Ground-state properties of deformed odd-mass nuclei within the Higher Tamm–Dancoff approximation

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INTRODUCTION

MOTIVATIONS

- Aim: spectroscopy of odd-mass deformed nuclei, including K-isomers states and isospin properties
- Unified Model for axially deformed odd nuclei
  - collective degrees of freedom (d.o.f.) coupled to intrinsic d.o.f. in a way preserving the discrete symmetries of intrinsic deformation
  - for odd nuclei with good K

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

$\mathcal{R}_y$ = y-signature operator (symmetry axis = z axis)
$D^I_{M,K} =$ Wigner rotation matrix
$\phi_K =$ intrinsic state, e.g., in the Higher Tamm-Dancoff Approximation *(highly truncated shell model based on the Hartree–Fock solution)*

Introduction

Outline

1. Theoretical framework:
   - Hartree-Fock approximation for axially deformed odd nuclei (time-reversal symmetry broken)
   - Inclusion of $T = 0$ and $T = 1$ pairing correlations within HTDA (particle number conserved)
2. Results around ^{24}Mg and ^{48}Cr:
   - Effect of time-reversal symmetry breaking on s.p. spectra
   - Effects of core polarization and pairing correlations on some GS properties:
     - magnetic moment
     - isospin mixing
     - isovector odd-even binding-energy difference

Hartree-Fock approach to odd nuclei

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

Hartree-Fock calculation for even-even nuclei:

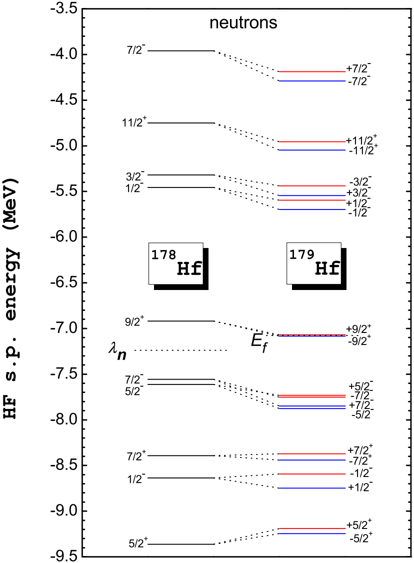
- Skyrme effective interaction (SIII, SLy4)
- axial and intrinsic parity symmetries assumed

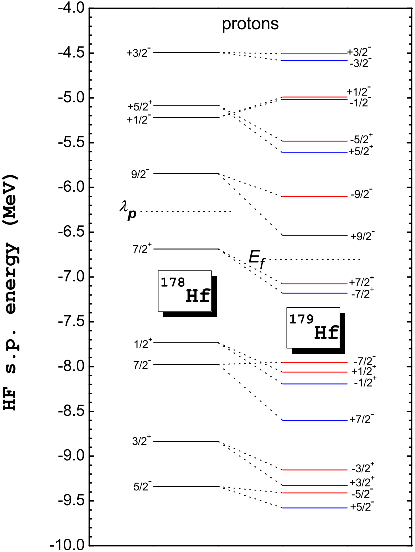
$\Rightarrow$ HF solution $|\Phi_0\rangle$

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

- Choose the lowest-energy K^π s.p. state unoccupied in $|\Phi_0\rangle$
  $\Rightarrow$ rank n among K^π states by increasing energy
- Solve the HF equations for the odd nucleus with occupation set to 1 for the K^π s.p. state of rank n
  $\Rightarrow$ HF solution $|\Phi_{K^\pi}\rangle$ (no pairing), Kramers degeneracy of s.p. spectrum suppressed

HF S.P. SPECTRA





HTDA APPROACH TO ODD NUCLEI

BRIEF DESCRIPTION

Highly truncated shell model on a Hartree-Fock solution:

1. HF solution $|\Phi_{K^\pi}\rangle$ with blocked K^π s.p. state
2. many-body basis: *n*-particle–*n*-hole excitations on $|\Phi_{K^\pi}\rangle$ (*type depending on correlations to be described*)
3. diagonalization of HTDA hamiltonian in the many-body basis
   $\Rightarrow$ correlated ground state $|\Psi_{K^\pi}\rangle$

