Impact of methods and symmetries on quasi-particle excitations in mean-field theory.

ECT* workshop on odd nuclei

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Table of contents

The means: `MOCCa`.

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MOCCa

- 3D Lagrange mesh code

MOCCa

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MOCCa

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- Skyrme NLO and N2LO
- SLy5s1 in this presentation
- Full HFB
- ! 16 different symmetry combinations

Single-particle symmetry operators

$$D_{2h}^{TD} = \{\hat{P}, \hat{R}_{x/y/z}, \hat{S}_{x/y/z}, \check{T}, \check{R}^{T}_{x,y,z}, \check{S}^{T}_{x,y,z}\}$$

Single-particle symmetry operators

$$D_{2h}^{TD} = \{ \overbrace{\underbrace{\hat{P}}_{\text{H}}, \underbrace{\hat{R}_{x/y/z}, \hat{S}_{x/y/z}}_{\text{AH}}}^{\text{Linear}}, \overbrace{\underbrace{\check{T}}_{\text{AH}}, \underbrace{\check{R}^{T}_{x,y,z}, \check{S}^{T}_{x,y,z}}_{\text{H}}}^{\text{Antilinear}} \} \,.$$

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Many-body operators differ:

		$\mathcal{D}_{2h}^{T}$	$\mathcal{D}_{2h}^{TD}$
$\check{\mathcal{T}}^2$	=	1	-1
$\left[\hat{\mathcal{R}}_\mu, \hat{\mathcal{R}}_\nu\right]$	=	0	$\epsilon_{\mu\nu\kappa}\hat{\mathcal{R}}_\kappa - \delta_{\mu\nu}$

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Subgroups $\leftrightarrow$ Generator sets $\leftrightarrow$ Symmetries of the spwfs

Single-particle symmetry operators

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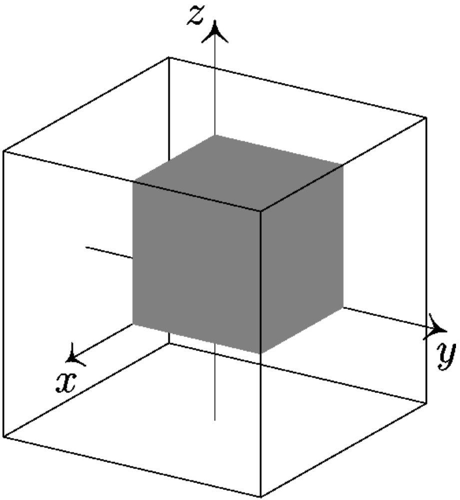
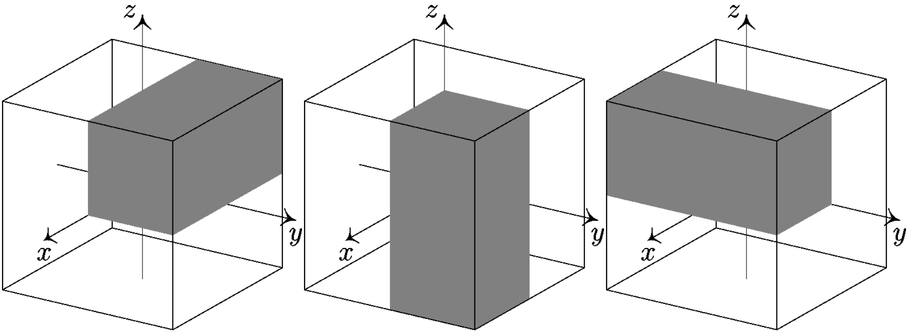
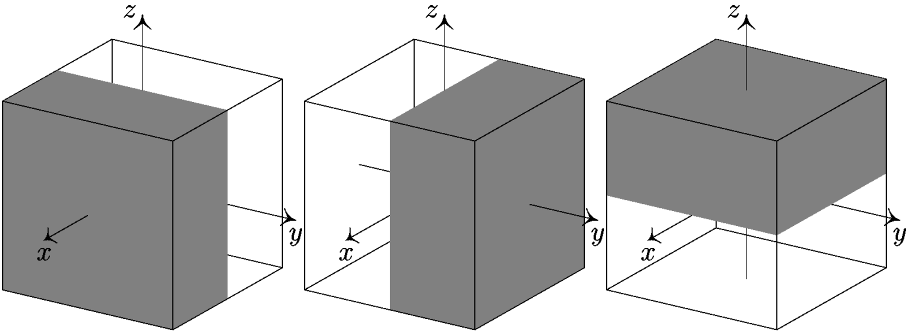
Subgroups	$\leftrightarrow$	Generator sets	$\leftrightarrow$	Symmetries of the spwfs
D_{2h}^T	$\leftrightarrow$	$G\left\{\check{\mathcal{T}}, \hat{\mathcal{P}}, \hat{\mathcal{R}}_z, \check{\mathcal{S}}_y^T\right\}$	$\leftrightarrow$	Kramers, P, η, phase choice

MOCCa's implementation



MOCCa's implementation

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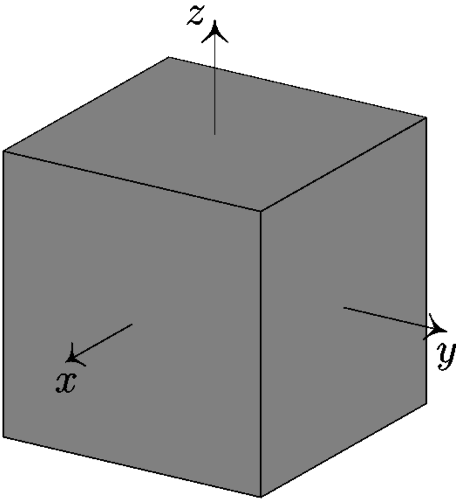

Operator of the hour:

$$\hat{\vec{\mathcal{J}}}$$

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It is heavily restricted by symmetries

$$\check{T} \text{ conserved} \qquad \langle \hat{\vec{\mathcal{J}}} \rangle = 0$$

Angular momentum and symmetries

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$$\begin{array}{lll} \check{T} \text{ conserved} & \langle \hat{\vec{\mathcal{J}}} \rangle = 0 & \\ \hat{\mathcal{R}}_\mu \text{ conserved} & \langle \hat{\vec{\mathcal{J}}}_\nu \rangle = 0 & \nu \neq \mu \\ \check{\mathcal{R}}^T_\mu \text{ conserved} & \langle \hat{\vec{\mathcal{J}}}_\mu \rangle = 0 & \end{array}$$

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\end{aligned}$$

One only degree of freedom that is available in a run-of-the-mill calculation

$$\langle \hat{\vec{\mathcal{J}}}_z \rangle$$

Methods, or how to block qps.

