Time-odd effects on single-particle spectra of odd-mass nuclei in the Skyrme–Hartree–Fock approach

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Introduction

Motivations

- Aim: spectroscopy of odd-mass deformed nuclei, including isomeric states in the Higher Tamm-Dancoff Approximation *(highly truncated shell model based on the Hartree–Fock solution)*
- Unified Model for axially deformed odd nuclei
  - collective degrees of freedom (d.o.f.) coupled to intrinsic d.o.f. in a symmetry-preserving way that depends on the discrete symmetries of intrinsic deformation
  - for odd nuclei with time-reversal breaking one-body hamiltonian:

$$\Psi_{IMK} \propto (1 + \mathcal{R}_y) D^I_{M,K} \phi_K$$

with $\mathcal{R}_y$ = y-signature operator (symmetry axis = z axis)

Introduction

Motivations

- First step here: single-particle spectra within Hartree-Fock approach (including polarization of the underlying even-even core but no pairing) and physical consequences

Outline

- Theoretical framework:

  self-consistent one-body hamiltonian in the time-reversal symmetry breaking Hartree-Fock approach

- Results for deformed odd nuclei:
  - *Effects of time-reversal symmetry breaking on single-particle spectra*
  - *Core polarization contribution to single-particle magnetic moments*

THEORETICAL FRAMEWORK:

HARTREE-FOCK APPROACH TO ODD NUCLEI

Hartree-Fock approach to odd nuclei

Description of the even-even (N, Z) core

Hartree-Fock-BCS calculation for even-even nucleus around $A = 100$:

- Skyrme SIII effective interaction (good spectroscopic properties)
- constant pairing matrix elements in BCS
- axial and intrinsic parity symmetries assumed

$\Rightarrow$ BCS ground state with realistic deformation

Hartree-Fock approach to odd nuclei

Description of $(N+1, Z)$ and $(N, Z+1)$ nuclei

- Extract lowest-energy Slater determinant $|\Phi_0\rangle$ from BCS ground state of even-even core
- Create one neutron or one proton in the lowest-energy K^π unoccupied single-particle state on $|\Phi_0\rangle \Rightarrow$ Slater determinant $|\Phi_K\rangle$ (no pairing)
- Some arbitrariness:
  - choice of K^π (possibly also experimental $J^{/pi}$)
  - description as one-particle state over (N, Z) core instead of one-neutron-hole state in $(N+2, Z)$ core or one-proton-hole in $(N, Z+2)$ core

Hartree-Fock approach to odd nuclei

One-body hamiltonian

- One-body density matrix from Slater determinant $|\Phi_K\rangle$ no longer time-reversal invariant
- Currents

$$\mathbf{j}_q = \frac{1}{2i} \sum_{k \in |\Phi_K\rangle}^{(q)} \left(\phi_k^* \boldsymbol{\nabla} \phi_k - \phi_k \boldsymbol{\nabla} \phi_k^* \right)$$

and spin-vector density matrix components

$$\boldsymbol{\rho}_q = \sum_{k \in |\Phi_K\rangle}^{(q)} \phi_k^* \boldsymbol{\sigma} \phi_k$$

for each charge state q (n or p)

HARTREE-FOCK APPROACH TO ODD NUCLEI

ONE-BODY HAMILTONIAN

- Skyrme-Hartree-Fock hamiltonian in **r**-space

$$h_{\mathrm{HF}}^{(q)} = -\frac{\hbar^2}{2m}\nabla f_q \cdot \nabla + U_q - i\hbar(\nabla V_q^{so} \times \nabla)\cdot\boldsymbol{\sigma} + \frac{1}{2} i\hbar(\boldsymbol{\alpha}_q \cdot \nabla + \nabla \cdot \boldsymbol{\alpha}_q) - \hbar \mathbf{S}_q \cdot \boldsymbol{\sigma}$$

with

$$\hbar\boldsymbol{\alpha}_q = 2(B_3\mathbf{j} + B_4\mathbf{j}_q) - B_9(\nabla \times \boldsymbol{\rho} + \nabla \times \boldsymbol{\rho}_q)$$

$$\hbar\mathbf{S}_q = B_9(\nabla \times \mathbf{j} + \nabla \times \mathbf{j}_q) - 2(B_{10}\boldsymbol{\rho} + B_{11}\boldsymbol{\rho}_q) - 2\rho^\gamma(B_{12}\boldsymbol{\rho} + B_{13}\boldsymbol{\rho}_q)$$

