Chiral and wobbling modes in collective Hamiltonian

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Outline

- Introduction
- Theoretical framework
- Chiral mode in collective Hamiltonian
- Wobbling mode in collective Hamiltonian
- Summary and perspective
Undoubtedly, the investigation of chiral and wobbling modes in atomic nuclei has become one of the hottest topics in nuclear physics.
“Standard” models

- **Triaxial PRM**
  - ✔ Lab frame; quantal model; with quantum tunneling;
  - ✗ Phenomenological

- **Tilted axis cranking (TAC)**
  - ✔ Intrinsic frame; microscopic; self-consistent; mean-field approximation
  - ✗ Semi-classical; no quantum tunneling;

- **Other models**
  - ■ Projected shell model
  - ■ IBFFM
  - ■ Pairing truncated shell model

Frauendorf & Meng, NPA617, 131 (1997)
Peng et al., PRC 68, 044324 (2003)
Koike et al., PRL 93, 172502 (2004)
Zhang et al., PRC 75, 044307 (2007)
Qi et al., PLB 675, 175 (2009)
Lawrie & Shirinda, PLB 689, 66 (2010)
Frauendorf and Döna, PRC 89, 014322 (2014)

...
Descriptions of excitations beyond mean field approximation: RPA

- **TAC + RPA for chiral mode**
  - ✔ Beyond mean field;
  - ✔ Available for chiral vibration
  - ✗ No available for chiral rotation as its small amplitude harmonic vibration approximation;

  *Mukhopadhyay et al., PRL 99, 172501 (2007)*
  *Almehed et al., PRC 83, 054308 (2011)*

- **Cranking + RPA for wobbling mode**
  - ✔ Beyond mean field;
  - ✔ Available for wobbling excitations
  - ✗ Anharmonic behavior in wobbling;

  *Mikhailov & Janssen, PLB 72, 303 (1978)*
  *Marshalek, NPA 331, 429 (1979)*
  *Shimizu & Matsuyanagi, PTP 70, 144 (1983)*
  *Matsuzaki et al., PRC 65, 041303(R) (2002)*

It is thus necessary to search a unified method for studying both chiral and wobbling modes.
Collective Hamiltonian

- Collective Hamiltonian, in terms of a few numbers of collective coordinates and momenta, is an effective method for describing various collective processes which involve small velocities.

- Bohr Hamiltonian describes the collective rotational and vibrational degrees of freedom with the five collective intrinsic variables $\beta$, $\gamma$, and Euler angles $\Omega$ with great successes.

- Based on self-consistent (covariant) density functional theory, five-dimensional collective Hamiltonian has been extensively applied to various mass regions and achieved great successes on the studies of the low-lying excited spectra, shape evolution/transition.

In present work, the collective Hamiltonian for chiral and wobbling modes based on cranking mean field is introduced.
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Collective Hamiltonian

- **Microscopic basis**  Collective Hamiltonian, which aims to describe large amplitude collective motions, can be obtained by
  
  - **Generate coordinate method (GCM)**  Hill&Wheeler, PR 89, 1102 (1953); Ring&Schuck1980
  
  - **Adiabatic time-dependent Hartree-Fock (ATDHF) method**  Baranger&Kumar, NPA 122, 241 (1968); Ring&Schuck1980,
  
  - **Adiabatic self-consistent coordinate method (ASCC)**  Marumori et al., PTP 64, 1294 (1980); Matsuo et al., PTP 103, 959 (2000); Hinohara et al., PRC 82, 064313 (2010); Matsuyanagi et al., JPG 37, 064018 (2010);

  - **Starting point:** time-dependent Hartree-Fock (TDHF) equation
  
  - **Assumptions:**  adiabatic approximation, i.e., the collective motion is slow or collective momenta are small (can be large)
  
  - **Procedure:**  expand the TDHF equations with respect to the collective momenta up to second order

  \[
  \mathcal{H}(q,p) = \langle \phi(q,p)|\hat{H}|\phi(q,p)\rangle = \frac{1}{2} \sum_{ij} B^{ij}(q)p_ip_j + V(q)
  \]

  \[
  B^{ij}(q) = \left. \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} \right|_{p=0} \\
  V(q) = \mathcal{H}(q,p)|_{p=0}
  \]
For chiral and wobbling modes, the orientation angles of angular momentum can be chosen as collective coordinates.

\[(\theta, \varphi)\]

For simplicity, only one collective coordinate is considered here,

\[(\theta, \varphi) \rightarrow \varphi\]

The classical form of a collective Hamiltonian in terms of \(\varphi\) as,

\[\hat{H}_{\text{coll}} = \hat{T}_{\text{kin}}(\varphi) + V(\varphi) = \frac{1}{2}B\dot{\varphi}^2 + V(\varphi)\]

According to general Pauli quantization,

\[\hat{H}_{\text{coll}} = \hat{T}_{\text{kin}}(\varphi) + V(\varphi) = -\frac{\hbar^2}{2\sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} \frac{1}{\sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} + V(\varphi)\]
The collective potential $V(\varphi)$ could be extracted by minimizing the total Routhian surface, obtained by any TAC calculation, with respect to $\theta$ for given $\varphi$.

Mass parameter $B(\varphi)$ could be obtained from TAC calculations by cranking formula

\[
B(\varphi) = 2\hbar^2 \sum_{l \neq 0} \frac{(E_l - E_0)^3 \left| \langle l | \frac{\partial}{\partial \varphi} | 0 \rangle \right|^2}{\left[ (E_l - E_0)^2 - \hbar^2 \Omega^2 \right]^2}
\]

\[
= 2\hbar^2 \sum_{l \neq 0} \frac{(E_l - E_0) \left| \langle l | \hat{r} \left[ \frac{\partial}{\partial \varphi} \right] | 0 \rangle \right|^2}{\left[ (E_l - E_0)^2 - \hbar^2 \Omega^2 \right]^2}
\]
### Basis space

\[ \hat{H}_{\text{coll}} = \hat{T}_{\text{kin}}(\varphi) + V(\varphi) = -\frac{\hbar^2}{2 \sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} \sqrt{B(\varphi)} \frac{1}{\sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} + V(\varphi) \]

#### Symmetry

The collective Hamiltonian keeps the parity conservation with respect to \( \varphi \rightarrow -\varphi \).

