K-ISOMERIC STATES IN HEAVY, WELL-DEFORMED NUCLEI WITHIN A MICROSCOPIC FRAMEWORK

L. Bonneau[1], P. Quentin[1], N. Minkov[2], D. Ivanova[3,4], J. Bartel[5], H. Molique[5], Meng Hock Koh[6]

[1]CENBG, Bordeaux (France)
[2]INRNE, Sofia (Bulgaria)
[3]University Hospital "Saint Ekaterina", Sofia (Bulgaria)
[4]Military Medical Academy, Sofia (Bulgaria)
[5]IPHC, Strasbourg (France)
[6]UTM, Johor Bahru (Malaysia)

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cnrs IN2P3 Institut national de physique nucléaire et de physique des particules

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Introduction

Context

- K-isomerism as a way to probe details of nuclear mean field (single-particle spectra, deformation)
- recent theoretical efforts: DSM approach (N. Minkov et al.), covariant DFT approach (talk by G. Lalazissis)

Goals

1. Assess quality of spectroscopic results from selfconsistent mean-field approaches with pairing in deformed nuclei for quasiparticle-like configurations such as K-isomeric states
2. Study effects of symmetry breaking at the mean-field level on static properties of K-isomers
   - core polarization (Koopmans vs. selfconsistent blocking)
   - octupole degree of freedom

Outline:

1. Description of nuclei in states with finite seniority number[1]: mean-field approach with selfconsistent blocking and treatment of pairing correlations
2. Application to 2-qp K-isomeric states around $A \sim 154$ and $A \sim 236$ without parity breaking
3. Effect of octupole degree of freedom (parity breaking)

[1] number of unpaired nucleons

Skyrme-HFBCS approach

General features

- Variational principle applied to BCS-like trial wave functions:
  - For GS of even-even nuclei

$$|\mathrm{BCS}\rangle = \prod_{i>0}(u_i + v_i a_i^\dagger a_{\bar{i}}^\dagger)\,|0\rangle$$

  - Variation with respect to occupation amplitudes v_i and single-particle states $|i\rangle = a_i^\dagger|0\rangle$

$$\delta(\langle \mathrm{BCS}|\hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} - \lambda \hat{Q} \cdots |\mathrm{BCS}\rangle) = 0$$

    $\langle \mathrm{BCS}|\hat{H}|\mathrm{BCS}\rangle$ = Skyrme energy-density functional (here SIII + seniority residual interaction)
    $\hat{Q}$ = any additional constraint (multipole moments, center of mass position if parity breaking...)
- Selfconsistent determination of v_i and $|i\rangle$ by iterations
- In practice expansion of s.p. states on axially-deformed HO basis
  $\Rightarrow$ HF orbitals mix Nilsson quantum numbers

Skyrme-HFBCS approach

Selfconsistent symmetries

- axial symmetry (z axis)
- parity symmetry for the study in rare-earth nuclei only

Selfconsistent blocking of nucleons

Odd-mass, odd-odd or excited even-even nuclei:

- n and/or p close to Fermi level of underlying even-even core
- occupation equal to 1 for each single-particle state i with quantum numbers $\Omega_i^{\pi_i}$ such that $\sum_i \Omega_i = K$ et $\prod_i \pi_i = \pi$
- BCS solution with blocked states $\Rightarrow$ pairing quenching
- procedure embedded in the iterative HF process

SKYRME-HFBCS APPROACH

DEFINITION OF PAIRS OF CONJUGATE STATES

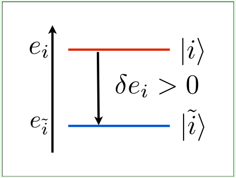
- Case of a time-reversal invariant solution:
  Kramers degeneracy $\Rightarrow$ *pairs of conjugate states* $(|i\rangle, |\bar{i}\rangle)$
- Case of a time-reversal breaking solution:
  pairs of conjugate states $(|i\rangle, |\tilde{i}\rangle)$ *such that*

$$\hat{h}_{\mathrm{HF}}|i\rangle = e_i|i\rangle \qquad \hat{J}_z|i\rangle = \Omega_i|i\rangle \quad \text{with } \Omega_i > 0$$

$$\hat{h}_{\mathrm{HF}}|\tilde{i}\rangle = e_{\tilde{i}}|\tilde{i}\rangle \qquad \hat{J}_z|\tilde{i}\rangle = \Omega_{\tilde{i}}|\tilde{i}\rangle \quad \text{with } \Omega_{\tilde{i}} = -\Omega_i < 0$$

$$\left|\langle\bar{i}|\widetilde{i}\rangle\right| \text{ maximum (close to 1 in practice)}$$

$$\delta e_i = e_i - e_{\tilde{i}}$$



ADJUSTMENT OF RESIDUAL INTERACTION IN BCS

Like-nucleon pairing residual interaction: $\langle i\bar{i}|\hat{V}|\widetilde{j\bar{j}}\rangle = \dfrac{G_0^{(q)}}{11 + N_q}$ $\quad q = \text{n or p}$

