Relativistic configuration-interaction density functional theory: chiral rotation in ^{130}Cs

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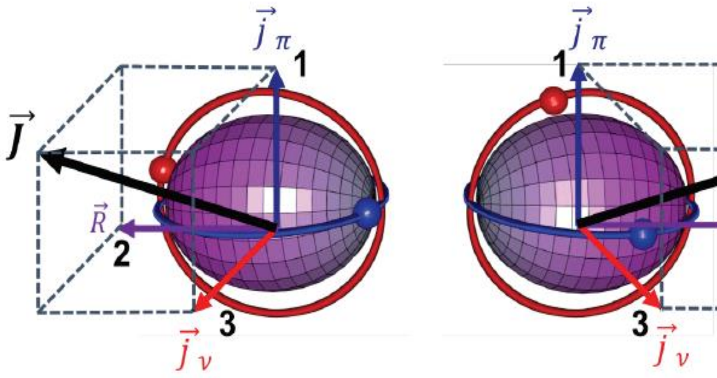
Outline

- Introduction
- Theoretical framework
- Numerical details
- Results and discussion
- Summary

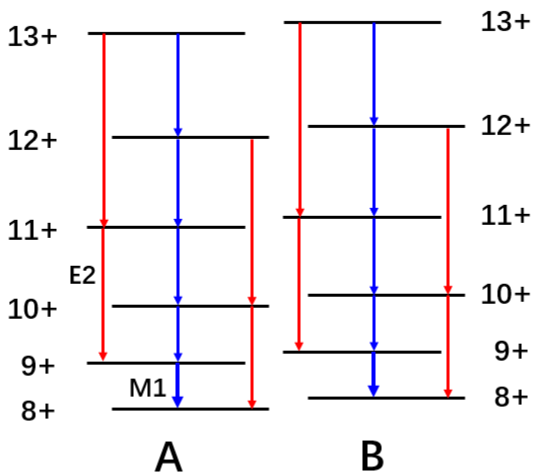
Nuclear chirality

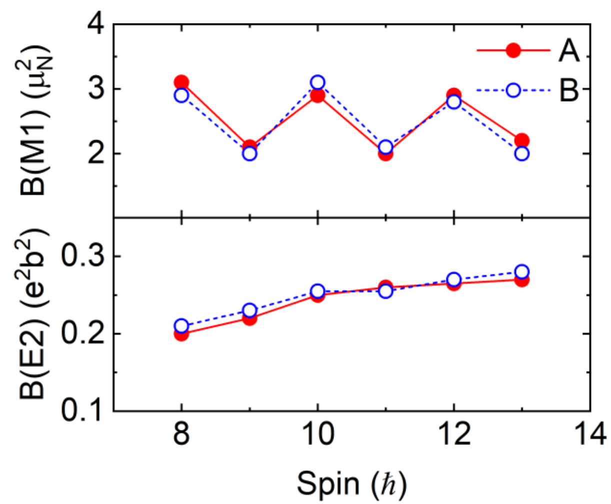
- Chirality in atomic nuclei was first suggested by Frauendorf and Meng in 1997 Frauendorf and Meng, NPA 617, 131 (1997)