$\mathbf{j} = \mathbf{j}_q + \mathbf{j}_{\bar{q}}$ (same for ρ); B_i = functions of Skyrme parameters

Hartree-Fock approach to odd nuclei

One-body hamiltonian

- Spin-vector densities $\boldsymbol{\rho}_q$ and spin fields $\mathbf{S}_q$ are in a plane containing the symmetry axis
- Currents $\mathbf{j}_q$ and $\boldsymbol{\alpha}_q$ fields are perpendicular to a plane containing the symmetry axis z

Hartree-Fock approach to odd nuclei

Perturbative expressions of polarizing fields

- Perturbatively, adding one nucleon to the even-even core creates charge-dependent polarizing fields.
- For a neutron-odd nucleus ($q = n$, $\overline{q} = p$) with SIII:

$$\hbar\boldsymbol{\alpha}_q \approx 2(B_3 + B_4)\mathbf{j}_n - 2B_9\nabla \times \boldsymbol{\rho}_n$$
$$\hbar\boldsymbol{\alpha}_{\overline{q}} \approx 2B_3\mathbf{j}_n - B_9\nabla \times \boldsymbol{\rho}_n$$

and

$$\hbar\mathbf{S}_q \approx -2B_9\nabla \times \mathbf{j}_n - 2(B_{10} + B_{11})\boldsymbol{\rho}_n$$
$$\hbar\mathbf{S}_{\overline{q}} \approx -B_9\nabla \times \mathbf{j}_n - 2(B_{10} + \rho B_{12})\boldsymbol{\rho}_n$$

RESULTS:

SINGLE-PARTICLE SPECTRA OF DEFORMED ODD NUCLEI

SINGLE-PARTICLE SPECTRA

LIFTING OF KRAMERS DEGENERACY

- Perturbative character of time-odd fields α and **S**
  $\Rightarrow$ "quasi Kramers-pairs" of opposite-K states ($|i\rangle$, $|\tilde{i}\rangle$):

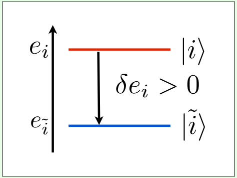
$$\hat{h}_{\mathrm{HF}}|i\rangle = e_i|i\rangle \qquad \hat{j}_z|i\rangle = K_i|i\rangle \quad \text{with } K_i > 0$$

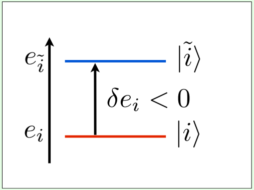
$$\hat{h}_{\mathrm{HF}}|\tilde{i}\rangle = e_{\tilde{i}}|\tilde{i}\rangle \qquad \hat{j}_z|\tilde{i}\rangle = K_{\tilde{i}}|\tilde{i}\rangle \quad \text{with } K_{\tilde{i}} = -K_i < 0$$

$$\langle\tilde{i}|\hat{s}_z|\tilde{i}\rangle \approx -\langle i|\hat{s}_z|i\rangle$$