HTDA APPROACH TO ODD NUCLEI

MANY-BODY BASIS

HTDA ground state $|\Psi\rangle$ expanded on 2p-2h "quasi-paired" excitations ($T_z = -1$, 0 and 1) created on $|\Phi_{K^\pi}\rangle$:

$$|\Psi\rangle = \chi_0 |\Phi_{K^\pi}\rangle + \sum_i \chi_i |\Phi_i\rangle$$

$$|\Phi_i\rangle = a^\dagger_\beta a^\dagger_{\widetilde{\beta}} a_{\widetilde{b}} a_b |\Phi_{K^\pi}\rangle \, ,$$

with $|\widetilde{b}\rangle$ such that

$$\hat{H}_{\mathrm{HF}} |\widetilde{b}\rangle = e_{\widetilde{b}} |\widetilde{b}\rangle \; (e_{\widetilde{b}} \neq e_b)$$

$$\hat{J}_z |\widetilde{b}\rangle = -K_b \hbar |\widetilde{b}\rangle$$

$$\langle \overline{b} | \widetilde{b} \rangle \quad \text{maximum (close to 1).}$$

HTDA approach to odd nuclei

HTDA Hamiltonian

- Given a 2-body density-dependent interaction $\hat{V}$:

$$\hat{H} = \hat{K} + \hat{V}$$
$$= \underbrace{\hat{K} + \hat{V}_{\mathrm{HF}} - \langle \Phi_{K^\pi} | \hat{V} | \Phi_{K^\pi} \rangle + E_R}_{\hat{H}_0} + \underbrace{\hat{V} - \hat{V}_{\mathrm{HF}} + \langle \Phi_{K^\pi} | \hat{V} | \Phi_{K^\pi} \rangle - E_R}_{\hat{V}_{\mathrm{res}}}$$

(E_R = rearrangement energy)

- Approximation for the nuclear part:
  $\hat{V} \approx \delta$ interaction in $\hat{V}_{\mathrm{res}}$ ($T = 0$ and $T = 1$ pairing)

Magnetic moments

Magnetic moments in the Unified Model

$$\mu = \underbrace{g_R \frac{I(I+1)-K^2}{I+1}\,\mu_N}_{\mu_{\rm coll}} + \underbrace{g_K \frac{K^2}{I+1}}_{\mu_{\rm intr}}$$

with $g_K = \langle\Phi_K|\hat{\mu}_z|\Phi_K\rangle/K$, $|\Phi_K\rangle$ intrinsic state

Intrinsic contribution

- Single-particle model:
  $\mu_{\rm intr} \approx \mu_{\rm odd} = \frac{K}{I+1}\left(g_\ell\langle\hat{\ell}_z\rangle_{\rm odd} + g_s s_{\rm odd}\right)\mu_N$
- HF: g_s renormalized by core polarization

$$g_s^{\rm (eff)} = g_s^{(q)} + \sum_{q'=n,p}\left(1 - \frac{g_\ell^{(q')}}{g_s^{(q')}}\right)\frac{g_s^{(q')}\langle\Phi_K|\hat{s}_z|\Phi_K\rangle_{\rm core}^{(q')}}{s_{\rm odd}},$$

Magnetic moments

Spin quenching of magnetic moments

Nucleus	$(J^\pi)_{\rm exp}$	$(K^\pi)_{\rm th}$	$s_{\rm odd}$	Spin quenching factor
^{49}Cr	$5/2^-$	$5/2^-$	0.429	0.742
^{49}Mn	$5/2^-$	$5/2^-$	0.429	0.843
^{99}Sr	$3/2^+$	$3/2^+$	0.333	0.842
^{99}Y	$5/2^+$	$5/2^+$	0.432	0.840
^{103}Mo	$3/2^+$	$3/2^+$	0.355	0.763
^{103}Tc	$5/2^+$	$3/2^-$	0.486	0.803
^{175}Yb	$7/2^-$	$7/2^-$	−0.421	0.693
^{175}Lu	$7/2^+$	$7/2^+$	−0.479	0.794
^{179}Hf	$9/2^+$	$9/2^+$	0.437	0.700
^{179}Ta	$7/2^+$	$9/2^-$	0.479	0.821
^{235}U	$7/2^-$	$7/2^-$	0.364	0.717
^{235}Np	$5/2^+$	$5/2^-$	-0.386	0.823

On average $\frac{g_s^{\rm (eff)}}{g_s} = 1 - \eta \approx 0.78$ (close to empirical value ~ 0.7)

