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Quantum Chirality

量子手性研究新进展

ATOMKI seminar

Jie MENG（孟 杰）

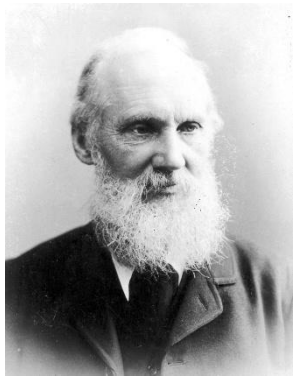
School of Physics, Peking University（北京大学物理学院）

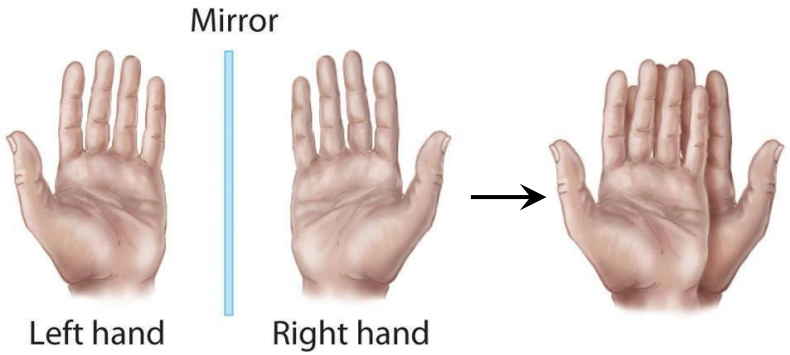
Email: mengj@pku.edu.cn

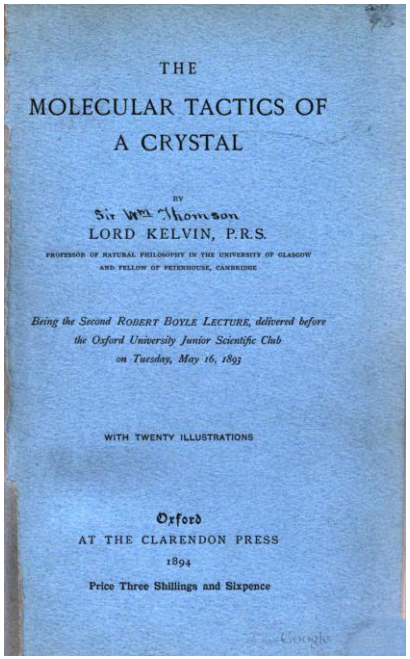
手性 Chirality

Definition / 定义

Chirality: A system is chiral if it cannot be superimposed onto its mirror image by any combination of translations and rotations.






THE
MOLECULAR TACTICS OF
A CRYSTAL

BY
Sir Wm. Thomson
LORD KELVIN, P.R.S.

PROFESSOR OF NATURAL PHILOSOPHY IN THE UNIVERSITY OF GLASGOW
AND FELLOW OF PETERHOUSE, CAMBRIDGE

Being the Second ROBERT BOYLE *LECTURE, delivered before the Oxford University Junior Scientific Club on Tuesday, May 16, 1893*

WITH TWENTY ILLUSTRATIONS

Oxford
AT THE CLARENDON PRESS
1894
Price Three Shillings and Sixpence

"I call any geometrical figure, or group of points, chiral, and say that it has chirality if its image in a plane mirror, ideally realized, cannot be brought to coincide with itself."

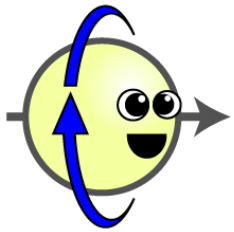
Lord Kelvin

The Molecular Tactics of a Crystal

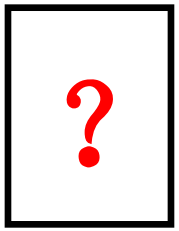
Press: Oxford, UK, 1894; section 22, footnote p. 27

手性 Chirality

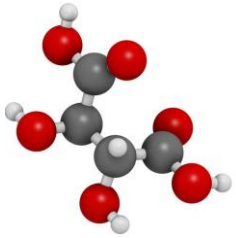
- **Chirality is an important phenomenon in sciences**



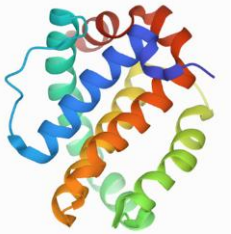
Neutrino



Nucleus



Molecule



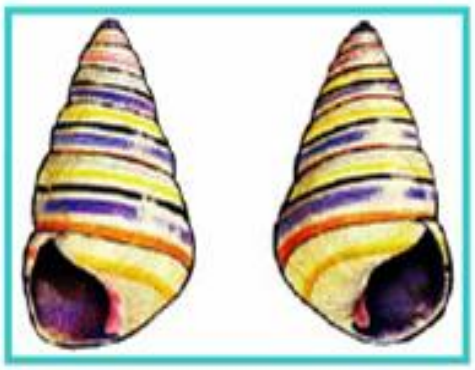
Biomolecule

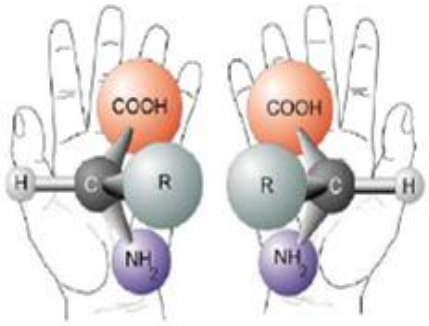


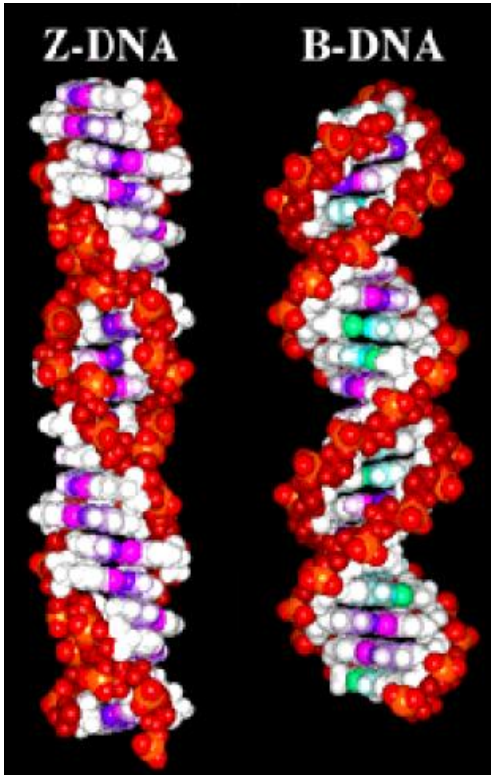
Organism



Galaxy

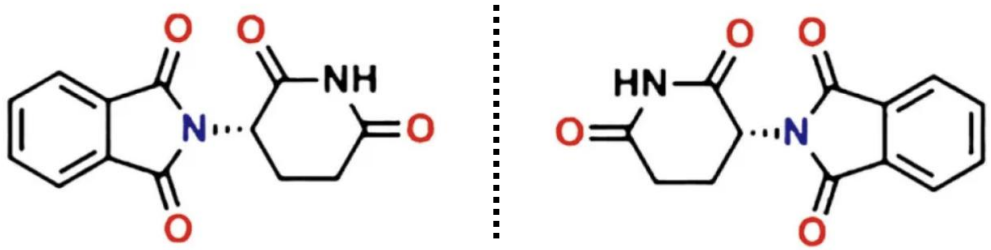






"Thalidomide" tragedy

- The tragedy occurred in Europe in the 60s of the 20th century: about 12,000 "seal limb deformity" babies were born around the world due to pregnant women taking "response stop", and promoted the reform of the modern drug regulatory system



(L) Poison (R) Ssedative



THALIDOMIDE AND CONGENITAL ABNORMALITIES

SIR,—Congenital abnormalities are present in approximately 1·5% of babies. In recent months I have observed that the incidence of multiple severe abnormalities in babies delivered of women who were given the drug thalidomide (' Distaval ') during pregnancy, as an antiemetic or as a sedative, to be almost 20%.

These abnormalities are present in structures developed from mesenchyme—i.e., the bones and musculature of the gut. Bony development seems to be affected in a very striking manner, resulting in polydactyly, syndactyly, and failure of development of long bones (abnormally short femora and radii).

Have any of your readers seen similar abnormalities in babies delivered of women who have taken this drug during pregnancy?

Hurstville, New South Wales. W. G. MCBRIDE.

*** In our issue of Dec. 2 we included a statement from the Distillers Company (Biochemicals) Ltd. referring to " reports from two overseas sources possibly associating thalidomide (' Distaval ') with harmful effects on the fœtus in early pregnancy ". Pending further investigation, the company decided to withdraw from the market all its preparations containing thalidomide.—ED.L.