#### Basis states

**Basis states with positive parity:**

\[ \psi_n(\varphi) = \sqrt{\frac{2}{\pi}} \frac{\cos(2n - 1)\varphi}{B^{1/4}(\varphi)}, \quad n \geq 1 \]

**Basis states with negative parity:**

\[ \psi_n(\varphi) = \sqrt{\frac{2}{\pi}} \frac{\sin 2n\varphi}{B^{1/4}(\varphi)}, \quad n \geq 1 \]

These basis states fulfill the box boundary condition:

\[ \psi_n(\pi/2) = \psi_n(-\pi/2) = 0 \]
minimize $E' = \langle h' \rangle - \frac{1}{2} \sum_{k=1}^{3} J_k \omega_k^2$

$\hat{h}' = \hat{h}_{\text{def}} - \vec{\omega} \cdot \vec{j}$

$B = 2\hbar^2 \sum_{l \neq 0} \frac{(E_l - E_0) \left| \frac{\partial \hat{\omega}}{\partial \varphi} \langle l | \hat{\omega} | 0 \rangle \right|^2}{\left[ (E_l - E_0)^2 - \hbar^2 \Omega^2 \right]^2}$

$\hat{H}_{\text{coll}} = -\frac{\hbar^2}{2 \sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} \frac{1}{\sqrt{B(\varphi)}} \frac{\partial}{\partial \varphi} + V(\varphi)$

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For chiral modes, we consider a system of a high-j particle and a high-j hole coupled to a triaxial rotor.

\[
\hat{h}' = \hat{h}_{\text{def}} - \mathbf{\omega} \cdot \hat{\mathbf{j}},
\]

\[\mathbf{\omega} = (\omega \sin \theta \cos \varphi, \omega \sin \theta \sin \varphi, \omega \cos \theta),\]

\[
\hat{h}_{\text{def}} = \frac{1}{2} C \left\{ \left( \hat{j}_3^2 - \frac{j(j + 1)}{3} \right) \cos \gamma + \frac{1}{2\sqrt{3}} \left( \hat{j}_+^2 + \hat{j}_-^2 \right) \sin \gamma \right\},
\]

\[
E'(\theta, \varphi) = \langle h' \rangle - \frac{1}{2} \sum_{k=1}^{3} J_k \omega_k^2, \quad J_k : \text{moments of inertia},
\]

Parameters:

Configurations: \[\pi(1h_{11/2})^1 \otimes \nu(1h_{11/2})^{-1}\]

Single-j shell Hamiltonian coefficients: \[C_\pi = 0.25 \text{ MeV} \quad C_\nu = -0.25 \text{ MeV}\]

Triaxial deformation: \[\gamma = -30^\circ\]

Moment of inertia: \[J_0 = 40\hbar^2/\text{MeV}\]

Potential energy surface mesh points are represented as:

\[\theta_i = (i - 1) \times 1^\circ, (i = 1, \ldots, 91),\]

\[\varphi_j = (j - 91) \times 1^\circ, (j = 1, \ldots, 181).\]
Total Routhian surfaces

Minima: $\varphi = 0 \rightarrow \varphi \neq 0$; one $\rightarrow$ two

Rotating mode: planar $\rightarrow$ aplanar
With the increase of rotational frequency, the potential barrier $\Delta V$ increases.
For the case of chiral rotation, the chiral vibration frequency is taken as \( \Omega=0 \).

\[
B = 2\hbar^2 \sum_{l \neq 0} \frac{\left| \frac{\partial \tilde{\omega}}{\partial \varphi} \langle l | \hat{J} | 0 \rangle \right|^2}{(E_l - E_0)^3}
\]
Energy spectra

- Energy levels become paired
- Tunneling penetration probability is more and more suppressed
- MχD picture can be obtained Droste et al., EPJA 42, 79 (2009); Chen et al., PRC 82, 067302 (2010); Hamamoto, PRC 88, 024327 (2013).
Chiral patterns

- Wave function and probability distributions

- Wave function
  - symmetric for level 1 and antisymmetric for level 2
  - chiral symmetry broken in the aplanar TAC solutions is restored
  - from chiral vibration to chiral rotation
Going beyond mean field, collective Hamiltonian gives the partner band and well reproduce the PRM results.

The success of the collective Hamiltonian guarantees its application for realistic TAC calculations.
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For **longitudinal and transverse wobblers**, we consider a system of a high-j particle coupled to a triaxial rotor.

\[
\hat{h}' = \hat{h}_{\text{def}} - \boldsymbol{\omega} \cdot \hat{j},
\]

\[
\boldsymbol{\omega} = (\omega \sin \theta \cos \varphi, \omega \sin \theta \sin \varphi, \omega \cos \theta),
\]

\[
\hat{h}_{\text{def}} = \frac{1}{2} C \left\{ (\hat{j}_3^2 - \frac{j(j+1)}{3}) \cos \gamma + \frac{1}{2\sqrt{3}} (\hat{j}_+^2 + \hat{j}_-^2) \sin \gamma \right\},
\]

\[
E'(\theta, \varphi) = \langle h' \rangle - \frac{1}{2} \sum_{k=1}^{3} \mathcal{J}_k \omega_k^2, \quad \mathcal{J}_k : \text{moments of inertia},
\]

Minimizing the total Routhian with respect to \( \theta \) for given \( \varphi \), the collective potential \( V(\varphi) \) is finally obtained.

