Continuation Method for Spin-1 BEC and Zeeman effect

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Outline

- Spin-1 BEC
  - Continuous normalized gradient flow (CNGF)
  - Pseudo-arclength continuation method (PACM)
- Spin-1 BEC in magnetic field
- Numerical Results
- Conclusions
1. Spin-1 BEC
- Model

\[ E[\Psi] = \int_{\mathbb{R}^3} \left\{ \frac{\hbar^2}{2M_a} |\nabla \Psi|^2 + V_{ext}(r)|\Psi|^2 + \frac{1}{2} c_n |\Psi|^4 + \frac{1}{2} c_s (\Psi^* S \Psi)^2 \right\} \, dr, \]

- \( \hbar \) : Planck constant
- \( M_a \) : atomic mass
- \( V_{ext} \) : external trapping potential
  - consider a harmonic trap: \( V_{ext}(r) = \frac{M_a}{2} (\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \)
  - \( \omega_x, \omega_y \) and \( \omega_z \) : trap frequencies
- \( \Psi = (\psi_1, \psi_0, \psi_{-1})^T \) : three-component wave function
- \( S = (S_x, S_y, S_z) \) : spin-1 Pauli operator
1. Spin-1 BEC
- Model

\[ E[\Psi] = \int_{\mathbb{R}^3} \left\{ \frac{\hbar^2}{2M_a} |\nabla \Psi|^2 + V_{\text{ext}}(r) |\Psi|^2 + \frac{1}{2} c_n |\Psi|^4 + \frac{1}{2} c_s (\Psi^* S \Psi)^2 \right\} \, dr, \]

\[
c_n = \frac{4\pi \hbar^2}{3M_a} (a_0 + a_2) \\
c_s = \frac{4\pi \hbar^2}{3M_a} (a_2 - a_0) 
\]

<table>
<thead>
<tr>
<th>Interaction</th>
<th>&gt; 0</th>
<th>&lt; 0</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c_n)</td>
<td>spin-independent</td>
<td>repulsive</td>
</tr>
<tr>
<td>(c_s)</td>
<td>spin-exchange</td>
<td>anti-ferromagnetic</td>
</tr>
</tbody>
</table>

- \(a_0(a_2)\): the s-wave scattering length
1. Spin-1 BEC
- Model

- $n_m = |\psi_m|^2$ : density of each component
- $n = n_1 + n_0 + n_{-1}$ : total density
- $N_m = \int n_m dr$ : population of each hyperfine state
- $N = N_1 + N_0 + N_{-1}$ : total number of atoms
- $M = N_1 - N_{-1}$ : magnetization
Three coupled Gross–Pitaevskii equations

\[
\begin{align*}
(\mu + \lambda)\psi_1 &= \tilde{H}_n\psi_1 + g_s(n_1 + n_0 - n_{-1})\psi_1 + g_s\bar{\psi}_{-1}\psi_0^2, \\
\mu\psi_0 &= \tilde{H}_n\psi_0 + g_s(n_1 + n_{-1})\psi_0 + 2g_s\bar{\psi}_{-1}\psi_0\psi_1, \\
(\mu - \lambda)\psi_{-1} &= \tilde{H}_n\psi_{-1} + g_s(n_0 + n_{-1} - n_1)\psi_{-1} + g_s\bar{\psi}_1\psi_0^2,
\end{align*}
\]

\[N_1 + N_0 + N_{-1} = 1\]

and

\[N_1 - N_{-1} = M\]

\[\tilde{H}_n = -\frac{\nabla^2}{2} + \tilde{V}_{\text{ext}}(r) + g_n n \quad \text{and} \quad \tilde{V}_{\text{ext}}(r) = \frac{1}{2\omega^2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)\]

\[g_n = \frac{4\pi(a_0 + 2a_2)}{3d_s}N \quad \text{and} \quad g_s = \frac{4\pi(a_2 - a_0)}{3d_s}N\]
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)


\[
\partial_t \phi_1(x, t) = \left[ \frac{1}{2} \nabla^2 - V(x) - (\beta_n + \beta_s) (|\phi_1|^2 + |\phi_0|^2) - (\beta_n - \beta_s) |\phi_{-1}|^2 \right] \phi_1
\]

(2.13) \quad -\beta_s \phi_{-1}^2 + [\mu_\Phi(t) + \lambda_\Phi(t)] \phi_1 = -H_1 \phi_1 + [\mu_\Phi(t) + \lambda_\Phi(t)] \phi_1,

\[
\partial_t \phi_0(x, t) = \left[ \frac{1}{2} \nabla^2 - V(x) - (\beta_n + \beta_s) (|\phi_1|^2 + |\phi_{-1}|^2) - \beta_n |\phi_0|^2 \right] \phi_0
\]

(2.14) \quad -2\beta_s \phi_{-1} \phi_0 \phi_1 + \mu_\Phi(t) \phi_0 = -H_0 \phi_0 + \mu_\Phi(t) \phi_0,

\[
\partial_t \phi_{-1}(x, t) = \left[ \frac{1}{2} \nabla^2 - V(x) - (\beta_n + \beta_s) (|\phi_{-1}|^2 + |\phi_0|^2) - (\beta_n - \beta_s) |\phi_1|^2 \right] \phi_{-1}
\]

