Ground States of Spin-1 Bose-Einstein Condensates w/o magnetic field

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[1] Characterization of the ground states of spin-1 Bose-Einstein condensates, ArXiv 11020832v2, 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

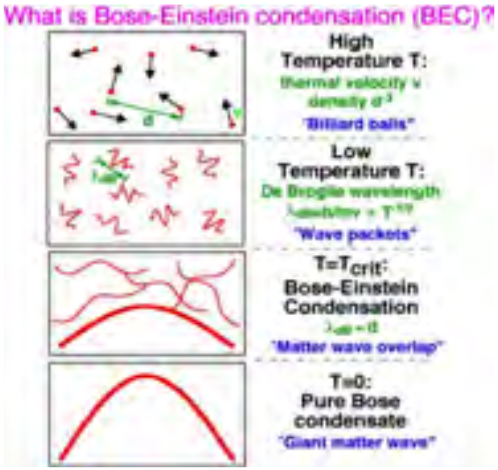
[3] Exploring ground states and excited states of spin-1 Bose-Einstein condensates by continuation methods, Journal of Computational Physics,230 (2011) 2222-2236.

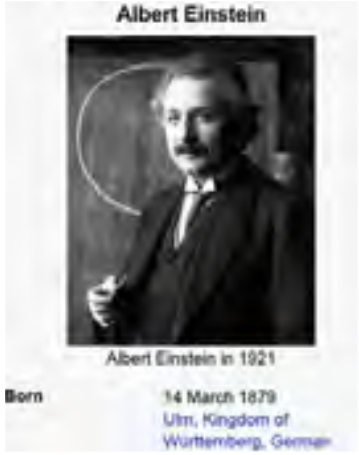
[4] A Complete Study of the Ground State Phase Diagrams of Spin-1 Bose-Einstein Condensates in a Magnetic Field via Continuation Methods, Preprint, CCMSC, NCTU (2014).

Outline

What are BECs? Theory

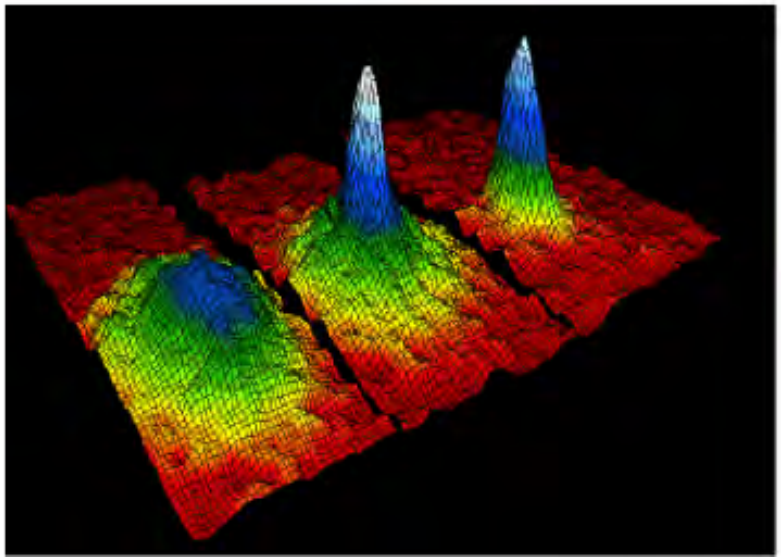
- Boson particles are those particles whose total spin are integers. Alkali atoms are bosons.
- Two identical bosons can occupy the same state.
- Bosons are confined at very low temperature, their de Broglie wave length are long enough. They are coherent and the lowest quantum state become apparent,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





What are BECs? Experiment

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



Eric A. Cornell Wolfgang Ketterle Carl E. Wieman

The Nobel Prize in Physics 2001 was awarded jointly to Eric A. Cornell, Wolfgang Ketterle and Carl E. Wieman *"for the achievement of Bose-Einstein condensation in dilute gases of alkali atoms, and for early fundamental studies of the properties of the condensates"*.

Mean field model for BECs

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

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

- Ultracold and dilute gases, the mean field approximation:

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

- 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-Pitaeviskii equation

- Hamiltonian:

$$\boxed{H = \frac{\hbar^2}{2M_a}|\nabla\psi|^2 + V(x)|\psi|^2 + \frac{\beta}{2}|\psi|^4}\ ,\ \beta = gN$$

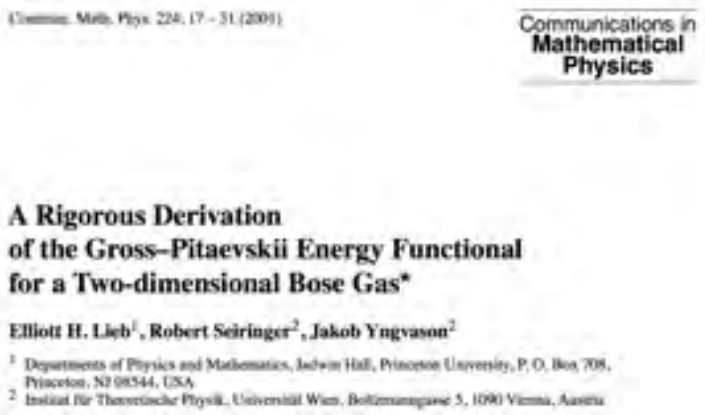
- Energy $\mathbb{E}[\psi] = \int H\, dx$.
- Gross-Pitaevskii equation: $i\hbar\partial_t\psi = \delta\mathbb{E}/\delta\psi^*$.

$$\boxed{i\hbar\partial_t\psi = -\frac{\hbar^2}{2M_a}\nabla^2\psi + V(x)\psi + \beta|\psi|^2\psi}$$

