

TAURUS applied to EDF

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Acknowledgements

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Luis. M. Robledo (UAM)

Benjamin Bally (CEA-Saclay)

Nathalie Pillet (CEA-DAM)

Samuel. A. Giuliani (UAM) Jaime Martínez-Larraz (UAM)

- ① Introduction
- ② The project TAURUS
- ③ Gogny EDF
- ④ Proton-Neutron pairing
- ⑤ Conclusions and Research Plan

Landscape of nuclear physics paths

The nuclear problem is a two-part problem. Even with a **nuclear interaction**, exact wave functions and energies cannot be obtained for the general **many-body problem** :

- The number of configurations for the many-body Hilbert space skyrockets.
- Non-storable amount of 2,3,...-body matrix elements.

The most widely used *solutions* to attack these problems :

- **Valence-space (Shell Model) calculations.**
- **Approximate methods (variational).**

Landscape of nuclear physics paths

Self-Consistent Mean Field

- Variational approximation using trial wave functions for EDF.
 - Small set of parameters for the interaction, adjusted from the data of finite nuclei.
 - Precise description of ground state properties.
 - Spectroscopy and dynamics through **Beyond Mean Field**.
-

Shell Model

- Exact diagonalization within a valence space.
- Interactions highly fitted for the valence space shell and the replication of the s.p.e.
- Precise description of spectroscopy and transitions.
- Intrinsic shapes from EM-moments and spectra.

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TAURUS for SCMF and BMF, other sister methods :

- Monte Carlo Shell Model ¹
- Discrete NonOrthogonal Shell Model (DNO-SM) ²
- PGCM ³
- ... many others with the same philosophy ; solving the many-body nuclear problem using variational methods that mix non-orthogonal wave functions.

-
1. T.Otsuka, M.Honma, T.Mizusaki, N.Shimizu, Y.Utsuno, Prog. Part. Nucl. Phys., 47 (2001), p. 319
 2. D.D.Dao, F.Nowacki Phys. Rev. C 105 (2022), 054314
 3. Z.-C. Gao, M. Horoi, Y.S. Chen, Phys. Rev. C 92(6), 064310 (2015), C.F. Jiao, J. Engel, J.D. Holt, Phys. Rev. C 96(5), 054310 (2017), TAURUS, M. Frosini (2021)

Mean Field and Beyond Mean Field techniques. PGCM

- Trial wave functions on collective variables

$$|\Psi_{\sigma}^{\Lambda}\rangle = \sum_{i,K} f_{\sigma K}^{\Lambda}(a_i) P_{MK}^J P^{\pi} P^Z P^N |\Phi(a_i)\rangle$$

Using a *basis* of projected states $|\Phi^{\Lambda}(a_i)\rangle$, being $\Lambda \equiv (JM\pi ZN)$

Coordinates a are usually the mean value of multipole deformations, pairing content, etc

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Coordinates a are usually the mean value of multipole deformations, pairing content, etc

- $f_{\sigma K}^{\Lambda}(a)$ weights are obtained from **HWG equations**, by minimizing the expectation value of the energy of $|\Psi_{\sigma}^{\Lambda}\rangle$

$$\delta \frac{\langle \Psi_{\sigma}^{\Lambda} | H | \Psi_{\sigma}^{\Lambda} \rangle}{\langle \Psi_{\sigma}^{\Lambda} | \Psi_{\sigma}^{\Lambda} \rangle} = 0 \rightarrow \mathcal{H}f = E\mathcal{N}f \quad \begin{cases} \mathcal{H}_{iK,jK'}^{\Lambda} = \langle \Phi(a_i) | \hat{H} P_{KK'}^J P^{\pi} P^Z P^N | \Phi(a_j) \rangle \\ \mathcal{N}_{iK,jK'}^{\Lambda} = \langle \Phi(a_i) | P_{KK'}^J P^{\pi} P^Z P^N | \Phi(a_j) \rangle \end{cases}$$

- Selection of states by the physical relevance in the set $\{a\}$, also excluding linear dependencies between states $|\Phi(a)\rangle$.

Mean Field and Beyond Mean Field techniques. Starting point from HFB

- The Hartree-Fock-Bogoliubov method is a self-consistent mean-field approach based on the variational method.
- Intrinsic state $|\Phi(a)\rangle$ is built by the product of Bogoliubov quasiparticles β (q.p. vacuum)

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \quad \beta_k |\Phi(a)\rangle = 0 \quad \forall k$$

$$U = \begin{pmatrix} U_{pp} & U_{p\textcolor{blue}{n}} \\ U_{\textcolor{blue}{n}p} & U_{nn} \end{pmatrix} \quad V = \begin{pmatrix} V_{pp} & V_{p\textcolor{blue}{n}} \\ V_{\textcolor{blue}{n}p} & V_{nn} \end{pmatrix}$$

- HFB (and constrained-HFB) equations are solved with the gradient method

$$\delta \frac{\langle \Phi(a) | H | \Phi(a) \rangle}{\langle \Phi(a) | \Phi(a) \rangle} = \delta_{U,V} (E_{HFB}) = 0$$

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- HFB (and constrained-HFB) equations are solved with the gradient method

$$\delta \frac{\langle \Phi(a) | H | \Phi(a) \rangle}{\langle \Phi(a) | \Phi(a) \rangle} = \delta_{U,V} (E_{HFB}) = 0$$

- The general HFB solutions normally break the Hamiltonian symmetries.