W. G. Mcbride ,The Lancet, **278** (1961) 1358

Nobel Prize in Chemistry

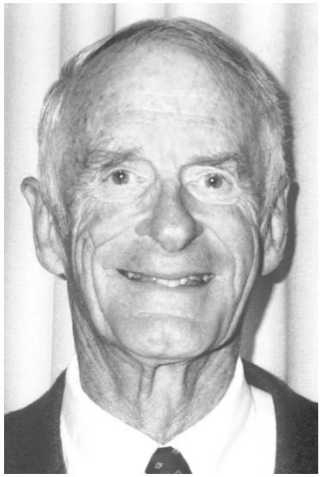


Photo: Pressens Bild. Nobel Foundation archive.

William S. Knowles

Prize share: 1/4



Photo: Pressens Bild. Nobel Foundation archive.

Ryoji Noyori

Prize share: 1/4

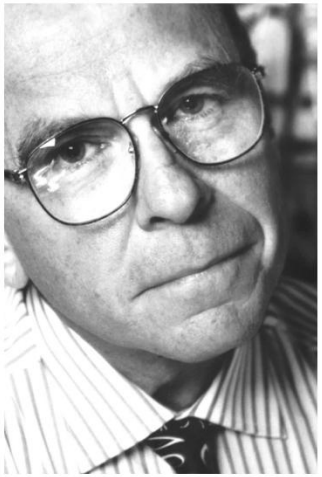


Photo: Pressens Bild. Nobel Foundation archive.

K. Barry Sharpless

Prize share: 1/2



© Nobel Prize Outreach. Photo: Stefan Bladh.

Benjamin List

Prize share: 1/2



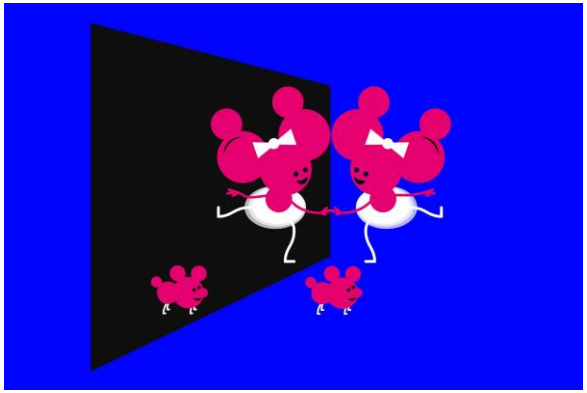
© Nobel Prize Outreach. Photo: Risdon Photography

David W.C. MacMillan

Prize share: 1/2

The Nobel Prize in Chemistry 2001 was divided, one half jointly to William S. Knowles and Ryoji Noyori "for their work on chirally catalysed hydrogenation reactions" and the other half to K. Barry Sharpless "for his work on chirally catalysed oxidation reactions"

The Nobel Prize in Chemistry 2021 was awarded jointly to Benjamin List and David W.C. MacMillan "for the development of asymmetric organocatalysis"





Ill. Niklas Elmehed © Nobel Prize Outreach

Henri B. Kagan

Prize share: 1/2



Ill. Niklas Elmehed © Nobel Prize Outreach

Kenso Soai

Prize share: 1/2

Nobel Prize in Chemistry 2026

Henri B. Kagan Université Paris-Sud, France

Kenso Soai Tokyo University of Science, Japan

"for the discovery of non-linear effects and autocatalysis in asymmetric organic synthesis"

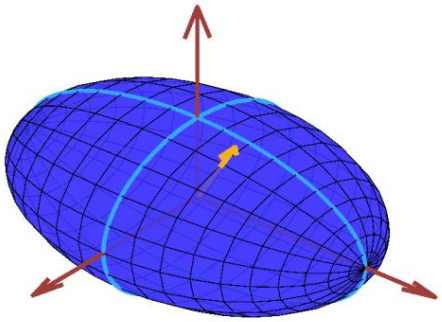
They made chemistry choose a mirror image

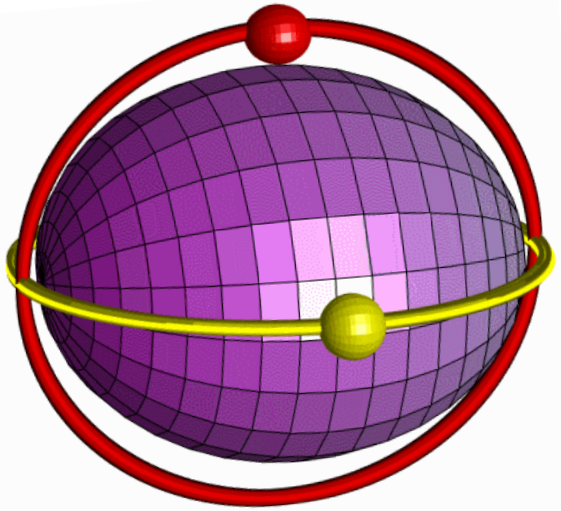
Chirality

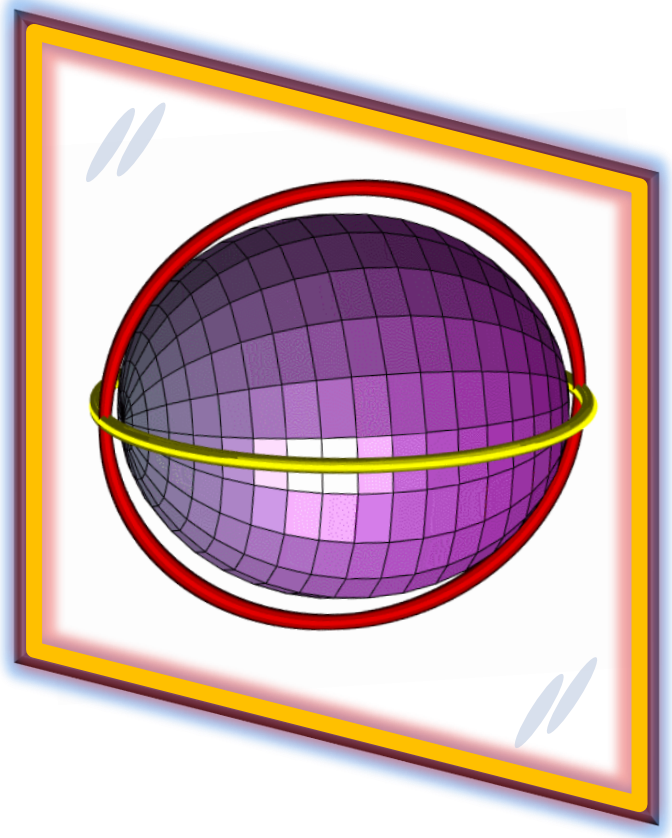
- Classical Examples:
  - Hands
  - Screws: left- and right-handed screws.
  - Molecules: such as amino acids and sugars.
- The famous "Thalidomide" tragedy occurred because its left-handed molecule had a sedative effect, while its right-handed molecule caused birth defects.
- Classically, a chiral object is typically stable in its specific chiral state.

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Quantum Chirality







courtesy of X.H. Wu

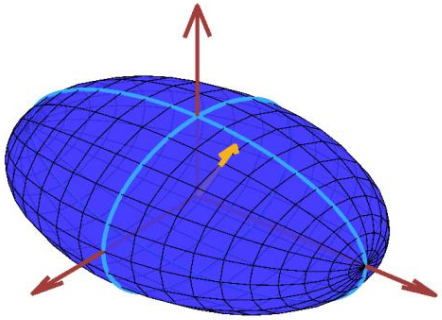
Chiral symmetry breaking in intrinsic frame