For **simple wobbler**, the simple triaxial rotor does not couple any particles, the total Routhian is degenerated to

\[
E'(\theta, \varphi) = -\frac{1}{2} \sum_{k=1}^{3} \mathcal{J}_k \omega_k^2:
\]

and similarly the total Routhian is obtained by minimizing the total Routhian with respect to \( \theta \) for given \( \varphi \).
Mass parameter

For a harmonic oscillator:

\[ \Omega = \sqrt{\frac{\text{stiffness}}{\text{mass}}} = \sqrt{\frac{C}{B}} \Rightarrow B = \frac{C}{\Omega^2} \]

➢ For simple wobbler, harmonic approximation (HA) adopted,

\[ V(\varphi) = -\frac{1}{2} \omega^2 (J_1 \cos^2 \varphi + J_2 \sin^2 \varphi) \]
\[ \approx -\frac{1}{2} J_1 \omega^2 + \frac{1}{2} \omega^2 (J_1 - J_2) \varphi^2, \quad \text{for} \ \varphi \to 0^\circ. \quad C = \omega^2 (J_1 - J_2) \]

\[ \hbar \Omega_{\text{wob}} = 2I \sqrt{\left( \frac{\hbar^2}{2J_2} - \frac{\hbar^2}{2J_1} \right) \left( \frac{\hbar^2}{2J_3} - \frac{\hbar^2}{2J_1} \right)} \]
\[ = \frac{\hbar^2 I}{J_1} \sqrt{\frac{(J_1 - J_2)(J_1 - J_3)}{J_3 J_2}} \]
\[ = \hbar \omega \sqrt{\frac{(J_1 - J_2)(J_1 - J_3)}{J_3 J_2}}. \]

\[ B = \frac{J_2 J_3}{J_1 - J_3} \]
For longitudinal and transverse wobblers, harmonic frozen alignment (HFA) approximation Frauendorf&Donau2014PRC adopted,

\[ J_1^*(\omega) = \frac{J_1 \omega + j}{\omega} = J_1 + \frac{j}{\omega} \text{ effective moment of ineritia} \]

\[ V(\varphi) = \langle \hat{h}_{\text{def}} \rangle - \omega j \cos \varphi - \frac{1}{2} \omega^2 (J_1 \cos^2 \varphi + J_2 \sin^2 \varphi) \]

\[ \approx \langle \hat{h}_{\text{def}} \rangle - \omega j (1 - \frac{\varphi^2}{2}) - \frac{1}{2} J_1 \omega^2 + \frac{1}{2} \omega^2 (J_1 - J_2) \varphi^2, \text{ for } \varphi \to 0 \]

\[ = \langle \hat{h}_{\text{def}} \rangle - \frac{1}{2} \omega j - \frac{1}{2} \left( J_1 + \frac{j}{\omega} \right) \omega^2 + \frac{1}{2} \omega^2 \left[ \left( J_1 + \frac{j}{\omega} \right) - J_2 \right] \varphi^2 \]

\[ = \langle \hat{h}_{\text{def}} \rangle - \frac{1}{2} \omega j - \frac{1}{2} J_1^* \omega^2 + \frac{1}{2} \omega^2 \left[ J_1^*(\omega) - J_2 \right] \varphi^2 \quad C = \omega^2 (J_1^*(\omega) - J_2) \]

\[ B(\omega) = \frac{J_2 J_3}{J_1^*(\omega) - J_3} = \frac{J_2 J_3}{(J_1 - J_3) + \frac{j}{\omega}} \]

\[ \hbar \Omega_{\text{wob}} = \sqrt{\frac{J_1^*(\omega) - J_2}{B(\omega)}} \hbar \omega \]

\[ = \hbar \sqrt{\frac{[(J_1 - J_3)\omega + j] [(J_1 - J_2)\omega + j]}{J_2 J_3}} \]
Numerical details

- Deformation parameters: \( \beta = 0.25, \gamma = -30^\circ \)

  1, 2, and 3-axis respectively correspond to short (s), intermediate (i), and long (l) axis.

- Configuration for longitudinal and transverse wobblers: \( \pi (1 h_{11/2})^1 \)

- Moment of inertia:
  - Simple and longitudinal wobblers: rigid body type, \( \mathcal{J}_{1}^{\text{rig}} \) maximal
    \[
    \mathcal{J}_k^{\text{rig}} = \mathcal{J}_0^{\text{rig}} \left[ 1 - \sqrt{\frac{5}{4\pi}} \beta \cos(\gamma - \frac{2\pi}{3} k) \right], \quad \mathcal{J}_0^{\text{rig}} = \frac{256\pi}{15} \hbar^2 / \text{MeV}
    \]
  - Transverse wobbler: irrotational flow type, \( \mathcal{J}_{2}^{\text{irr}} \) maximal
    \[
    \mathcal{J}_k^{\text{irr}} = \mathcal{J}_0^{\text{irr}} \sin^2(\gamma - \frac{2\pi}{3} k), \quad \mathcal{J}_0^{\text{irr}} = 40 \hbar^2 / \text{MeV}
    \]
Wobbling for a triaxial rotor

\[
E'(\theta, \varphi) = -\frac{1}{2} \sum_{k=1}^{3} J_k \omega_k^2
\]

\[
B = \frac{J_2 J_3}{J_1 - J_3}
\]

Chen, Zhang, Zhao, and Meng, PRC 90, 044306 (2014)

- Symmetrical: \( \theta = 90^\circ, \varphi = 0^\circ \)
- Minima: \( \varphi = 0^\circ \)
- Stiffness: larger

Increasing trend of wobbling frequency
Collective Hamiltonian excellently reproduces the TRM results.
Collective potential

Longitudinal wobbler

- Symmetrical: $\varphi = 0^\circ$
- Minima: $(\theta = 90^\circ, \varphi = 0^\circ)$
- Stiffness: larger

Transverse wobbler

- Symmetrical: $\varphi = 0^\circ$
- Minima: from $\varphi = 0^\circ$ to $\varphi \neq 0^\circ$
- Potential barrier: increase
Increasing trend of wobbling frequency
HFA results gradually deviate from PRM with increasing $n$.
Collective Hamiltonian excellently reproduces the PRM results.