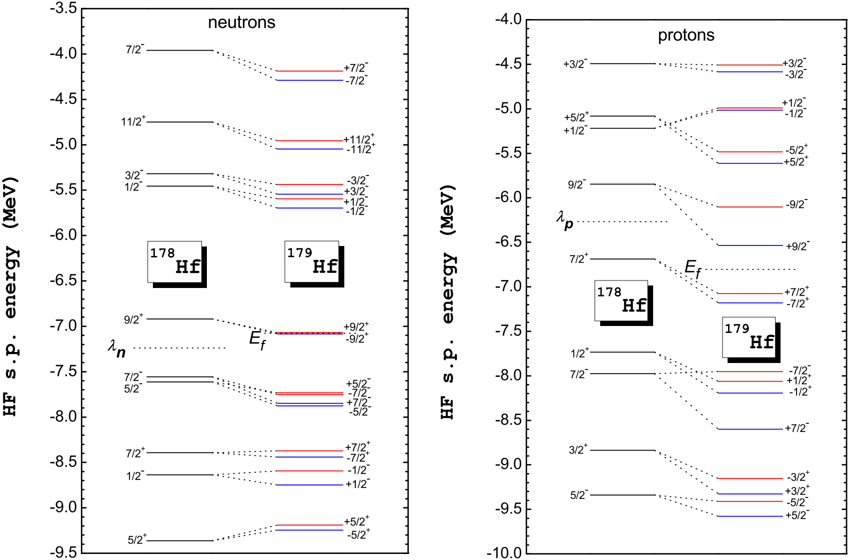
- Energy splitting between partners of a quasi-Kramers pair:

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





Single-particle spectra



Single-particle spectra

Correlation between energy splitting and spins

- General trend across nuclid chart: correlation between
  - energy splitting between quasi-Kramers partners, δe_i;
  - expectation values of $\hat{s}_z$ for odd nucleon, s_{odd}, and for positive-K partner of quasi-Kramers pair i, $s(i)$

$$s_{\text{odd}} s(i) \delta e_i \begin{cases} > 0 & \text{for } q \text{ charge state (same as odd nucleon)} \\ < 0 & \text{for } \overline{q} \text{ charge state} \end{cases}$$

In the $(s_{\text{odd}} s(i), \delta e_i)$ plane, results lie in

- upper right and lower left quadrants for q charge state
- lower right and upper left quadrants for $\overline{q}$ charge state

For better visual representation, spread results upon multiplying abscissa $\text{sign}\big(s_{\text{odd}} s(i)\big)$ *by* $|\Lambda(i)| \equiv |\langle i|\hat{\ell}_z|i\rangle|$

Single-particle spectra

Correlation between energy splitting and spins

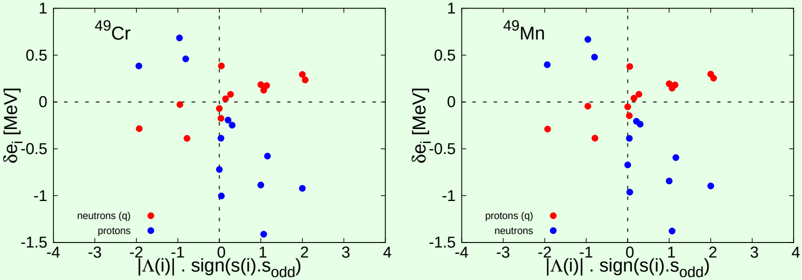
Calculated results:

Nucleus	$(J^\pi)_{\rm exp}$	$(K^\pi)_{\rm th}$	$s_{\rm odd}$
^{49}Cr	$5/2^-$	$5/2^-$	0.429
^{49}Mn	$5/2^-$	$5/2^-$	0.429
^{99}Sr	$3/2^+$	$5/2^-$	0.386
^{99}Y	$5/2^+$	$5/2^+$	0.432
^{103}Mo	$3/2^+$	$3/2^+$	0.366
^{103}Tc	$5/2^+$	$3/2^-$	0.486
^{175}Yb	$7/2^-$	$7/2^-$	-0.421
^{175}Lu	$7/2^+$	$7/2^+$	-0.479
^{179}Hf	$9/2^+$	$9/2^+$	0.437
^{179}Ta	$7/2^+$	$9/2^-$	0.479
^{235}U	$7/2^-$	$7/2^-$	0.364
^{235}Np	$5/2^+$	$7/2^-$	-0.386