Reminder: two-basis method

HF-states $\psi_l^{(\mathrm{iter})}(l = 1, \ldots N)$

Reminder: two-basis method

h, Δ: HFB equations

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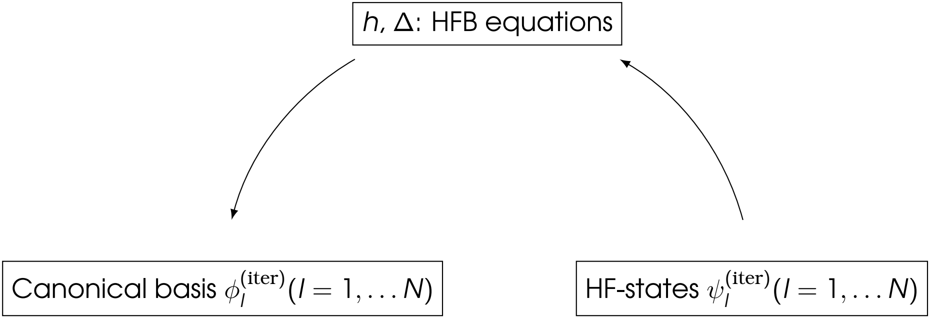
Reminder: two-basis method

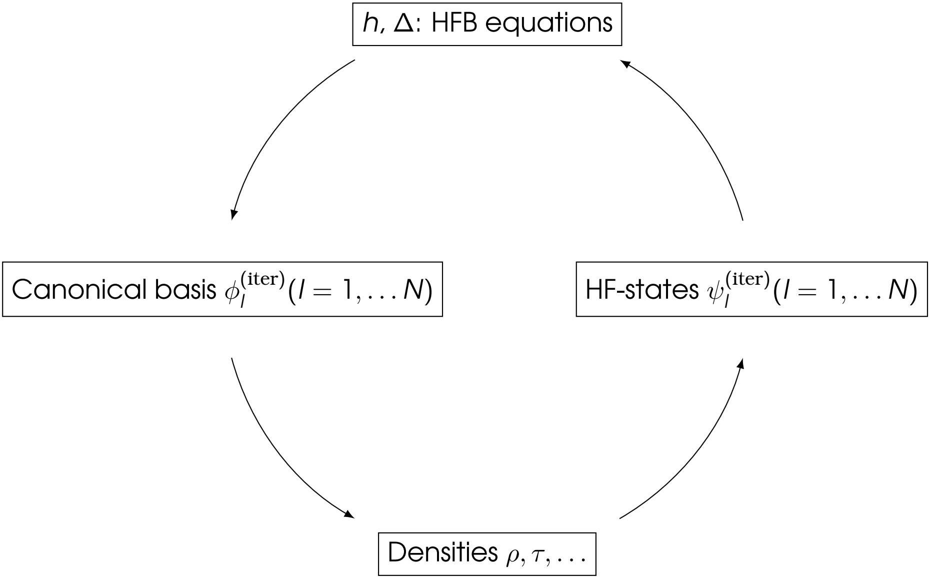


Reminder: two-basis method

h, Δ: HFB equations

Canonical basis $\phi_l^{(\mathrm{iter})}(l = 1, \ldots N)$

HF-states $\psi_l^{(\mathrm{iter})}(l = 1, \ldots N)$


h, Δ: HFB equations
Canonical basis $\phi_l^{(\mathrm{iter})}(l = 1, \ldots N)$
HF-states $\psi_l^{(\mathrm{iter})}(l = 1, \ldots N)$
Densities $\rho, \tau, \ldots$

HFB equations in the HF basis

Assume

- **HF basis** of dimension **N**
- h diagonal in this basis

Bogoliubov transformation from particles to quasiparticles

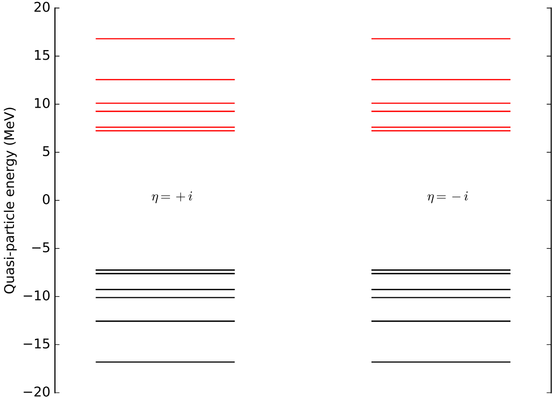
$$\text{Dimension 2N} \left\{ \begin{pmatrix} \hat{\beta} \\ \hat{\beta}^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} \hat{c} \\ \hat{c}^\dagger \end{pmatrix} \right.$$

Where the U, V matrices are determined by

$$\mathcal{H} \begin{pmatrix} U \\ V \end{pmatrix} = \underbrace{\begin{pmatrix} h & \Delta \\ -\Delta & -h \end{pmatrix}}_{\text{Dimension 2N}} \begin{pmatrix} U \\ V \end{pmatrix} = E^{qp} \begin{pmatrix} U \\ V \end{pmatrix} .$$

Inherent symmetry:

$$U_l \leftrightarrow V_l^*$$
$$V_l \leftrightarrow U_l^*$$
$$E_l^{qp} \leftrightarrow -E_l^{qp}$$
$$\hat{\beta}_l \leftrightarrow \hat{\beta}_l^\dagger$$