Rare-earth region: 2 independent fits of $G_0^{(\tau_i)}$ (Nor et al., PRC99 (2019))

- directly on 3-point binding-energy differences centered on odd-A nucleus

$$\Delta_3^{(n)} = \frac{(-1)^N}{2}\Big[E(N+1,Z) + E(N-1,Z) - 2E(N,Z)\Big]$$

- on moments of inertia

$$\frac{\hbar^2}{2\mathcal{I}_{\text{Bel}} \times \alpha} = \frac{1}{6}\, E^*_{\text{exp}}(2_1^+)$$

where $\alpha =$ corrective factor for Thouless–Valatin effects

$\Rightarrow$ very close resulting optimal values $G_0^{(n)} = 16.20$ and $G_0^{(p)} = 15.05$

note that $G_0^{(p)}/G_0^{(n)} = 0.93$ consistent with expected Coulomb anti-pairing effect

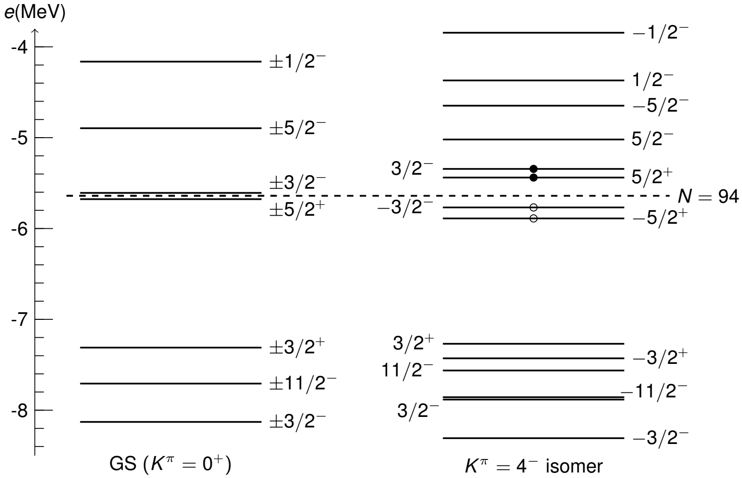
Adjustment of residual interaction in BCS

Like-nucleon pairing residual interaction: $\langle i\bar{i}|\hat{V}|\widetilde{j\bar{j}}\rangle = \dfrac{G_0^{(q)}}{11 + N_q}$ $\quad q = $ n or p

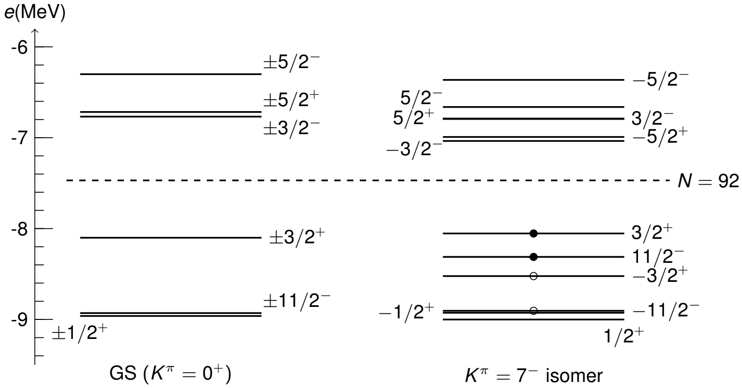
Actinide region: preliminary calibration of $G_0^{(n)}$ on moment of inertia for a small sample of nuclei, with $G_0^{(p)} = 0.9 \times G_0^{(n)}$ as for rare earths
$\Rightarrow G_0^{(n)} = 16$, $G_0^{(p)} = 14.5$ (slightly smaller than in rare-earth region)

Nucleus	$\dfrac{\hbar^2}{2\mathcal{I}_{\rm Bel} \times \alpha}$ (keV)	$\frac{1}{6}\, E^*_{\rm exp}(2^+_1)$ (keV)
^{234}U	7.41	7.25
^{236}U	8.16	7.53
^{236}Pu	7.01	7.43
^{238}Pu	7.48	7.34