(2.15) \quad -\beta_s \phi_0^2 \phi_1 + [\mu_\Phi(t) - \lambda_\Phi(t)] \phi_{-1} = -H_{-1} \phi_{-1} + [\mu_\Phi(t) - \lambda_\Phi(t)] \phi_{-1}.
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)

\[
\mu_\Phi(t) = \frac{R_\Phi(t) D_\Phi(t) - M_\Phi(t) F_\Phi(t)}{N_\Phi(t) R_\Phi(t) - M_\Phi^2(t)}, \quad \lambda_\Phi(t) = \frac{N_\Phi(t) F_\Phi(t) - M_\Phi(t) D_\Phi(t)}{N_\Phi(t) R_\Phi(t) - M_\Phi^2(t)},
\]

with

\[
N_\Phi(t) = \int_{\mathbb{R}^d} \left[ |\phi_{-1}(x, t)|^2 + |\phi_0(x, t)|^2 + |\phi_1(x, t)|^2 \right] dx,
\]

(2.17)

\[
M_\Phi(t) = \int_{\mathbb{R}^d} \left[ |\phi_1(x, t)|^2 - |\phi_{-1}(x, t)|^2 \right] dx,
\]

(2.18)

\[
R_\Phi(t) = \int_{\mathbb{R}^d} \left[ |\phi_1(x, t)|^2 + |\phi_{-1}(x, t)|^2 \right] dx,
\]

(2.19)

\[
D_\Phi(t) = \int_{\mathbb{R}^d} \left\{ \sum_{j=-1}^{1} \left( \frac{1}{2} |\nabla \phi_j|^2 + V(x) |\phi_j|^2 \right) + 2(\beta_n - \beta_s) |\phi_1|^2 |\phi_{-1}|^2 + \beta_n |\phi_0|^4 \\
+ (\beta_n + \beta_s) \left[ |\phi_1|^4 + |\phi_{-1}|^4 + 2 |\phi_0|^2 (|\phi_1|^2 + |\phi_{-1}|^2) \right] \\
+ 2 \beta_s \left( \bar{\phi}_{-1} \phi_0^2 \phi_1 + \phi_{-1} \phi_0^2 \phi_1 \right) \right\} dx,
\]

(2.20)

\[
F_\Phi(t) = \int_{\mathbb{R}^d} \left\{ \frac{1}{2} (|\nabla \phi_1|^2 - |\nabla \phi_{-1}|^2) + V(x) (|\phi_1|^2 - |\phi_{-1}|^2) \\
+ (\beta_n + \beta_s) \left[ |\phi_1|^4 - |\phi_{-1}|^4 + |\phi_0|^2 (|\phi_1|^2 - |\phi_{-1}|^2) \right] \right\} dx.
\]

(2.21)
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)

**Theorem 2.2.** For any given initial data

\begin{equation}
\Phi(x, 0) = (\phi_1(x, 0), \phi_0(x, 0), \phi_{-1}(x, 0))^T := \Phi^{(0)}(x), \quad x \in \mathbb{R}^d,
\end{equation}

satisfying

\begin{equation}
N_\Phi(t = 0) := N_\Phi^{(0)} = 1, \quad M_\Phi(t = 0) := M_\Phi^{(0)} = M,
\end{equation}

the CNGF (2.13)–(2.15) is mass and magnetization conservative and energy-diminishing, i.e.,

\begin{equation}
N_\Phi(t) \equiv N_\Phi(t = 0) = 1, \quad M_\Phi(t) \equiv M_\Phi(t = 0) = M, \quad t \geq 0,
\end{equation}

\begin{equation}
E(\Phi(\cdot, t)) \leq E(\Phi(\cdot, s)) \quad \text{for any} \ t \geq s \geq 0.
\end{equation}
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)

To prove

\[ \frac{dN_\Phi(t)}{dt} = 2\mu_\Phi(t)N_\Phi(t) + 2\lambda_\Phi(t)M_\Phi(t) - 2D_\Phi(t) \]
\[ = 2N_\Phi(t) \frac{R_\Phi(t)D_\Phi(t) - M_\Phi(t)F_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M^2_\Phi(t)} + 2M_\Phi(t) \frac{N_\Phi(t)F_\Phi(t) - M_\Phi(t)D_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M^2_\Phi(t)} - 2D_\Phi(t) \]
\[ (2.28) \quad = 2D_\Phi(t) - 2D_\Phi(t) \equiv 0, \quad t \geq 0. \]

\[ \frac{dM_\Phi(t)}{dt} = 2\mu_\Phi(t)M_\Phi(t) + 2\lambda_\Phi(t)R_\Phi(t) - 2F_\Phi(t) \]
\[ = 2M_\Phi(t) \frac{R_\Phi(t)D_\Phi(t) - M_\Phi(t)F_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M^2_\Phi(t)} + 2R_\Phi(t) \frac{N_\Phi(t)F_\Phi(t) - M_\Phi(t)D_\Phi(t)}{N_\Phi(t)R_\Phi(t) - M^2_\Phi(t)} - 2F_\Phi(t) \]
\[ (2.31) \quad = 2F_\Phi(t) - 2F_\Phi(t) \equiv 0, \quad t \geq 0. \]