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Quantum Chirality

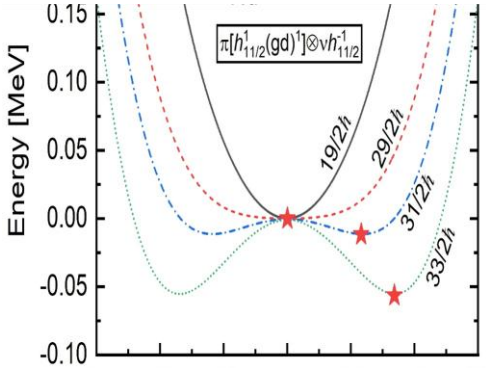
01 / Space Representation

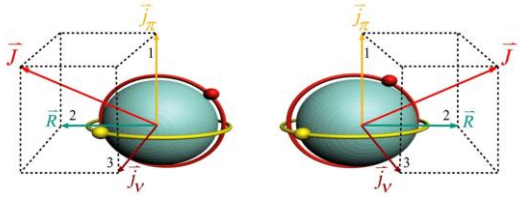
Space → Angular Momentum Space



02 / Intrinsic Frame

Chirality in intrinsic frame: degenerate spectra

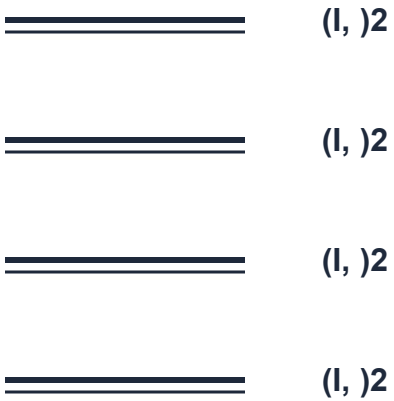




03 / Quantum Effects

Quantum Tunneling

Near-degenerate spectra appear → **Experimental signal**

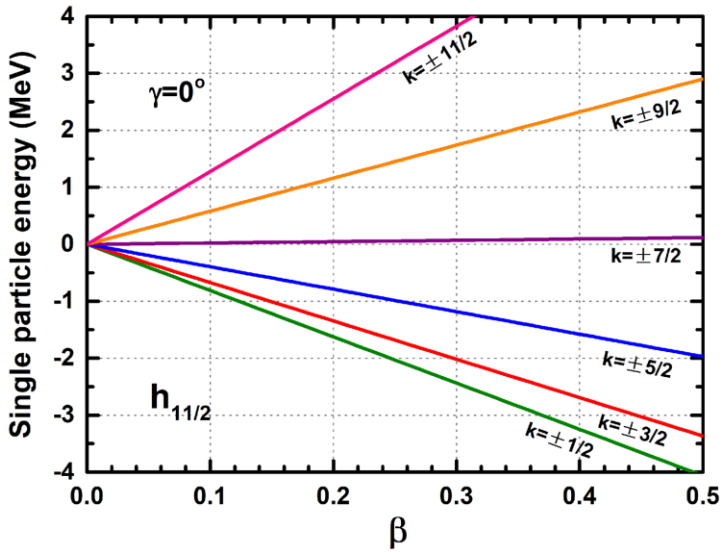


Chiral Geometry: AM Orientation

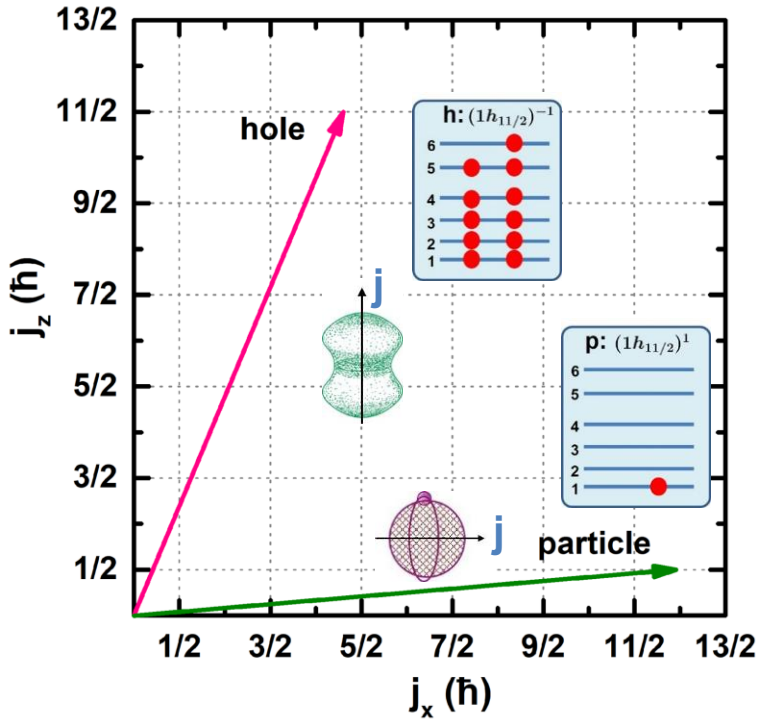
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Valence Orbitals: Particle & Hole

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



Orientation of Spin

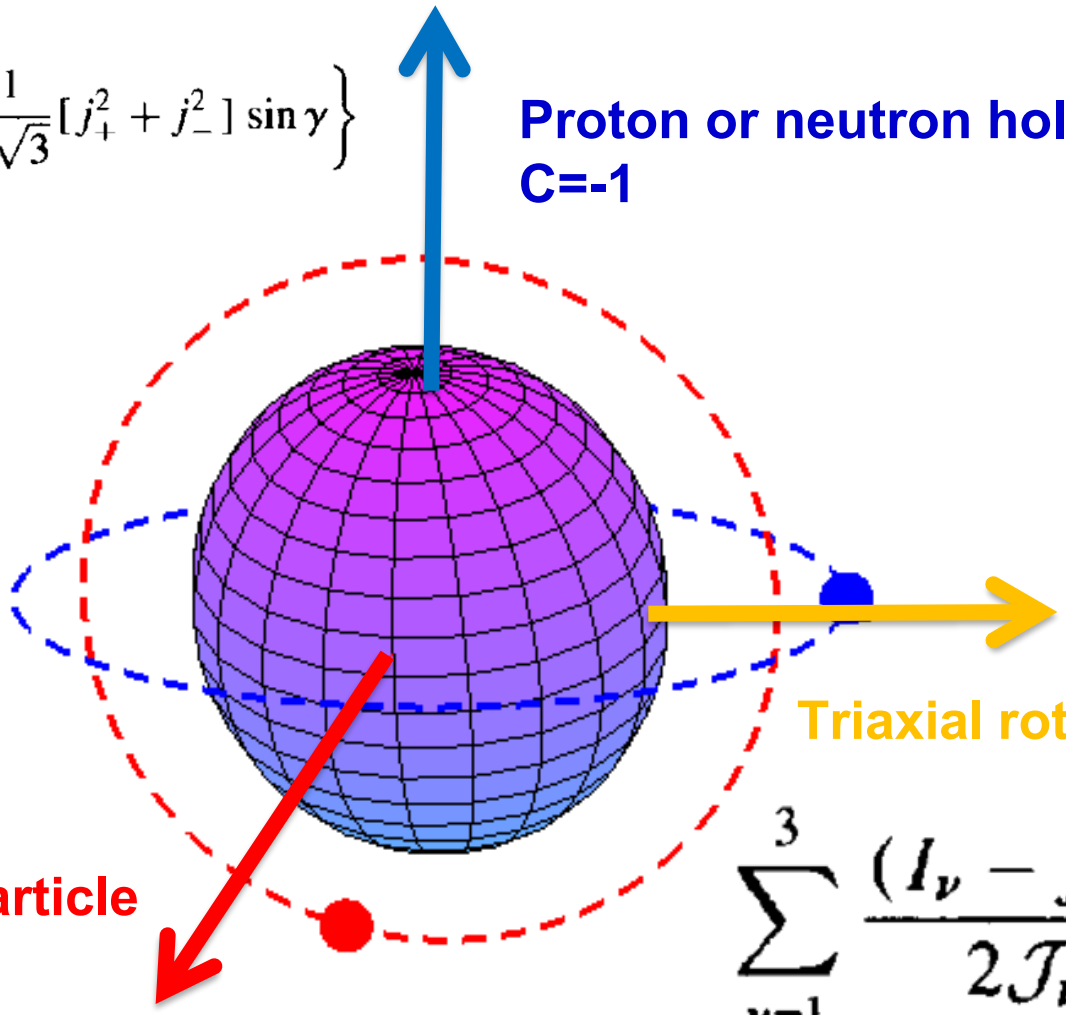


By QB Chen

Quantum Chirality: Geometry

Triaxial Particle-core Model

$$h = \frac{1}{2}C\left\{\left(j_3^2 - \frac{j(j+1)}{3}\right)\cos\gamma + \frac{1}{2\sqrt{3}}[j_+^2 + j_-^2]\sin\gamma\right\}$$



$$\sum_{\nu=1}^{3}\frac{(I_\nu - j_\nu)^2}{2\mathcal{J}_\nu}$$

$$\mathcal{J}_\nu = \mathcal{J}\sin\left(\gamma - \frac{2\pi}{3}\nu\right)^2 \qquad \gamma = -30°$$

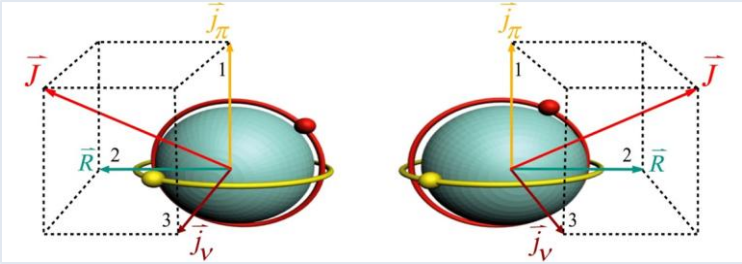
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Quantum Chirality

Classical Approximation

Classical Vector Approximation

The operator of the total angular momentum is replaced by the classical vector representation.