Decreasing trend of wobbling frequency
The onset of transitions from the transverse to longitudinal wobbling motions in PRM is not reproduced since the boundary condition used.

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⇒ Summary and perspective
Summary

Based on cranking mean field, by introducing the collective coordinate $\phi$, a collective Hamiltonian is constructed for chiral and wobbling modes.

As it goes beyond the mean-field approximation and includes the quantum tunneling effect, the collective Hamiltonian restores the breaking chiral symmetry and describes chiral vibration and rotation in a unified model.

For wobbling mode, the collective Hamiltonian confirms that the wobbling frequency increases with the rotational frequency in simple and longitudinal wobblers while decreases in transverse one. These variation trends are related to the stiffness of the collective potential.

Perspective

Combine to microscopic TAC for realistic nucleus;

Two dimensional calculations; (preliminary results are obtained)

Thank you for your attention!
Two dimensional Collective Hamiltonian (2DCH)

- In the previous study, the collective Hamiltonian is restricted along $\varphi$ direction.

In the following, a two dimensional collective Hamiltonian (2DCH) is constructed with the collective coordinate $(\theta, \varphi)$, and preliminary results for chiral modes are shown.
**Two dimensional Collective Hamiltonian (2DCH)**

- **Construction of 2DCH**
  - collective coordinate: orientation angles of nucleus \((\theta, \varphi)\)
  
  ![Diagram of orientation angles](Image)

- collective Hamiltonian:

\[
\hat{H}_{\text{coll}} = \hat{T}_{\text{kin}}(\varphi) + V(\varphi)
\]

\[
= -\frac{\hbar^2}{2\sqrt{w}} \left[ \frac{\partial}{\partial \varphi} \frac{B_{\theta\theta}}{\sqrt{w}} \frac{\partial}{\partial \varphi} - \frac{\partial}{\partial \varphi} \frac{B_{\varphi\theta}}{\sqrt{w}} \frac{\partial}{\partial \theta} - \frac{\partial}{\partial \theta} \frac{B_{\varphi\varphi}}{\sqrt{w}} \frac{\partial}{\partial \varphi} + \frac{\partial}{\partial \theta} \frac{B_{\varphi\varphi}}{\sqrt{w}} \frac{\partial}{\partial \theta} \right] + V(\theta, \varphi)
\]

with mass tensor \(w = B_{\varphi\varphi}B_{\theta\theta} - B_{\varphi\theta}B_{\theta\varphi}\)
Two dimensional Collective Hamiltonian (2DCH)

Construction of 2DCH

- collective potential: based on TAC

\[ E'(\theta, \varphi) = \langle \hat{h}' \rangle - \frac{1}{2} \sum_{k=1}^{3} J_k \omega_k^{2} \]

\[ \hat{h}_{\text{def}}^{\pi(\nu)} = \pm \frac{1}{2} C \left\{ \left( \hat{j}_3^2 - \frac{j(j+1)}{3} \right) \cos \gamma + \frac{1}{2\sqrt{3}} (\hat{j}_+^2 + \hat{j}_-^2) \sin \gamma \right\}. \]

- mass parameter: cranking formula

\[ B_{\varphi \varphi} = 2 \sum_{\alpha \beta} \frac{\left| \langle \alpha | \frac{\partial \omega}{\partial \varphi} \cdot \hat{j} | \beta \rangle \right|^2}{(\varepsilon_{\alpha} - \varepsilon_{\beta})^3}, \quad B_{\theta \theta} = 2 \sum_{\alpha \beta} \frac{\left| \langle \alpha | \frac{\partial \omega}{\partial \theta} \cdot \hat{j} | \beta \rangle \right|^2}{(\varepsilon_{\alpha} - \varepsilon_{\beta})^3}, \]

\[ B_{\varphi \theta} = B_{\theta \varphi} = 2 \sum_{\alpha \beta} \frac{\langle \alpha | \frac{\partial \omega}{\partial \varphi} \cdot \hat{j} | \beta \rangle \langle \beta | \frac{\partial \omega}{\partial \theta} \cdot \hat{j} | \alpha \rangle}{(\varepsilon_{\alpha} - \varepsilon_{\beta})^3}. \]

The solutions of 2DCH could be found in appendix.
Two dimensional Collective Hamiltonian (2DCH)

- **Basis states with different symmetry (under box boundary condition)**
  
  1DCH-box:
  
  \[
  \psi^{(1)}_n(\varphi) = \sqrt{\frac{2}{\pi}} \frac{\cos(2n - 1)\varphi}{B^{1/4}_{\varphi\varphi}}, \quad n \geq 1
  \]
  
  \[
  \psi^{(2)}_n(\varphi) = \sqrt{\frac{2}{\pi}} \frac{\sin 2n\varphi}{B^{1/4}_{\varphi\varphi}}, \quad n \geq 1.
  \]

  2DCH-box:
  
  \[
  \psi^{(1)}_{mn}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2}} \frac{\sin(2m - 1)\theta \cos(2n - 1)\varphi}{w^{1/4}}, \quad m, n \geq 1,
  \]
  
  \[
  \psi^{(2)}_{mn}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2}} \frac{\sin(2m - 1)\theta \sin 2n\varphi}{w^{1/4}}, \quad m, n \geq 1,
  \]
  
  \[
  \psi^{(3)}_{mn}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2}} \frac{\sin 2m\theta \cos(2n - 1)\varphi}{w^{1/4}}, \quad m, n \geq 1,
  \]
  
  \[
  \psi^{(4)}_{mn}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2}} \frac{\sin 2m\theta \sin 2n\varphi}{w^{1/4}}, \quad m, n \geq 1,
  \]
  
  in which \( w = \det B = B_{\varphi\varphi}B_{\theta\theta} - B_{\varphi\theta}B_{\theta\varphi} \).
Two dimensional Collective Hamiltonian (2DCH)