N, Z (particle number conservation)	Pairing condensate
J, J_z (rotational invariance)	Axial deformations
Π (parity invariance)	Octupolar deformations
\mathcal{T} (time-reversal invariance)	Cranking / odd-mass nuclei

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The project TAURUS







- Numerical suite for symmetry-projected variational calculations.
Theory for **A** Unified descRiption of nUclear **S**tructure



- Codes by B.Bally (CEA), T.R. Rodríguez (UCM)
 - Adrián Sánchez-Fernández (YU-uk)
- Marie Skłodowska-Curie Actions individual fellowship (2019-2021)

The project TAURUS. Details

- Family of symmetry-projected variational calculations :
 - `taurus_vap` : Constrained HFB/PN-VAP calculation
 - `taurus_pav` : PAV symmetry projections from an HFB/VAP results.
 - `taurus_mix` : configuration-mixing from PAV results by solving the HWG equation.
 - Other codes/scripts related to the previous codes.
- PN-VAP code is publically available
Repository : https://github.com/project-taurus/taurus_vap⁴
- Features :
 - Spherical HO basis : $|n, l, s = 1/2, j, m_j; t = 1/2, m_t\rangle$
 - No model space predefined (extracted and allocated from the Hamiltonian).
 - Hamiltonians for SM (s.p.e. + 2-body) or more general J-scheme $\langle ab || \hat{H} || cd \rangle_J$. Including 0,1 and 2-body Hamiltonians.
 - Real general Bogoliubov quasiparticle-states $|\Phi\rangle$.

4. B. Bally, T.R. Rodríguez, A. Sánchez-Fernández, Eur.Phys.J. A (2021) 57 :69      

The project TAURUS. taurus_vap Details

- Minimization schemes : VAP-NP / HFB
- Gradient methods for the minimization.
- $|\Phi\rangle$ breaks all the symmetries, one can preserve some of them by choosing between several options of symmetry-conserving seeds.
- **Constraints.** It constraints the Bogoliubov states

$$\delta \left(\frac{\langle \Phi(a_i) | \hat{H} \hat{P}^N \hat{P}^Z | \Phi(a_i) \rangle}{\langle \Phi(a_i) | \hat{P}^N \hat{P}^Z | \Phi(a_i) \rangle} - \lambda_Q \frac{\langle \Phi(a_i) | \hat{Q} | \Phi(a_i) \rangle}{\langle \Phi(a_i) | \Phi(a_i) \rangle} \right) = 0$$

- Multipole deformations $\hat{Q}_{\lambda\mu} (\lambda = [1, 4] \quad 0 \leq \mu \leq |\lambda|)$, also separable by (p, n) or (*isoscalar, isovector*)
- Angular momentum $\hat{J}_x, \hat{J}_y, \hat{J}_z$
- Pairing content : $[P^\dagger]_{MM_T}^{JT}, \Delta$
- RMS radius : $\langle \hat{r}_\tau^2 \rangle$, also $\tau = p, n$ or *isoscalar, isovector*

Advantages of TAURUS over traditional BMF solvers



- It can implement any type of Hamiltonian interaction.
- Can treat even-even, even-odd, and odd-odd nuclei on the same footing.
- General HFB (real) transformation allows the inclusion of proton-neutron mixing.

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \quad \beta_k |\Phi(a)\rangle = 0 \quad \forall k$$

$$U = \begin{pmatrix} U_{pp} & U_{pn} \\ U_{np} & U_{nn} \end{pmatrix} \quad V = \begin{pmatrix} V_{pp} & V_{pn} \\ V_{np} & V_{nn} \end{pmatrix}$$

- Study many constraints (deformations, intrinsic rotations, pairing).
- Particle-number, parity, and rotational symmetries can be simultaneously broken (and restored afterward).

Downside : This generality comes at the cost of calculation time.

The project TAURUS. Results

- Valence-space calculation with shell model

Hamiltonians

B. Bally, T.R. Rodríguez, A. Sánchez-Fernández,

Phys.Rev.C (2019) 100, 044308

Phys.Rev.C (2021) 103, 024315

Phys.Rev.C (2021) 104, 054306

- No-core calculations with chiral Hamiltonian

M. Frosini, T. Duguet, J-P.Ebran, B. Bally, T. Mongelli,

T.R.Rodríguez, R.Roth, V. Somà

Eur.Phys. J.A (2022) 58 : (62,63,64)

- Ab-initio* nuclear matrix elements for $0\nu\beta\beta$ decay

J.M.Yao, B.Bally, J.Engel, R.Wirth, T.R.Rodríguez, H.Hergert

Phys.Rev.Lett (2020) 124.232501

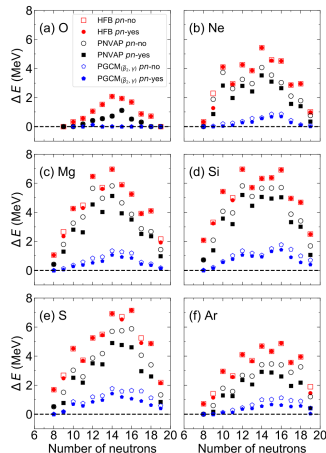
A.M.Romero, J.Yao, B.Bally, T.R.Rodríguez, J.Engel

Phys.Rev.C (2021) 104.054317

- Single-beta decay¹ and M1 transitions²

¹V.Vijayan MSc Thesis and ²J. Martínez-Larraz PhD thesis,

articles pending.