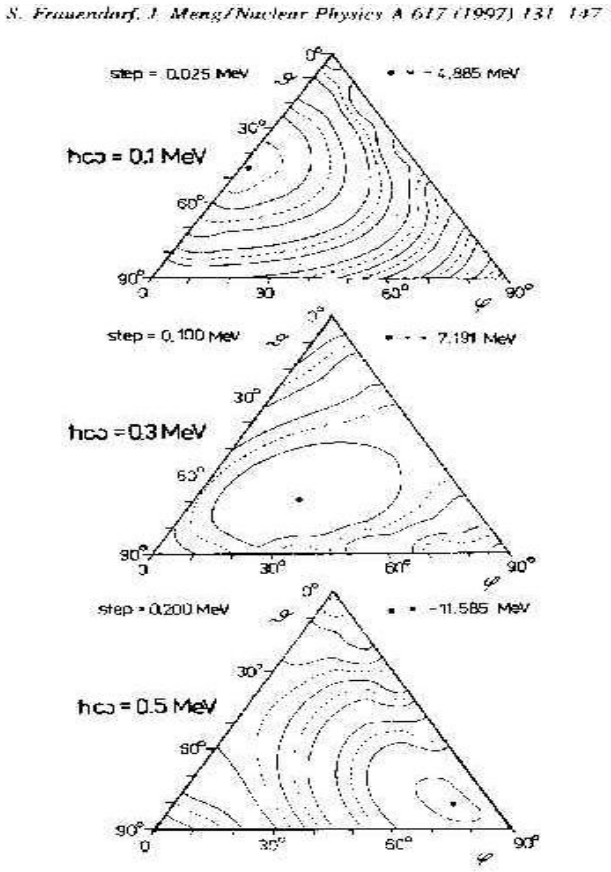
$$h' = h_{\text{def}} - \boldsymbol{\omega} \cdot \boldsymbol{j},$$

$$\boldsymbol{\omega} = (\omega \sin\vartheta \sin\varphi, \omega \sin\vartheta \cos\varphi, \omega \cos\vartheta),$$

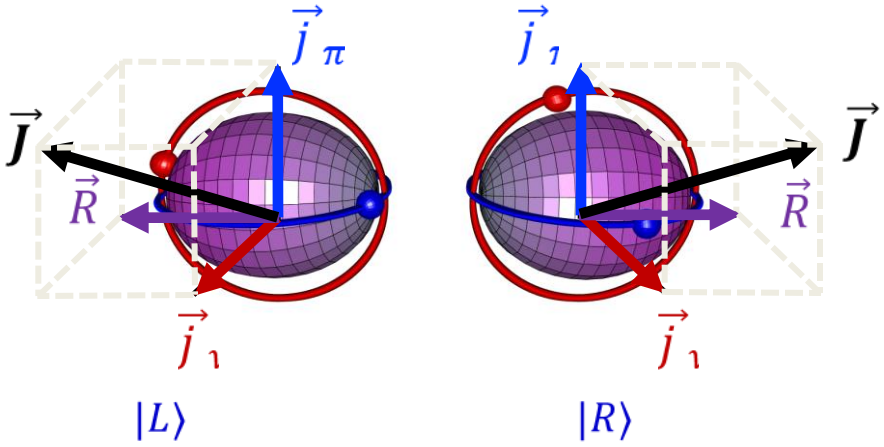
$$h = \frac{1}{2} C \left\{ \left(j_3^2 - \frac{j(j+1)}{3} \right) \cos\gamma + \frac{1}{2\sqrt{3}} [j_+^2 + j_-^2] \sin\gamma \right\}$$

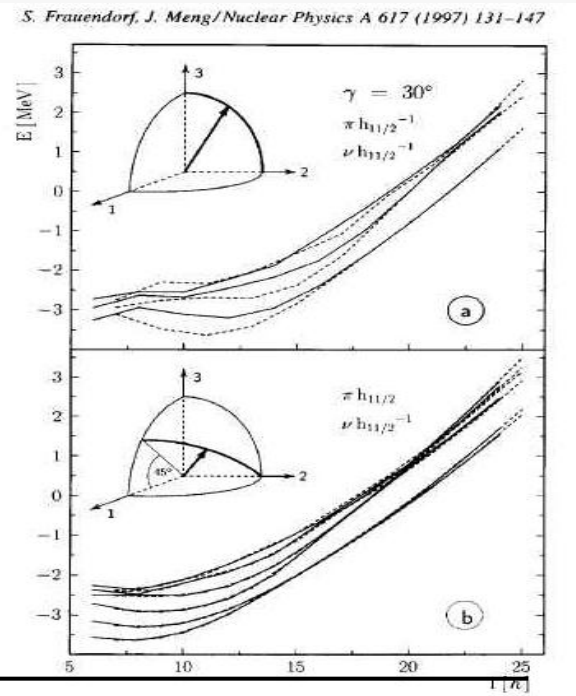
- **Proton particle:** C = 1
- **Neutron hole:** C = -1

Classical Energy Surfaces



Quantum Chirality



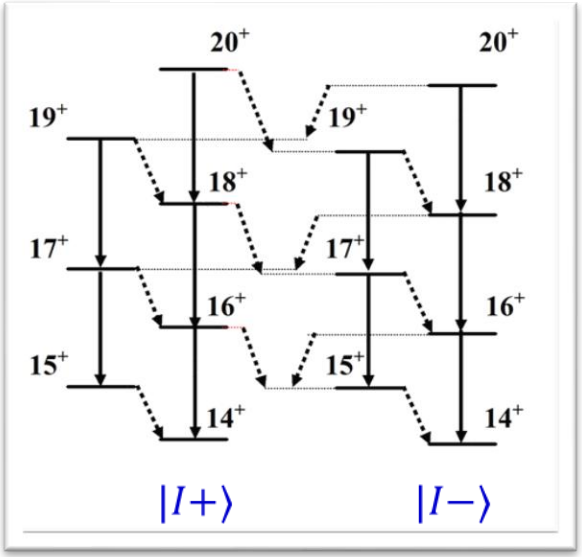


S. Frauendorf and J. Meng, NPA 617 (1997) 131

Experimental signal

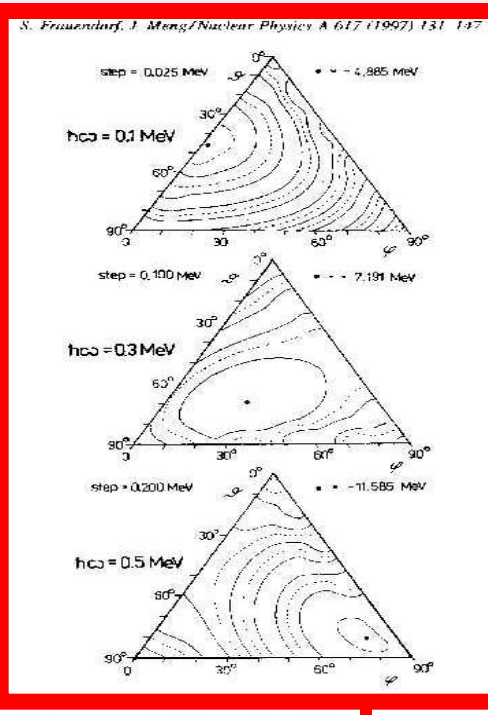
$$|I+\rangle = \frac{1}{\sqrt{2}}\Big[|L\rangle + |R\rangle\Big]$$

$$|I-\rangle = \frac{i}{\sqrt{2}}\Big[|L\rangle - |R\rangle\Big]$$



Quantum Chirality: atomic nuclei

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ELSEVIER

Nuclear Physics A 617 (1997) 131–147

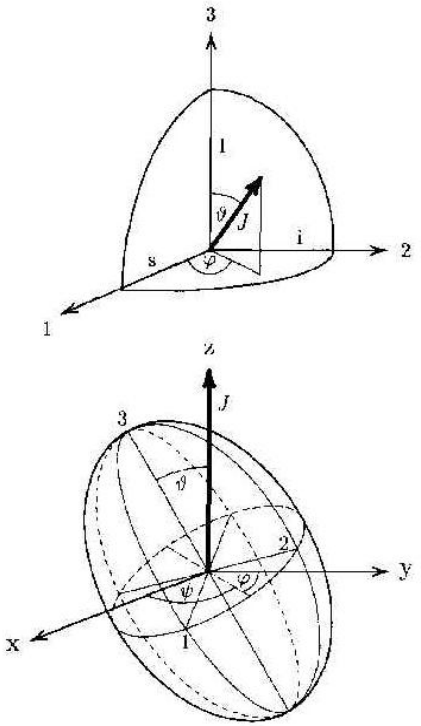
NUCLE PHYSIC

$(I,\pi)^2$ $(I,\pi)^2$ $(I,\pi)^2$ $(I,\pi)^2$ $(I,\pi)^2$

Tilted rotation of triaxial nuclei

S. Frauendorf, Jie Meng [1]

Institut für Kern- und Hadronenphysik, Forschungszentrum Rossendorf e.V., PF 510119, 01314 Dresden, Germany

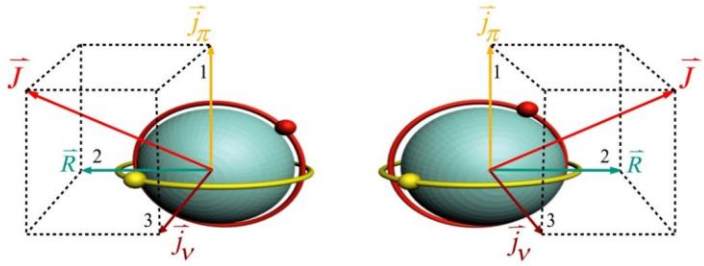


Abstract

The Tilted Axis Cranking theory is applied to the model of two particles coupled to a triaxial rotor. Comparing with the exact quantal solutions, the interpretation and quality of the mean field approximation is studied. Conditions are discussed when the axis of rotation lies inside or outside the principal planes of the triaxial density distribution. The planar solutions represent $\Delta I = 1$ bands, whereas the aplanar solutions represe parity. The two bands differ by the chirality momentum vector. The transition from planar and the mean field calculations. Its physical o

PACS: ...