- ψ 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


Commun. Math. Phys. 224, 17 – 31 (2001)

Communications in Mathematical Physics

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]

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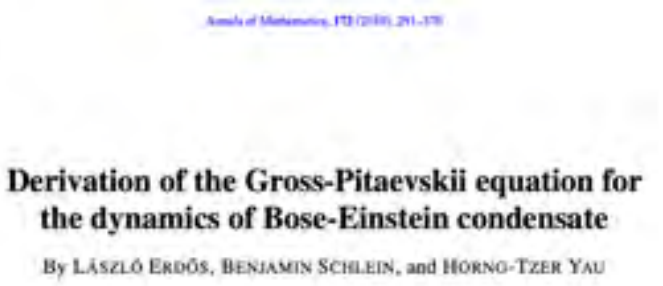
[2] Institut für Theoretische Physik, Universität Wien, Boltzmanngasse 5, 1090 Vienna, Austria


Annals of Mathematics, 172 (2010), 291–370

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 (ψ_1, ψ_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 Ψ, the spin vector $F = \Psi^\dagger \mathbf{F} \Psi \in \mathbb{R}^3$, which is just like a magnetic dipole moment.
- $\mathbf{F} = (F_x, F_y, F_z)$ 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:

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

- $|\Psi|^2 \cdot |\Psi|^2$: spin-independent interaction
- $|\Psi^\dagger \mathbf{F}\Psi|^2$: spin-spin interaction (spin-exchange).
- The total energy $\mathbb{E}[\Psi] = \int H\, dx$.
- The G-P equation

$$i\hbar\partial_t\Psi = \frac{\delta\mathbb{E}}{\delta\Psi^\dagger}$$

Physical parameters

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

	interaction	> 0	< 0
$c_n = \frac{4\pi\hbar^2(a_0+2a_2)}{3M_a}$	spin-independent	repulsive	attractive
$c_s = \frac{4\pi\hbar^2(a_2-a_0)}{3M_a}$	spin-exchange	antiferromagnetic	ferromagnetic

	c_n	c_s	
^{87}Rb	7.793	-0.0361	ferromagnetic
^{23}Na	15.587	0.4871	anti-ferromagnetic

Spinor BEC in uniform magnetic field

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

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

- Gauge invariant: energy is invariant under transform

$$\Psi \to e^{i\phi} R_z(\alpha)\Psi$$

- This leads to two conservation laws:
  - Total number of atoms

$$\boxed{\int (|\psi_1|^2 + |\psi_0|^2 + |\psi_{-1}|^2)\, dx = N}$$

  - Total magnetization

$$\boxed{\int (|\psi_1|^2 - |\psi_{-1}|^2)\, dx = M}$$

The ground state problem

Ground state problem

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

where

- $\mathbb{E}[\Psi] = \int H\,dx$
- $H = H_{kin} + H_{pot} + H_n + H_s + H_{Zee}$
- $n_j = |\psi_j|^2$,
- $n = n_1 + n_0 + n_{-1}$
- $m = n_1 - n_{-1}$

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

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

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

- 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:

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

- Spin-exchange interaction

	interaction	$c_s < 0$(ferro)	$c_s > 0$(antiferro)
(n_1, n_{-1})	$-c_s n_1 n_{-1}$	repulsive	attractive
(n_0, n_1)	$c_s n_0 n_1$	attractive	repulsive
(n_0, n_{-1})	$c_s n_0 n_{-1}$	attractive	repulsive

Spinor BECs, theory and experiments

VOLUME 81, NUMBER 4 PHYSICAL REVIEW LETTERS 27 JULY 1998

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}Na, ^{39}K, and ^{87}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}He-A. [S0031-9007(98)06714-3]

PACS numbers: 03.75.Fi, 05.30.Jp

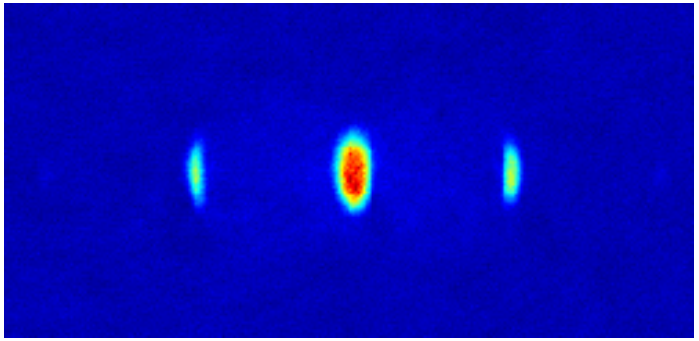


Figure : University of Hamburg 2006: First 1D-lattice at the spinor experiment. As a first step towards the exploration of magnetism of spinor quantum gases in periodic potential we have successfully loaded a BEC into a standing wave potential using a Ti:Sa laser at 830nm. The figure shows an absorbtion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

Outline

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

$$
\begin{aligned}
(\mu+\lambda)\psi_1 &= \tilde{H}_n\psi_1 + c_s(n_1+n_0-n_{-1})\psi_1 + c_s\bar{\psi}_{-1}\psi_0^2 \\
\mu\psi_0 &= \tilde{H}_n\psi_0 + c_s(n_1+n_{-1})\psi_0 + 2c_s\psi_{-1}\bar{\psi}_0\psi_1 \\
(\mu-\lambda)\psi_{-1} &= \tilde{H}_n\psi_{-1} + c_s(n_0+n_{-1}-n_1)\psi_{-1} + c_s\bar{\psi}_1\psi_0^2
\end{aligned}
$$

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

$$\boldsymbol{F}(\boldsymbol{x},\tau) = \boldsymbol{0}$$

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

- The solution is a curve $\boldsymbol{x}(\tau)$, or $\boldsymbol{u}(\tau) := [\boldsymbol{x}(\tau), \tau]$.