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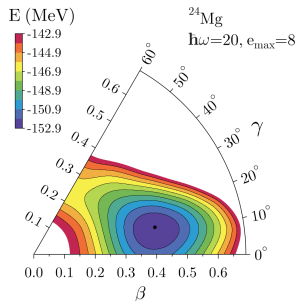
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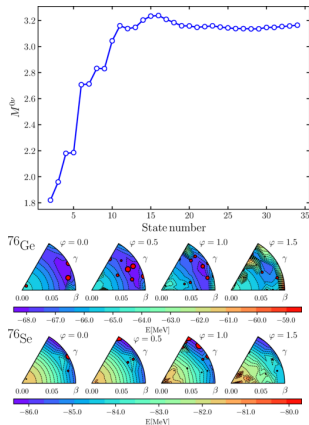
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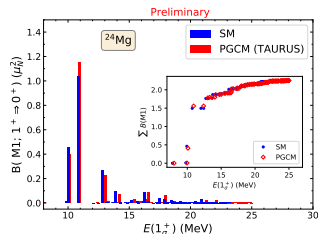
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TAURUS applied to EDF

Topic

- TAURUS has been designed only for Hamiltonians and not for EDF.
- We want to extend the scope of TAURUS to include EDF.

Why?

- Current EDF solvers are highly optimized to their underlying interaction, usually by assuming symmetry restrictions.
- `taurus_vap` allows us to explore more topics than traditional EDF solvers.
 - Symmetry breaking, more collective coordinates can be explored.
 - Study pn-pairing.
 - It works in the same way for even-even and odd-mass nuclei, one can extend the EDF methods to odd-mass nuclei straightforwardly.

Downside (again) : This generality comes at the cost of calculation time.

TAURUS applied to EDF

- Taking advantage of the Hamiltonian implementation, it is reasonable to extend it for "Hamiltonian-like" EDFs. In our case Gogny.
- Construction of the fields from two-body Hamiltonian, via matrix elements $\langle ab || V || cd \rangle_J$.⁵

$$\begin{aligned}\rho_{\delta\beta} &= \langle \Phi | c_{\beta}^{\dagger} c_{\delta} | \Phi \rangle & \kappa_{\gamma\delta} &= \langle \Phi | c_{\delta} c_{\gamma} | \Phi \rangle \\ \Gamma_{\alpha\gamma} &= \sum \langle \alpha\beta | v | \overline{\gamma\delta} \rangle \rho_{\delta\beta} & \Delta_{\alpha\beta} &= \sum \langle \alpha\beta | v | \overline{\gamma\delta} \rangle \kappa_{\gamma\delta} \\ & & H^{20}(U, V; t, \Gamma, \Delta)\end{aligned}$$

- For EDF derived from a Hamiltonian

$$\langle \hat{a}\hat{b} || V || \hat{c}\hat{d} \rangle_J \longrightarrow \langle \alpha\beta | v | \overline{\gamma\delta} \rangle \longrightarrow \left(\begin{matrix} \rho, \kappa \\ \Gamma, \Delta \end{matrix} \right) \longleftrightarrow H^{20}$$

- Applying interactions with no Hamiltonian expression, append the fields of the EDF.

$$\Gamma = \Gamma^{Hamil} + \Gamma^{EDF} \quad \Delta = \Delta^{Hamil} + \Delta^{EDF}$$

5. Note : Greek letters refer to uncoupled states $|\alpha\rangle \equiv |a(m_{t_a}), m_j = \alpha\rangle$

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Benchmarks with HFBaxial code.

Results for axial-octupole and triaxial-octupole TES.

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Gogny EDF

- The Gogny interaction is a phenomenological finite range force with a density-dependent term.

$$\begin{aligned}
 & \sum_{i=1,2} e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu_i^2} (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau) \\
 & + \frac{e^2 \delta(\tau_z^1 p, \tau_z^2 p)}{|\mathbf{r}_1 - \mathbf{r}_2|} + i W_0 (\sigma_1 + \sigma_2) \mathbf{k}^\dagger \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} \\
 & + t_3 (1 + x_0 P^\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^\alpha \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right)
 \end{aligned}$$

- The family of D1 interactions includes a finite range part, letting the treatment of the pairing and HF together (*ph* and *pp* parts).
- In this work we use D1S parametrization⁶, (good description of nuclear properties involving pairing).
- Fitted without accounting for the *pn* mixing.

6. J.F.Berger, M.Girod and D.Gogny, *Comp.Phys.Comm.*, **63** (1991) 365

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Fields

- Implementation for these matrix elements for the Gogny interaction in the SHO basis, including the 1B and 2B center-of-mass corrections⁷.
- DD term was chosen to be zero-range, involves the evaluation of the *rearrangement term* $\langle \Phi | \delta v[\rho] / \delta \rho_{kk'} | \Phi \rangle$
- DD term is isospin-dependent, but the parameterizations impose $x_0 = 1$ to avoid any pairing from this source.
- 2B antisymmetrized DD matrix elements (SHO) $\bar{v}_{\alpha\beta\gamma\delta}^{DD}$, being

$$x_{abcd} = \delta_{ac}^{\tau} \delta_{bd}^{\tau'} - x_0 \delta_{ad}^{\tau} \delta_{bc}^{\tau'}$$

$$t_3 \int dr^3 \rho^{\alpha}(\mathbf{r}) \mathcal{R}_{abcd}(r) \left[\mathcal{Y}_{\alpha\gamma} \mathcal{Y}_{\beta\delta}(\hat{\Omega}) x_{abcd} - \mathcal{Y}_{\alpha\delta} \mathcal{Y}_{\beta\gamma}(\hat{\Omega}) x_{abdc} \right]$$

$\rho(\mathbf{r})$ could lead symmetry breaking matrix elements (i.e. $l_a + l_b \neq l_c + l_d$ or $\alpha + \beta \neq \gamma + \delta$)