Courtesy of X. H. Wu

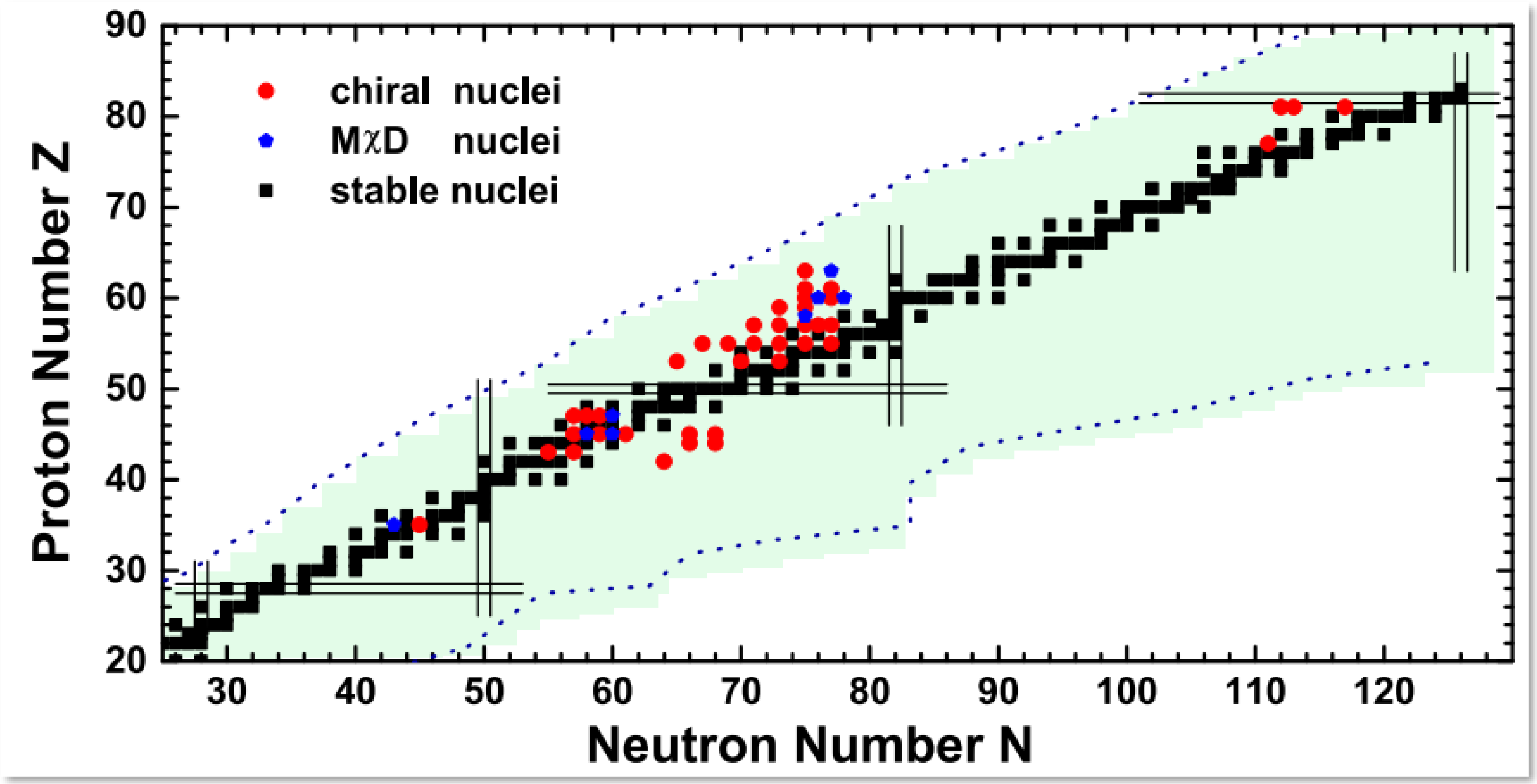
Intrinsic frame





Laboratory frame

Experimental progress



- More than 60 chiral doublet bands have been reported in mass regions 80, 100, 130, and 190.

Xiong and Wang, ADNDT 125, 193-225 (2019)

Theoretical progress

☐ Particle rotor model

Frauendorf and Meng, NPA 617, 131 (1997), Koike et al., PRL 93, 172502 (2004)

Peng et al., PRC 68, 044324 (2003), Zhang et al., PRC 044307 (2007)

Qi et al., PLB 675, 175 (2009), Chen et al., PLB 782, 744 (2018)

☐ Generalized coherent state model

Raduta et al., JPG 43, 095107 (2016)

☐ Interacting boson fermion-fermion model

Tonev et al., PRL 96, 052501 (2006), Tonev et al., PRC 76, 044313 (2007)

Brant et al., PRC 78, 034301 (2008)

Phenomenological approaches, parameters fitted to the data

Theoretical progress

- Tilted axis cranking (TAC) model

Frauendorf and Meng, NPA 617, 131 (1997),   Dimitrov et al., PRL 84, 5732 (2000)

- TAC + random phase approximation

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

- TAC + collective Hamiltonian method

Chen et al., PRC 87, 024314 (2013),   Chen et al., PRC 94, 044301 (2016)

- Projected shell model

Chen et al., PLB 785, 211 (2018),   YKW et al., PRC 99, 054303 (2019)

Single-*j* or pairing plus quadrupole-quadrupole model

Nuclear chirality in density functional theory

- Nonrelativistic density functional theory (DFT) + TAC

Olbratowski et al., PRL 93, 052501 (2004), Olbratowski et al., PRC 73, 054308 (2006)

- Relativistic DFT+ TAC

Zhao, PLB 773, 1 (2017), Zhao et al., PRC 99, 054319 (2019), Wang and Meng, PLB 841, 137923 (2023)

- Time-dependent relativistic DFT

Ren et al., PRC 105, L011301 (2022)

Angular momentum and transition probabilities are treated in a semiclassical way

Chirality in a fully microscopic and quantal way based on DFT is highly desirable

The present work

- Relativistic Configuration-interaction Density functional (ReCD) theory is adopted to study the nuclear chirality:
  - ✓ ReCD combines the advantages of configuration-interaction shell model and relativistic DFT ⇒ Simultaneous description of chiral doublet bands based on microscopic two-body interactions
  - ✓ The broken rotational symmetry is restored by three dimensional angular momentum projection technique ⇒ quantal description of spectra and transition probabilities

Relativistic DFT

- Relativistic Lagrangian density and Hamiltonian:

$$(\bar{\psi}\mathcal{O}\Gamma\psi), \quad \mathcal{O} \in \{1, \tau\}$$

$$\Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_\mu\gamma_5, \sigma_{\mu\nu}\}$$

$$\Rightarrow$$

$$\mathcal{L} = \mathcal{L}^{\text{free}} + \mathcal{L}^{\text{4f}} + \mathcal{L}^{\text{der}} + \mathcal{L}^{\text{hot}} + \mathcal{L}^{\text{em}}$$

$$\hat{H} = \int d\boldsymbol{r}\mathcal{H}(\boldsymbol{r})$$

- Relativistic density functional:

$$E \equiv \langle\Phi|\hat{H}|\Phi\rangle = \int d\boldsymbol{r}\left\{\sum_{i=1}^{A}\psi_i^\dagger(\boldsymbol{\alpha}\cdot\boldsymbol{p}+\beta m)\psi_i + \frac{1}{2}\alpha_S\rho_s^2 + \frac{1}{3}\beta_S\rho_s^3 + \frac{1}{4}\gamma_S\rho_s^4 + \frac{1}{2}\delta_S\rho_s\Delta\rho_s \right.$$
$$\left. + \frac{1}{2}\alpha_V j_\mu j^\mu + \frac{1}{4}\gamma_V(j_\mu j^\mu)^2 + \frac{1}{2}\delta_V j_\mu\Delta j^\mu + \frac{1}{2}\alpha_{TV}\vec{j}_\mu\vec{j}^\mu + \frac{1}{2}\delta_{TV}\vec{j}_\mu\Delta\vec{j}^\mu + \frac{1}{2}e^2A_\mu j_p^\mu\right\}$$