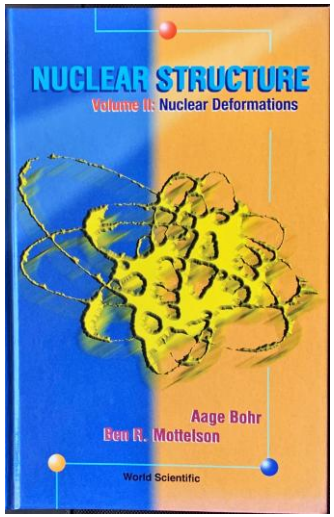
Keywords: Tilted axis cranking; Triaxiality; Chirality



[1] Also at Institute of Theoretical Physics, Chinese Academy of Science, Beijing 100080, PR China. Present address: Alexander von Humboldt fellow, Physik-Department der Technischen Universität München, D-85747 Garching, Germany.

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Axial deformed system




A. N. Bohr


B. R. Mottelson


J. Rainwater

Nobel Prize in Physics 1975

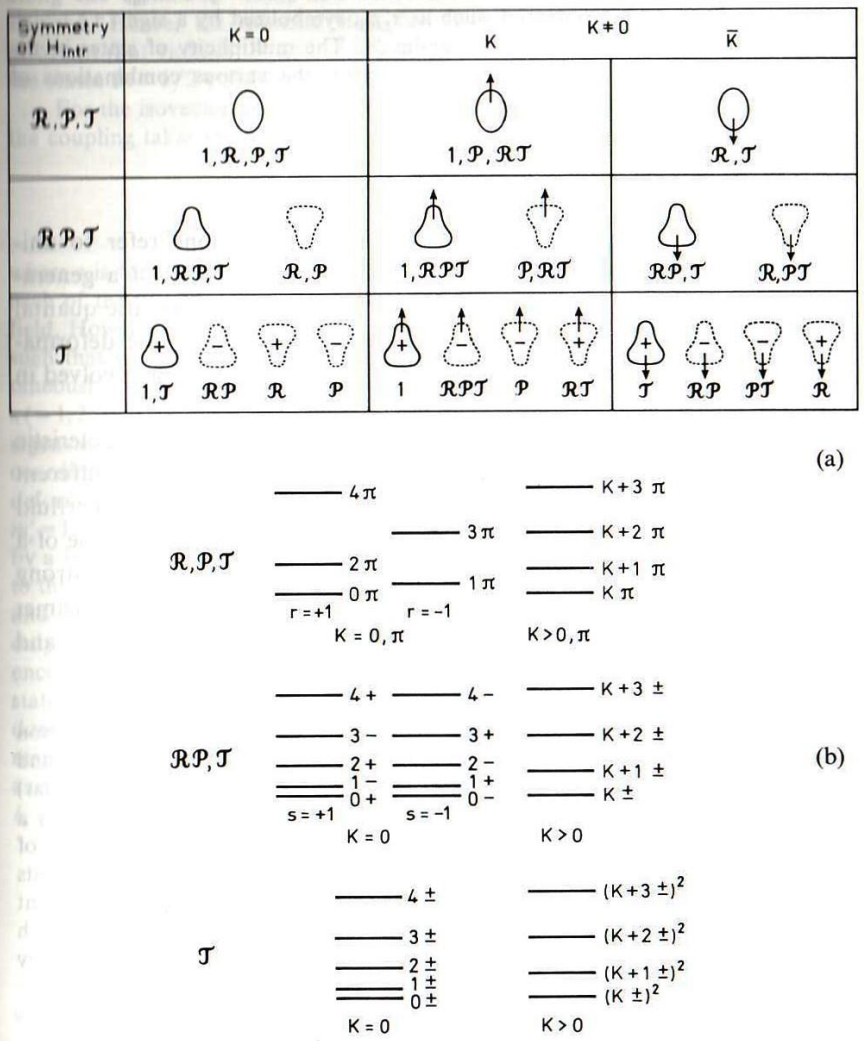
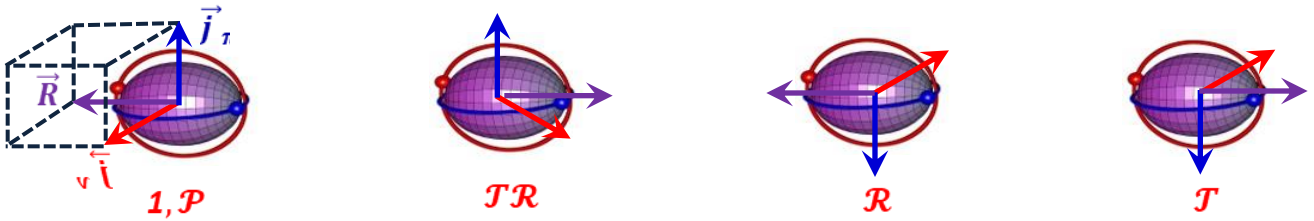


Figure 4-2 Rotational spectra for axially symmetric systems with different combinations of $\mathcal{R}$, $\mathcal{P}$, and $\mathcal{T}$ invariance. The intrinsic states are illustrated in Fig. 4-2a and the associated rotational spectra in Fig. 4-2b; the quantum numbers $I\pi$ are given to the right of the energy levels.

A. Bohr, B. Mottelson, Nuclear Structure II, Benjamin, New York (1975), p.19

Triaxial deformed nucleus

Symmetry of H_{intr}: $\mathcal{R}, \mathcal{P}$

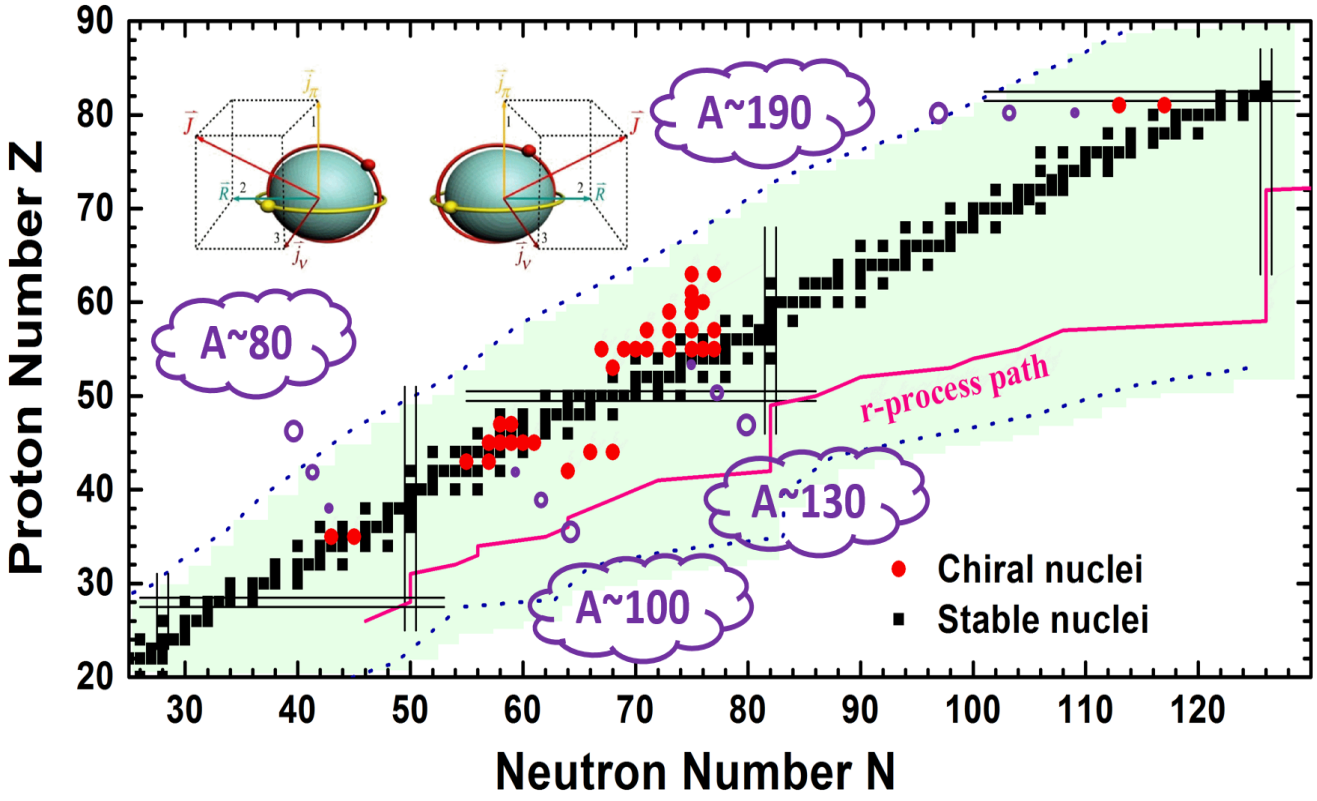
Intrinsic States	
Rotational Spectra	$(I+3,\pi)^2$ $(I+2,\pi)^2$ $(I+1,\pi)^2$ $(I,\pi)^2$

"The system with the symmetries $\mathcal{R}$ and $\mathcal{P}$ hasn't been discussed in Nuclear Structure, which corresponds to the nuclear chirality."

