Then
   \[
   q \int u_0^2 \geq 2c_s \int u_0^2 (u_1 - u_{-1})^2.
   \]
3 Take $q^n \to 0$, $u^n \to u^\infty$ with $u^n \in \mathbb{G}_{M,q^n}$

$$q^n \int (u_0^n)^2 \gtrsim \int \Omega (u_0^1 - u_{-1}^n)^2 \gtrsim \int (u_0^n)^2 \gtrsim \int (u_0^n)^2.$$ 

- $u^n \to u^\infty$ uniformly and $u^\infty \in \mathbb{G}_{M,0}$;
- We have known that $u_1^\infty > u_{-1}^\infty$ when $q = 0$;
- $u^n$ are exponential decay at far field;

4 $\int (u_0^n)^2 = 0$ if $n$ is large enough.
Outline

1. Part 1: Background BECs and spinor BECs
   - What are BECs?
   - Mean field model: Gross-Pitaevskii equation

2. Part 2: Numerics for Ground States of Spin-1 BECs
   - Numerical investigation: no external magnetic field
   - Numerical investigation: in uniform magnetic field

3. Part 3: Analysis for Ground States of Spin-1 BECs
   - Existence and Uniqueness
   - Characterization of the ground states
   - Phase transition diagram

4. Conclusion
Summary of analytic results

- **Existence of ground state** for the case: trap potential with $c_n > 0, |c_s| < c_n$

- **Uniqueness**: for 2C ground state $(c_n, c_s, q > 0)$

- **Characterization of ground states** $(q = 0)$
  - For $c_s < 0$, SMA
  - For $c_s > 0$, 2C $(M \neq 0)$ and SMA $(M = 0)$

- **Characterization of ground states** $(c_n, c_s > 0, q > 0)$
  - If $M = 0$, then nematic state (NS) $(0, 1, 0)$
  - If $0 < M \leq 1$, then $u_{-1} < u_1$

- **Phase transition**: for $c_s > 0$, there exists $q_{2C \rightarrow 3C}(M)$

- **A key lemma**: Mass redistribution reduces kinetic energy.
Thank you for your attention.