- Relativistic Hartree-Bogoliubov (RHB) equation:

$$\begin{pmatrix} h_D - \lambda & \Delta \\ -\Delta^* & -h_D^* + \lambda \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

$$h_D = \boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta(m+S) + V$$

$$\Delta_{\mu\nu} = \frac{1}{2}\sum_{\delta\gamma}\langle\mu\nu|V^{pp}|\delta\gamma\rangle_a\kappa_{\delta\gamma}$$

- Intrinsic ground-state for odd-odd nucleus: $|\Phi_{\pi_0\nu_0}\rangle = \hat{\beta}^\dagger_{\pi_0}\hat{\beta}^\dagger_{\nu_0}|\Phi_0\rangle$

ReCD theory

- Wavefunction in ReCD theory:

$$|\Psi^I_\alpha\rangle = \sum_{K=-I}^{I} \sum_{\kappa} f^{I\alpha}_{K\kappa} \hat{P}^I_{MK} |\Phi_\kappa\rangle$$

- Configuration space:

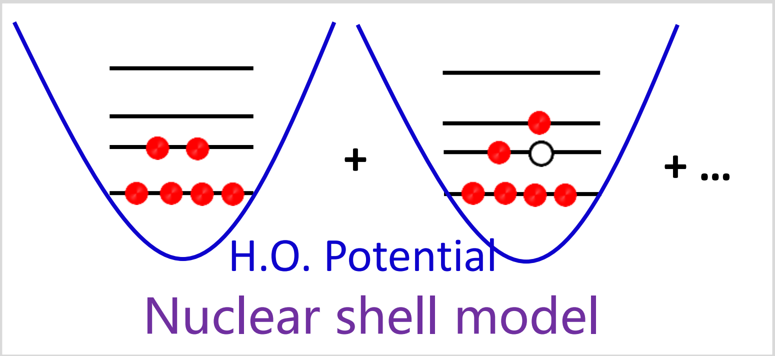
$$|\Phi_\kappa\rangle \in \{|\Phi_{\pi_0\nu_0}\rangle, \hat{\beta}^\dagger_{\pi_i}\hat{\beta}^\dagger_{\nu_j}|\Phi_0\rangle, \hat{\beta}^\dagger_{\pi_i}\hat{\beta}^\dagger_{\nu_j}\hat{\beta}^\dagger_{\nu_k}\hat{\beta}^\dagger_{\nu_l}|\Phi_0\rangle, \hat{\beta}^\dagger_{\pi_i}\hat{\beta}^\dagger_{\nu_j}\hat{\beta}^\dagger_{\pi_k}\hat{\beta}^\dagger_{\pi_l}|\Phi_0\rangle\}.$$

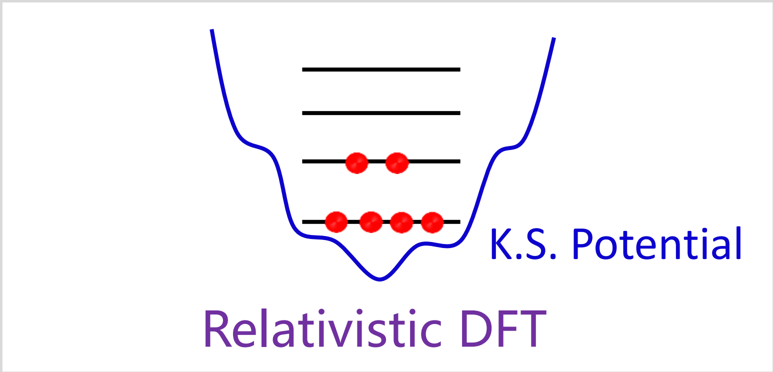
- Hill-Wheeler equation:

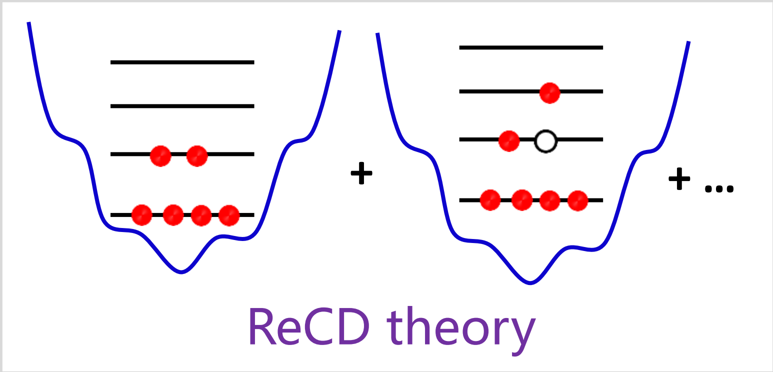
$$\sum_{K'\kappa'} \{\mathcal{H}^I_{KK';\kappa\kappa'} - E^I_\alpha \mathcal{N}^{I\alpha}_{KK';\kappa\kappa'}\} f^{I\alpha}_{K'\kappa'} = 0$$