J. Meng, Y. P. Wang, The 25th anniversary for nuclear chirality, Chirality and wobbling in atomic nuclei (2024)

49 Chiral candidate nuclei

- More than 62 chiral doublets bands have been reported in the A~80, 100, 130, and 190 mass regions.
- Multiple chiral doublets (MχD) were predicted in 2006 and observed in in 9 candidate nuclei.



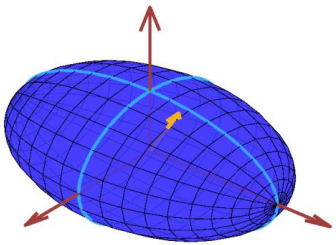
Xiong & Wang, ATOMIC DATA AND NUCLEAR DATA TABLES 125 (2019)193 .

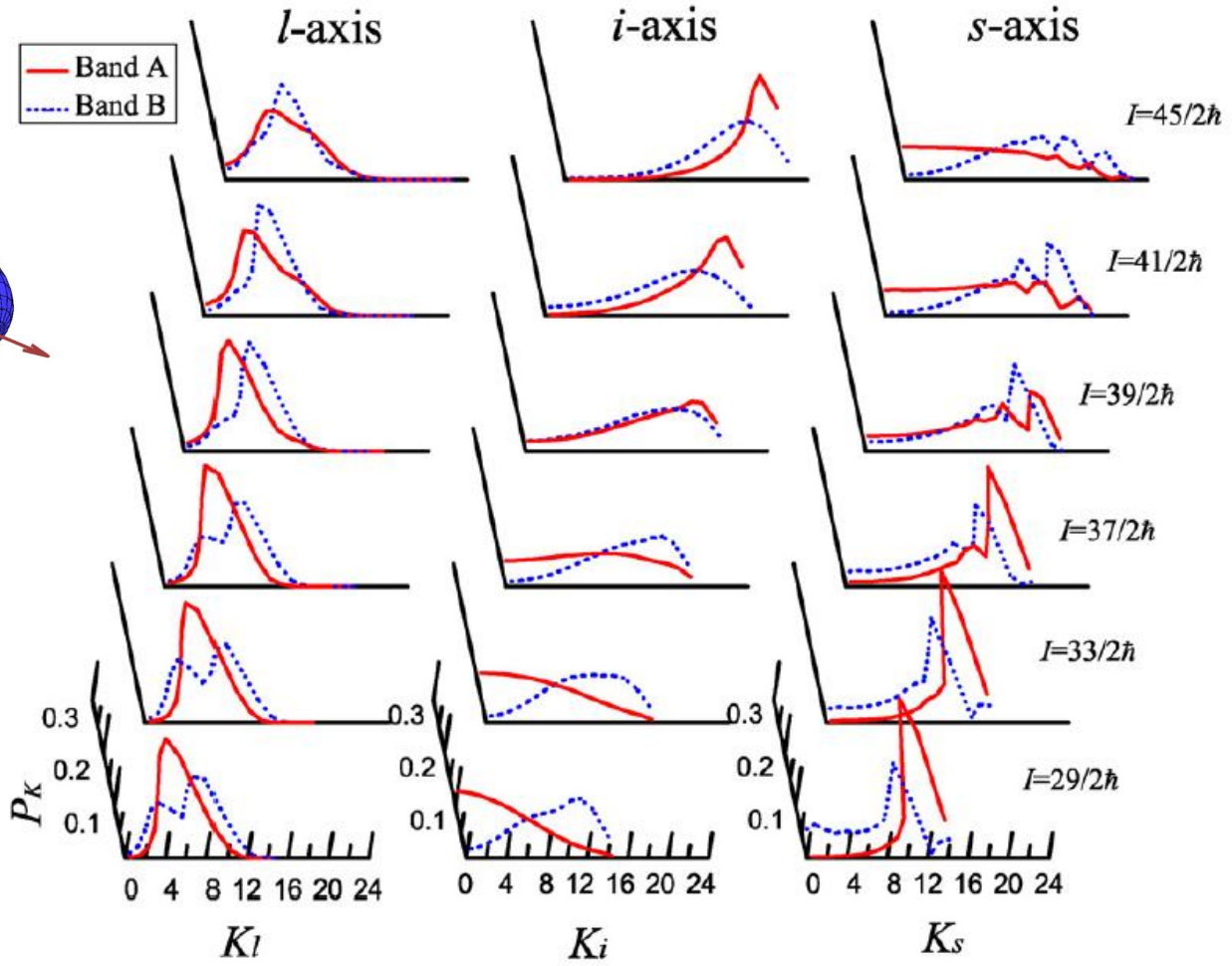
Quantum Chirality

Quantum chiral features: **K-Plot**

Triaxial Particle-core Model

B. Qi et al. / Physics Letters B 675 (2009) 175–180





Quantum Chiral Features: K-Plot

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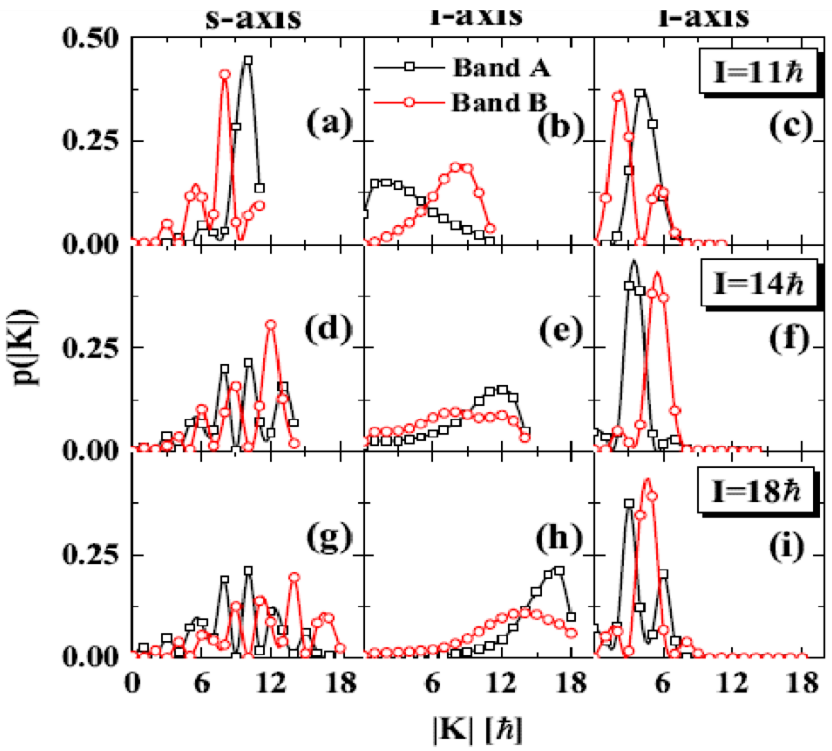
Angular Momentum Projected Shell Model

Key Insight

Evolution of Chiral Modes

The transition from chiral vibration near the band head to static chirality at higher spins is clearly exhibited in the ^{128}Cs doublet bands.