7. github.com/miguelde lafuente1/2B_MatrixElements.git

DD-considerations

Fields

$$\Gamma_{\alpha\gamma} = \sum \langle \alpha\beta | v | \overline{\gamma\delta} \rangle \rho_{\delta\beta}$$

$$\Delta_{\alpha\beta} = \sum \langle \alpha\beta | v | \overline{\gamma\delta} \rangle \kappa_{\gamma\delta}$$

$$\partial\Gamma_{ij} = \frac{1}{4} \sum \langle \alpha\beta | \frac{\partial v}{\partial \rho} \phi_i^* \phi_j \delta_{ij}^\tau | \overline{\gamma\delta} \rangle D_{\alpha\beta\gamma\delta}$$

$$D_{\alpha\beta\gamma\delta} = 2\rho_{\delta\beta}\rho_{\gamma\alpha} - \kappa_{\alpha\beta}^* \kappa_{\gamma\delta}$$

$$\rho = \begin{pmatrix} \rho_{pp} & \rho_{pn} \\ \rho_{np} & \rho_{nn} \end{pmatrix} \quad \kappa = \begin{pmatrix} \kappa_{pp} & \kappa_{pn} \\ \kappa_{np} & \kappa_{nn} \end{pmatrix}$$

Isospin contributions to the density-dependent term.

$\Gamma_{\alpha\gamma}^{\tau_a\tau_c}$	$\langle \alpha_{\tau_a} \beta_{\tau_b} \gamma_{\tau_c} \delta_{\tau_d} \rangle$	$\rho_{\delta\beta}^{\tau_d\tau_b}$
pp	pn pn	nn
nn	pn pn	pp
pn	pn np	pn

$\Delta_{\alpha\beta}^{\tau_a\tau_b}$	$\langle \alpha_{\tau_a} \beta_{\tau_b} \gamma_{\tau_c} \delta_{\tau_d} \rangle$	$\kappa_{\gamma\delta}^{\tau_c\tau_d}$
pp	pp pp	pp
nn	nn nn	nn
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DD-considerations

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pp	$pn \quad pn$	nn
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$\Delta_{\alpha\beta}^{\tau_a\tau_b}$	$\langle \alpha_{\tau_a} \beta_{\tau_b} \quad \gamma_{\tau_c} \delta_{\tau_d} \rangle$	$\kappa_{\gamma\delta}^{\tau_c\tau_d}$
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pn	$pn \quad pn$	pn

It doesn't apply for $x_0 = 1$

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Evaluating the optimal oscillator length.

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Benchmark 1 : Evaluating the optimal oscillator length.

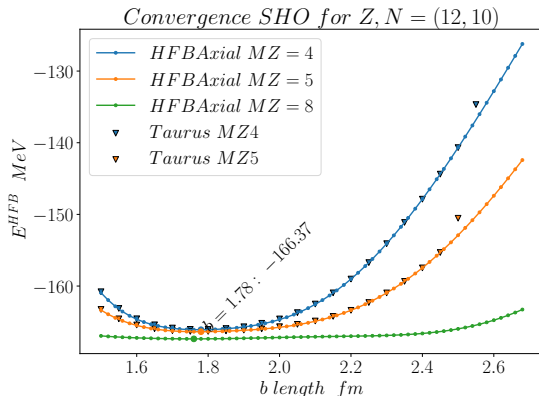
Validations with the axial HFB code⁸ (D1S interaction implemented)

$$b = \frac{\hbar c}{\sqrt{(mc^2)\hbar\omega}}$$

No-core calculation details :

- 1b,2b COM
- $\langle Q_{10} \rangle = 0$
- Coulomb on
- HO Shells= 4, 5

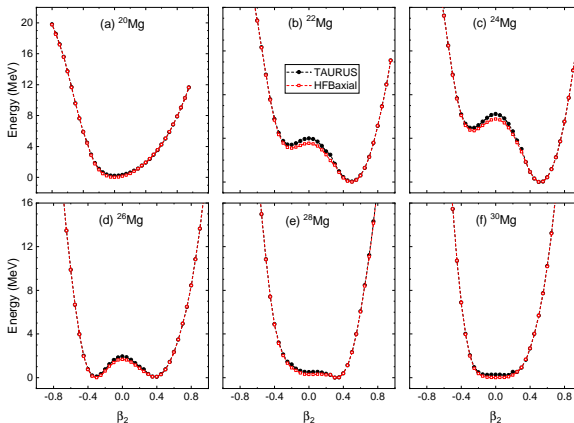
Reevaluating the BB matrix elements for TAURUS at each b.



8. L. M. Robledo, HFBaxial code, (2002)

Benchmark 2 : Axial quadrupole and octupole TES.

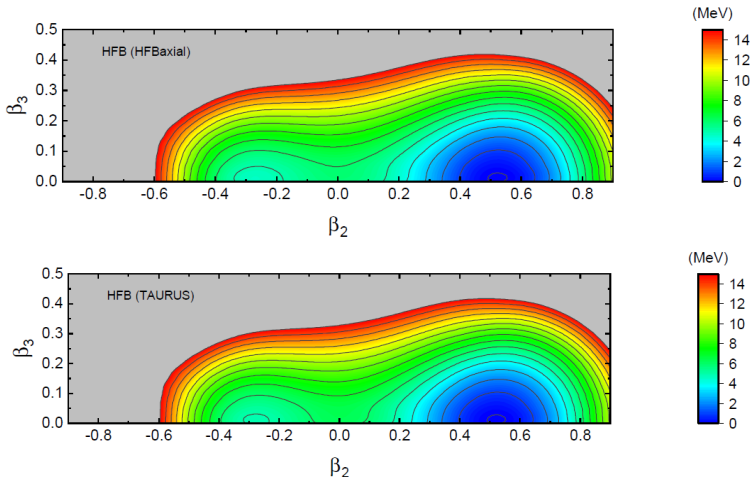
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- Mg energy deformation surfaces $E_{HFB}(\beta_{20})$



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9. L. M. Robledo, HFBaxial code, (2002)

① Introduction

② The project TAURUS

③ Gogny EDF

Benchmarks with HFBaxial code.