- Transition probabilities:

$$\frac{1}{2I_i+1} |\langle \Psi^{I_f} || \hat{O}_\lambda || \Psi^{I_i} \rangle|^2$$







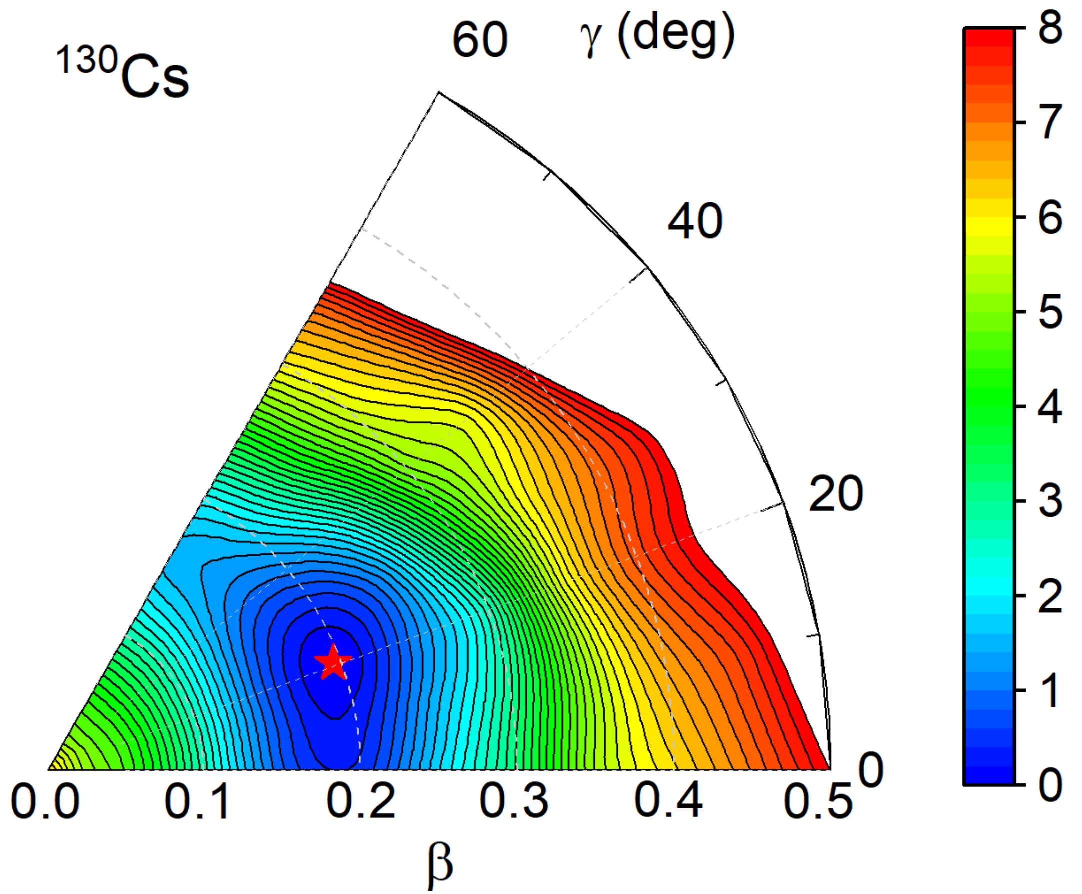
Numerical details

- Nucleus: ^{130}Cs
- Major shells: 10
- Density functional: PC-PK1

  Zhao, Li, Yao, and Meng, PRC 82, 054319 (2010)
- Pairing interaction: Separable pairing force