\[ \frac{dE(\Phi(t))}{dt} = \mu_\Phi(t) \frac{dN_\Phi(t)}{dt} + \lambda_\Phi(t) \frac{dM_\Phi(t)}{dt} - 2 \int_{\mathbb{R}^d} \left[ |\partial_t \phi_{-1}|^2 + |\partial_t \phi_0|^2 + |\partial_t \phi_1|^2 \right] d\mathbf{x} \]
\[ = -2 \int_{\mathbb{R}^d} \left[ |\partial_t \phi_{-1}|^2 + |\partial_t \phi_0|^2 + |\partial_t \phi_1|^2 \right] d\mathbf{x} \leq 0, \quad t \geq 0. \]
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)

Fig. 2. Time evolution of the mass $N$ and magnetization $M$ (left) and energy $E$ (right) for the discretization (3.32)–(3.34) with $\beta_n = 87.16$ and $\beta_s = -1.7481$ and initial data (4.2) with $\alpha = 0.1$. 
1. Spin-1 BEC
- Continuous normalized gradient flow (CNGF)

- Ground state and the corresponding energy of spin-1 BECs.
- However, at each time step, a nonlinear system must be solved.
  - CNGF or imaginary time method:
    - Time independent problem $$\rightarrow$$ Virtual time dependent problem
  - The computational cost is very expensive.
  - Only ground state solution can be achieved.
1. Spin-1 BEC
   - Pseudo-arclength continuation method (PACM)


- Yueh-Cheng Kuo, Wen-Wei Lin, Shih-Feng Shieh, and Weichung Wang,
1. Spin-1 BEC
- Pseudo-arclength continuation method (PACM)

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

- \( \tilde{H}_n = -\frac{\nabla^2}{2} + V_{\text{ext}}(r) + g_n n \)
- \( g_n = \frac{4\pi(a_0+2a_2)}{3d_s} N \)
- \( g_s = \frac{4\pi(a_2-a_0)}{3d_s} N \)
- Mass: \( N_1 + N_0 + N_{-1} = 1 \)
- Magnetization: \( N_1 - N_{-1} = M \) with \( -1 \leq M \leq 1 \)
- Potential: \( V_{\text{ext}}(r) = \frac{1}{2}(\gamma_x^2 x^2 + \gamma_y^2 y^2 + \gamma_z^2 z^2) \)

with \( \gamma_x = \frac{\omega_x}{\omega_m}, \gamma_y = \frac{\omega_y}{\omega_m} \) and \( \gamma_z = \frac{\omega_z}{\omega_m} \)
1. Spin-1 BEC
- Pseudo-arclength continuation method (PACM)

- The coupling constants depend on scattering lengths and total number of atoms.
- Scattering lengths can be tuned by Feshbach resonance.
- Continuation method:
  1. Fix \( N \) and change scattering lengths to vary \( g_n \), \( g_s \) or only \( g_s \).
  2. Fix scattering lengths and change \( N \) to vary \( g_n \), \( g_s \).
- Define the solution curve:
  \[ C = \{ u(s) = (v(s), \tau(s)) \mid G(u(s)) = 0, \ s \in \mathbb{R} \} \]
  \[ g_n = \frac{4\pi(a_0 + a_2)}{3d_s} N \]
  \[ g_s = \frac{4\pi(a_2 - a_0)}{3d_s} N \]
1. Spin-1 BEC
- Pseudo-arclength continuation method (PACM)

\[
\begin{align*}
(\mu + \lambda)\psi_1 &= \tilde{H}_n \psi_1 + g_s (n_1 + n_0 - n_{-1}) \psi_1 + g_s \bar{\psi}_{-1} \psi_0^2, \\
\mu \psi_0 &= \tilde{H}_n \psi_0 + g_s (n_1 + n_{-1}) \psi_0 + 2g_s \psi_{-1} \bar{\psi}_0 \psi_{+1}, \\
(\mu - \lambda)\psi_{-1} &= \tilde{H}_n \psi_{-1} + g_s (n_0 + n_{-1} - n_1) \psi_{-1} + g_s \bar{\psi}_{-1} \psi_0^2,
\end{align*}
\]

\[
\int (n_1 + n_0 + n_{-1}) \, dr = 1
\]

\[
\int (n_1 - n_{-1}) \, dr = M
\]

- Rewrite three coupled time-independent GPEs as :

  \- \( \tau \) : the continuation parameter

  \[
  G(v, \tau) = 0 \quad \text{where} \quad v = (\psi_1, \psi_0, \psi_{-1}, \mu, \lambda)^T \in \mathbb{R}^{3n+2}
  \]

  \- \( n \) : the number of grid points
1. Spin-1 BEC

- Pseudo-arclength continuation method (PACM)

➢ To trace the solution curve: the prediction-correction process

✓ Prediction vector: tangent vector of the solution curve at current sol.