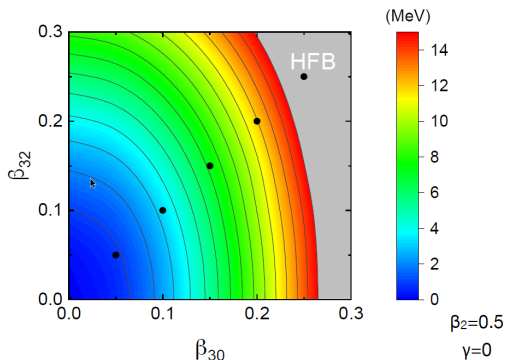
Results for axial-octupole and triaxial-octupole TES.

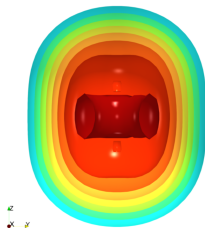
④ Proton-Neutron pairing

⑤ Conclusions and Research Plan

Exploration of octupole degrees of freedom with TAURUS (D1S)

HFB Energy Surfaces: axial and triaxial octupolarity



$\beta_{32}=0.00$ 

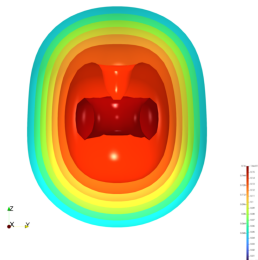
Exploration of octupole degrees of freedom with TAURUS (D1S)

$$\beta_2=0.5$$

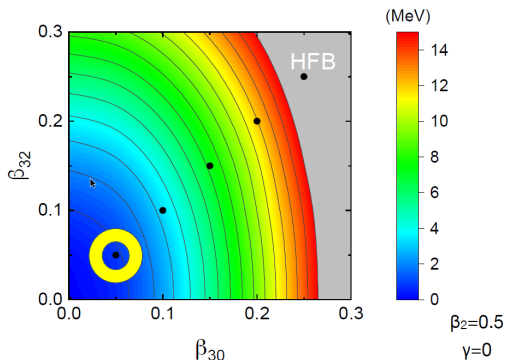
$$\gamma=0$$

$$\beta_{30}=0.05$$

$$\beta_{32}=0.05$$



HFB Energy Surfaces: axial and triaxial octupolarity



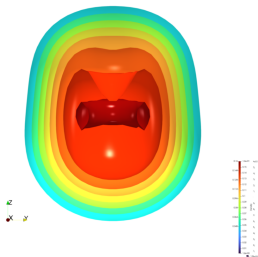
Exploration of octupole degrees of freedom with TAURUS (D1S)

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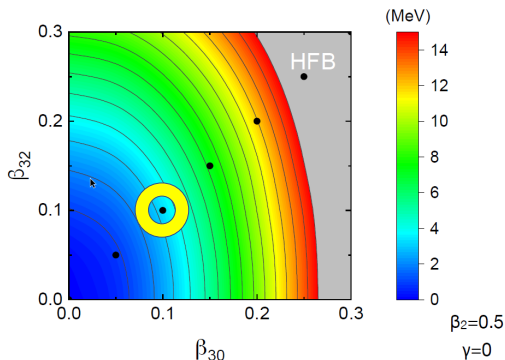
$$\gamma=0$$

$$\beta_{30}=0.10$$

$$\beta_{32}=0.10$$



HFB Energy Surfaces: axial and triaxial octupolarity



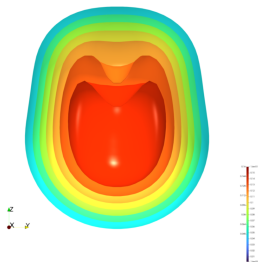
Exploration of octupole degrees of freedom with TAURUS (D1S)

$$\beta_2=0.5$$

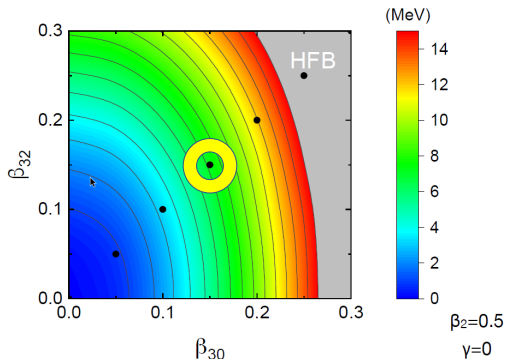
$$\gamma=0$$

$$\beta_{30}=0.15$$

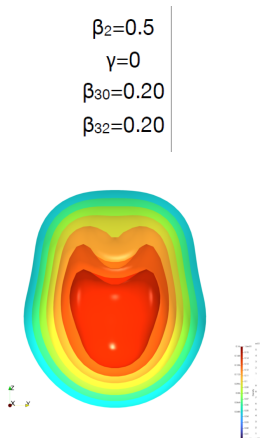
$$\beta_{32}=0.15$$



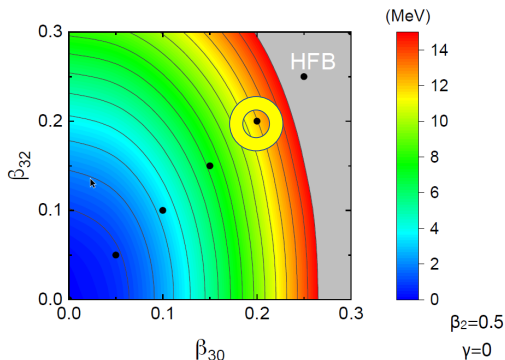
HFB Energy Surfaces: axial and triaxial octupolarity