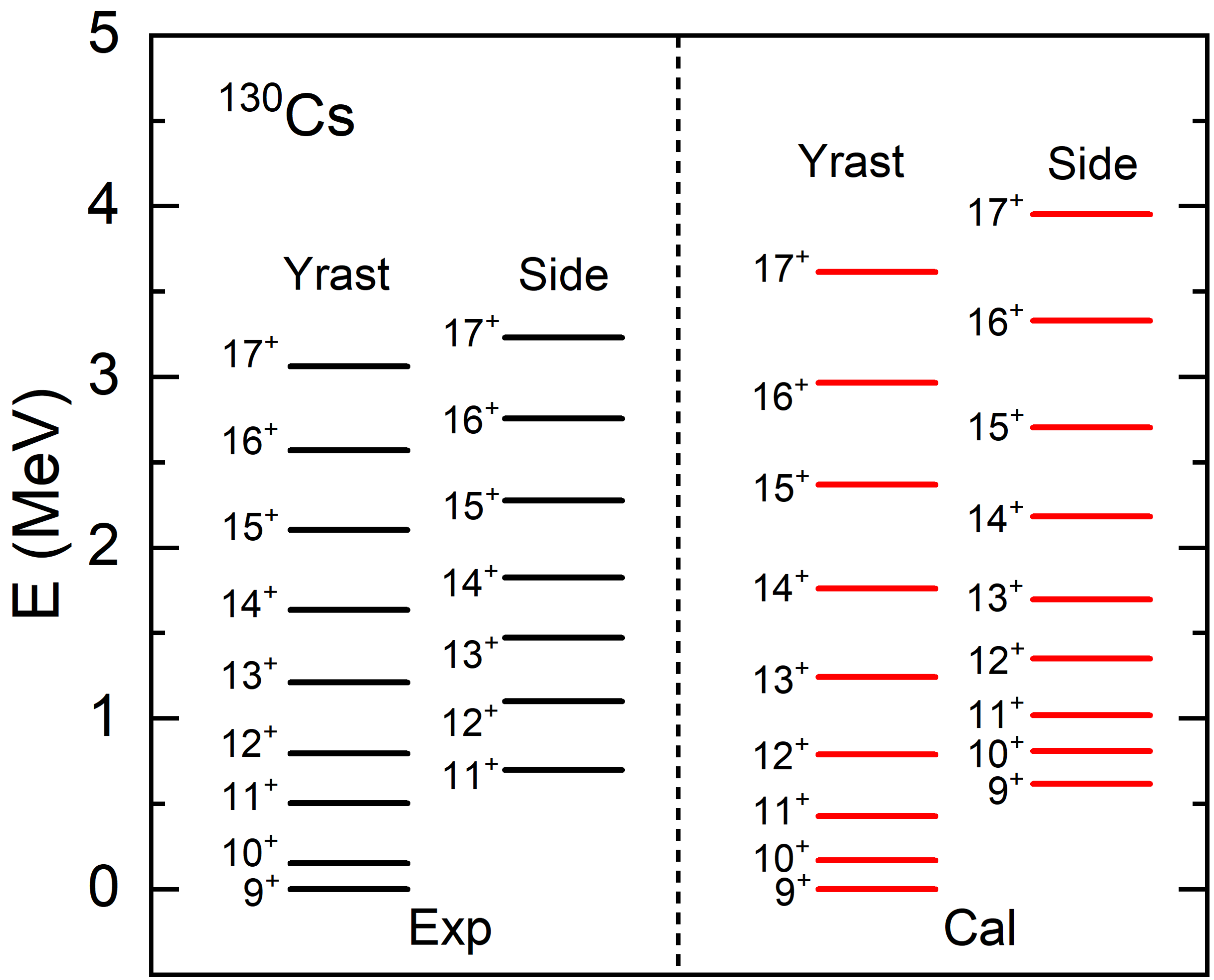
  Tian, Ma, and Ring, PLB 676, 44 (2009)
- Integral grids of Euler angles: $(\psi, \theta, \phi) = (20,20,20)$
- Quasiparticle excitation energy cutoff: E_{cut} = 5.0 MeV

Potential energy surface



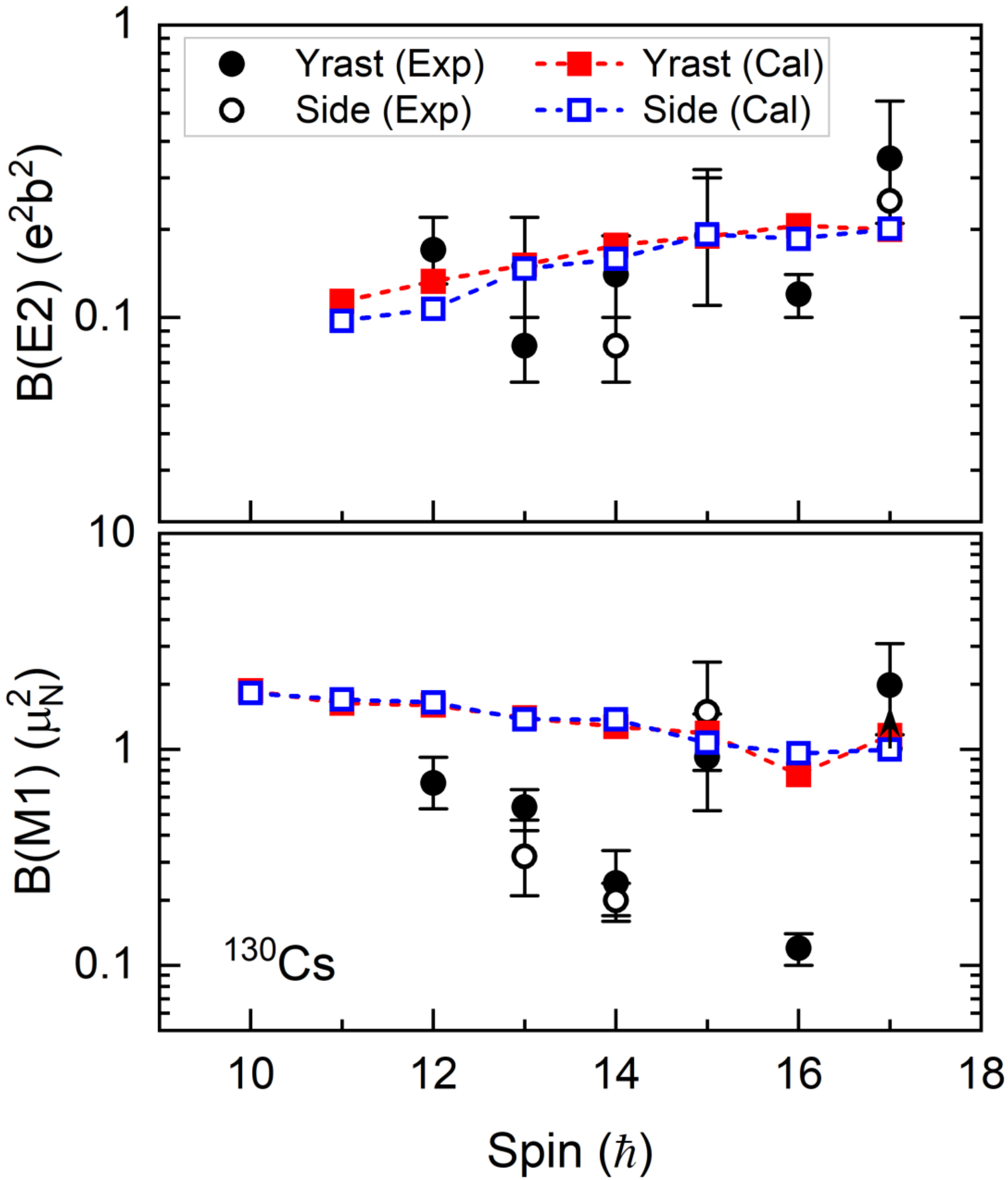
- The deformation parameters β and γ are predicted to be 0.195 and $20.58°$