Magnetic moments

Intrinsic contribution

- HTDA: $\mu_{\text{intr}} = \mu_{\text{HF}} + \mu_{\text{corr}}$ with

$$\mu_{\text{corr}} = \sum_{i \neq 0} \chi_i^2 \left(\langle \beta_i | \hat{\mu}_z | \beta_i \rangle + \langle \widetilde{\beta}_i | \hat{\mu}_z | \widetilde{\beta}_i \rangle - \langle b_i | \hat{\mu}_z | b_i \rangle - \langle \tilde{b}_i | \hat{\mu}_z | \tilde{b}_i \rangle \right)$$

given that

$$|\Psi\rangle = \chi_0 |\Phi_{K^\pi}\rangle + \sum_i \chi_i |\Phi_i\rangle$$

$$|\Phi_i\rangle = a^\dagger_{\beta_i} a^\dagger_{\widetilde{\beta}_i} a_{\widetilde{b}_i} a_{b_i} |\Phi_{K^\pi}\rangle \,,$$

HTDA calculations

Valence space

- Around ^{24}Mg: [e_F-17.5 MeV ; e_F+10 MeV]
  - 5 hole levels: $(1/2^-)_1$, $(3/2^-)_1$, $(1/2^-)_2$, $(1/2^+)_2$, $(3/2^+)_2$
  - 6 particle levels: $(5/2^+)_1$, $(1/2^+)_3$, $(1/2^+)_4$, $(1/2^-)_3$, $(3/2^-)_2$, $(3/2^+)_2$
- Around ^{48}Cr: [e_F-13.5 MeV ; e_F+10 MeV]
  - 8 hole levels: $(1/2^+)_2$, $(3/2^+)_2$, $(5/2^+)_1$, $(1/2^+)_3$, $(1/2^+)_4$, $(3/2^+)_2$, $(1/2^-)_4$, $(3/2^-)_3$
  - 8 particle levels: $(5/2^-)_1$, $(7/2^-)_1$, $(1/2^-)_5$, $(1/2^-)_6$, $(3/2^-)_4$, $(1/2^+)_5$, $(3/2^-)_5$, $(3/2^+)_3$

Residual interaction strength

$T = 1$ channel: $V_0^{(T=1)} = -300 \text{ MeV.fm}^3$ (justified a posteriori)

$T = 0$ channel: $V_0^{(T=0)} = x.V_0^{(T=1)}$

Magnetic moments

Intrinsic contribution

With $x = 0$ (no $T = 0$ pairing)

Nucleus	^{23}Na($K^\pi = \frac{3}{2}^+$)	^{23}Mg($\frac{3}{2}^+$)	^{25}Mg($\frac{5}{2}^+$)	^{25}Al($\frac{5}{2}^+$)
$\langle \hat{\mu}_z \rangle^{(n)}_{\mathrm{HF}}$	−0.0947	−1.4718	−1.7350	−0.1196
$\langle \hat{\mu}_z \rangle^{(n)}_{\mathrm{HTDA}}$	−0.1179	−1.4495	−1.7009	−0.1497
$\langle \hat{\mu}_z \rangle^{(p)}_{\mathrm{HF}}$	3.2634	0.1137	0.1472	4.5817
$\langle \hat{\mu}_z \rangle^{(p)}_{\mathrm{HTDA}}$	3.2175	0.1609	0.2191	4.5103
$\frac{K}{K+1} \langle \hat{\mu}_z \rangle_{\mathrm{HF}}$		−0.815		
$\frac{K}{K+1} \langle \hat{\mu}_z \rangle_{\mathrm{HTDA}}$		−0.709		
μ_{exp}		(−)0.5364(3)[a]		

[a] Kukuda et al., Hyperfine Interactions 78 (1993)

[b] A. Bohr and B. Mottelson (1975)

⇒ Correlations increase the $\bar{q}$ core contribution and decrease the contribution from the q states in absolute value

With $x = 1.2$ (Satula et al., PLB 393, 1997, with BCS+LN): $\mu_{\mathrm{HTDA}} = -0.57$

Isospin mixing

^{24}Mg: impact of Coulomb treatment and pairing

With $x = 0$

$\alpha^2 \approx \frac{\langle \mathbf{T}^2\rangle - \lvert T_z\rvert(\lvert T_z\rvert+1)}{2(\lvert T_z\rvert+1)}$ (%)	exact	Slater
HF	0.174	0.177
HTDA($\hat{V}_{\mathrm{res}}(\mathrm{Coul}) \neq 0$)	0.213	0.199
HTDA($\hat{V}_{\mathrm{res}}(\mathrm{Coul}) = 0$)	0.206	0.193

With $x = 1.25$:

$$\alpha^2(\mathrm{Slater}, \hat{\mathrm{V}}_{\mathrm{res}}(\mathrm{Coul}) = 0) = 0.23\%$$