Inherent HFB symmetry: multiple vacua

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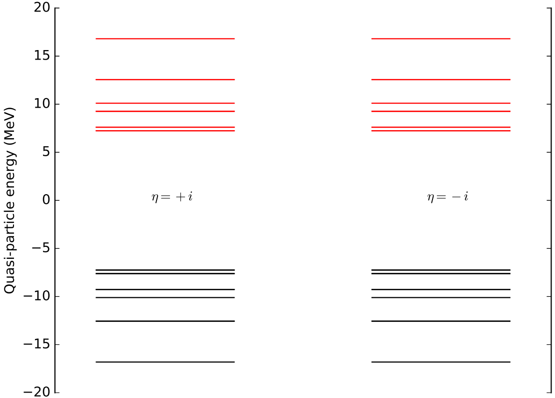

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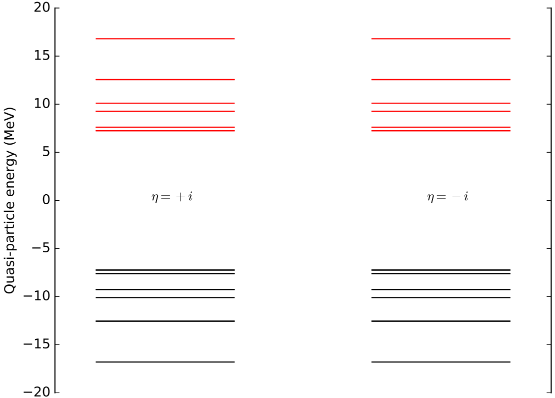
$$P \leftrightarrow P$$
$$\eta \leftrightarrow -\eta$$



Antilinear, hermitian symmetries come to the rescue.

$$\hat{\mathcal{R}}_{x/y/z}, \hat{\mathcal{S}}_{x/y/z}$$

Block structure of the HFB equations

Symmetries simplify the HFB equations
Hermitian, linear

$$\mathcal{H}_{\text{HFB}} = \begin{pmatrix} h_{++} & 0 & \Delta_{++} & 0 \\ 0 & h_{--} & 0 & \Delta_{--} \\ \Delta_{++} & 0 & -h_{++} & 0 \\ 0 & \Delta_{--} & 0 & -h_{--} \end{pmatrix}$$

$$\begin{pmatrix} U_+ \\ 0 \\ V_+ \\ 0 \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ U_- \\ 0 \\ V_- \end{pmatrix}$$

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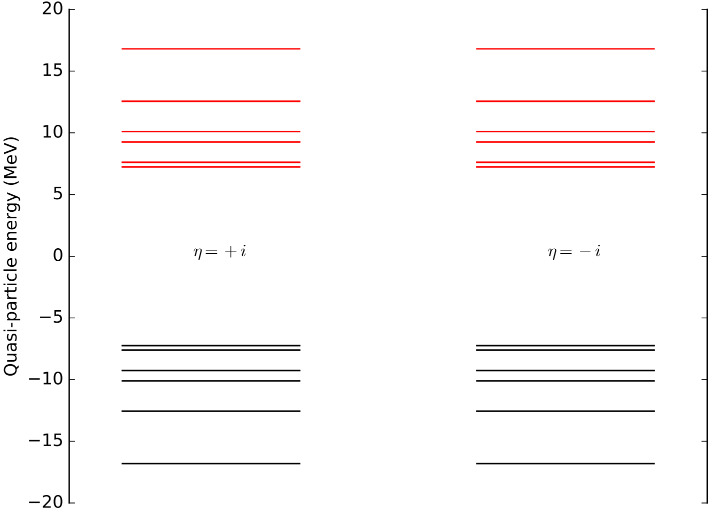
Antihermitian, linear

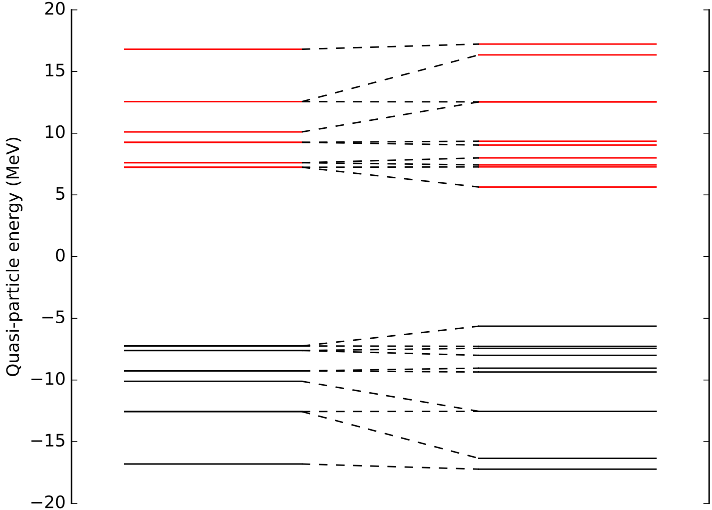
$$\mathcal{H}_{\mathrm{HFB}} = \begin{pmatrix} h_{++} & 0 & 0 & \Delta_{+-} \\ 0 & h_{--} & -\Delta^T_{+-} & 0 \\ 0 & -\Delta^T_{+-} & -h_{++} & 0 \\ \Delta_{+-} & 0 & 0 & -h_{--} \end{pmatrix} \qquad \begin{pmatrix} U_+ \\ 0 \\ 0 \\ V_- \end{pmatrix} \text{ or } \begin{pmatrix} 0 \\ U_- \\ V_+ \\ 0 \end{pmatrix}$$