Energy spectra



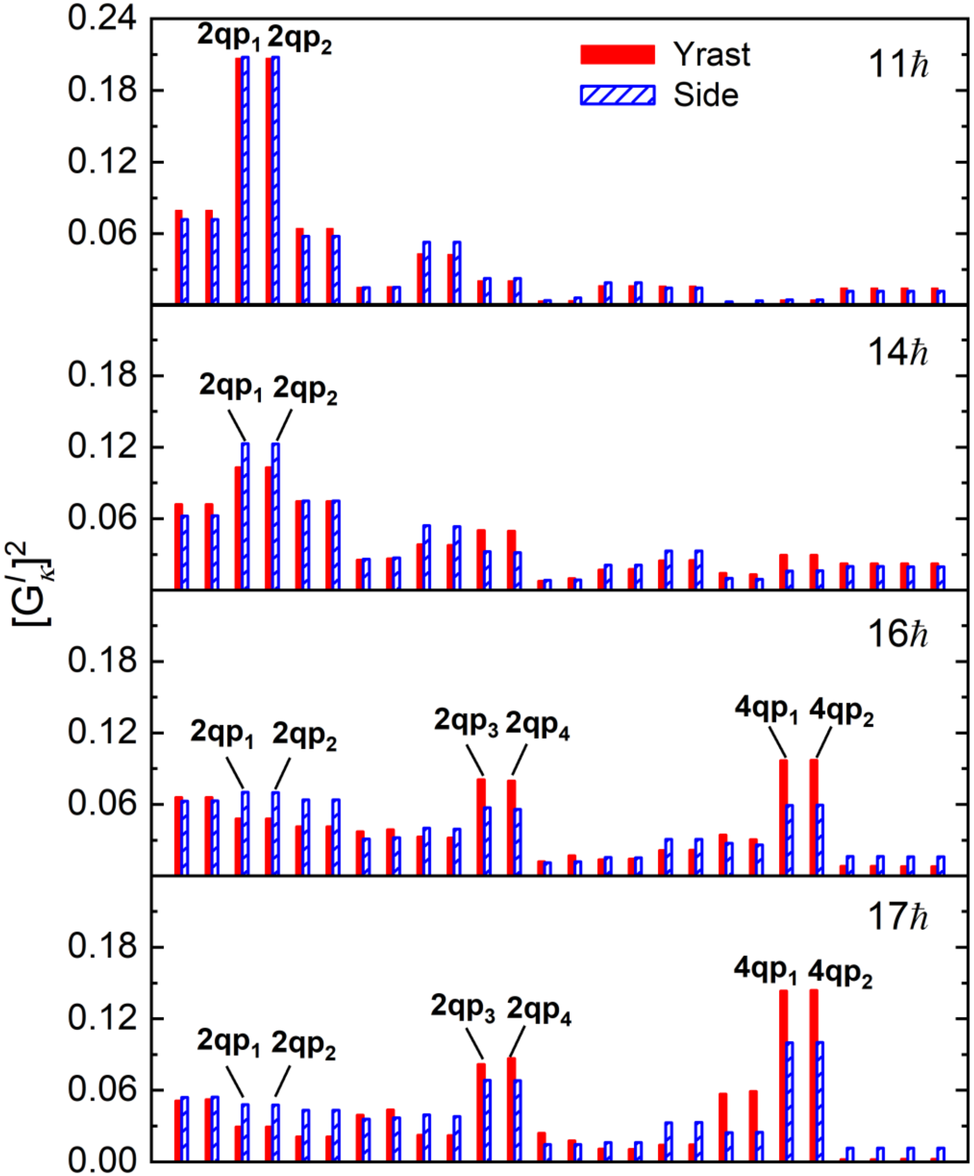
- The energy spectra for both the yrast and side bands in ^{130}Cs are reproduced satisfactorily by the ReCD calculations