Polar angle plots



Chiral geometry in symmetry-restored states: Chiral doublet bands in 128Cs

Authors: F. Q. Chen (陈芳祁), Q. B. Chen (陈启博), Y. A. Luo (罗延安), J. Meng (孟杰), and S. Q. Zhang (张双全)

Source: *Phys. Rev. C 96, 051303(R) – Published 20 November 2017*

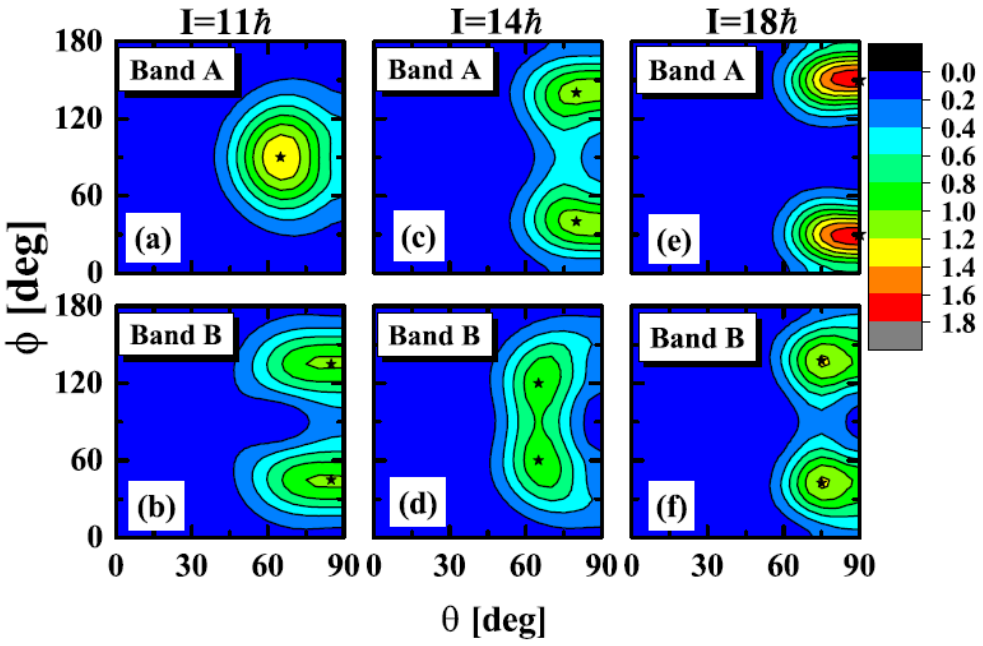
Quantum Chiral Features: Azimuthal Plot

Angular Momentum Projected Shell Model

Key Analysis

AM Orientation Examination

Azimuthal plots for I = 11, 14, and 18 are utilized to examine the orientation of the angular momentum (AM) in the restored states.



Chiral geometry in symmetry-restored states: Chiral doublet bands in 128Cs

Authors: F. Q. Chen (陈芳祁), Q. B. Chen (陈启博), Y. A. Luo (罗延安), J. Meng (孟杰), and S. Q. Zhang (张双全)

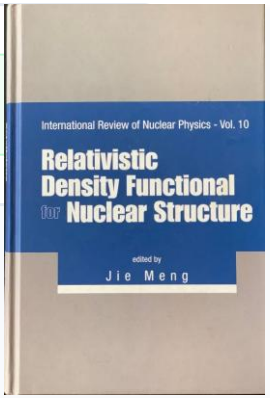
Source: *Phys. Rev. C 96, 051303(R) – Published 20 November 2017*

Relativistic DFT: Microscopic predictive tool for chirality (MχD)

Possible existence of multiple chiral doublets in ^{106}Rh

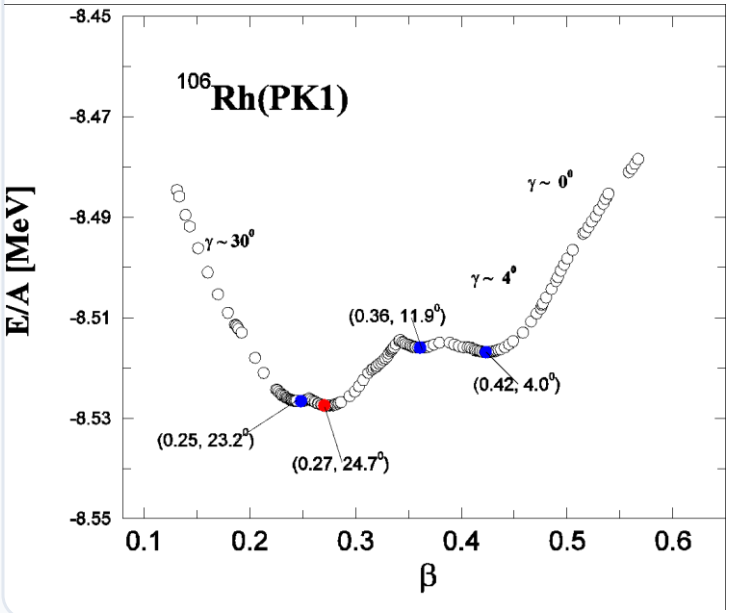
First configuration-fixed constrained triaxial relativistic mean field (RMF) calculation.

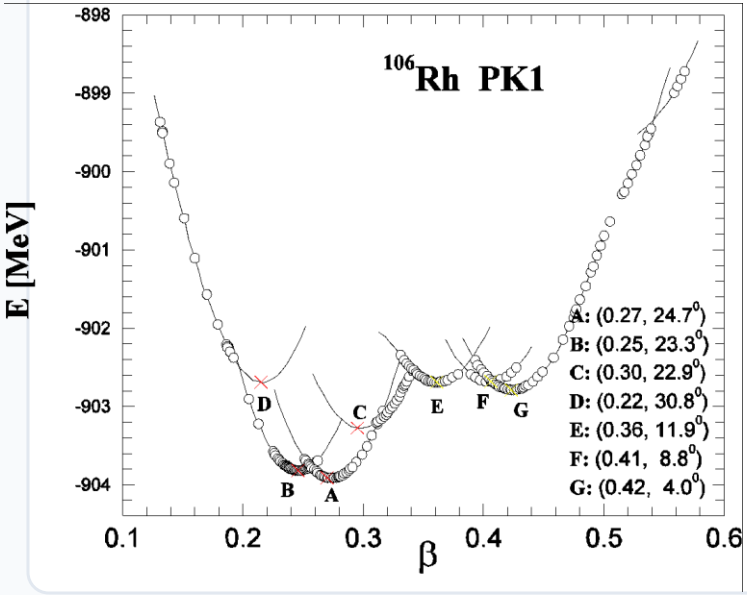
J. Meng, J. Peng, S. Q. Zhang, and S.-G. Zhou — Phys. Rev. C 73, 037303 (2006)



MχD

Energy per Nucleon (E/A) vs β

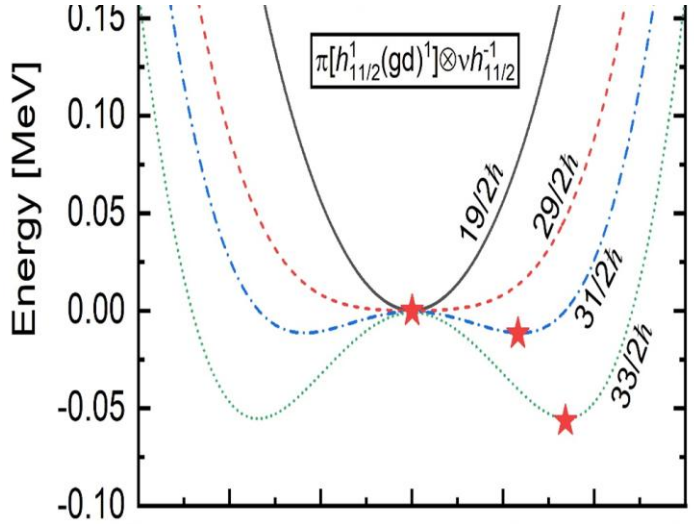


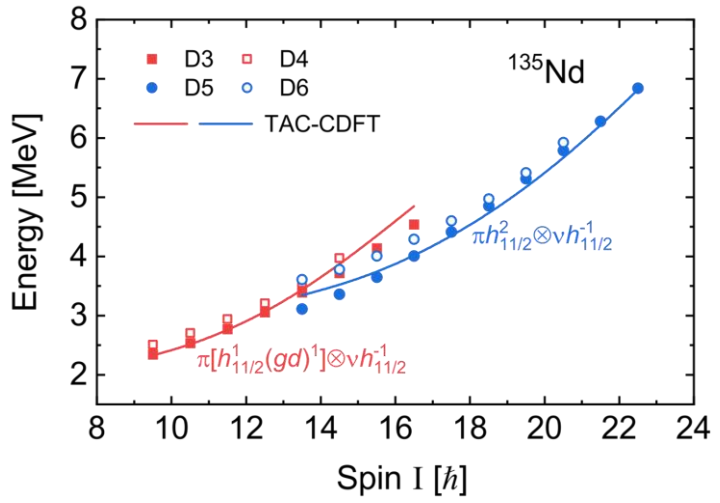


TAC - DFT in 3D Lattice for Chirality

Microscopic predictive tool for chirality (MχD)