Solve the linear system:

\[ \mathcal{D}G(u_i(s)) \dot{u}(s) = 0 \]

- \( u_i(s) = (v_i(s), \tau_i(s)) \): current sol. lying on \( C \).
- \( \dot{u}(s) = (\dot{v}(s), \dot{\tau}(s)) \): tangent vector of \( C \) at \( u_i(s) \).
- \( \mathcal{D}G(u_i(s)) = [G_v(u_i(s)) \ G_\tau(u_i(s))] \in \mathbb{R}^{(3n+2) \times (3n+3)} \): Jacobian matrix of \( G \) at \( u_i(s) \).

Normalize the prediction vector.

✓ Euler predictor:

\[ u^+ = u_i + \eta \dot{u} \quad \text{or} \quad \begin{bmatrix} v^+(s) \\ \tau^+(s) \end{bmatrix} = \begin{bmatrix} v_i(s) \\ \tau_i(s) \end{bmatrix} + \eta \begin{bmatrix} \dot{v}(s) \\ \dot{\tau}(s) \end{bmatrix} \]

where \( \eta \) is the stepsize of the search direction.
Corrector:

✓ solve the nonlinear system by Newton's method

\[
\begin{align*}
G(u(s)) &= 0, \\
P_t(u(s)) &= 0,
\end{align*}
\]

where

\[
P_t(u(s)) = \dot{u}(s)^\top u(s) - \dot{u}(s)^\top u^+(s) = 0
\]

is the hyperplane whose normal vector is the prediction vector.

✓ Jacobian matrix in kth iteration is

\[
J_{i,k} = \begin{bmatrix} G_v & G_\tau \\ \frac{\partial P_t}{\partial v} & \frac{\partial P_t}{\partial \tau} \end{bmatrix} = \begin{bmatrix} G_v & G_\tau \\ \dot{v}(s)^\top & \dot{\tau}(s) \end{bmatrix}
\]

✓ a new approximate solution at the solution curve

\[
u_{i,k+1}(s) = u_{i,k}(s) - J_{i,k}^{-1} \begin{bmatrix} G(u_{i,k}(s)) \\ P(u_{i,k}(s)) \end{bmatrix}
\text{ or }
\begin{bmatrix} v_{i,k+1}(s) \\ \tau_{i,k+1}(s) \end{bmatrix} = \begin{bmatrix} v_{i,k}(s) \\ \tau_{i,k}(s) \end{bmatrix} - J_{i,k}^{-1} \begin{bmatrix} G(v_{i,k}(s), \tau_{i,k}(s)) \\ P_t(v_{i,k}(s), \tau_{i,k}(s)) \end{bmatrix}.
\]
Detections of bifurcation:

- monitor the singularity of the Jacobian matrix
- Compute the smallest eigenvalue of Jacobian matrix, say $\mu_i$
- $\mu_{i-1}, \mu_i$ change signs $\rightarrow$ detect the singular point
- At the bifurcation point,
  the corresponding singular vector $\rightarrow$ prediction vector
1. Spin-1 BEC
- Pseudo-arclength continuation method (PACM)

Find the initial point of a continuation method

- At $\tau = 0$, i.e. no coupling interactions

  → compute the smallest eigenpair of linear Schrödinger equation, $u_0$

  → However, $DG(u_0)$ is singular.

- Mass and magnetization conservation:

  \[
  \begin{align*}
  N_1 + N_0 + N_{-1} &= 1 \\
  N_1 - N_{-1} &= M \text{ with } -1 \leq M \leq 1
  \end{align*}
  \]

  → infinite many choices of population of each component
1. Spin-1 BEC
   - Pseudo-arclength continuation method (PACM)

✓ For a sufficient small $\tau$ → Newton method → only two types of solutions

- Two-component solution (2C)
  $$(N_1, N_0, N_{-1}) = \left( \frac{1 + M}{2}, 0, \frac{1 - M}{2} \right)$$

- Three-component solution (3C)
  $$(N_1, N_0, N_{-1}) = \left( \frac{1 - N_0 + M}{2}, \frac{1 - M^2}{2}, \frac{1 - N_0 - M}{2} \right)$$

✓ Equilibrium property:

- PRL 99, 020404 (2007) and PRA 80, 023602 (2009)
1. Spin-1 BEC
- Pseudo-arclength continuation method (PACM)

\[ 2|0\rangle \iff |1\rangle + |-1\rangle \]

<table>
<thead>
<tr>
<th>( c_s )</th>
<th>Interaction</th>
<th>Reaction</th>
<th>Ground state</th>
</tr>
</thead>
<tbody>
<tr>
<td>Negative (e.g., ( ^{87}\text{Rb} ))</td>
<td>Ferromagnetic</td>
<td>( 2</td>
<td>0\rangle \iff</td>
</tr>
<tr>
<td>Positive (e.g., ( ^{23}\text{Na} ))</td>
<td>Anti-ferromagnetic</td>
<td>( 2</td>
<td>0\rangle \rightarrow</td>
</tr>
</tbody>
</table>
Atomic Parameters:

<table>
<thead>
<tr>
<th></th>
<th>$a_0$</th>
<th>$a_2$</th>
<th>$c_n$</th>
<th>$c_s$</th>
<th>Interaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{87}$Rb</td>
<td>101.8</td>
<td>100.4</td>
<td>7.793</td>
<td>-0.0361</td>
<td>ferromagnetic</td>
</tr>
<tr>
<td>$^{23}$Na</td>
<td>50.0</td>
<td>55.0</td>
<td>15.587</td>
<td>0.4871</td>
<td>anti-ferromagnetic</td>
</tr>
</tbody>
</table>

- Since $a_0$ and $a_2$ are comparable, $c_s$ is actually small.
- Small spin-dependent interactions are nonnegligible.
- Sign of $c_s$ → different ground-state structure.