Pseudo arclength continuation method-2

- PACM: Continuation method to find $\boldsymbol{u}(\cdot)$ by iteration from $\boldsymbol{u}_i$ to $\boldsymbol{u}_{i+1}$ with $\boldsymbol{F}(\boldsymbol{u}_i) = \boldsymbol{0}$ and $\boldsymbol{F}(\boldsymbol{u}_{i+1}) = \boldsymbol{0}$:
- Prediction:
  - Find tangent: $\dot{\boldsymbol{u}}_i = [\dot{\boldsymbol{x}}_i, \dot{\tau}_i]$ by solving

    $$\mathcal{D}\boldsymbol{F}(\boldsymbol{u}_i(s))\dot{\boldsymbol{u}}_i = \boldsymbol{0}, \mathcal{D}\boldsymbol{F}(\boldsymbol{u}_i(s)) = [\boldsymbol{F}_{\boldsymbol{x}}(\boldsymbol{u}_i(s)), \boldsymbol{F}_{\tau}(\boldsymbol{u}_i(s))]\,.$$

  - Euler predictor: $\boldsymbol{u}_{i+1}^{(1)} = \boldsymbol{u}_i + \delta_i \dot{\boldsymbol{u}}_i$
- Correction:
  - Orthogonal projection

    $$\begin{cases} \boldsymbol{F}(\boldsymbol{u}_{i+1}) = \boldsymbol{0}, \\ (\boldsymbol{u}_{i+1} - \boldsymbol{u}_{i+1}^{(1)}) \cdot \dot{\boldsymbol{u}}_i = 0, \end{cases}$$

  - Solved by Newton's method

Pseudo arclength continuation method-3

- Initialization
  - Starting from $(c_n, c_s) = (0, 0)$: the linear eigenvalue problem:
$$(-\frac{\hbar^2}{2M_a}\nabla^2 + V)\tilde{\psi} = \tilde{\mu}\tilde{\psi}.$$
  - Define a single mode approximation solution by
$$\tilde{\Psi} = (\gamma_1, \gamma_0, \gamma_{-1})\tilde{\psi}$$
where
$$\gamma = (1 + M, \sqrt{2(1 - M^2)}, 1 - M)/2 \qquad \text{(3C)}$$
$$\gamma = (\sqrt{1 + M}, 0, \sqrt{1 - M})/\sqrt{2} \qquad \text{(2C)}$$
  - Find the initial state $\boldsymbol{x}_0$ by solving $\boldsymbol{F}(\boldsymbol{x}, 0) = \boldsymbol{0}$ by Newton's method with initial $(\tilde{\Psi}, \tilde{\mu}, 0, 0)$.

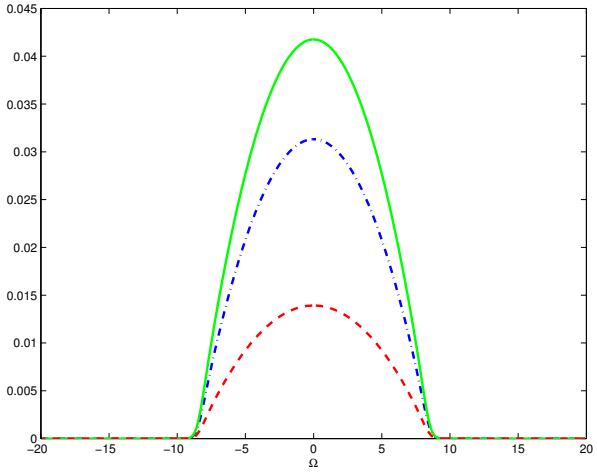
Numerical investigation: no external magnetic field

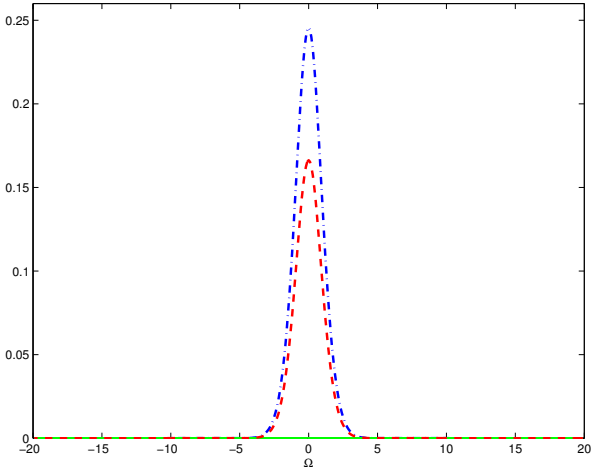
Goal: Study the structures of ground state and excited states as c_s varies.

- Experiment 1 (^{87}Rb: Ferromagnetic)
  - $V = 0,\ M = 0.2$
  - $c_s \in (-0.5, -0.2)$
- Experiment 2 (^{23}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: $\mathcal{A}_1 = \{\mathbf{u} \in \mathcal{A} \,|\mathbf{u} = (\gamma_1, \gamma_0, \gamma_{-1})\rho\}$
- 2C: $\mathcal{A}_2 = \{\mathbf{u} \in \mathcal{A} \,|u_0 \equiv 0\}$





Numerical investigation: uniform magnetic field

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

$$H_{Zee} = \sum_{j=-1}^{1} E_j(B) n_j$$
$$= q(n_1 + n_{-1}) + p(n_1 - n_{-1}) + E_0 n$$

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

$$\boxed{\mathbb{E}[\Psi] = \int \left(H + q(n_1 + n_{-1})\right) dx + E_0 N + pM}$$

$$H = H_{kin} + H_{pot} + H_n + H_s$$

- Ground state problem

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

- Important observation: $q \uparrow \;\Rightarrow\; n_{\pm 1} \downarrow$

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 ϵ, M, perform Pseudo Arclength Continuity Method with continuation parameter: q ranging from 0 to 0.5.