Choosing a vacuum

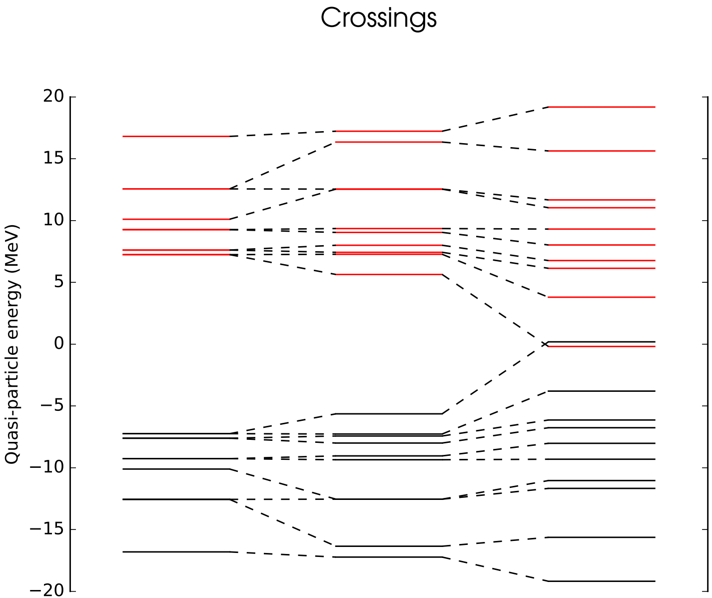
Time-reversal invariant



Lifting the degeneracy



Choosing a vacuum



Consequences of choosing wrong

$|\Psi_1\rangle$ $|\Psi_2\rangle = \hat{\beta}_1^\dagger |\Psi_1\rangle$

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Disaster for any numerical solver.

Signature broken HFB

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Solution: Avoid making a choice.

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$$|\Psi(Z)\rangle = \left[-\frac{1}{2} \sum_{ij} Z_{ij} \beta_i^\dagger \beta_j^\dagger \right] |\Psi_{\text{sym}}\rangle \, . \qquad E(Z, \Psi_0) = \frac{\langle \Psi(Z) | \hat{\mathcal{H}}_{\text{HFB}} | \Psi(Z) \rangle}{\langle \Psi(Z) | \Psi(Z) \rangle} \, .$$

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Minimizing the energy with respect to Z_{ij} gives rise to an iterative scheme

$$\begin{aligned} U^{(\text{iter}+1)} &= U^{(\text{iter})} - \epsilon V^{*,(\text{iter})} \left(\mathcal{H}^{20}_{\text{HFB}} - \lambda \mathcal{N}^{20} \right)^* , \\ V^{(\text{iter}+1)} &= V^{(\text{iter})} - \epsilon U^{*,(\text{iter})} \left(\mathcal{H}^{20}_{\text{HFB}} - \lambda \mathcal{N}^{20} \right)^* . \end{aligned}$$

Methods of blocking

Direct Blocking

1. Get initial false vacuum, i.e. U_0, V_0.
2. Calculate h, Δ
3. Diagonalize (Lapack) $\mathcal{H}$
4. Identify blocked quasiparticle.
5. Calculate $\rho, \kappa, \ldots$
6. Update mean-field.
7. Go to step 2.

Thouless Blocking

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Identify qp every iteration.

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Identify qp only once.

Comparison Thouless vs Direct blocking

	Direct	Thouless
Identification of qp	Every iteration	Once
Antihermitian symmetry	Necessary	Not necessary
Lowest energy?	Maybe	Guaranteed
Multiple states	Yes	Only lowest
Fire and forget	No	Yes

Equivalence

		E (MeV)	$\langle \hat{\mathcal{J}}_z \rangle$ ($\hbar$)
^{25}Mg	Thouless	-202.3515**38**	0.018
	Direct	-202.3515**40**	0.018
^{65}Ge	Thouless	-548.14**8448**	1.40**3**
	Direct	-548.14**7910**	1.40**4**
^{178}Lu	Thouless	-1423.092**18**	0.9**77**
	Direct	-1423.092**02**	0.9**81**
^{223}Th	Thouless	-1695.2**7024**	$-$3.5**71**
	Direct	-1695.2**6991**	$-$3.5**52**

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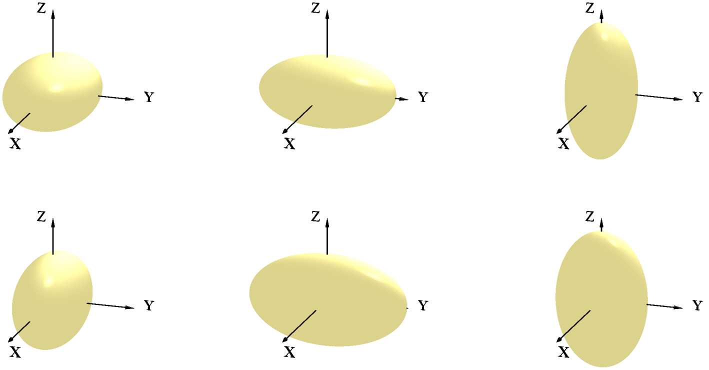
! Note that it is not necessary trivial to find the same minimum with both methods.

The influence of symmetries.

Orientations of the nucleus



Orientations

Orientation	Energy (MeV)	q (fm^2)	$\gamma(^\circ)$	$\langle \hat{M}_{10} \rangle$	$\langle \hat{\mathcal{J}}_z \rangle$
		^{24}Mg			
$(X > Y = Z)$	$-196.8152083\mathbf{7}$	$67.933857\mathbf{5}$	$0.024\mathbf{2}$	0.000	0.000
$(Y > X = Z)$	$-196.8152083\mathbf{7}$	$67.933857\mathbf{5}$	$0.024\mathbf{1}$	0.000	0.000
$(Z > X = Y)$	$-196.8152083\mathbf{8}$	$67.933857\mathbf{8}$	$0.024\mathbf{1}$	0.000	0.000