- Rb (Rubidium), Na (Sodium)
1. Spin-1 BEC
- PACM ~ Simulation.1 87Rb

- $^{87}$Rb
- $V_{ext}(x) = \frac{1}{2}x^2$
- Interaction: repulsive, ferromagnetic
- Parameters: $M = 0.2$, $g_n = 0.08716N$ and $g_s = -0.0017481N$
- Fix the scattering lengths $a_0$ and $a_2$
  
  vary the total number of atom $N$
- Continuation parameters: $g_n$ and $g_s$ with $\tau = 10^{-5} \sim 10^4$
- Initial solution:
  
  - 3C (0.36, 0.48, 0.16) $\rightarrow$ Ground state
  - 2C (0.6, 0.0, 0.4) $\rightarrow$ Excited state

\[ g_n = \frac{4\pi(a_0+2a_2)}{3d_s} N \]
\[ g_s = \frac{4\pi(a_2-a_0)}{3d_s} N \]
1. Spin-1 BEC

- PACM ~ Simulation.1  87Rb

Comparison of PACM and CNGF for computing the ground state energy of spin-1 $^{87}$Rb BEC with $M = 0.2$. In addition, the excited state energies obtained by PACM are also listed in the last columns. The numbers in parentheses are the computed absolute errors of Eq. (10) in 2-norm.

<table>
<thead>
<tr>
<th>$N$</th>
<th>CNGF [14]</th>
<th>CNGF-base</th>
<th>PACM Ground state ($\tilde{N}_{3C}$)</th>
<th>PACM Excited state ($\tilde{N}_{2C}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100</td>
<td>1.77618</td>
<td>1.77417</td>
<td>1.77409 (6.45 × 10^{-14})</td>
<td>1.79437 (6.27 × 10^{-14})</td>
</tr>
<tr>
<td>200</td>
<td>2.70597</td>
<td>2.70265</td>
<td>2.70259 (6.44 × 10^{-14})</td>
<td>2.73573 (5.65 × 10^{-14})</td>
</tr>
<tr>
<td>500</td>
<td>4.86973</td>
<td>4.86360</td>
<td>4.86357 (6.15 × 10^{-14})</td>
<td>4.92547 (6.72 × 10^{-14})</td>
</tr>
<tr>
<td>1000</td>
<td>7.67568</td>
<td>7.66675</td>
<td>7.66672 (5.70 × 10^{-14})</td>
<td>7.75977 (6.27 × 10^{-14})</td>
</tr>
<tr>
<td>5000</td>
<td>22.30065</td>
<td>22.31135</td>
<td>22.31134 (6.56 × 10^{-14})</td>
<td>22.42107 (7.43 × 10^{-14})</td>
</tr>
<tr>
<td>10,000</td>
<td>35.21286</td>
<td>35.40153</td>
<td>35.40073 (7.74 × 10^{-14})</td>
<td>35.51103 (8.40 × 10^{-14})</td>
</tr>
</tbody>
</table>
1. Spin-1 BEC

- PACM ~ Simulation.1  87Rb

- Blue dash-dotted : 1
- Green solid : 0
- Red dotted : -1

Fig. 2. Densities of the ground state of spin-1 $^{87}$Rb BEC with different number of atoms $N = 100$ (top left), $N = 1000$ (top right), $N = 5000$ (bottom left) and $N = 10000$ (bottom right). The $m = 1$, 0, and $-1$ components are depicted by blue dash-dotted, green solid and red dashed lines, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)
1. Spin-1 BEC
- PACM ~ Simulation.1  87Rb

\[
(N_1, N_0, N_{-1}) = \left( \frac{1 - N_0 + M}{2}, \frac{1 - M^2}{2}, \frac{1 - N_0 - M}{2} \right)
\]
1. Spin-1 BEC

- PACM ~ Simulation.2  23Na

- $^{23}\text{Na}$

- $V_{ext}(x) = \frac{1}{2}x^2$

- Interaction: repulsive, antiferromagnetic

- Parameters: $M = 0 \sim 0.8$, $g_n = 0.0241$ and $g_s = 0.00075$

- Fix the scattering lengths $a_0$ and $a_2$

  vary the total number of atom $N$

- Continuation parameters: $g_n$ and $g_s$ with $\tau = 10^{-5} \sim 10^4$

- Initial solution:

  $- 3C \left( \frac{1-N_0+M}{2}, \frac{1-M^2}{2}, \frac{1-N_0-M}{2} \right) \rightarrow \text{Excited state}$

  $- 2C \left( \frac{1+M}{2}, 0, \frac{1-M}{2} \right) \rightarrow \text{Ground state}$
1. Spin-1 BEC
- PACM ~ Simulation.2  23Na

Comparison of the PACM and CNGF for computing the ground state energy of spin-1 $^{23}$Na BEC for different magnetization $M$.