Single-particle spectra

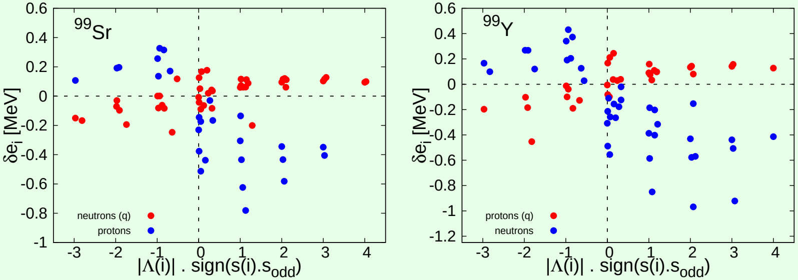
Correlation between energy splitting and spins

- Mass region $A = 50$



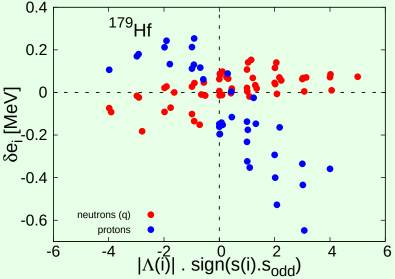
Correlation between energy splitting and spins

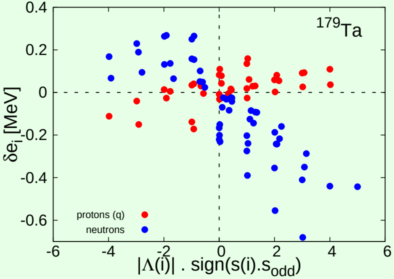
- Mass region $A = 100$



CORRELATION BETWEEN ENERGY SPLITTING AND SPINS

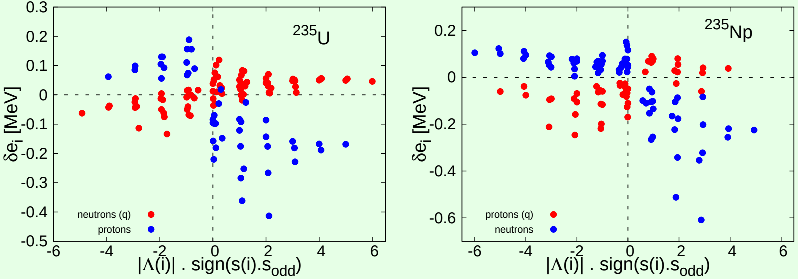
- Mass region $A = 180$





CORRELATION BETWEEN ENERGY SPLITTING AND SPINS

- Mass region $A = 235$



Single-particle spectra

Correlation between energy splitting and spins

- Interpretation: "spin-alignment" core polarization

  Upon integrating over space the spin-field component along symmetry axis z

$$S_q = \int d\mathbf{r}\, \mathbf{S}_q.\mathbf{e}_z \ ,$$

we find an "anti-alignment" for $\langle \mathbf{s} \rangle_{\rm odd}$ *and* $\mathbf{S}_q$*:*