Example: neutron single-particle spectra of ^{154}Nd with HF(SIII)+BCS(G)



Example: neutron single-particle spectra of ^{156}Gd with HF(SIII)+BCS(G)



2QP K-ISOMERS IN RARE-EARTH NUCLEI AROUND $A \sim 154$

Magnetic diple moment of $K = I$ bandhead (in μ_N unit):

$$\mu = \frac{K}{K+1}(g_R + \langle\hat{\mu}_z\rangle) \qquad \text{with } \hat{\mu}_z = g_\ell \hat{L}_z + g_s \hat{S}_z$$

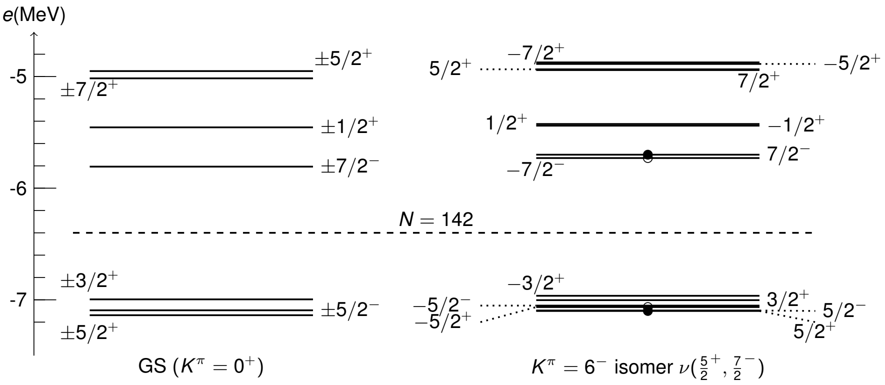
without empirical attenuation factor for g_s because selfconsistent blocking (SCB) effectively quenches g_s (L. B. et al. PRC91 (2015))

Nucleus	K^π	config.	β_2	E_{2qp}	E^*_{SCB}	E^*_{exp}	$\langle\hat{\mu}_z\rangle$	g_R	μ
^{154}Nd	4^-	$\nu(\frac{5}{2}^+, \frac{3}{2}^-)$	0.32	1.681	1.165	1.298	−1.962	0.476	−1.189
^{156}Nd	5^-	$\nu(\frac{5}{2}^+, \frac{5}{2}^-)$	0.32	1.955	1.447	1.431	−0.117	0.475	0.298
^{156}Sm	5^-	$\nu(\frac{5}{2}^+, \frac{5}{2}^-)$	0.31	1.929	1.659	1.398	−0.097	0.358	0.217
		$\pi(\frac{5}{2}^+, \frac{5}{2}^-)$	0.32	1.988	1.233		4.925		4.402
^{156}Gd	7^-	$\nu(\frac{11}{2}^-, \frac{3}{2}^+)$	0.31	2.642	3.115	2.138	−2.189	0.269	−1.680

($Z/A \approx 0.39$ for these nuclei)

- SCB decreases isomer excitation energy E^* with respect to E_{2qp}
- Good agreement of SCB calculations with experimental E^*
- Exception: ^{156}Gd
- 2 candidate config. found in ^{156}Sm, distinguished by magnetic moment

Example: neutron single-particle spectra of ^{234}U with HF(SIII)+BCS(G)



2QP K-ISOMERS IN ACTINIDE NUCLEI AROUND $A \sim 236$

Considered isomers:

Nucleus	K^π	config.
^{234}U	6^-	$\nu(\frac{7}{2}^-, \frac{5}{2}^+)$
^{236}U	4^-	$\nu(\frac{7}{2}^-, \frac{1}{2}^+)$
		$\pi(\frac{5}{2}^-, \frac{3}{2}^+)$
^{236}Pu	5^-	$\pi(\frac{5}{2}^-, \frac{5}{2}^+)$
^{238}Pu	4^-	$\nu(\frac{7}{2}^-, \frac{1}{2}^+)$

HF(SIII)+BCS(G) results:

Nucleus	K^π	β_2	E^*_{SCB}	E^*_{exp}	$\langle \hat{\mu}_z \rangle$	g_R	μ
^{234}U	6^-	0.25	1.595	1.421	-0.190	0.303	0.097
^{236}U	4^-_n	0.25	1.067	1.052	3.528	0.322	3.080
	4^-_p	0.25	1.457		-0.239		0.066
^{236}Pu	5^-	0.26	1.236	1.185	4.899	0.365	4.387
^{238}Pu	4^-	0.26	1.071	–	-0.216	0.379	0.130