- Basis states with different symmetry (without box boundary condition)

1DCH-peri.:

\[ \psi_{n}^{(1)}(\varphi) = \sqrt{\frac{2}{\pi(1 + \delta_{n0})}} \frac{\cos 2n\varphi}{B_{\varphi\varphi}^{1/4}}, \quad n \geq 1, \quad (34) \]

\[ \psi_{n}^{(2)}(\varphi) = \sqrt{\frac{2\sin 2n\varphi}{\pi B_{\varphi\varphi}^{1/4}}}, \quad n \geq 1. \quad (35) \]

2DCH-peri.:

\[ \psi_{mn}^{(1)}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2(1 + \delta_{m0}) (1 + \delta_{n0})}} \frac{\cos 2m\theta \cos 2n\varphi}{w^{1/4}}, \quad m \geq 0, n \geq 0, \quad (36) \]

\[ \psi_{mn}^{(2)}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2(1 + \delta_{m0})}} \frac{\cos 2m\theta \sin 2n\varphi}{w^{1/4}}, \quad m \geq 0, n \geq 1, \quad (37) \]

\[ \psi_{mn}^{(3)}(\theta, \varphi) = \sqrt{\frac{4}{\pi^2(1 + \delta_{n0})}} \frac{\sin 2m\theta \cos 2n\varphi}{w^{1/4}}, \quad m \geq 1, n \geq 0, \quad (38) \]

\[ \psi_{mn}^{(4)}(\theta, \varphi) = \sqrt{\frac{4 \sin 2m\theta \sin 2n\varphi}{\pi^2 w^{1/4}}}, \quad m, n \geq 1, \quad (39) \]

in which \( w = \det B = B_{\theta\theta}B_{\phi\phi} - B_{\theta\phi}B_{\phi\theta} \).
Numerical details

- **Configurations:** $\pi(1h_{11/2})^1 \otimes \nu(1h_{11/2})^{-1}$

- **Single-j shell Hamiltonian coefficients:** $C_\pi = 0.25, \quad C_\nu = -0.25$

- **Triaxial deformation:** $\gamma = -30^\circ$

- **Moments of inertia:**

  $\mathcal{J}^\text{irr}_k = \mathcal{J}^\text{irr}_0 \sin^2 \left( \gamma - \frac{2\pi}{3} k \right), \quad \mathcal{J}^\text{irr}_0 = 40 \ h^2/\text{MeV}$
Collective potential

- Symmetrical with respect to $\varphi=0^\circ$ and $\theta=90^\circ$

- The minimum changes from $\theta, \varphi=64^\circ$ to $\theta, \varphi=90^\circ$ (2-axis)
Mass parameter

- $B_{\theta\theta}$ and $B_{\varphi\varphi}$ are symmetrical with respect to $\varphi=0^\circ$ and $\theta=90^\circ$
- $B_{\theta\varphi}$ is antisymmetrical with respect to $\varphi=0^\circ$ and $\theta=90^\circ$
Mass parameter

- $B_{\theta\theta}$ and $B_{\varphi\varphi}$ are symmetrical with respect to $\varphi=0^\circ$ and $\theta=90^\circ$
- $B_{\theta\varphi}$ is antisymmetrical with respect to $\varphi=0^\circ$ and $\theta=90^\circ$
The solutions in “−” block are all the same

In “+” block, solutions without box boundary condition are lower in energy
Energy spectra in 2DCH

- With or without box boundary condition

- The solutions in “– –” block are all the same

- In “+ +” block, solutions without box boundary condition are lower in energy
Collective energy spectra are richer in 2DCH

For each 1DCH level, one can find the corresponding in 2DCH
Comparison of wave functions in 1DCH and 2DCH

- Under box boundary condition

For the corresponding levels in 1DCH and 2DCH, their wave functions are similar with collective coordinate $\varphi$. 

\[ \hbar\omega = 0.50 \text{ MeV (box)} \]
Probability distributions in 2DCH

• Under box boundary condition

For the corresponding levels, the wobbling number in $\theta$ is zero.

Similar conclusions can be drawn for other frequencies.
Collective energy spectra are richer in 2DCH

For each 1DCH level, one can find the corresponding in 2DCH
Comparison of wave functions in 1DCH and 2DCH

- Without box boundary condition

For the corresponding levels in 1DCH and 2DCH, their wave functions are similar with collective coordinate $\varphi$. 

\[ \hbar \omega = 0.50 \text{ MeV} \]
Probability distributions in 2DCH

- Without box boundary condition

- For the corresponding levels, the wobbling number in $\theta$ is zero.

- Similar conclusions can be drawn for other frequencies.
Excitation energy

- Excitation energy in different blocks

- Excitation energy in each block first decreases, then increases gradually.
• Lowest excitation energy in different blocks

- Excitation energy in each block first decreases, then increases gradually.
Under box boundary condition, the energy between doublet bands gradually decreases to zero.

Without box boundary condition, the energy between doublet bands first decreases, then increases.

**Excitation energy**

- **Lowest excitation energy** (i.e., $\Delta E$ between doublet bands)
A two dimensional collective Hamiltonian which includes the full dynamical motions of nuclear orientations is constructed and applied for the chiral modes.

The collective potential and mass parameters in the collective Hamiltonian are obtained based on TAC approach.

The collective Hamiltonian are solved by the basis expansions with (or without) box boundary conditions to investigate the boundary dependence for the solutions.