$$s_{\rm odd} S_q < 0 \ ,$$

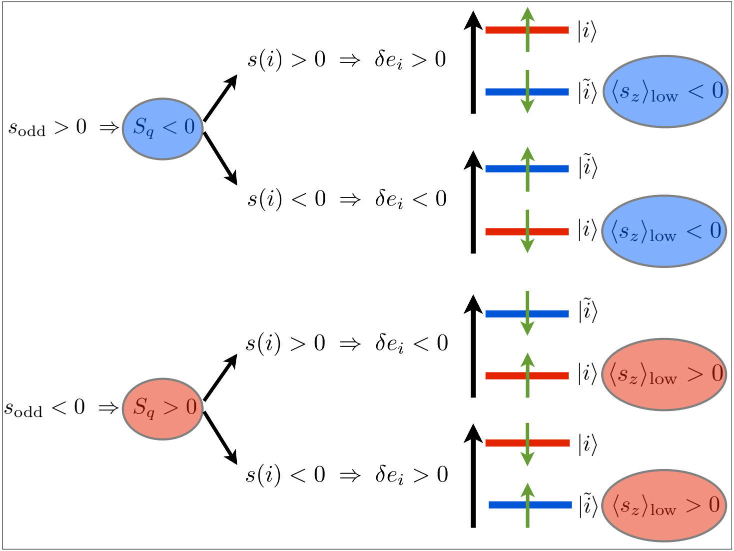
hence

$$\boxed{s(i)\delta e_i S_q < 0} \ ,$$

which translates into the "alignment" of spin-field $\mathbf{S}_q$ *and* $\langle \mathbf{s} \rangle_{\rm low}$ *for lowest partner of quasi-Kramers pair (since* $s(i)s(\tilde{i}) < 0$*).*

SINGLE-PARTICLE SPECTRA

For q charge state: S_q and $\langle \hat{s}_z \rangle_{\rm low}$ have the same sign



Single-particle spectra

Correlation between energy splitting and spins

- *For $\overline{q}$ charge state: "alignment" of* $\mathbf{s}_{\mathrm{odd}}$ *and* $\mathbf{S}_{\overline{q}}$

$$s_{\mathrm{odd}} S_{\overline{q}} < 0 \,,$$

hence

$$\boxed{s(i)\delta e_i S_{\overline{q}} < 0}$$

$\Rightarrow$ *same conclusion for $\overline{q}$ charge state as for q charge state*

Results:

Single-particle magnetic moments of odd deformed nuclei

Single-particle magnetic moments

Magnetic moment operator

$$\hat{\boldsymbol{\mu}} = (g_\ell \hat{\boldsymbol{\ell}} + g_s \hat{\mathbf{s}})\mu_N$$

with $\mu_N = \frac{e\hbar}{2m_p c}$ (nuclear magneton) and following values for orbital and spin gyromagnetic ratios

Particle	g_ℓ	g_s
neutron	0	-3.826
proton	1	5.586

SINGLE-PARTICLE MAGNETIC MOMENTS

MAGNETIC MOMENTS IN INDEPENDENT-PARTICLE MODEL

In the Slater determinant $|\Phi_K\rangle$:

$$\begin{aligned}\mu_{\text{ind}} &= \frac{K}{I+1}\langle\Phi_K|\hat{\mu}_z|\Phi_K\rangle \\ &= \frac{K}{I+1}\sum_{i\in|\Phi_k\rangle}\langle i|\hat{\mu}_z|i\rangle \\ &= (\mu_{\text{int}})_{\text{sp}} + (\mu_{\text{int}})_{\text{core}}\end{aligned}$$

Single-particle model: neglect core contribution

$$\Rightarrow \quad \mu_{\text{ind}} \approx (\mu_{\text{ind}})_{\text{sp}} = \frac{K}{I+1}\left(g_\ell\langle\hat{\ell}_z\rangle_{\text{odd}} + g_s s_{\text{odd}}\right)$$

Single-particle magnetic moments

Magnetic moments in independent-particle model

- Good approximation for light nuclei with spin-saturated magic core (up to ^{16}O)
- In nuclei with spin-unsaturated core, quenching of spin contribution, especially in deformed nuclei:

$$(\mu_{\mathrm{ind}})_{\mathrm{sp}}^{(\mathrm{eff})} = \frac{K}{I+1}\left(g_\ell \langle \hat{\ell}_z \rangle_{\mathrm{odd}} + g_s^{(\mathrm{eff})} s_{\mathrm{odd}}\right)\mu_N$$

with $g_s^{(\mathrm{eff})} \approx 0.7 g_s$ to account for discrepancy with experimental values