<table>
<thead>
<tr>
<th>$M$</th>
<th>CNGF [15]</th>
<th>PACM</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_{2C} = (\frac{1+M}{2}, 0, \frac{1-M}{2})$</td>
<td>$N_{3C} = (\frac{1-N_0+M}{2}, \frac{1-M}{2}, \frac{1-N_0-M}{2})$</td>
</tr>
<tr>
<td>0</td>
<td>15.2485</td>
<td>15.2485</td>
</tr>
<tr>
<td>0.2</td>
<td>15.2599</td>
<td>15.2599</td>
</tr>
<tr>
<td>0.4</td>
<td>15.2945</td>
<td>15.2945</td>
</tr>
<tr>
<td>0.6</td>
<td>15.3537</td>
<td>15.3536</td>
</tr>
<tr>
<td>0.8</td>
<td>15.4405</td>
<td>15.4404</td>
</tr>
</tbody>
</table>
1. Spin-1 BEC
- PACM ~ Simulation.2 23Na

- Ground state $\rightarrow$ 2C solution

- Total number of atom: 10,000
1. Spin-1 BEC

- PACM ~ Simulation.3 \( g_s < g_n < 0 \), attractive, ferromagnetic

- \( g_s < g_n < 0 \)

- Interaction: attractive, ferromagnetic

- A vanishing potential: \( V_{ext} = 0 \)

- Parameters: \( M = 0.2, g_n = -1 \) and \( g_s = -0.2 \sim -5 \)
1. Spin-1 BEC
- PACM ~ Simulation.3 $g_s < g_n < 0$, attractive, ferromagnetic

**Step.1**
- Parameters: $g_n = -1$ and $g_s = -0.2$
- Continuation parameter: $g_n \rightarrow \tau g_n$ and $g_s \rightarrow \tau g_s$
- $C_1 = \{ u | G(u) = 0, \text{with } 10^{-4} \leq \tau \leq 1 \}$
- Initial solution:
  * 3C (0.36, 0.48, 0.16)
  * 2C (0.6, 0, 0.4)

**Step.2**
- Parameters: $g_n = -1$ and $g_s = -0.2$
- Continuation parameter: Fix $g_n$ and vary $g_s \rightarrow \tau g_s$
- $C_2 = \{ u | G(u) = 0, \text{with } 1 \leq \tau \leq 25 \}$
- Initial solution:
  * The target points in **Step.1**.
  * 3C (0.36, 0.48, 0.16) $\rightarrow$ Ground state
  * 2C (0.6, 0, 0.4) $\rightarrow$ Excited state $\rightarrow$ Bifurcation
1. Spin-1 BEC
- PACM ~ Simulation.3 $g_s < g_n < 0$, attractive, ferromagnetic

![Graph]

**Fig. 3.** The energy curves of $c_3^{(2)}$ starting from the points satisfying $\tilde{N}_{2c}$ and $\tilde{N}_{3c}$. 
1. Spin-1 BEC
- PACM ~ Simulation.3  \( g_s < g_n < 0 \)

- Ground state \( \rightarrow \) 3C solution
1. Spin-1 BEC
- PACM ~ Simulation.3 \( g_s < g_n < 0 \)

- Excited state → 2C solution
  - component separation
1. Spin-1 BEC

- PACM ~ Simulation.3 \( g_s < g_n < 0 \)

- Excited state \( \rightarrow \) two-component solution
  - component separation
1. Spin-1 BEC
   - PACM ~ Simulation.3 \( g_s < g_n < 0 \)

✓ Population transfer
- An atom in the \( m_F = 1 \) state may scatter with another atom in the \( m_F = 0 \) state.
1. Spin-1 BEC
- PACM ~ Simulation
$g_s < g_n < 0$

- Component separation
- Population transfer
1. Spin-1 BEC
   - PACM ~ Simulation.4  $g_n < 0$ : attractive, $g_s > 0$ antiferro.

   - $g_n < 0$ and $g_s > 0$
   - Interaction : attractive, antiferromagnetic
   - External potential : $V_{ext} = 0.05x^2$
   - Parameters : $M = 0.2$, $g_n = -1$ and $g_s = 0.2 \sim 5$

**Step.1**
- Parameters : $g_n = -1$ and $g_s = 0.2$
- Continuation parameter : $g_n \rightarrow \tau g_n$ and $g_s \rightarrow \tau g_s$
- $C_1 = \{u|G(u) = 0, \text{with } 10^{-4} \leq \tau \leq 1\}$
- Initial solution :
  * 3C (0.6, 0, 0.4)
  * 2C (0.36, 0.48, 0.16)

**Step.2**
- Parameters : $g_n = -1$ and $g_s = 0.2$
- Continuation parameter : Fix $g_n$ and vary $g_s \rightarrow \tau g_s$
- $C_2 = \{u|G(u) = 0, \text{with } 1 \leq \tau \leq 25\}$
- Initial solution :
  * The target points in **Step.1**.
  * 2C (0.6, 0, 0.4) → Ground state
  * 3C (0.36, 0.48, 0.16) → Excited state → Bifurcation
1. Spin-1 BEC
- PACM ~ Simulation.4  \( g_n < 0 \) : attractive, \( g_s > 0 \) antiferro.