The lower bands are well reproduced but NOT the upper bands





Semi-classical Approximation

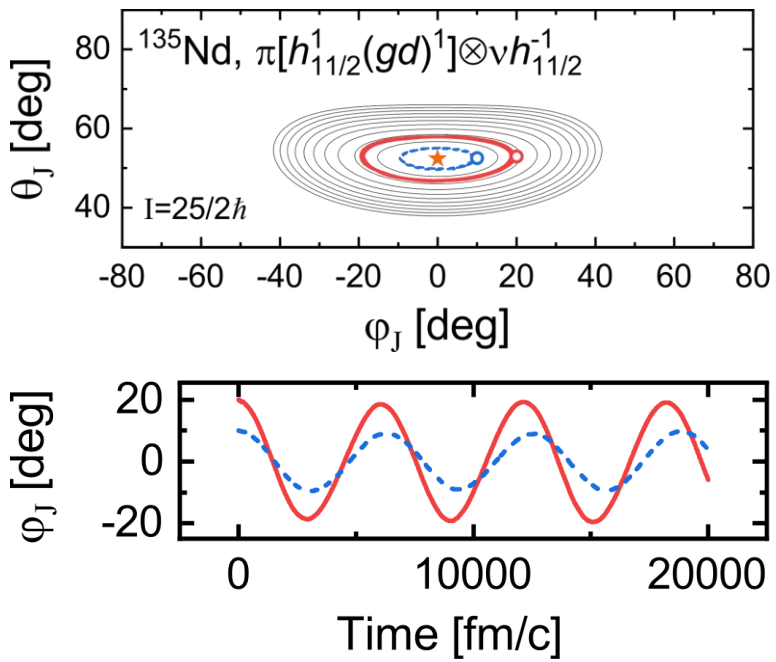
References & Literature

Upper Bands Limit: Zhao, PLB **773**, 1 (2017)

DFT Analysis: Ren, Zhao, Meng, PRC, **105**, L011301 (2022)

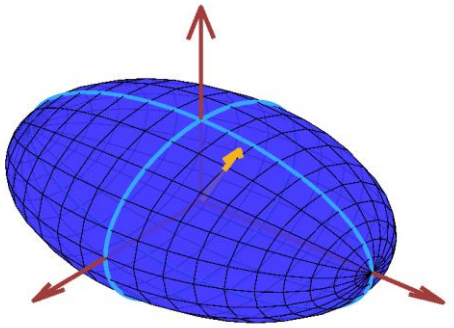
Quantum Chirality in Time-Dependent DFT

Chiral Precession Dynamics



Precession periods across sectors are roughly **identical**.

Body-Fixed Frame



3D Nuclear Ellipsoid

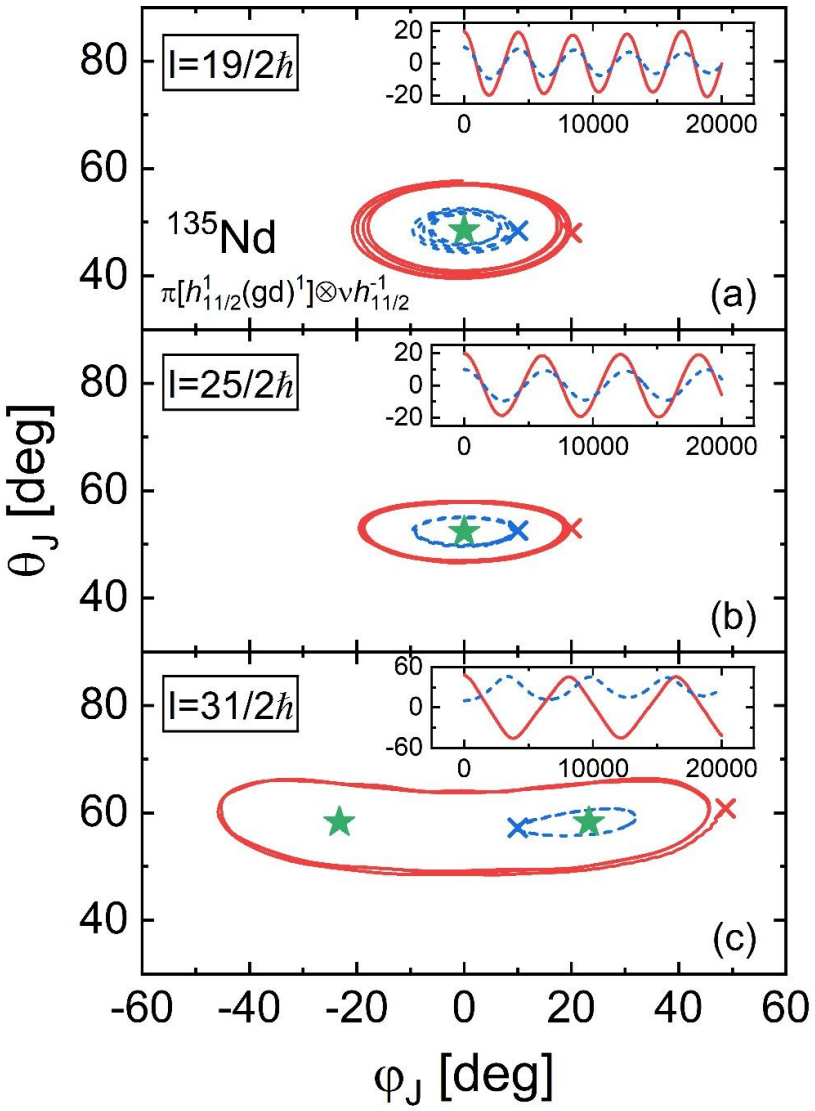
Visual representation of the nuclear shape and axes rotation within the body-fixed coordinate system.

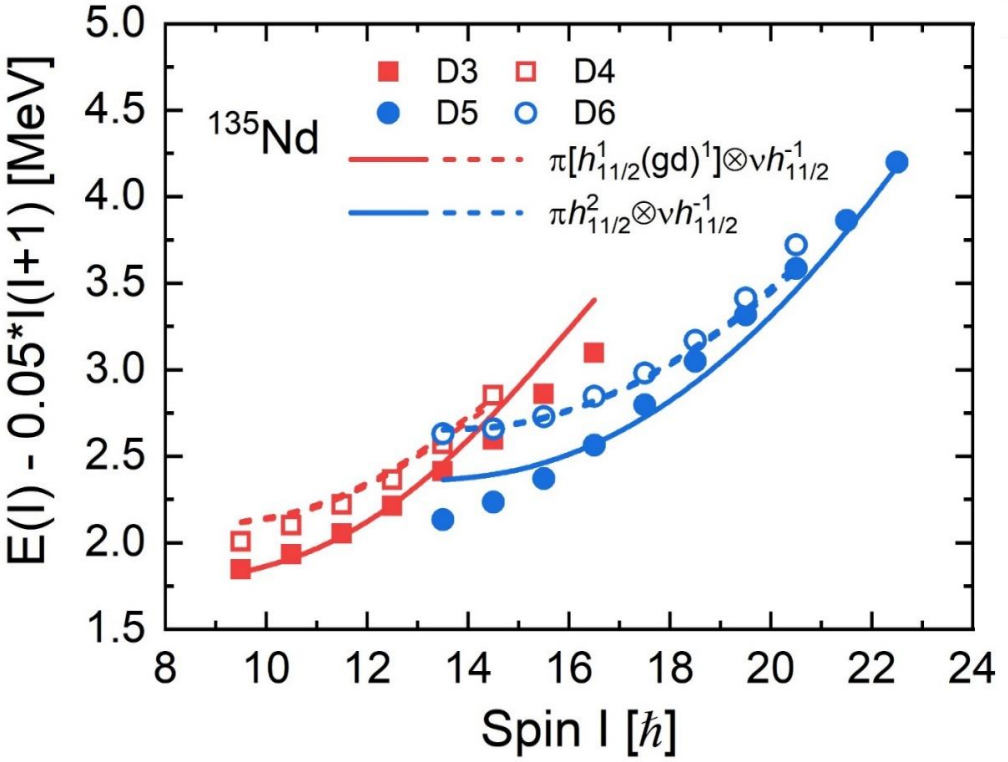
- **Chiral Precession**

References & Literature

[1] Ren, Zhao, Meng, PRC, **105**, L011301 (2022) | **[2]** Li, Zhao, Meng, PLB 856 (2024) 138877

Quantum chirality in Time-depend DFT





The first fully microscopic and self-consistent description for the ***chiral twin bands*** in the framework of DFTs.

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Summary & Perspectives

Key takeaways and future outlook on nuclear chirality research

01

Active Hot Topic

Chirality in atomic nuclei remains a highly active topic in modern nuclear physics, pushing and extending our tknowledge boundaries.

02

Great Progress

Significant theoretical and experimental breakthroughs in nuclear chirality have been successfully achieved globally.

03

Future Outlook

Continuous efforts to explore and understand the deep quantum nature of nuclear chirality are highly encouraged and appreciated.

Open Oquestions:

- Energy splitting versus angular momentum
- Orbitals higher than h11/2 for chiral nuclei
- Large-scale relativistic DFT calculations to predict new chiral nuclei
- Spontaneousl symmetry breaksing with …
- Wobbling and chiral rotation
- Quantum tunneling effect…

Thank you !

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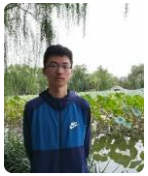
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Teng Qu



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Peng Guo



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