Transition probabilities



- The B(E2) and B(M1) values are reproduced satisfactorily
- No effective charges are used in the calculation
- Transition probabilities for yrast and side bands are predicted to be similar
- The calculated staggering behaviors for M1 transitions for states with spin larger than $14\hbar$ are much weaker than data

Composition of wavefunctions



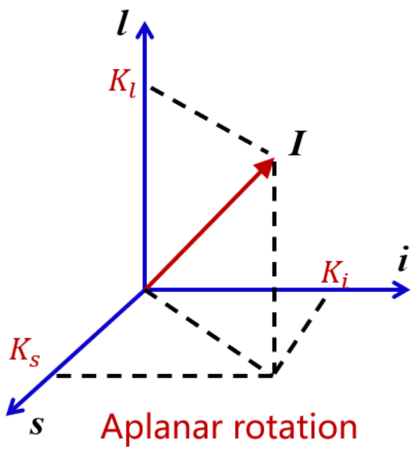
$$G^I_\kappa = \sum_K \sum_{\kappa' K'} N^{1/2}_{\kappa K;\kappa' K'} F^I_{\kappa' K'}$$

Label	Configuration
2qp1	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;9/2})$
2qp2	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-9/2})$
2qp3	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;5/2})$
2qp4	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-5/2})$
4qp1	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;9/2}h_{11/2;7/2}h_{11/2;-7/2})$
4qp2	$\pi(h_{11/2;1/2}) \otimes \nu(h_{11/2;-9/2}h_{11/2;7/2}h_{11/2;-7/2})$

- Four qp configurations begin to play dominant roles for states with $I = 16\hbar$ and $17\hbar$

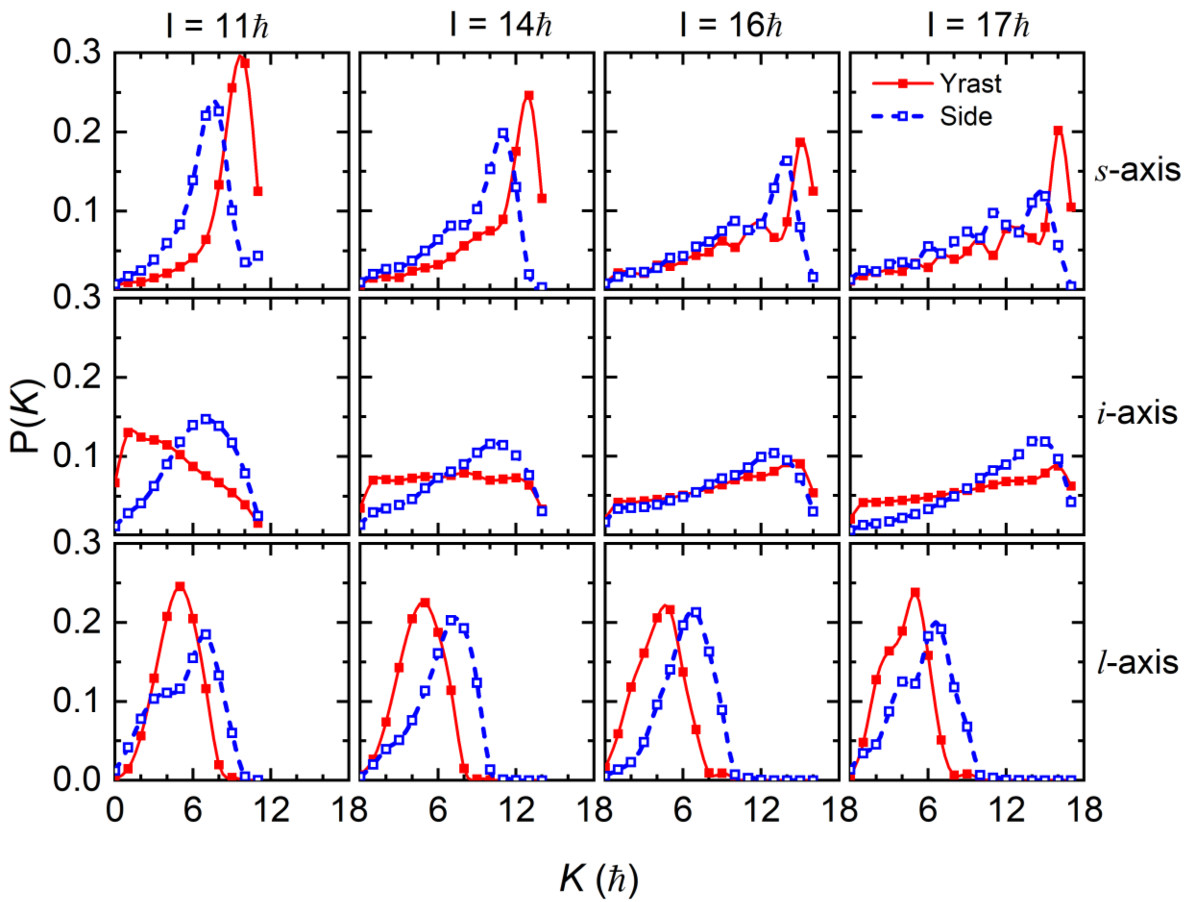
Chiral geometry: K-plot

A-plot: *the probability distribution of angular momentum components on three axes of the intrinsic frame*



$$G_{\kappa K} = \sum_{\kappa' K'} N^{1/2}_{\kappa K;\kappa' K'} F_{\kappa' K'}$$