Fig. 9. The energy curves of \( c_2^{(d)} \) starting from the points satisfying \( \tilde{N}_{2c} \) and \( \tilde{N}_{3c} \).
1. **Spin-1 BEC**
   - PACM ~ Simulation 4 \( g_n < 0 \), \( g_s > 0 \)
1. Spin-1 BEC
- PACM ~ Simulation.4 \( g_n<0, g_s>0 \)
1. Spin-1 BEC
- PACM ~ Simulation.4  \( g_n < 0 \), \( g_s > 0 \)
1. Spin-1 BEC
- PACM ~ Simulation.4 $g_n < 0$, $g_s > 0$
1. Spin-1 BEC
- PACM ~ Simulation.4 \( g_n < 0, g_s > 0 \)
2. Spin-1 BEC in magnetic field
- Model

\[ i\hbar \partial_t \psi_1 = \left[ H + E_1 + c_0 n + c_2 (n_1 + n_0 - n_{-1}) \right] \psi_1 + c_2 \bar{\psi}_{-1} \psi_0^2, \]  
\[ \text{Eq. (1)} \]

\[ i\hbar \partial_t \psi_0 = \left[ H + E_0 + c_0 n + c_2 (n_1 + n_{-1}) \right] \psi_0 + 2c_2 \psi_{-1} \bar{\psi}_0 \psi_1, \]  
\[ \text{Eq. (2)} \]

\[ i\hbar \partial_t \psi_{-1} = \left[ H + E_{-1} + c_0 n + c_2 (n_{-1} + n_0 - n_1) \right] \psi_{-1} + c_2 \psi_0^2 \bar{\psi}_1, \]  
\[ \text{Eq. (3)} \]

\[ E_l \ (l = -1, 0, 1) \] is the Zeeman energy of spin component \( m_F = l \) in the uniform magnetic field.
2. Spin-1 BEC in magnetic field

- Model

\[ p_0 = \frac{1}{2}(E_1 - E_{-1}) \approx -\frac{\mu_B B}{2}, \]

\[ q_0 = \frac{1}{2}(E_1 + E_{-1} - 2E_0) \approx \frac{\mu_B^2 B^2}{4E_{\text{hfs}}}. \]

\[ p = \frac{p_0}{\hbar \omega_m}, \]

\[ q = \frac{q_0}{\hbar \omega_m}. \]

In order to minimize any possible numerical error that can be caused by large Zeeman energy when (1)-(2) are solved numerically, we shift the energy level and set the zero energy to be \( E_0 \), which is equivalent to replacing

\[ \psi_l \rightarrow \psi_l \exp(-\frac{iE_0 t}{\hbar}). \]
2. Spin-1 BEC in magnetic field
- Model

\[ \mu_1 \phi_1 = \left[ H + q + p + \beta_n n + \beta_s (n_1 + n_0 - n_{-1}) \right] \phi_1 + \beta_s \bar{\phi}_{-1} \phi_0^2, \tag{14} \]
\[ \mu_0 \phi_0 = \left[ H + \beta_n n + \beta_s (n_1 + n_{-1}) \right] \phi_0 + 2\beta_s \phi_{-1} \bar{\phi}_0 \phi_1, \tag{15} \]
\[ \mu_{-1} \phi_{-1} = \left[ H + q - p + \beta_n n + \beta_s (n_{-1} + n_0 - n_1) \right] \phi_{-1} + \beta_s \phi_0^2 \bar{\phi}_1. \tag{16} \]

Here $\mu_1$, $\mu_0$, and $\mu_{-1}$ are the chemical potentials of the three components and they satisfy

\[ \mu_1 = \mu + \lambda, \quad \mu_0 = \mu, \quad \mu_{-1} = \mu - \lambda, \tag{17} \]
2. Spin-1 BEC in magnetic field

- CNGF


**FIG. 3:** Ground state of $^{23}$Na with $M = 0.3$ in harmonic potential: (a) $q = 0.1$, (b) $q = 0.5$, and harmonic plus optical lattice potential: (c) $q = 0.1$, (d) $q = 0.5$. 
2. Spin-1 BEC in magnetic field