Exploration of octupole degrees of freedom with TAURUS (D1S)



HFB Energy Surfaces: axial and triaxial octupolarity

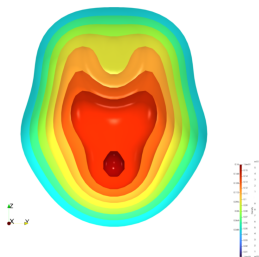


$\beta_2=0.5$

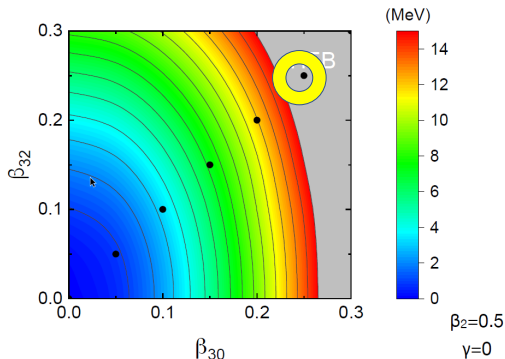
$\gamma=0$

$\beta_{30}=0.25$

$\beta_{32}=0.25$



HFB Energy Surfaces: axial and triaxial octupolarity



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Testing behavior with pn-mixing channels
- ⑤ Conclusions and Research Plan

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Testing behaviour with pn-mixing channels

Definitions

- Static correlations in nuclei : formation of Cooper pairs for like-particles ($T = 1, M_T = \pm 1$).
- Pairs depend on the overlap, $Z \approx N$ nuclei requires extending the theory for pn pairs.
- pn pairs can be **isoscalar** ($T = 0, J = 1$) and **isovector** ($T = 1, M_T = 0; J = 0$).

Pair coupling operator (one-body operator)

$$\delta_{M_J M_T}^{JT} = \langle \Phi | \frac{1}{2} ([P^\dagger] + [P]) | \Phi \rangle$$

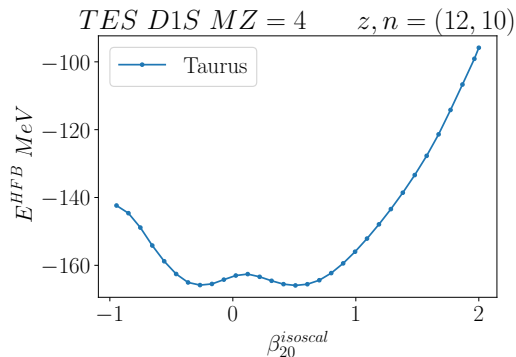
$$[P^\dagger]_{M_J M_T}^{JT} = \frac{1}{\sqrt{2}} \sum_a \sqrt{2j_a + 1} [c_a^\dagger c_a^\dagger]_{M_J M_T}^{JT}$$

What are we expecting ?

- Overall stability under the original D1S interaction.
- Behaviour of the energy surfaces.
- Not having isovector/isoscalar minima.

Pairing Calculations

- No-core calculation
 - 1b,2b COM
 - $\langle Q_{10} \rangle = 0$
 - Coulomb on
 - HO Shells = 4, 5
- Optimal oscillator length.
- Getting the unconstrained minimum.
- Constraint each δ_{JM}^{TM} from the minimum, while leaving the other δ and $\beta_{\lambda\mu}$ free

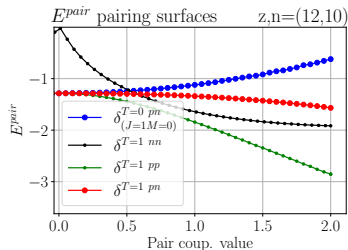
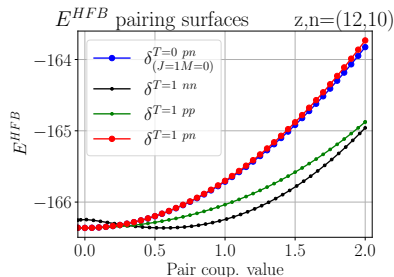


Analysis for Mg isotopes ($MZ_{max} = 5$)

General $N \neq Z$
case :

- $E^{HFB}(\text{isovector-pn/isoscalar}) > E^{HFB}(\text{pp/nn})$

- $E^{pair}(\text{isovector-pn/isoscalar}) > E^{pair}(\text{pp/nn})$

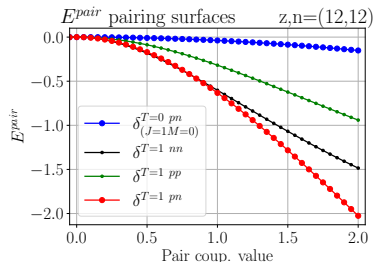
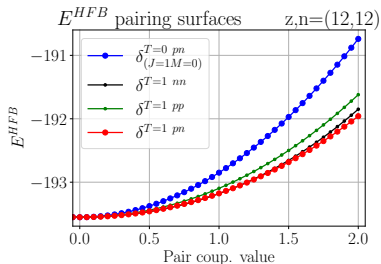


Analysis for Mg isotopes ($MZ_{max} = 5$)

$N = Z$ case :