Single-particle magnetic moments

Spin quenching of magnetic moments

- Origin of the quenching: spin core polarization effect

$$\mu_{\text{ind}} \equiv (\mu_{\text{ind}})_{\text{sp}} + (\mu_{\text{ind}})_{\text{core}}$$
$$= \frac{K}{I+1}\left[g_\ell \langle \hat{\ell}_z \rangle_{\text{odd}} + g_s \left(1 - R + \frac{\langle \Phi_K | g_\ell \hat{\ell}_z | \Phi_K \rangle_{\text{core}}}{g_s s_{\text{odd}}}\right) s_{\text{odd}}\right] \mu_N$$

with

$$R = -\frac{\langle \Phi_K | g_s \hat{s}_z | \Phi_K \rangle_{\text{core}}}{g_s s_{\text{odd}}}$$

and for low spin-mixing in odd-particle states ($|s_{\text{odd}}| \lesssim \frac{1}{2}$)

$$\left| \langle \Phi_K | g_\ell \hat{\ell}_z | \Phi_K \rangle_{\text{core}} \right| \ll |g_s s_{\text{odd}}|$$

hence $\mu_{\text{ind}} = (\mu_{\text{ind}})_{\text{sp}}^{(\text{eff})}$ with $g_s^{(\text{eff})} \approx (1-R) g_s$

SINGLE-PARTICLE MAGNETIC MOMENTS

SPIN QUENCHING OF MAGNETIC MOMENTS

Calculated results: $g_s^{(\mathrm{eff})}/g_s$ close to empirical value ~ 0.7

Nucleus	$(J^\pi)_{\mathrm{exp}}$	$(K^\pi)_{\mathrm{th}}$	s_{odd}	Spin quenching factor
^{49}Cr	$5/2^-$	$5/2^-$	0.429	0.695
^{49}Mn	$5/2^-$	$5/2^-$	0.429	0.835
^{99}Sr	$3/2^+$	$5/2^-$	0.386	0.670
^{99}Y	$5/2^+$	$5/2^+$	0.432	0.835
^{103}Mo	$3/2^+$	$3/2^+$	0.366	0.786
^{103}Tc	$5/2^+$	$3/2^-$	0.486	0.803
^{175}Yb	$7/2^-$	$7/2^-$	-0.421	0.656
^{175}Lu	$7/2^+$	$7/2^+$	-0.479	0.775
^{179}Hf	$9/2^+$	$9/2^+$	0.437	0.649
^{179}Ta	$7/2^+$	$9/2^-$	0.479	0.815
^{235}U	$7/2^-$	$7/2^-$	0.364	0.673
^{235}Np	$5/2^+$	$7/2^-$	-0.386	0.784

Conclusions

- Hartree–Fock hamiltonian for odd-nuclei breaks time-reversal invariance ⇒ Kramers degeneracy removed
- Perturbative character of time-reversal symmetry breaking + axial symmetry ⇒ quasi-Kramers pairs with opposite K-values
- Correlation between energy splitting and expectation values of $\hat{s}_z$ in a given quasi-Kramers pair and for the odd nucleon, interpreted as alignment of spin of favored partner and spin field (“spin paramagnetic” core polarization)
- Spin core polarization quenches the spin contribution to magnetic moment in independent-particle model (reproduction of empirical quenching factor)

Perspectives

- Further tests of the polarization rule (more nuclei, other Skyrme forces)
- Include pairing correlations within the Higher Tamm-Dancoff Approximation (highly truncated shell model based on the Hartree–Fock solution)
- Study extensively in the Bohr and Mottelson Unified Model the influence of core polarization on spectroscopic properties (magnetic moments, transitions; Coriolis coupling...)
- Extension to a more general class of time-reversal breaking intrinsic solutions, as K-isomers