Antiferromagnetic systems: $\epsilon = 0.5$

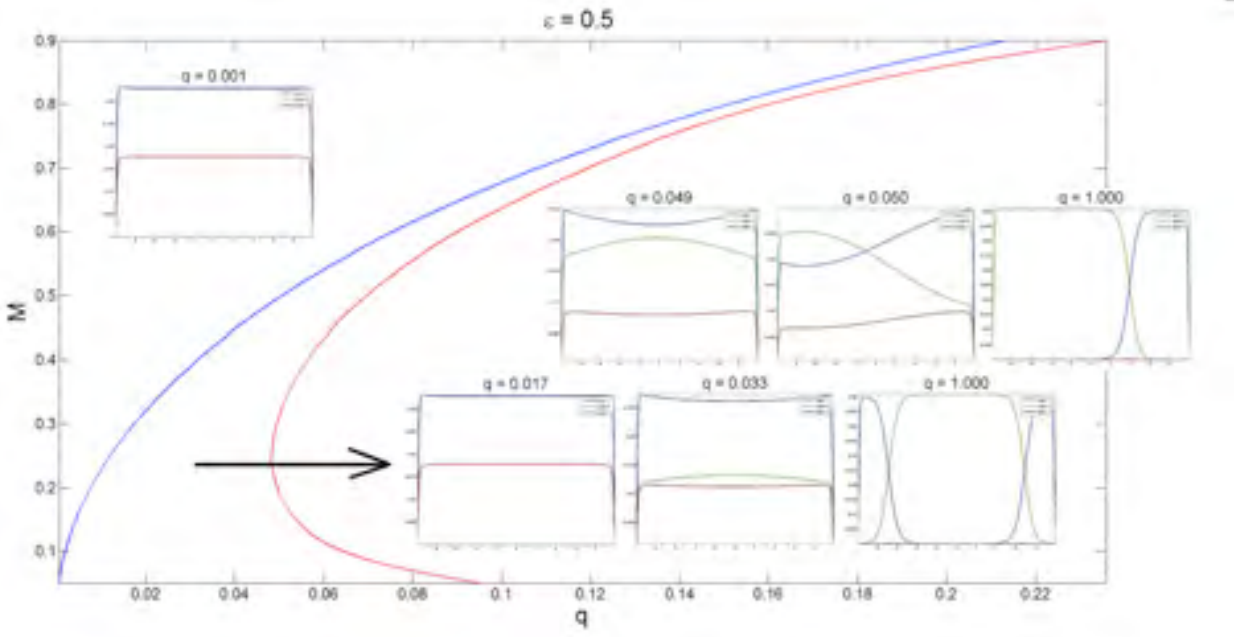
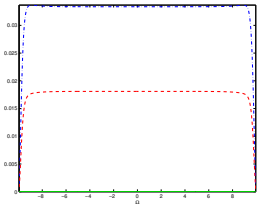
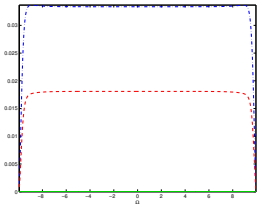
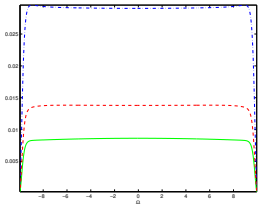
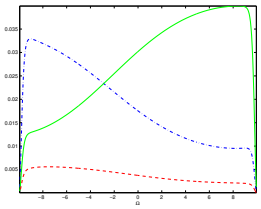
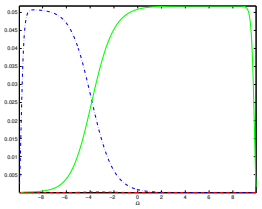
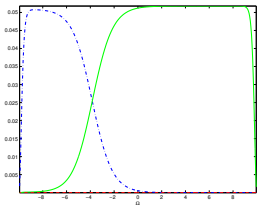


Figure : $\epsilon = 0.5$. Blue line is the transition: 2C $\rightarrow$ 3C (symmetric). Red line is the transition: 3C (symmetric) $\rightarrow$ NS+2C.

Table : (Case 1) Ground state patterns of antiferromagnetic BEC (^{23}Na) with $M = 0.3$ in the constant potential.

	$q = -1$	$q = 0$	$q = 0.02582$
State	2C	2C	3C
Profile			

	$q = 0.1115$	$q = 1$	$q = 3$
State	2C+NS	2C+NS	MS+NS
Profile			

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 ϵ, M, perform Pseudo Arclength Continuity Method with continuation parameter: q ranging from 0 to -0.5.