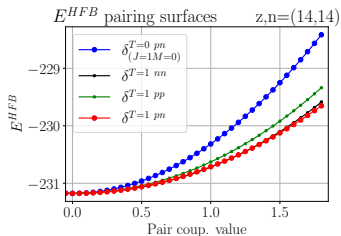
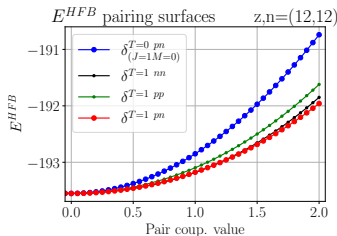
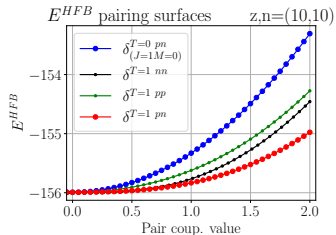
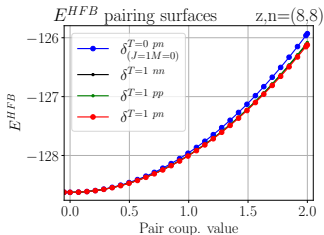
- $$E^{HFB}(\text{isovector-pn}) \leq E^{HFB}(\text{pp/nn}) < E^{HFB}(\text{isoscalar})$$

- $$E^{pair}(\text{isovector-pn}) \leq E^{pair}(\text{pp/nn}) < E^{pair}(\text{isoscalar})$$



Analysis for even-even $N = Z$ nuclei ($MZ_{max} = 5$)

$$E^{HFB}(\text{isovector-pn}) \leq E^{HFB}(\text{pp/nn}) < E^{HFB}(\text{isoscalar})$$



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Appx.

TAURUS for EDF and pn-pairing

Conclusions

- For the first time, we explore the proton-neutron channel of the D1S interaction.
- Satisfactory outcome from the extension of the original D1S to *pn*-mixing wave functions at MF level.
- The interaction shows a consistent behavior when *pn* wave functions are employed in these light nuclei.
 - *pn* channels are not favoured for $N \neq Z$ (as expected).
 - *pn*-isovector channel is favored for $N = Z$ isotopes.

Perspectives

- Many *pn* pairing physics occurs in rotating nuclei, investigate cranking with D1S interaction.
- Explore other density-dependent interactions with this framework.
- Projection to particle number $P^N P^Z |\Phi\rangle$
 - Pairing condensates lose out the particle number as a good quantum number.
 - Restoring it might lead a real *pn* minimum.
 - It is necessary to access **odd-odd** nuclei at MF level.

Recap. of TAURUS



- It can implement any type of Hamiltonian interaction.
- Can treat even-even, even-odd, and odd-odd nuclei on the same footing.
- General HFB (real) transformation allows the inclusion of proton-neutron mixing.

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l \quad \beta_k |\Phi(a)\rangle = 0 \quad \forall k$$

$$U = \begin{pmatrix} U_{pp} & U_{p\textcolor{blue}{n}} \\ U_{\textcolor{blue}{n}p} & U_{nn} \end{pmatrix} \quad V = \begin{pmatrix} V_{pp} & V_{p\textcolor{blue}{n}} \\ V_{\textcolor{blue}{n}p} & V_{nn} \end{pmatrix}$$

- Study many constraints (deformations, intrinsic rotations, pairing).
- Particle-number, parity, and rotational symmetries can be simultaneously broken (and restored afterward).

Thank you !

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Appendix

- The wave function employs the product of quasiparticles β , then nuclear states are the quasiparticle vacua :

$$|\Phi\rangle = \prod_{k=1} \beta_k |-\rangle \rightarrow \beta_k |\Phi\rangle = 0 \quad \forall k$$

- β is defined with the most general linear transformation between operators c, c^\dagger of a certain base $\{|i\rangle\}$

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l$$

- HFB equations are solved with the gradient method, constraining observables through Lagrange multipliers

$$\delta(E'_{HFB}) = 0$$

$$E'_{HFB} = \langle \Phi(q) | \hat{H} - \lambda_N \hat{N} - \lambda_Z \hat{Z} - \lambda_q \hat{Q} | \Phi(q) \rangle$$

where q are multipole deformations, pairing content, radius,...

Appendix

D1S interaction

The case for the D1 family interactions includes a finite range part in the form of Brink-Boeker, characterizing nuclei where pairing plays an important role (*ph* and *pp* treated with the same interaction).¹⁰

$$\begin{aligned}
 & \sum_{i=1,2} e^{-(\mathbf{r}_1 - \mathbf{r}_2)^2 / \mu_i^2} (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau) \\
 & + \frac{e^2 \delta(\tau_z^1 p, \tau_z^2 p)}{|\mathbf{r}_1 - \mathbf{r}_2|} + i W_0 (\sigma_1 + \sigma_2) \mathbf{k}^\dagger \times \delta(\mathbf{r}_1 - \mathbf{r}_2) \mathbf{k} \\
 & + t_3 (1 + x_0 P^\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^\alpha \left(\frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \right)
 \end{aligned}$$

10. J.Dechargé, D.Gogny. D1S parametrization.

Appendix

- Implementation for these matrix elements for the Gogny interaction in the SHO basis, including the 1B and 2B center-of-mass corrections¹⁰.
- DD term was chosen to be zero-range, involves the evaluation of the *rearrangement term* $\langle \Phi | \delta v[\rho] / \delta \rho_{kk'} | \Phi \rangle$
- DD term is isospin-dependent, but the parameterizations impose $x_0 = 1$ in order to avoid any pairing from this source.
- 2B antisymmetrized DD matrix elements for SHO $\bar{v}_{\alpha\beta\gamma\delta}^{DD}$, being

$$x_{abcd} = \delta_{ac}^{\tau} \delta_{bd}^{\tau'} - x_0 \delta_{ad}^{\tau} \delta_{bc}^{\tau'}$$

$$t_3 \int dr^3 \rho^{\alpha}(\mathbf{r}) \mathcal{R}_{abcd}(r) \left[\mathcal{Y}_{\alpha\gamma} \mathcal{Y}_{\beta\delta}(\hat{\Omega}) x_{abcd} - \mathcal{Y}_{\alpha\delta} \mathcal{Y}_{\beta\gamma}(\hat{\Omega}) x_{abdc} \right]$$