Isospin mixing

Spurious mixing correction

With $x = 0$

α^2(%)	^{23}Mg	^{23}Na	^{25}Mg	^{25}Al
HF(Slater)	0.609	0.597	0.515	0.558
HTDA($\hat{V}_{\rm res}(\rm Coul) = 0$)	0.664	0.629	0.578	0.675
$e = 0$ (no Coulomb):				
HF	0.503	0.503	0.425	0.425
HTDA	0.554	0.554	0.500	0.500

Approximate correction for spurious mixing: subtract $\alpha^2(e = 0)$

Isospin mixing

^{23}Mg: effect of core polarization

HF(Slater) and HTDA with $V_{\mathrm{res}}(\mathrm{Coul}) = 0$

α^2(%)	polarization+correction	Koopmans
$x = 0$	0.13	0.11
$x = 1.25$	0.21	0.17

$\Rightarrow$ Koopmans approximation seems to slightly underestimate α^2

GS properties within HTDA

Isovector odd-even binding-energy difference

Definition: $\delta \equiv \Delta_n^{(3)}(N,Z) - \Delta_p^{(3)}(N,Z)$,
with the 3-point odd-even binding-energy difference

$$\Delta_n^{(3)}(N,Z) = \frac{(-1)^N}{2}\left[E(N+1,Z) + E(N-1,Z) - 2\,E(N,Z)\right] .$$

Within HTDA:
$E(N,Z) = \langle\Phi_0(N,Z)|\hat{H}|\Phi_0(N,Z)\rangle + \underbrace{\langle\Psi(N,Z)|\hat{H}_0 + \hat{V}_{\rm res}|\Psi(N,Z)\rangle}_{E_{\rm corr}}$,

so $\Delta_n^{(3)}(N,Z) = \Delta_n^{(3)}(\mathrm{HF}) + \Delta_n^{(3)}(\mathrm{corr})$ and $\delta(\mathrm{HTDA}) = \delta(\mathrm{HF}) + \delta(\mathrm{corr})$.
Koopmans approximation: $\Delta_n^{(3)}(\mathrm{HF}) \approx \frac{(-1)^N}{2}(e_\nu - e_n)$, hence:
$\delta \approx \frac{(-1)^N}{2}\,[\underbrace{(e_\nu - e_n) - (e_\pi - e_p)}_{\Delta e_{\rm IV}}] + \Delta_n^{(3)}(\mathrm{corr}) - \Delta_p^{(3)}(\mathrm{corr})$.

$\delta(\mathrm{Koopmans}, N=Z) \approx \Delta_n^{(3)}(\mathrm{corr}) - \Delta_p^{(3)}(\mathrm{corr})$ (isospin symmetry weakly broken).

GS PROPERTIES WITHIN HTDA

ISOVECTOR ODD-EVEN BINDING ENERGY DIFFERENCE

Values of δ in MeV for two even-even core nuclei with SIII and $V_0^{(T=0)} = 0$, $V_0^{(T=1)} = -300$ MeV.fm^{-3}

Core	^{24}Mg	^{48}Cr
δ(Koopmans)	0.033	−0.004
δ(HF)	−0.132	−0.137
δ(corr)	0.023	0.011
δ(HTDA)	−0.109	−0.126
δ(exp)	−0.110	−0.136

$\Rightarrow$ importance of core polarization (HF variational solution instead of Koopmans approximation) at least in light nuclei, correlations bring a small correction

GS properties within HTDA

Isovector odd-even mass difference

Values of δ in MeV for ^{24}Mg even-even core with SLy4 and $V_0^{(T=0)} = 0$, $V_0^{(T=1)} = -300\,\mathrm{MeV.fm}^{-3}$

Core	^{24}Mg
δ(Koopmans)	0.035
δ(HF)	−0.136
δ(corr)	0.047
δ(HTDA)	−0.089
δ(exp)	−0.110

$\Rightarrow$ conclusion insensitive to Skyrme parametrizations (to be checked with other parametrizations)

CONCLUSIONS

1. Core polarization:
   - quenches the spin contribution to intrinsic magnetic moment (reproduction of empirical quenching factor)
   - increases slightly isospin mixing (with approximate correction for spurious mixing)
   - accounts for isovector odd-even mass difference
2. Pairing correlations:
   - decrease in absolute value the magnetic moment (very sensitive to $T = 0$ pairing)
   - increase the isospin mixing

$\Rightarrow$ with the same strength for $T = 1$ and $T = 0$ pairing, and core polarization, $\alpha^2(N = Z \pm 1) \lesssim \alpha^2(N = Z)$