Ferromagnetic systems: $\epsilon = 0.5$

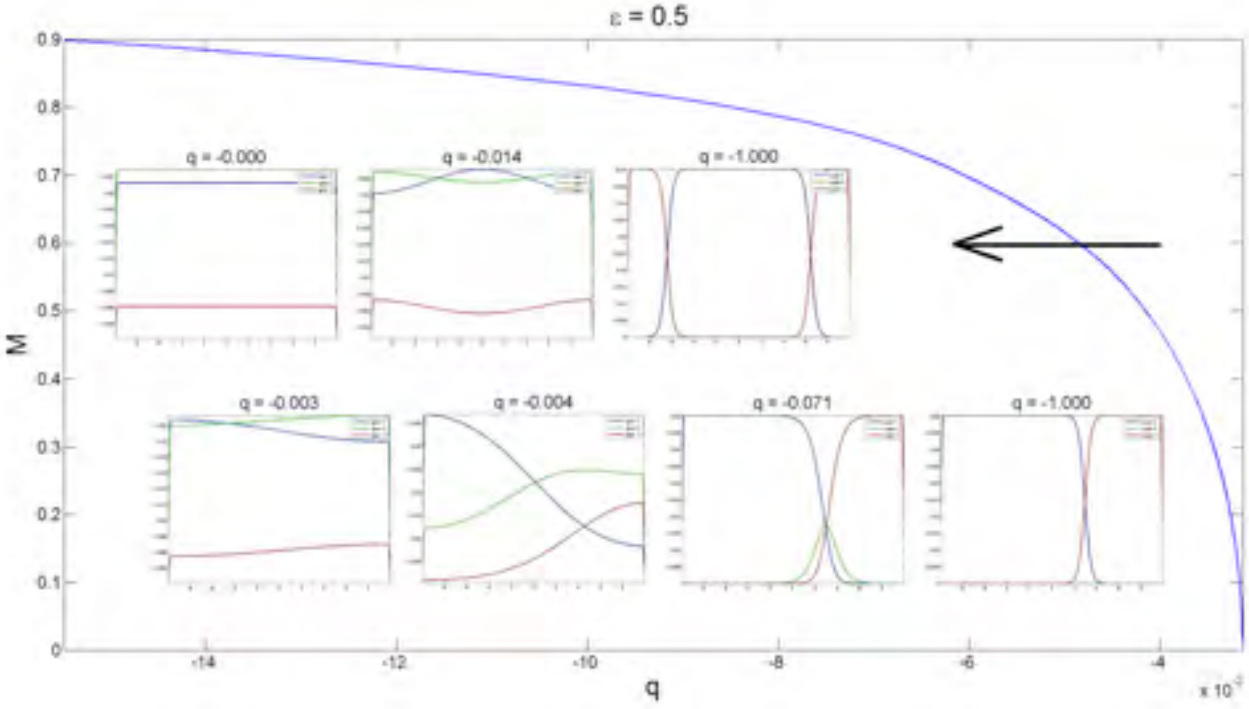
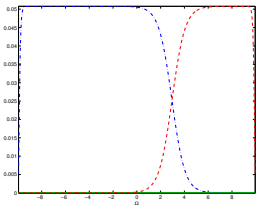
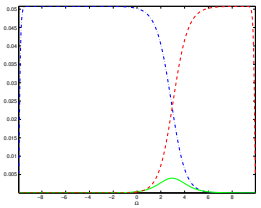
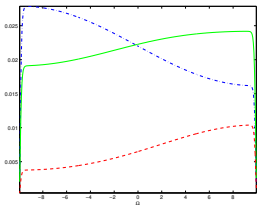
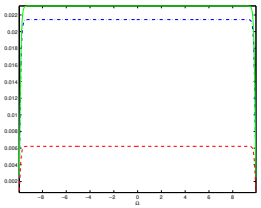
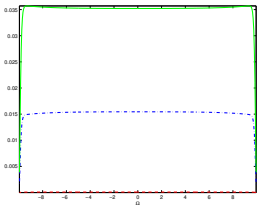
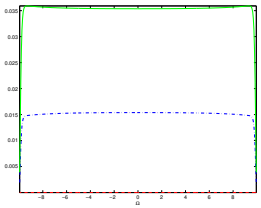


Figure : $\epsilon = 0.5$. Blue line is the transition: 3C (symmetric) $\rightarrow$ NS+2C.

Table : (Case 3) Ground state patterns of ferromagnetic BEC (^{87}Rb) with $M = 0.3$ in the constant potential.

	$q = -1$	$q = -0.2035$	$q = -0.01416$
State	MS+MS	MS+MS+NS	2C+NS
Profile			

	$q = 0$	$q = 1$	$q = 5$
State	3C	3C	2C$_{\{1,0\}}$
Profile			

Experimental Results: Phase transition 2C → 3C

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Phase diagram of spin-1 antiferromagnetic Bose-Einstein condensates

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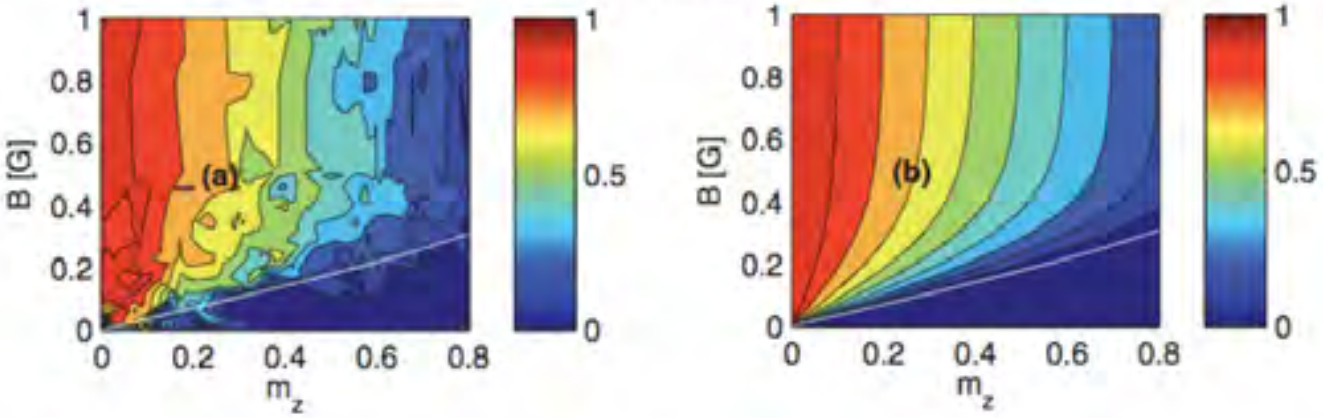


FIG. 3. (Color online) (a) Experimental phase diagram showing the population n_0 of the $m = 0$ Zeeman state versus magnetization and applied magnetic field B. The plot shows a contour interpolation through all data points, with magnetization ranging from 0 to 0.8. T white line is the predicted critical 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 $T = 0$ K.