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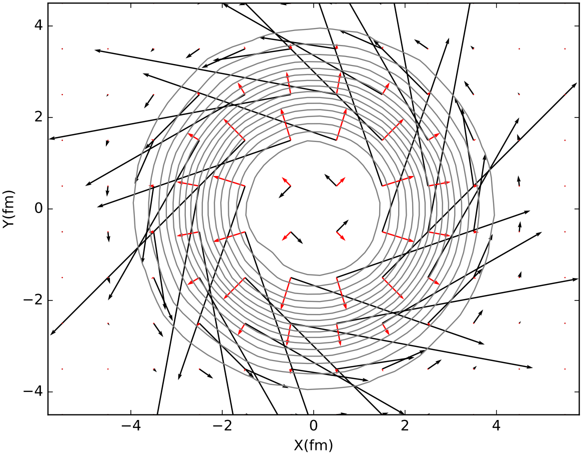
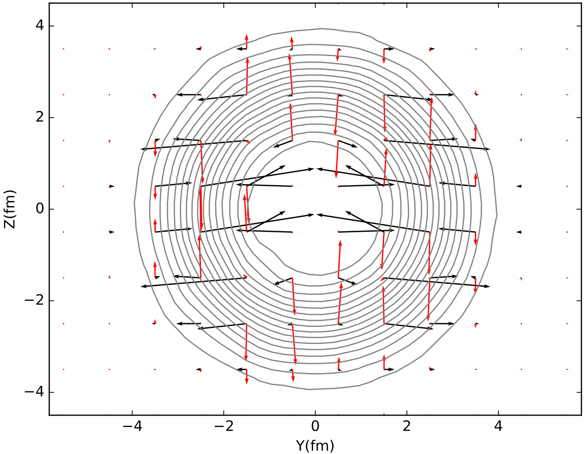
$(Z > X = Y)$	-196.8152083**8**	67.933857**8**	0.024**1**	0.000	0.000

		^{25}Mg			
$(X > Y = Z)$	-202.351538**45**	85.845055**9**	0.719	-0.012	0.018
$(Y > X = Z)$	-202.351538**39**	85.845055**8**	0.719	-0.012	0.018
$(Z > X = Y)$	-202.295653**32**	85.71151**92**	0.000	-0.690	1.490

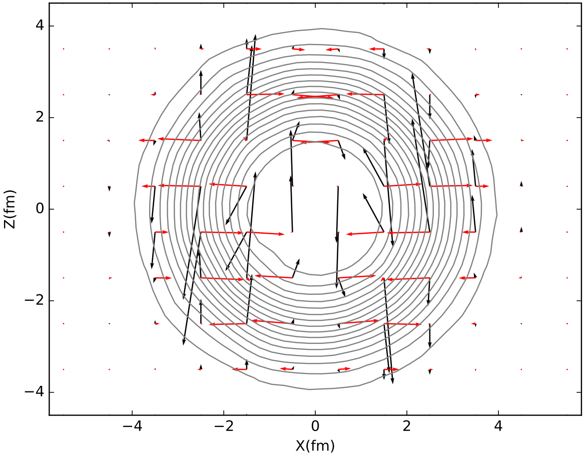
^{24}Mg, $(Z > X = Y)$ around the Z-axis, $\vec{j}$ and $\vec{s}$



^{24}Mg, $(X > Y = Z)$ around the X-axis, $\vec{j}$ and $\vec{s}$



^{24}Mg, ($Y > X = Z$) around the Y-axis, $\vec{j}$ and $\vec{s}$



Symmetries and orientation

Orientation	Energy (MeV)	q (fm^2)	$\gamma(^\circ)$	$\langle \hat{M}_{10} \rangle$	$\langle \hat{\mathcal{J}}_z \rangle$
		^{64}Ge			
$(X > Y > Z)$	-543.08859**88**	269.27**50**	29.927**27**	0.000	0.000
$(Y > X > Z)$	-543.08859**88**	269.27**49**	29.927**33**	0.000	0.000
$(Z > X > Y)$	-543.08859**72**	269.27**50**	29.927**74**	0.000	0.000
$(X > Z > Y)$	-543.08859**88**	269.27**50**	29.927**25**	0.000	0.000
$(Y > Z > X)$	-543.08859**86**	269.27**50**	29.927**24**	0.000	0.000
$(Z > Y > X)$	-543.08859**89**	269.27**51**	29.927**23**	0.000	0.000

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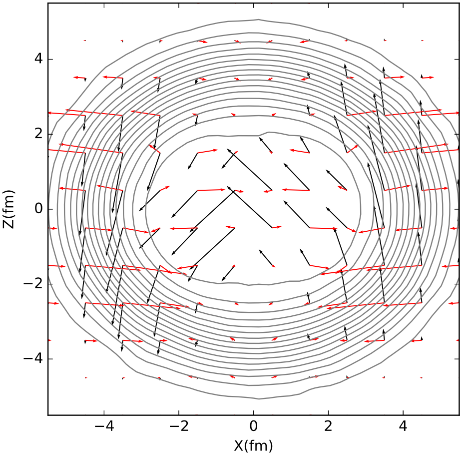
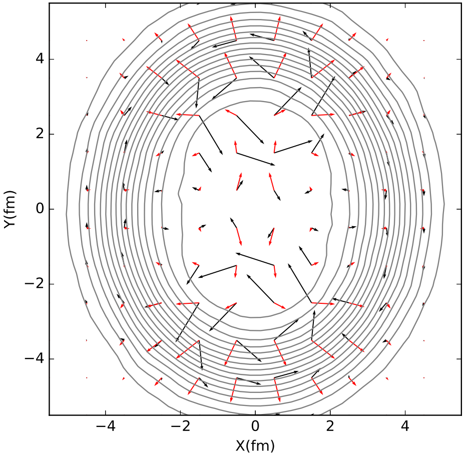
$(X > Y > Z)$	−543.0885988	269.2750	29.92727	0.000	0.000
$(Y > X > Z)$	−543.0885988	269.2749	29.92733	0.000	0.000
$(Z > X > Y)$	−543.0885972	269.2750	29.92774	0.000	0.000
$(X > Z > Y)$	−543.0885988	269.2750	29.92725	0.000	0.000
$(Y > Z > X)$	−543.0885986	269.2750	29.92724	0.000	0.000
$(Z > Y > X)$	−543.0885989	269.2751	29.92723	0.000	0.000
		^{65}Ge			
$(X > Y > Z)$	−548.1544126	260.2480	38.51258	0.0208	1.371
$(Y > X > Z)$	−548.1544108	260.2485	38.51364	0.0208	1.371
$(Z > X > Y)$	−548.1274486	261.0480	37.73917	−0.0025	−0.421
$(X > Z > Y)$	−548.1134288	260.4935	22.08575	0.0032	0.043
$(Y > Z > X)$	−548.1134993	260.4933	22.08613	0.0032	0.043
$(Z > Y > X)$	−548.1274993	261.0481	37.69863	−0.0026	−0.423