IMPACT OF OCTUPOLE DEGREE OF FREEDOM ON K-ISOMERS

Case of ^{234}U

- DSM calculations of $E_{2qp}(\beta_2, \beta_3)$ suggest octupole deformed 6^- isomer (N. Minkov and P. Walker, Phys. Scr. 89 (2014))
- HF(SIII)+BCS(G) calculations: blocked configuration $\nu(\frac{5}{2}, \frac{7}{2})$ nearest to Fermi level with parity and time-reversal symmetry breaking

K^π	β_2	β_3	Single-particle $\langle\hat{\pi}\rangle$	$E^*_{\rm SCB}$(MeV)	$E^*_{\rm exp}$	μ
0^+	0.25	0.00	—	0	0	0
6^-	0.25	0.05	$\langle\pi\rangle(\frac{5}{2}) = +0.086$ $\langle\pi\rangle(\frac{7}{2}) = -0.775$	1.481	1.421	-0.081
	0.25	set to 0	—	1.595		0.097

Multipole deformation parameters β_ℓ calculated as $\beta_\ell = \frac{4\pi}{3} \frac{\langle r^\ell Y_\ell^0 \rangle}{r_0^\ell A^{1+\ell/3}}$ *($r_0 = 1.2$ fm)*

Very strong parity mixing in the $\Omega = 5/2$ blocked state

Parity projection is expected to yield virtually no effect according to, e.g., T.V. Nhan Hao, P. Quentin and L. B., PRC86 (2012)

Conclusions:

- Rather good reproduction of excitation energies of K-isomers around $A \sim 154$ and $A \sim 236$ thanks to good spectroscopic properties of SIII and good pairing strength
- Important effect of selfconsistent blocking
- Sizeable effect of octupole deformation in ^{234}U isomeric state $K^{\pi} = 6^{-}$

Perspectives:

- Investigate impact of particle-number conservation in pairing treatment on isomer excitation energies
- Extend search for octupole effects on 2qp K-isomers around ^{154}Nd, ^{254}No and ^{270}Ds
- Apply this approach to K-isomers in odd-mass and odd-odd nuclei

BACKUP SLIDES

PHENOMENOLOGICAL EFFECTIVE "INTERACTION"

Skyrme two-body interaction + density-dependent term in momentum space:

$$\widetilde{v}_{\mathrm{Sk}}(\mathbf{k},\mathbf{k}') = \underbrace{t_0(1+x_0\hat{P}_\sigma) + \frac{t_3}{6}\widetilde{\rho^\alpha}(\mathbf{K})(1+x_3\hat{P}_\sigma) + \frac{t_1}{2}(1+x_1\hat{P}_\sigma)(\mathbf{k}^2+\mathbf{k}'^2)}_{^1S_0\ (S=0,\ T=1)\ \textit{and}\ ^3S_1\ (S=1,\ T=0)}$$

$$+ \underbrace{t_2(1+x_2\hat{P}_\sigma)\,\mathbf{k}\cdot\mathbf{k}'}_{^1P_1\ (S=T=0)\ \textit{and}\ ^3P_J\ (S=T=1)} + \underbrace{i\,W\,(\hat{\boldsymbol{\sigma}}_1+\hat{\boldsymbol{\sigma}}_2)\cdot(\mathbf{k}\times\mathbf{k}')}_{^3P_J\ (S=T=1)}$$

$$+ \underbrace{\frac{t_o}{2}\left[3\Big((\hat{\boldsymbol{\sigma}}_1\cdot\mathbf{k})\,(\hat{\boldsymbol{\sigma}}_2\cdot\mathbf{k}') + (\hat{\boldsymbol{\sigma}}_1\cdot\mathbf{k}')\,(\hat{\boldsymbol{\sigma}}_2\cdot\mathbf{k})\Big) - 2(\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2)\,\mathbf{k}\cdot\mathbf{k}'\right]}_{^3P_J\ (S=T=1)}$$

$$+ \underbrace{\frac{t_e}{2}\left[3(\hat{\boldsymbol{\sigma}}_1\cdot\mathbf{k})(\hat{\boldsymbol{\sigma}}_2\cdot\mathbf{k}) - (\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2)\,\mathbf{k}^2 + 3(\hat{\boldsymbol{\sigma}}_1\cdot\mathbf{k}')(\hat{\boldsymbol{\sigma}}_2\cdot\mathbf{k}') - (\hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2)\,\mathbf{k}'^2\right]}_{^3S_1-{}^3D_1\ (S=1,\ T=0)}$$