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: $q_{2C \to 3C}$, $q_{3C \to 2C+NS}$.
- For $q < q_{2C \to 3C}$, the 2C state is independent of q.
- For $q > q_{3C \to 2C+NS}$, 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 ϵ.

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: $q_{3C \to 2C+NS}$.
- For $q > q_{3C \to 2C+NS}$, 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}.

Outline

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

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

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

where $\rho = |\mathbf{u}|$.

Admissible class

- Function class

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

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

- Admissible class

$$\mathbb{A} = \{\mathbf{u} \in \mathbb{B} \,|\, \mathcal{N}[\mathbf{u}] = 1,\ \mathcal{M}[\mathbf{u}] = M\}$$

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

$$\mathbb{G}_{M,q} = \{\mathbf{u} \in \mathbb{A} \,|\, \mathcal{E}[\mathbf{u}] = E_g(M, q)\}$$

Existence

Theorem (Existence)

$\mathbb{G} \neq \emptyset$, i.e. there does exist a ground state. Furthermore, for each u_j, either $u_j \equiv 0$ or $u_j > 0$ 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 $H_n + H_s \leq C|\mathbf{u}|^4$.
- Strong maximum principle: $u_j > 0$ or $u_j \equiv 0$.

Uniqueness

Theorem

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

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

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

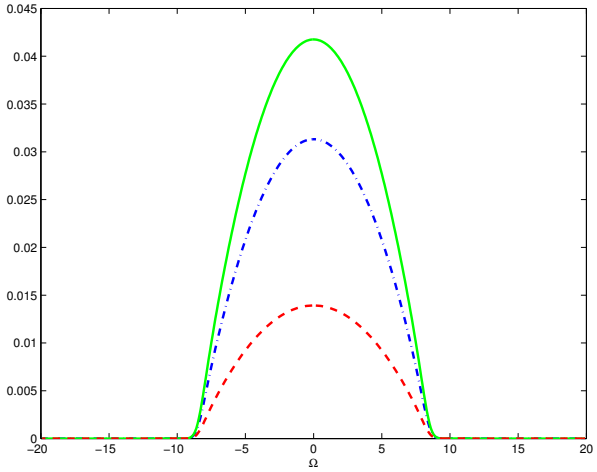
- $\int q(z_1^2 + z_{-1}^2)\, dx = qN$.

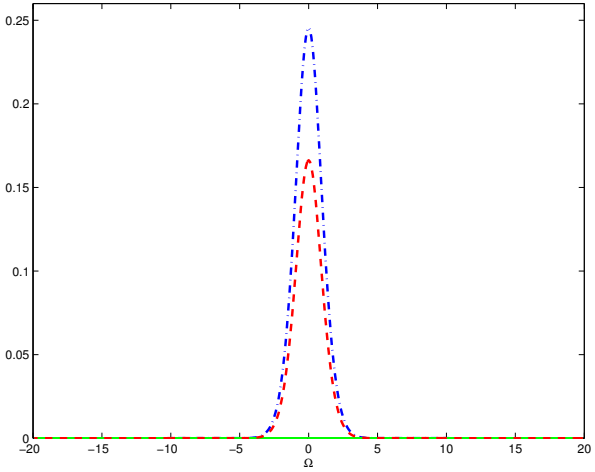
Remark. The ground states may not be unique in general!

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: $\mathcal{A}_1 = \{\mathbf{u} \in \mathcal{A} \,|\mathbf{u} = (\gamma_1, \gamma_0, \gamma_{-1})\rho\}$
- 2C: $\mathcal{A}_2 = \{\mathbf{u} \in \mathcal{A} \,|u_0 \equiv 0\}$





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* $\mathbf{u} \in \mathcal{A}$, *define* $\rho = |\mathbf{u}|$ *and*

$$\begin{cases} \gamma_1^\star &= \frac{1}{2}\left(1 + \frac{M}{N}\right) \\ \gamma_0^\star &= \sqrt{\frac{1}{2}\left(1 - \frac{M^2}{N^2}\right)} \\ \gamma_{-1}^\star &= \frac{1}{2}\left(1 - \frac{M}{N}\right). \end{cases}$$

Then $H(\boldsymbol{\gamma}^\star \rho) \leq H(\mathbf{u})$;

(ii) *if* $\mathbf{u} \in \mathbb{G} \cap (C^2(D))^3$, *then* $\mathbf{u} = \boldsymbol{\gamma}^\star \rho$.

Here, $\mathbb{G}$ 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 $(c_s > 0)$,

(i) *Given any* $\mathbf{u} \in \mathcal{A}$, *define* $\widetilde{\mathbf{u}} = (\widetilde{u}_1, \widetilde{u}_0, \widetilde{u}_{-1})$

$$\widetilde{u}_0 \equiv 0, \ \sum \widetilde{u}_j^2 = \sum u_j^2, \ \widetilde{u}_1^2 - \widetilde{u}_{-1}^2 = u_1^2 - u_{-1}^2$$