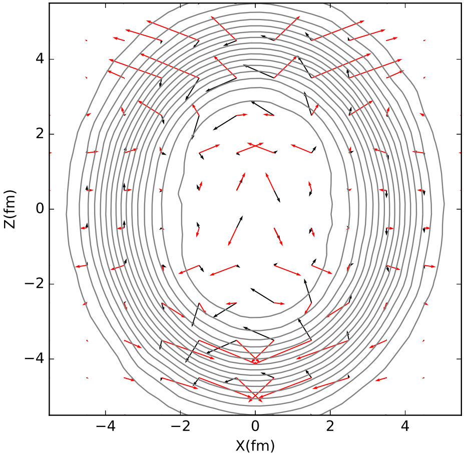
^{64}Ge, $(Y > Z > X)$ around the Y-axis, $\vec{j}$ and $\vec{s}$



^{64}Ge, $(Z > Y > X)$ around the Z-axis, $\vec{j}$ and $\vec{s}$



^{64}Mg, $(Y > X > Z)$ around the Y-axis, $\vec{j}$ and $\vec{s}$



What we are actually probing: Alispin

Consider the space spanned

$$\begin{pmatrix} a \\ b \end{pmatrix} = a\psi + b\bar{\psi}$$

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Symmetry considerations

- Symmetry of the energy if time-reversal is conserved.
- Breaks signature for non-special angles.

States related by alispin rotations

As an example, consider eigenstates of $\hat{J}_z$

$$|K\rangle \text{ and } |-K\rangle$$

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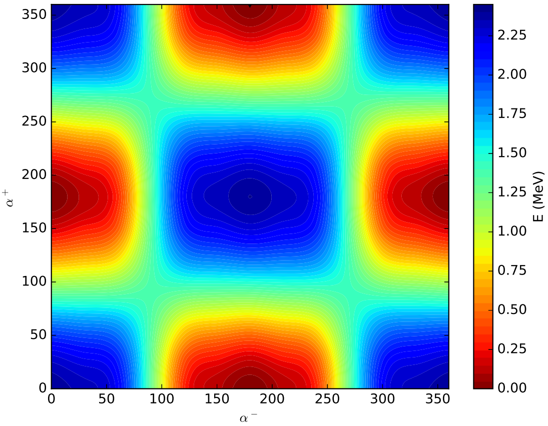
Note that this 'hides' mean-field angular momentum as

$$\langle 1_x|\hat{\mathcal{J}}_z|1_x\rangle = \langle 2_x|\hat{\mathcal{J}}_z|2_x\rangle = \langle 1_y|\hat{\mathcal{J}}_z|1_y\rangle = \langle 2_y|\hat{\mathcal{J}}_z|2_y\rangle = 0\,.$$

Non-selfconsistent energy of two-quasi-proton excitation in ^{20}Ne.

$$|\psi^{\pm}\rangle = \cos(\alpha_{\pm})|\psi^{\pm}\rangle + i\sin(\alpha_{\pm})|\bar{\psi}^{\pm}\rangle$$



Cranked Skyrme-HFB.

Optimize Routhian R instead of energy E

$$R = E - \omega \langle \hat{\mathcal{J}}_z \rangle$$

One-dimensional cranked-Skyrme HFB

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Three different ways (that I know of) to view it

1. Kamlah expansion to projection on angular momentum.
2. Mean-field equations in the rotating frame.
3. $\langle \hat{\mathcal{J}}_z \rangle$ as (semi-)generator coordinate, to be constrained.

Main advantage is the link with experiment

$$\hat{\mathcal{I}}^{(1)} = \frac{I}{\omega}$$

where I is the collective part of $\langle \hat{\mathcal{J}}_z \rangle$.
Experimentally

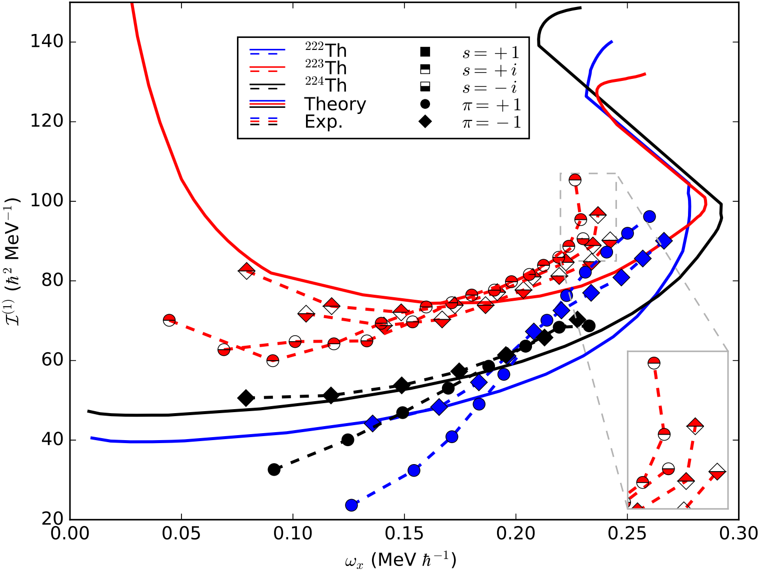
$$\omega = \frac{E(J+1) - E(J-1)}{I(J+1) - I(J-1)} \qquad \hat{\mathcal{I}}^{(1)} = \frac{I(J)}{\omega} \, .$$