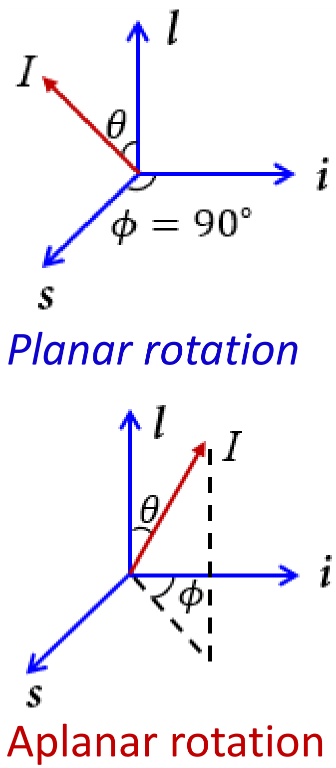
$$P(K) = \sum_{\kappa} |G_{\kappa K}|^2 + |G_{\kappa -K}|^2$$

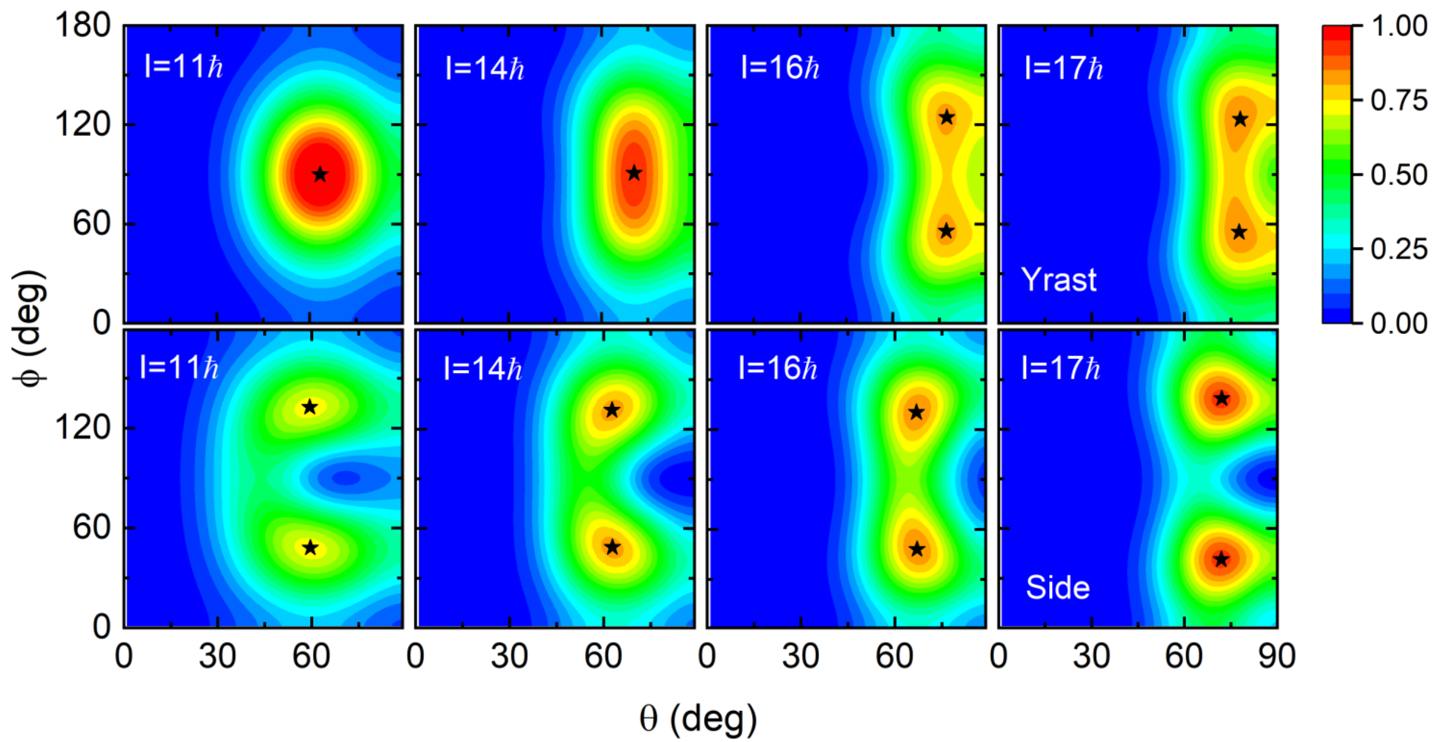


- The evolution from chiral vibration to static chirality is clearly shown

Chiral geometry: A-plot

Azimuthal plot (A-plot): *the probability distribution for the orientation of the angular momentum on the* (θ, ϕ) *plane*





- The chiral geometry revealed by A-plot is consistent with that obtained from K-plot

Summary

- ReCD theory is adopted to study the nuclear chirality in 130Cs:
  - ✓ The spectroscopic properties of chiral doublets are reproduced satisfactorily
  - ✓ The chiral geometries from chiral vibration to static chirality are illustrated through the A-plot and K-plot
  - ✓ The present work provides the first microscopic and quantal description for the chirality in atomic nuclei