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

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

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 ρ minimizes

$$\min_{f \in \mathcal{A}_s} \int_D |\nabla f|^2 + V f^2 + c_n f^4.$$

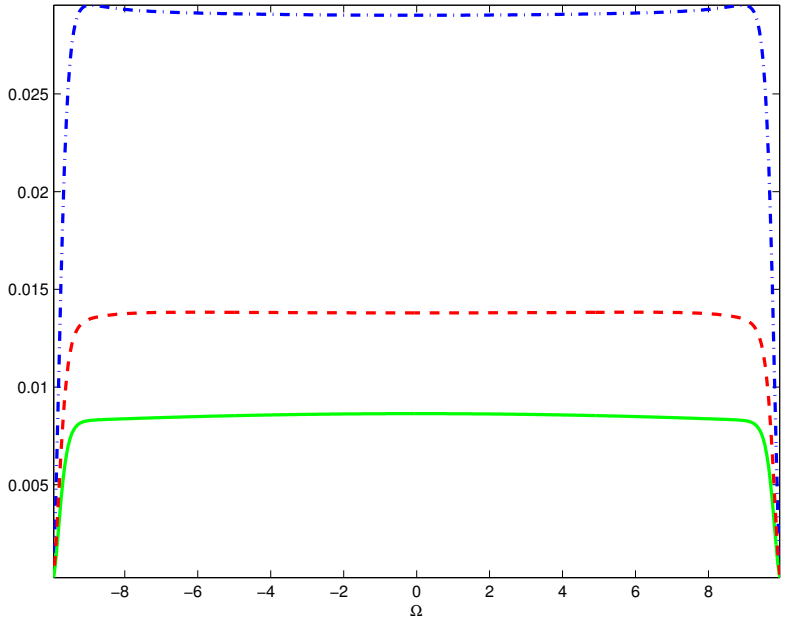
Characterization of ground state $c_s > 0$, $q > 0$

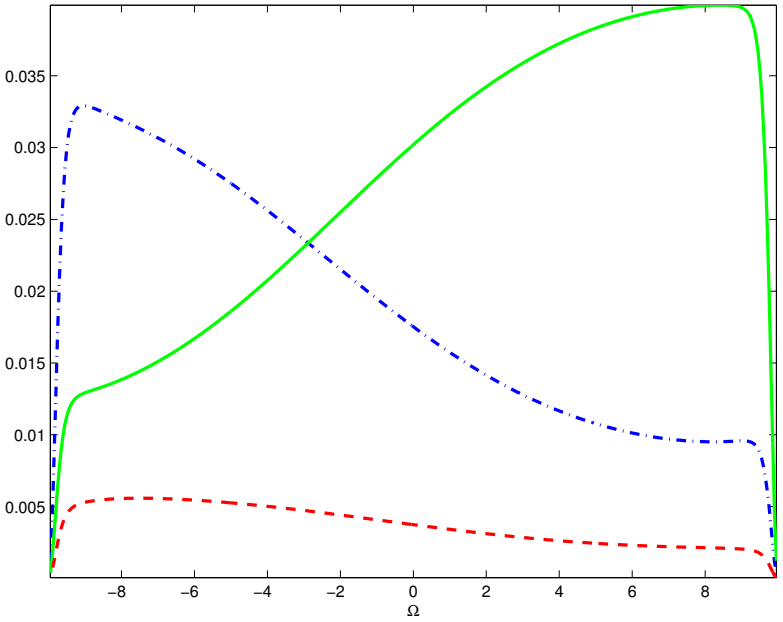
Proposition

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

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

(3) *For* $0 < M < 1$ *and* $q \geq 0$, $\mathbf{u} \in \mathbb{G}_{M,q}$ *satisfies* $u_{-1} < u_1$.