where $I(J)$ is

$$I(J) = J \qquad \text{(even-even systems)}$$

$$I(J) = \sqrt{(J+1/2)^2 - K^2} \qquad \text{(odd systems)} \, .$$

Octupole shape transition in ^{222}Th



Generalized cranking in 3D

$$R = E - \omega_x \langle \hat{\mathcal{J}}_x \rangle - \omega_y \langle \hat{\mathcal{J}}_y \rangle - \omega_z \langle \hat{\mathcal{J}}_z \rangle$$

which in general breaks symmetries

	Signatures	Simplexes	Time-simplexes
$\omega_x \neq 0$	$\hat{\mathcal{R}}_y, \hat{\mathcal{R}}_z$	$\hat{\mathcal{S}}_y, \hat{\mathcal{S}}_z$	$\check{S}^T_x$
$\omega_y \neq 0$	$\hat{\mathcal{R}}_x, \hat{\mathcal{R}}_z$	$\hat{\mathcal{S}}_x, \hat{\mathcal{S}}_z$	$\check{S}^T_y$
$\omega_z \neq 0$	$\hat{\mathcal{R}}_x, \hat{\mathcal{R}}_y$	$\hat{\mathcal{S}}_x, \hat{\mathcal{S}}_y$	$\check{S}^T_z$

Kerman-Onishi

Given a determined $\vec{\omega}$, at the minimum of the Routhian $R(\vec{\omega})$ one has $\langle \hat{\mathcal{J}} \rangle$ parallel to $\vec{\omega}$ i.e.

$$\vec{\omega} \parallel \langle \hat{\mathcal{J}} \rangle \, .$$

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- ! In the absence of any multipole constraint.
- ! This includes constraints on non-physical degrees of freedom.
- ! Does not specify anything else about the minimum!

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Usual strategy: Given $|\vec{\omega}|$ minimize for different orientations.

Calculation

- ^{24}Mg
- SLy5s1 functional
- HF/no pairing
- Y-axis is the symmetry axis
- $|\vec{\omega}| = 0.4$ MeV $\hbar^{-1}$
- Angle θ in the x-z plane

$\theta_{\vec{\omega}}(^\circ)$	$\theta_{\mathcal{J}}(^\circ)$	E(MeV)
20	20.000**6**	−198.2780**80**
40	40.000**3**	−198.2780**16**
60	59.999**8**	−198.2780**35**
80	79.999**8**	−198.2780**02**
100	100.000**2**	−198.2780**02**
120	120.000**2**	−198.2780**35**
140	139.999**7**	−198.2780**16**
160	159.999**4**	−198.2780**80**

What Kerman-Onishi does not tell you

The Kerman-Onishi theorem is a statement about the

Routhian,

and does not tell you anything about either

E, $\langle \vec{\mathcal{J}} \rangle$.

See Olivius and Bengtsson,
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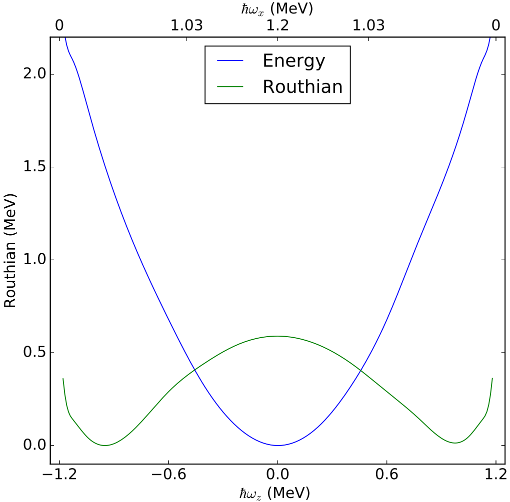


Routhian vs. Energy

One can decompose $\langle \vec{\mathcal{J}} \rangle$

$$\langle \vec{\mathcal{J}} \rangle = \langle \vec{\mathcal{J}} \rangle_{\parallel} + \langle \vec{\mathcal{J}} \rangle_{\perp}$$

Routhian vs. Energy

One can decompose $\langle \vec{\mathcal{J}} \rangle$

$$\langle \vec{\mathcal{J}} \rangle = \langle \vec{\mathcal{J}} \rangle_{\parallel} + \langle \vec{\mathcal{J}} \rangle_{\perp}$$

And then the Routhian becomes

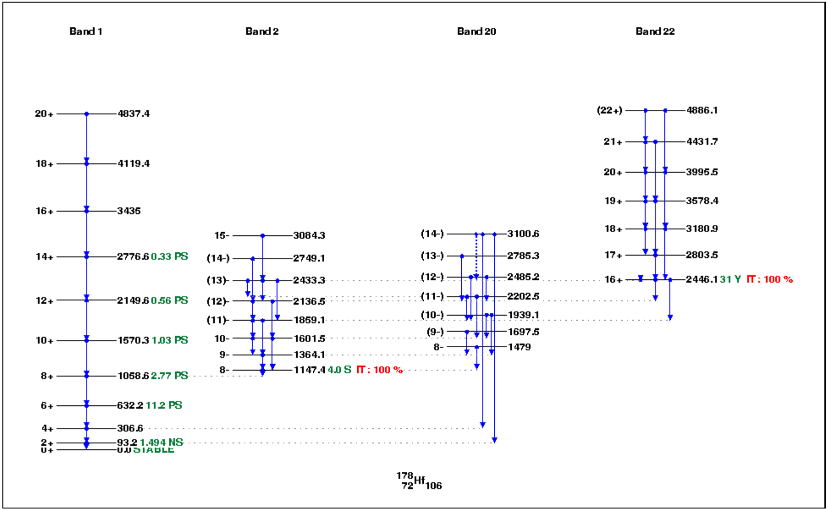
$$R = E - \vec{\omega} \cdot \langle \vec{\mathcal{J}} \rangle = E - \vec{\omega} \cdot \langle \vec{\mathcal{J}} \rangle_{\parallel} \, .$$

A Routhian is indifferent to

- Non-parallel angular momentum $\langle \vec{\mathcal{J}} \rangle_{\perp}$,
- Angular momentum hidden in alispin.

To an end; (Multi-)quasi-particle rotational bands.