- CNGF

FIG. 4: (Left) Relative population of each hyperfine component of $^{23}$Na in a harmonic potential (dotted line) and a harmonic plus optical lattice potential (solid line), subject to magnetic field a) $q = 0.02$, (b) $q = 0.1$, and (c) $q = 1.0$. (Right) Relative population of each hyperfine component of $^{23}$Na in a harmonic potential (dotted line) and a harmonic plus optical lattice potential (solid line), subject to magnetic field $q = 0.1$, for (i) $M = 0$, (ii) $M = 0.1$, (iii) $M = 0.3$, (iv) $M = 0.5$, (v) $M = 0.7$, and (vi) $M = 0.9$. 
2. Spin-1 BEC in magnetic field

\[-\text{PACM}\]

\[
\begin{align*}
(\mu + \lambda)\psi_1 &= \tilde{H}_n \psi_1 + (q + p)\psi_1 + g_s (n_1 + n_0 - n_{-1})\psi_1 + g_s \bar{\psi}_{-1} \psi_0^2, \\
\mu \psi_0 &= \tilde{H}_n \psi_0 + g_s (n_1 + n_{-1})\psi_0 + 2g_s \psi_{-1} \bar{\psi}_0 \psi_1, \\
(\mu - \lambda)\psi_{-1} &= \tilde{H}_n \psi_{-1} + (q - p)\psi_{-1} + g_s (n_0 + n_{-1} - n_1)\psi_{-1} + g_s \bar{\psi}_1 \psi_0^2,
\end{align*}
\]

where $p$ and $q$ are the linear Zeeman energy and the quadratic Zeeman energy, respectively.
2. Spin-1 BEC in magnetic field

To solve the problem defined in (1), we define $\tilde{\lambda} = \lambda - p$ and solve the following nonlinear eigenvalue problem by PACM.

\[
\begin{align*}
(\mu + \tilde{\lambda})\psi_1 &= \tilde{H}_n\psi_1 + q\psi_1 + g_s(n_1 + n_0 - n_{-1})\psi_1 + g_s\bar{\psi}_{-1}\psi_0^2, \\
\mu\psi_0 &= \tilde{H}_n\psi_0 + g_s(n_1 + n_{-1})\psi_0 + 2g_s\psi_{-1}\psi_0\psi_1, \\
(\mu - \tilde{\lambda})\psi_{-1} &= \tilde{H}_n\psi_{-1} + q\psi_{-1} + g_s(n_0 + n_{-1} - n_1)\psi_{-1} + g_s\bar{\psi}_1\psi_0^2.
\end{align*}
\]
3. Numerical Results
- PACM $\sim ^{23}\text{Na}$

- $M = 0.7, g_n = 240.8, g_s = 7.5, p = -9411.8, q = 1.0$

- Vary $g_n$, $g_s$ and $q$, $\tau = 0.00001 \sim 1$ (trace forward)

- Three initial solution
3. Numerical Results
- PACM $\sim ^{23}\text{Na}$
3. Numerical Results

- PACM ~ $^{23}\text{Na}$

- $M = 0.7, g_n = 240.8, g_s = 7.5, p = -9411.8, q = 1.0$

- Vary $g_n$, $g_s$ and $q$, $\tau = 0.00001\sim1$ (trace forward)

- Initial solution: 3C (\(N_0 = 0.052445992\))
3. Numerical Results
- PACM ~ $^{23}$Na
3. Numerical Results
- PACM ~ $^{23}\text{Na}$

- $M = 0.7$, $g_n = 240.8$, $g_s = 7.5$, $p = -9411.8$, $q = 1.0$
- Vary $q$, $\tau = 1\sim0.00001$ (trace backward)
- Initial solution : 3C
3. Numerical Results
- PACM $\sim ^{23}\text{Na}$

- Shift p

- Bifurcate at $\tau = 0.16621$
3. Numerical Results
- PACM $\sim ^{23}$Na
3. Numerical Results
- PACM \sim ^{23}\text{Na}
3. Numerical Results

- PACM $\sim ^{23}\text{Na}$
Thanks for your attention!
\[\begin{bmatrix} G_v & G_\tau \end{bmatrix} \begin{bmatrix} \dot{v}(s) \\ \dot{\tau}(s) \end{bmatrix} = 0\]

\[\Rightarrow \dot{v}(s) = G_v^{-1} \cdot G_\tau \cdot \dot{\tau}(s)\]

\[\Rightarrow \dot{v}(s) = G_v^{-1} \cdot G_\tau \quad (\text{choice } \dot{\tau}(s) = \frac{d\tau}{ds} = 1 )\]
Continuation method

Continuation method (Allgower, 1990)

- Homotopy method (1930)
- Example:

\[ F(x) = x^2 - x - 2 + \cos x = 0 \]

\[ F(x, \tau) = x^2 - x - 2 + \tau \cos x = 0 \]

\[ \begin{cases} 
F(x,0) = x^2 - x - 2 + 0 \cdot \cos x = 0 \Rightarrow x = 2 \text{ or } -1 \\
F(x,1) = x^2 - x - 2 + 1 \cdot \cos x = 0 
\end{cases} \]
Continuation method

Starting point: $\tau = 0$, $x = 2$

step.1 $F'(2,0) = 2 \cdot (2) - 1 - 0 \cdot \sin(-1) = 3$

step.2 Predictor $= 2 + \delta \cdot (3) = 2 + 0.01 \cdot (3) = 2.03$

step.3 Use Newton's method to solve

$F(x, 0.1) = 0$ with $\tau = 0.1$
Continuation method

\[ u_{i+1}^{(1)} = u_i + \delta_i \dot{u}_i \]

\[ F(x, \tau) = 0 \]

\( u_{i+1} \): predictor

\( u_{i+1} \): corrector