The obtained results by 2DCH are compared with those by 1DCH.

It is found that the calculations without the box boundary condition are more appropriate. An extreme case is when the minimum of the collective potential locates around the boundary.

In addition, the 2DCH solutions without the vibration in $\theta$ ($n_\theta=0$) are similar to 1DCH ones.
Backup
Adiabatic self-consistent collective coordinate method

- **Self-consistent collective coordinate (SCC) method** Marumori1977PTP, Marumori1980PTP
  - aim to describe large amplitude collective motion
  - treating the collective coordinates and momenta on the same footing
  - solved by perturbative expansion with respect to the amplitude of the collective motion.

- **Adiabatic self-consistent collective coordinate (ASCC) method** Matsuo2000PTP
  - solves the basic equations of the SCC method through the adiabatic expansion with respect to the collective momenta.
  - microscopic method for calculating collective potential and mass parameter.

- **Based on ASCC method**
  - collective Hamiltonian for quadrupole vibration was constructed Hinohara2010PRC.
  - shape coexistence/mixing phenomena in Se isotopes Hinohara2010PRC and shape transition in Cr isotopes Sato2012PRC.

In the following, collective Hamiltonian for describing three dimensional rotation will be derived on the basis of ASCC method.
SCC/ASCC method
Marumori1980PTP, Matsuo2000PTP, Matsuyangi2010JPG

Adiabatic approximation: expand SCC eq with respect to $p$

(I) State vector
\[ \delta \langle \phi(q) | e^{-i \tilde{G}} \hat{H} e^{i \tilde{G}} - \sum_k \frac{\partial \mathcal{H}}{\partial p_k} e^{-i \tilde{G}} \hat{P}_k e^{i \tilde{G}} - \sum_k \frac{\partial \mathcal{H}}{\partial q_k} \hat{Q}_k e^{i \tilde{G}} \rangle | \phi(q) \rangle = 0 \]

| $| \phi(q, p) \rangle = e^{i \tilde{G}} | \phi(q) \rangle$ |
| $\tilde{G} = \sum_k p_k \hat{Q}_k(q)$ |

(II) Infinitesimal generators
\[ \delta \langle \phi(q) | e^{-i \tilde{G}} \hat{H} e^{i \tilde{G}} - \sum_k \frac{\partial \mathcal{H}}{\partial p_k} (\hat{P}_k(q) - \sum_j p_j \frac{\partial \hat{Q}_j(q)}{\partial q_k}) - \sum_k \frac{\partial \mathcal{H}}{\partial q_k} \hat{Q}_k(q) | \phi(q) \rangle = 0 \]

\[ e^{\hat{A}} e^{\hat{B}} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \ldots \]

(III) Collective Hamiltonian
\[ \delta \langle \phi(q) | \hat{H} + i \sum_k p_k [\hat{H}, \hat{Q}_k(q)] - \frac{1}{2} \sum_{k,j} p_k p_j [[\hat{\tilde{H}}, \hat{Q}_k(q)], \hat{Q}_j(q)] \]
\[ - \sum_{k,l} B_{k,l}(q) p_j (\hat{P}_k(q) - \sum_l p_l \frac{\partial \hat{Q}_l(q)}{\partial q_k}) - \sum_k \left( \frac{\partial V(q)}{\partial q_k} + \frac{1}{2} \sum_{l} \frac{\partial B_{k,l}(q)}{\partial q_k} p_j p_l \right) \hat{Q}_k(q) | \phi(q) \rangle = 0 \]

\[ \mathcal{H} = \frac{1}{2} \sum_{i,j} B_{i,j}(q) p_i p_j + V(q) \]
Choose out the $0^{th}$, $1^{st}$, $2^{nd}$ equations with respect to $p$

(0$^{th}$) moving-frame HF eq
\[ \delta \langle \phi(q) | \hat{H} - \sum_k \frac{\partial V(q)}{\partial q_k} \hat{Q}_k(q) | \phi(q) \rangle = 0 \]
\[ \hat{H}_M = \hat{H} - \sum_k \frac{\partial V(q)}{\partial q_k} \hat{Q}_k(q) \]

(1$^{st}$) moving-frame RPA eq
\[ \delta \langle \phi(q) | i[\hat{H}, \hat{Q}_k(q)] - \sum_j B_{jk}(q) \hat{P}_j(q) | \phi(q) \rangle = 0 \]
\[ [\hat{Q}_k(q), \hat{Q}_j(q)] = 0 \]

(2$^{nd}$)
\[ \delta \langle \phi(q) | - \frac{1}{2} [\hat{H}, \hat{Q}_k(q)], \hat{Q}_j(q) ] + \sum_l B_{lj}(q) \frac{\partial \hat{Q}_k(q)}{\partial q_l} - \frac{1}{2} \sum_l \frac{\partial B_{jk}(q)}{\partial q_l} \hat{Q}_l(q) | \phi(q) \rangle = 0 \]

Rewrite ASCC eqs similar to RPA eqs

ASCC eqs
\[ \delta \langle \phi(q) | \hat{H}_M | \phi(q) \rangle = 0 \]
\[ \delta \langle \phi(q) | [\hat{H}_M, \hat{Q}_j(q)] - \frac{1}{i} \sum_k B_{jk}(q) \hat{P}_k(q) | \phi(q) \rangle = 0 \]
\[ \delta \langle \phi(q) | [\hat{H}_M, \frac{1}{i} \hat{P}_j(q)] - \sum_k C_{jk}(q) \hat{Q}_k(q) \]
\[ - \frac{1}{2} [\hat{H}_M, \sum_k \frac{\partial V(q)}{\partial q_k} \hat{Q}_k(q)], \sum_l B_{jl}^{-1}(q) \hat{Q}_l(q) ] | \phi(q) \rangle = 0 \]
\[ \langle \phi(q) | [\hat{Q}_j(q), \hat{P}_k(q)] | \phi(q) \rangle = i \delta_{jk} \]
\[ C_{jk}(q) = \left( \frac{\partial^2 V(q)}{\partial q_j \partial q_k} - \sum_l \Gamma_{lk}^l(q) \frac{\partial V(q)}{\partial q_l} \right) \]
\[ \Gamma_{lk}^l(q) = \frac{1}{2} \sum_n B_{kn}(q) \left( \frac{\partial B_{nl}^{-1}(q)}{\partial q_j} + \frac{\partial B_{nj}^{-1}(q)}{\partial q_l} - \frac{\partial B_{lj}^{-1}(q)}{\partial q_n} \right) \]