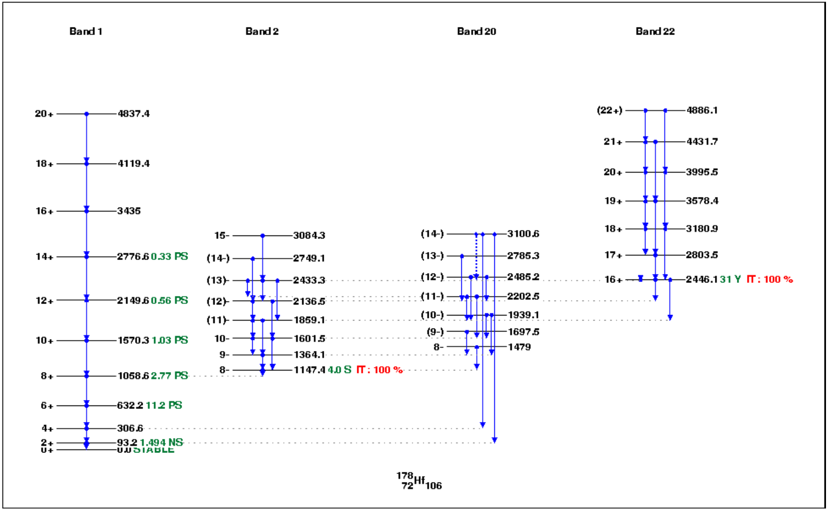
Two qp structures in ^{178}Hf



NNDC and A.B. Hayes, PRC 75, 034308 (2007).

Two qp structures in ^{178}Hf

$\nu(7/2^-, 9/2^+)$ $\pi(9/2^-, 7/2^+)$ Both



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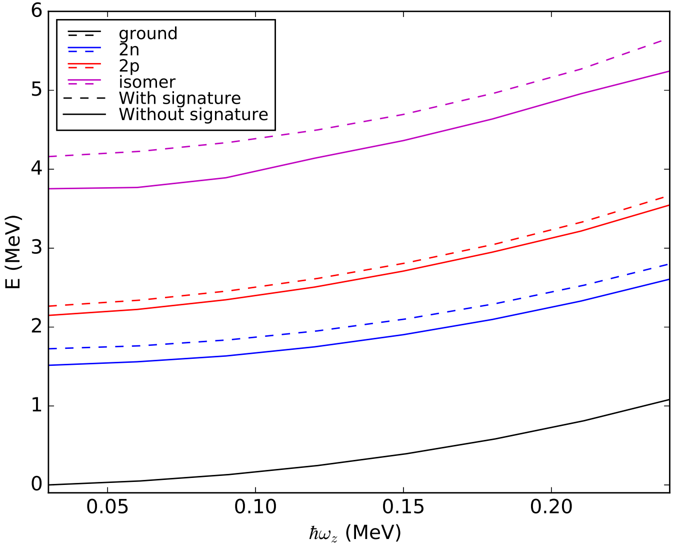
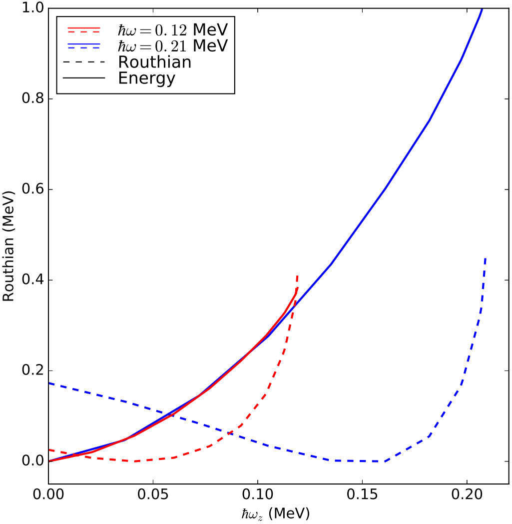
Multi-qp bands in ^{178}Hf



Multi-qp bands in ^{178}Hf

$\omega = 0$	With signature	Without
$\lvert\langle \hat{\mathcal{J}}(\hbar)\rangle\rvert$ $(\hbar)$	$\sqrt{\langle \hat{\mathcal{J}}_z\rangle^2}$	$\sqrt{\langle \hat{\mathcal{J}}_x\rangle^2 + \langle \hat{\mathcal{J}}_z\rangle^2}$
groundstate	0	0
2-neutron	1.76	6,39
2-proton	0.41	7.52
isomer	2.06	2.27

Multi-qp bands in ^{178}Hf



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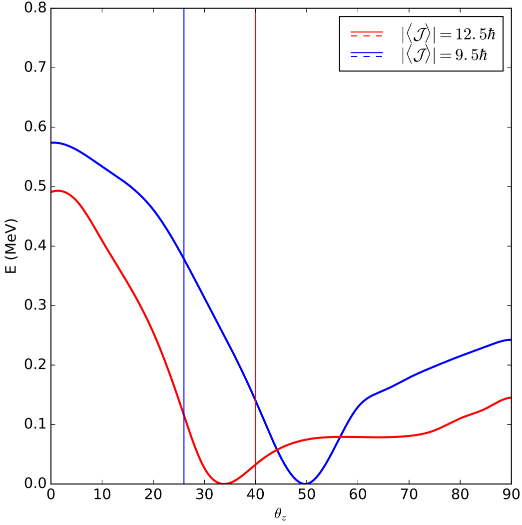

Conclusions

Antihermitian symmetries cause trouble.

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- Numerical cost increases;
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- More components of $\langle \hat{\mathcal{J}} \rangle$

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Pick the wrong one

- Symmetry choices are nontrivial;
- Alispin is a relevant degree of freedom;
- Limited $\langle \hat{\mathcal{J}} \rangle$

$\Longrightarrow$ Also trouble!

Thank you!

Collaborators

- M. Bender, CNRS
- P.-H. Heenen, ULB
- B. Bally, UAM

Parts based on notes by

- B. Avez

But also

- CC of the IN2P3, for the access to French computing resources.
- CECI, for the access to Belgian computing resources.
- You, for your attention.