ENERGY FUNCTIONAL

For a BCS-type product state $|\Psi\rangle$:

$$E[\Psi] = \int d\mathbf{r} \left(\mathcal{H}_{\rm kin}(\mathbf{r}) + \mathcal{H}_{\rm nucl}(\mathbf{r})\right) + E_{\rm Coul} + E_{\rm pair}$$

with

$$\mathcal{H}_{\rm kin}(\mathbf{r}) = \left(1 - \frac{1}{A}\right) \frac{\hbar^2}{2m} \tau \quad \text{(here, 1-body center-of-mass correction only)}$$

$$\mathcal{H}_{\rm nucl}(\mathbf{r}) = (B_1 + B_7 \rho^\alpha)\rho^2 + (B_{10} + B_{12}\rho^\alpha)\mathbf{s}^2 + B_3\,(\rho\,\tau - \mathbf{j}^2) + B_5\,\rho\,\Delta\rho \quad \text{(central)}$$

$$+ B_{14}\,(\overleftrightarrow{J}^2 - \mathbf{s}\cdot\mathbf{T}) + B_{18}\,\mathbf{s}\cdot\Delta\mathbf{s} \quad \text{(central + tensor)}$$

$$+ B_{16}\left[(\mathrm{Tr}\,\mathrm{J})^2 + \sum_{\mu,\nu} \mathrm{J}_{\mu\nu}\mathrm{J}_{\nu\mu} - 2\,\mathbf{s}\cdot\mathbf{F}\right] + B_{20}\,(\boldsymbol{\nabla}\cdot\mathbf{s})^2 \quad \text{(tensor)}$$

$$+ B_9 \left(\rho\,\boldsymbol{\nabla}\cdot\mathbf{J} + \mathbf{j}\cdot\boldsymbol{\nabla}\times\mathbf{s}\right) \quad \text{(spin-orbit)}$$

$$+ \sum_q \text{corresponding terms for the charge state } q \text{ alone}$$

$E_{\rm Coul} = E^{(dir)}_{\rm Coul}$ (exact) $+ E^{(exch)}_{\rm Coul}$ (Slater approximation)

$E_{\rm pair}$ calculated in BCS with a seniority force

Skyrme-HFBCS approach

Hartree–Fock Hamiltonian

$$\langle \mathbf{r}|\hat{h}^{(q)}_{\mathrm{HF}}|\phi_k\rangle = -\boldsymbol{\nabla}.\left(\frac{\hbar^2}{2m^*_q(\mathbf{r})}\boldsymbol{\nabla}[\phi_k](\mathbf{r})\right) + \Big(U_q(\mathbf{r}) + \delta_{q\,p}V_{\mathrm{Coul}}(\mathbf{r})\Big)[\phi_k](\mathbf{r})$$

$$+ i\,\mathbf{W}_q(\mathbf{r})\cdot\Big(\boldsymbol{\sigma}\times\boldsymbol{\nabla}[\phi_k](\mathbf{r})\Big)$$

$$\underbrace{-i\sum_{\mu,\nu}\left\{\Big(W^{(J)}_{q,\mu\nu}(\mathbf{r})\sigma_\nu\nabla_\mu[\phi_k](\mathbf{r})\Big) + \nabla_\mu\Big(W^{(J)}_{q,\mu\nu}(\mathbf{r})\sigma_\nu[\phi_k](\mathbf{r})\Big)\right\}}_{\text{from } \mathrm{J}_{\mu\nu} \text{ terms induced by central + tensor}}$$

$$+\boxed{\mathbf{S}_q(\mathbf{r})\cdot\boldsymbol{\sigma}[\phi_k](\mathbf{r})} - \frac{i}{2}\left\{\mathbf{A}_q(\mathbf{r})\cdot\boldsymbol{\nabla}[\phi_k](\mathbf{r}) + \boldsymbol{\nabla}\cdot\Big(\mathbf{A}_q(\mathbf{r})[\phi_k](\mathbf{r})\Big)\right\}$$

+spin-gradient couplings from central + tensor

whith the spin field $\mathbf{S}_q(\mathbf{r})$

$$\mathbf{S}_q(\mathbf{r}) = \boxed{2\big(B_{10} + B_{12}\,\rho^\alpha\big)\mathbf{s} + 2\big(B_{11} + B_{13}\,\rho^\alpha\big)\mathbf{s}_q - (B_{14}\,\mathbf{T} + B_{15}\,\mathbf{T}_q)}$$

$$-\,B_9\,\boldsymbol{\nabla}\times(\mathbf{j}+\mathbf{j}_q) + \text{terms deriving from central + tensor}$$