10. github.com/miguelde lafuente1/2B_MatrixElements.git

Appendix

Fields

$$\rho_{\delta\beta} = \langle \Phi | c_{\beta}^{\dagger} c_{\delta} | \Phi \rangle$$

$$\kappa_{\gamma\delta} = \langle \Phi | c_{\delta} c_{\gamma} | \Phi \rangle$$

$$\Gamma_{\alpha\gamma} = \sum \langle \alpha\beta | v | \gamma\delta \rangle \rho_{\delta\beta}$$

$$\Delta_{\alpha\beta} = \sum \langle \alpha\beta | v | \gamma\delta \rangle \kappa_{\gamma\delta}$$

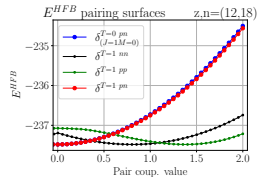
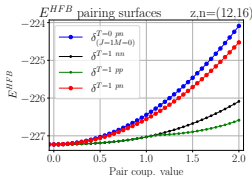
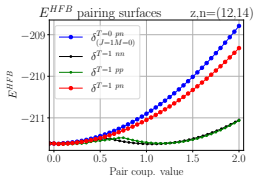
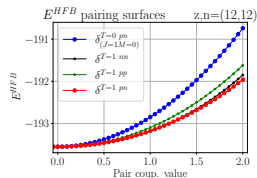
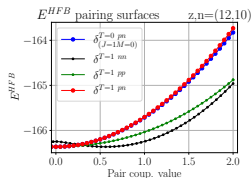
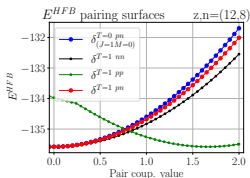
Isospin contributions to the density dependent term.

$\Gamma_{\alpha\gamma}^{\tau_a\tau_c}$	$\langle \alpha\tau_a \beta\tau_b \rangle$	$\gamma\tau_c \delta\tau_d \rangle$	$\rho_{\delta\beta}^{\tau_d\tau_b}$
<i>pp</i>	<i>pn</i>	<i>pn</i>	<i>nn</i>
<i>nn</i>	<i>pn</i>	<i>pn</i>	<i>pp</i>
<i>pn</i>	<i>pn</i>	<i>np</i>	<i>pn</i>

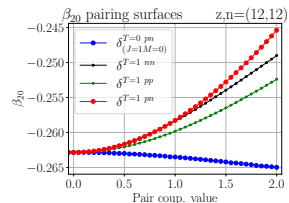
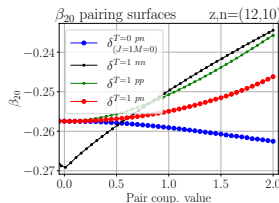
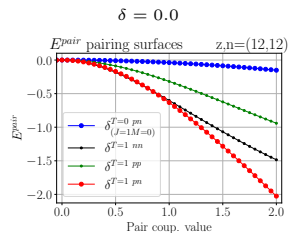
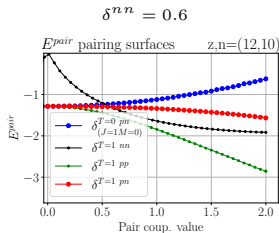
$\Delta_{\alpha\beta}^{\tau_a\tau_b}$	$\langle \alpha\tau_a \beta\tau_b \rangle$	$\gamma\tau_c \delta\tau_d \rangle$	$\kappa_{\gamma\delta}^{\tau_c\tau_d}$
<i>pp</i>	<i>pp</i>	<i>pp</i>	<i>pp</i>
<i>nn</i>	<i>nn</i>	<i>nn</i>	<i>nn</i>
<i>pn</i>	<i>pn</i>	<i>pn</i>	<i>pn</i>

It doesn't apply for $x_0 = 1$

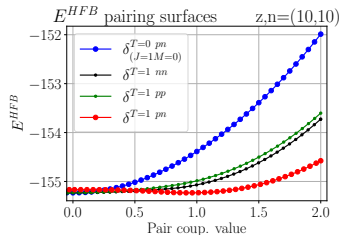
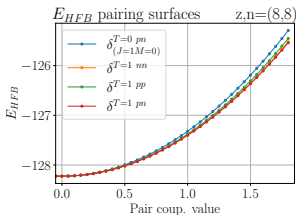
Appendix



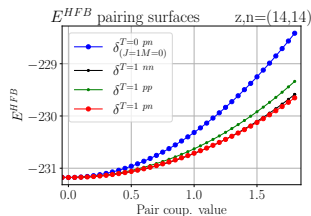
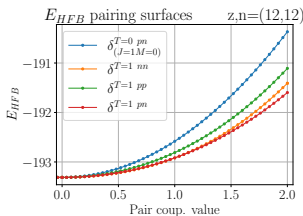
Appendix



Appendix



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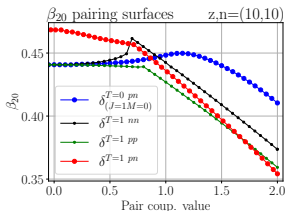
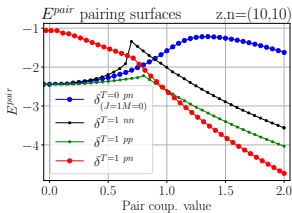


10. -0.06 MeV gain

Appendix

Neon 20 pn isovector minimum ($MZ_{max} = 4, 5$)

$$\delta^{T=1} pn = 0.95$$



$$\delta = 0.0$$