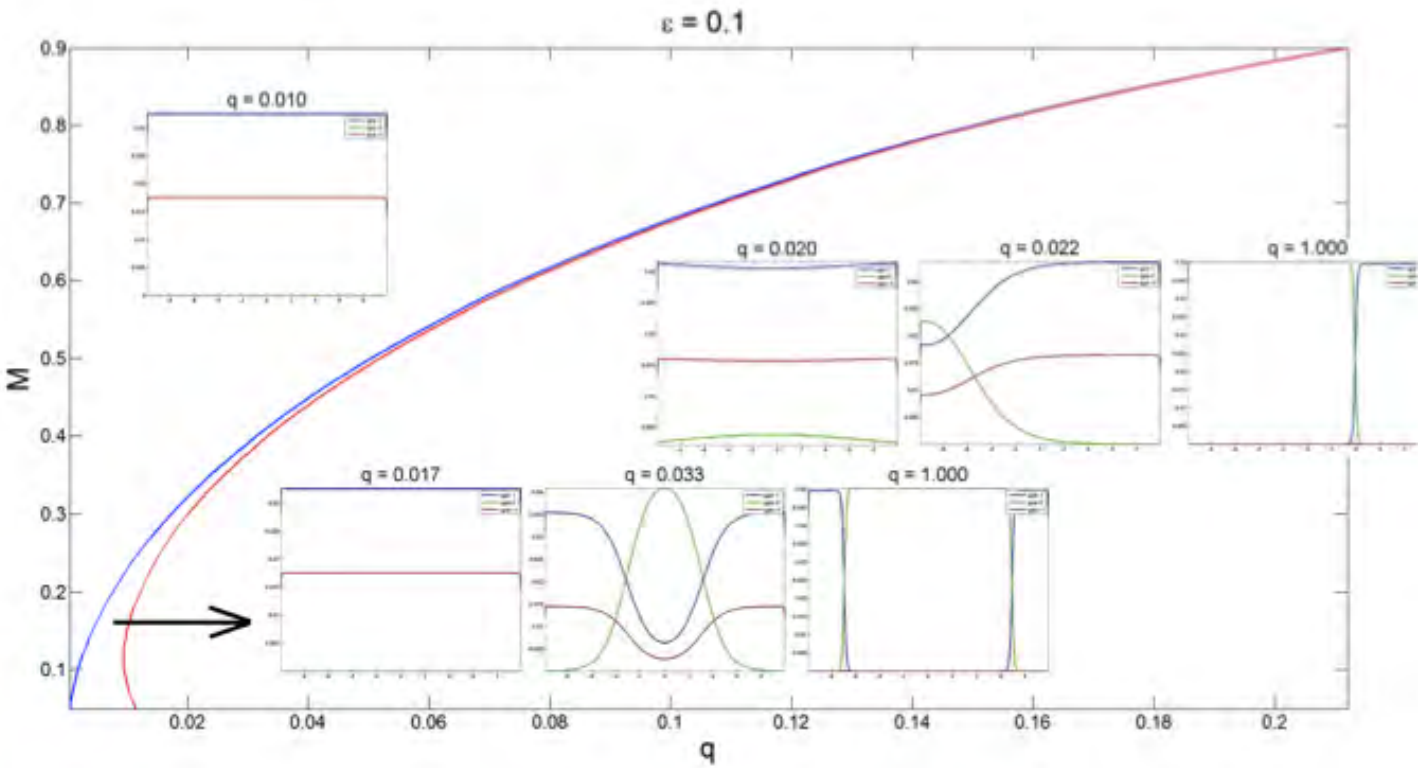




Phase transition from 2C to 3C

Theorem

For $0 < M < 1$, *there is a* $q_c(M) > 0$ *such that for* $q > q_c(M)$ *(resp.* $q < q_c(M)$*),* $\mathbf{u} \in \mathbb{G}_{M,q}$ *implies* $u_0 > 0$ *(resp.* $\mathbf{u} = \mathbf{z}^M$*).*



Key: Mass redistribution reduces kinetic energy

- Mass redistribution: $(u_1, ..., u_n) \to (v_1, ..., v_m)$ by

$$\boxed{v_\ell^2 = \sum_k b_{\ell k} u_k^2}, \; b_{\ell k} \geq 0, \sum_\ell b_{\ell k} = 1.$$

- Mass redistribution reduces kinetic energy

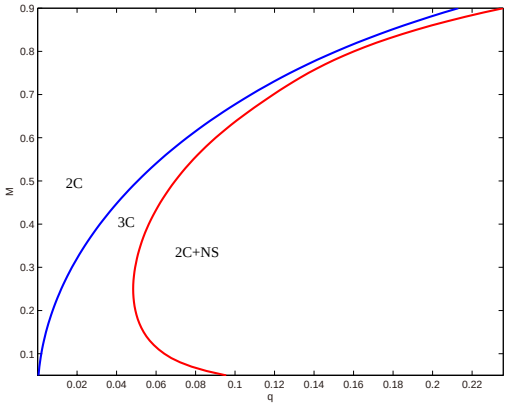
$$\boxed{|\nabla \mathbf{v}|^2 \leq |\nabla \mathbf{u}|^2}$$

- $|\nabla \mathbf{v}|^2 = |\nabla \mathbf{u}|^2$ if and only if $u_j \nabla u_k = u_k \nabla u_j$ for every $j \neq k$ with $b_{\ell j} b_{\ell k} \neq 0$ for at least one ℓ.
- Key step

$$\sum_k b_{\ell k} |\nabla u_k|^2 - |\nabla v_\ell|^2 = \begin{cases} \dfrac{1}{v_\ell^2} \displaystyle\sum_{j<k} b_{\ell j} b_{\ell k} |u_j \nabla u_k - u_k \nabla u_j|^2 & \text{on where } v_\ell > 0 \\ 0 & \text{on where } v_\ell = 0, \end{cases}$$

- For $m = 1$, see Lieb and Loss.

Recall: Phase transition from 2C to 3C



Proof.

1. Claim 1: For q large enough, $\mathbf{u} \in \mathbb{G}_{M,q}$ we have $u_0 > 0$.
2. Claim 2: Assume for some q there exists $\mathbf{u} \in \mathbb{G}_{M,q}$ with $u_0 > 0$, then for every $q' > q$, $\mathbf{v} \in \mathbb{G}_{M,q'}$ satisfies $v_0 > 0$.
3. Claim 3: There exist a $q > 0$ such that $\mathbf{u} \in \mathbb{G}_{M,q}$ implies $\mathbf{u} = \mathbf{z}$ (i.e. $u_0 = 0$).

Claim 1: For $q >> 1$, $\mathbf{u} \in \mathbb{G}_{M,q}$, we have $u_0 > 0$.

Proof.

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

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

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

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

4. q has an upper bound by

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

   RHS is independent of q.

Claim 3: $\exists q > 0$ such that $\mathbf{u} \in \mathbb{G}_{M,q} \Rightarrow u_0 = 0$.

1. For 3C, q has lower bound:

   Consider the redistribution to make $\mathcal{E}_{Zee}$ smaller:

$$\begin{cases} v_1^2 = u_1^2 + \frac{1}{2}u_0^2, \\ v_0^2 = 0, \\ v_{-1}^2 = u_{-1}^2 + \frac{1}{2}u_0^2. \end{cases}$$

2. This redistribution does not increase H_{kin} and leads to

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

   Then

$$q \int u_0^2 \geq 2c_s \int u_0^2 (u_1 - u_{-1})^2.$$

3 Take $q^n \to 0$, $\mathbf{u}^n \to \mathbf{u}^\infty$ with $\mathbf{u}^n \in \mathbb{G}_{M,q^n}$

$$q^n \int (u_0^n)^2 \gtrsim \int_\Omega (u_0^n)^2 (u_1^n - u_{-1}^n)^2 \gtrsim \int_\Omega (u_0^n)^2 \gtrsim \int (u_0^n)^2.$$

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

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

Outline

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 $q_{2C \to 3C}(M)$
- A key lemma: Mass redistribution reduces kinetic energy.

Thank you for your attention.