\[ \text{to be determined} \]
\[ | \phi(q) \rangle, \hat{P}_k(q), \hat{Q}_k(q), V(q), B_{jk}(q) \]
Chiral and wobbling modes

- The loss of axial symmetry in nuclei can lead to many interesting characteristics in the excited energy spectra, such as γ vibrational band, anomalous signature splitting, signature inversion, chiral symmetry breaking, and wobbling motion.

- The chiral and wobbling modes are regarded as fingerprints of stable triaxial nuclei.

- The wobbling motion within nuclear rotation was originally introduced by Bohr and Mottelson, and first observed experimentally in $^{163}\text{Lu}$. Bohr_Mottelson1975, Nuclear Structure Vol. II; Ødegård2001PRL, Jensen2002PRL

- Chirality was originally introduced by Frauendorf and Meng, and first observed experimentally in N=75 isotones. Frauendorf_Meng1997NPA; Starosta2001PRL

- Up to now, the investigation of chiral and wobbling modes in atomic nuclei has become one of the hottest topics in nuclear physics.
Chiral and wobbling modes

The investigation of chirality in atomic nuclei is one of the hottest topics in nuclear physics.

Originally suggested in 1997 chiral doublet bands

Firstly Observed in 2001
Wobbling for odd-A nuclei

- For a triaxial rotor coupled to a high-\(j\) quasiparticle

\[ J_3 \gg J_1, J_2 \]

Frauendorf and Dönau, PRC 89, 014322 (2014)
Matta, PRL 114, 082501 (2015)

- Longitudinal wobbler:
  \[
  j // J_{\text{max}} \\
  I \uparrow, \quad \hbar\Omega_{\text{wob}} \uparrow
  \]

- Transverse wobbler:
  \[
  j \perp J_{\text{max}} \\
  I \uparrow, \quad \hbar\Omega_{\text{wob}} \downarrow
  \]
Wobbling

- In *Bohr&Mottelson1975, Vol. II*, the concept of wobbling motion was first proposed for a rotating triaxial nuclei.

\[
\hat{H}_{\text{rot}} = \frac{\hat{I}_1^2}{2J_1} + \frac{\hat{I}_2^2}{2J_2} + \frac{\hat{I}_3^2}{2J_3}
\]

\[J_3 \gg J_1 \neq J_2, I \gg 1\]

- First experimental evidence: \(^{163}\text{Lu} \) Odegard et al., PRL 86, 5866 (2001)

- Theoretical investigations:
Success of Collective Hamiltonian

- Collective Hamiltonian, e.g. based on CDFT, has achieved great success on applications for shape evolution/transition.

Recent Progress on CDFT for Nuclear Low-lying Spectrum

1. Development of 3DAMP+GCM; Systematic study on $^{36,40}$Mg [1-4]
2. 3DAMP+GCM for low-lying states and np decoupling in C isotopes [5]
3. 3DAMP+GCM for the proton bubble structure in $^{24}$Si and $^{40}$Ar [6,7]
4. Development of CDFT based 5DCH; Systematic study on QPT in N=90 [8-10]
5. 5DCH for 2$^\text{nd}$ QPT and E(5) in Xe and Ba isotopes [11]
6. 5DCH for fission barrier and SD band in $^{26}$Pu [12]
7. 5DCH for shell erosion and shape transition in N=28 isotones [13]
8. 5DCH for shape transition and shape coexistence in A~100 [14,15]
9. 5DCH for enhanced collectivity in neutron-deficient Sn isotopes [16]
10. 5DCH for shape transition and shape coexistence of 118 isotopes [17,18]
11. 5DCH and 2DCH for double QPT in Th isotopes [19]
12. CDFT based QCCH; Study on Ra isotopes [20]
13. Systematic study on DCE for mass [21,22]
14. 5DCH for hypernuclei [23,24]

By Z. P. Li
Collective Hamiltonian

- **Collective Hamiltonian:**
  - **Goal:** to describe large amplitude collective motions, e.g., shape coexistence/mixing, nuclear fission/fussion etc.
  - **Microscopic basis:** adiabatic time-dependent Hartree-Fock (ATDHF) method
    - Baranger & Kumar, NPA 122, 241 (1968); Ring & Schuck 1980, or generate coordinate method (GCM) Hill & Wheeler, PR 89, 1102 (1953); Ring & Schuck 1980, or adiabatic self-consistent coordinate method (ASCC) Marumori et al., PTP 64, 1294 (1980); Matsu et al., PTP 103, 959 (2000); Hinohara et al., PRC 82, 064313 (2010); Matsuyanagi et al., JPG 37, 064018 (2010);
  - **Starting point:** time-dependent Hartree-Fock (TDHF) equation
  - **Assumptions:** adiabatic approximation, i.e., the collective motion is slow or collective momenta are small (can be large)
  - **Procedure:** expand the TDHF equations with respect to the collective momenta up to second order
  - **Form:** summation of kinetic and potential terms, characterized by mass parameter and collective potential
    \[ \mathcal{H}(q, p) = \langle \phi(q, p) | \hat{H} | \phi(q, p) \rangle = \frac{1}{2} \sum_{i,j} B^{ij}(q)p_i p_j + V(q) \]
    \[ B^{ij}(q) = \left. \frac{\partial^2 \mathcal{H}}{\partial p_i \partial p_j} \right|_{p=0} \quad V(q) = \left. \mathcal{H}(q, p) \right|_{p=0} \]
  - **Example:** Bohr Hamiltonian Bohr & Mottelson 1975, Vol. II
Collective Hamiltonian

- Collective Hamiltonian with collective potential $V(\bar{q})$ and mass parameters $B_{i,j}(\bar{q})$ constructed from the ASCC equations

**Classical form**

$$\mathcal{H} = \frac{1}{2} \sum_{i,j} B_{i,j}(\bar{q}) p_i p_j + V(\bar{q})$$

$$\frac{dq_k}{dt} = \frac{\partial H}{\partial p_k} = \sum_j B_{k,j} p_j$$

$$B_{i,j}(\bar{q}) = \frac{\partial^2 \mathcal{H}(\bar{q}, \bar{p})}{\partial p_i \partial p_j} \bigg|_{\bar{p} = 0} = \langle \phi(\bar{q}) | [\hat{H}, \hat{Q}_i(\bar{q})], \hat{Q}_j(\bar{q}) | \phi(\bar{q}) \rangle$$  \textbf{Mass parameter}

$$V(\bar{q}) = \langle \phi(\bar{q}, \bar{p}) | \hat{H} | \phi(\bar{q}, \bar{p}) \rangle \bigg|_{\bar{p} = 0} = \langle \phi(\bar{q}) | \hat{H} | \phi(\bar{q}) \rangle$$  \textbf{Collective potential}

**Quantal form**  \textbf{Pauli1933}

$$\hat{H}_{\text{kin}} = -\frac{\hbar^2}{2} \frac{1}{\sqrt{\det M}} \sum_{i,j} \frac{\partial}{\partial q_i} \sqrt{\det M} (M^{-1})_{i,j} \frac{\partial}{\partial q_j}$$  \textbf{Mass = $B^{-1}$}

- Solving the collective Hamiltonian, the energy spectra and corresponding collective wave function are yielded. With the obtained wave functions, other observables can be also obtained.
Collective Hamiltonian

- **Bohr Collective Hamiltonian:**
  - Collective coordinate
  \[ \alpha_{2\mu}, \beta, \gamma, \Omega(\phi, \theta, \varphi) \]
  - Classical Hamiltonian summation of kinetic and potential terms, characterized by mass parameter and collective potential
  \[ H = T_{\text{vib}}(\beta, \gamma) + T_{\text{rot}}(\beta, \gamma, \Omega) + V(\beta, \gamma) \]
  \[ T_{\text{vib}} = \frac{1}{2} B_{\beta\beta} \dot{\beta}^2 + \beta B_{\beta\gamma} \dot{\beta} \dot{\gamma} + \frac{1}{2} \beta^2 B_{\gamma\gamma} \dot{\gamma}^2 \]
  \[ T_{\text{rot}} = \frac{1}{2} \sum_{i=1}^{3} J_i \omega_i^2 \]
  - Pauli quantization
  \[ \hat{H}_\text{kin} = -\frac{\hbar^2}{2} \frac{1}{\sqrt{\det B}} \sum_{ij} \frac{\partial}{\partial q_i} \sqrt{\det B} (B^{-1})_{ij} \frac{\partial}{\partial q_i} \]
  - Bohr Hamiltonian *Bohr&Mottelson1975, Vol. II*
  \[ \hat{T}_{\text{vib}} = -\frac{\hbar^2}{2\sqrt{G}} \left( \frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^4 \sqrt{G} \frac{B_{\gamma\gamma}}{G_{\text{vib}}} \frac{\partial}{\partial \beta} + \frac{1}{\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \sqrt{G} \frac{B_{\beta\beta}}{G_{\text{vib}}} \frac{\partial}{\partial \gamma} \right) \]
  \[ -\frac{1}{\beta^4} \frac{\partial}{\partial \beta} \beta^3 \sqrt{G} \frac{B_{\beta\gamma}}{G_{\text{vib}}} \frac{\partial}{\partial \gamma} - \frac{1}{\beta \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \sqrt{G} \frac{B_{\beta\gamma}}{G_{\text{vib}}} \frac{\partial}{\partial \gamma} \]
Collective Hamiltonian results under box boundary conditions
($\hbar\omega = 0.9 \sim 0.1$ MeV)
2DCH 的能级比 1DCH 更丰富

1DCH 的能级能在 2DCH 中找到对应
1DCH与2DCH能对应的这些能级，它们在φ方向上的波函数行为是相似的。
1DCH与2DCH能对应上的这些能级，它们在θ方向上的振动模式为零声子模式

相似的结论对其他转动频率也类似
$\hbar\omega = 0.70 \text{ MeV (box)}$

2DCH (+ +) 2DCH (+ -)

Probability

$\theta$ (deg) $\theta$ (deg)
The diagram illustrates the energy levels for 1DCH and 2DCH systems with an energy resolution of $\hbar\omega = 0.30$ MeV (boxed). The energy levels are labeled with various transitions and parities ($P$) as follows:

- **Total** transitions are shown for $P_{\varphi}$ and $P_{\theta}$
- **1DCH** transitions are indicated with solid lines and labels 1, 2, and 3
- **2DCH** transitions are represented with dashed lines and purple labels

The parity assignments are as follows:
- $P_{\varphi} = +$ for solid lines
- $P_{\varphi} = -$ for dashed lines
- $P_{\theta} = +$ for transitions with a rightward arrow
- $P_{\theta} = -$ for transitions with a leftward arrow

The energy values are marked along the y-axis in MeV.
Collective Hamiltonian results without box boundary conditions
($\hbar\omega=0.9\sim0.1$ MeV)