Mumble, mumble odd nuclei, mumble, signature

ECT* workshop on odd nuclei

W. Ryssens[1], M. Bender[1] and P.-H. Heenen [2].

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`MOCCa`: The means . . .

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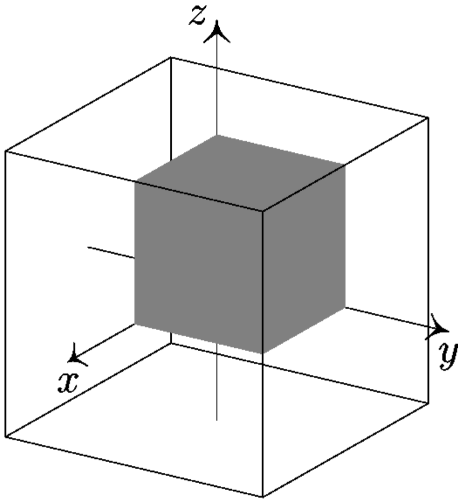
MOCCa

- Symmetries

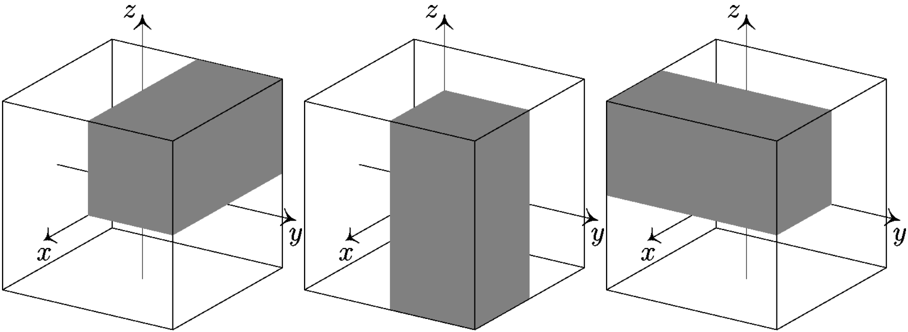
Symmetries

Symmetry groups for even-even and even-odd nuclei

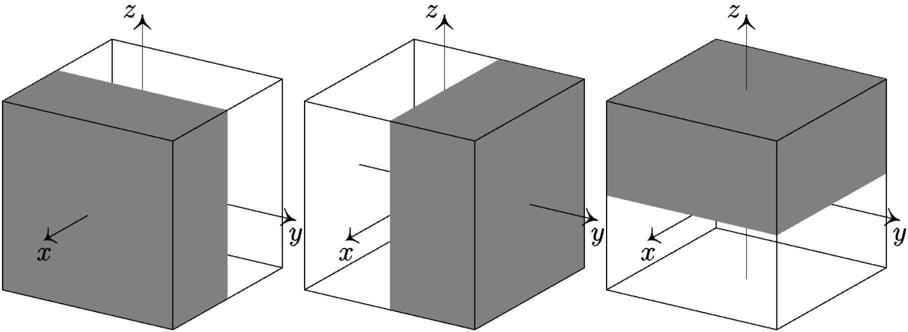
$\mathcal{D}_{2h}^{T}$ $\mathcal{D}_{2h}^{TD}$


z
x
y

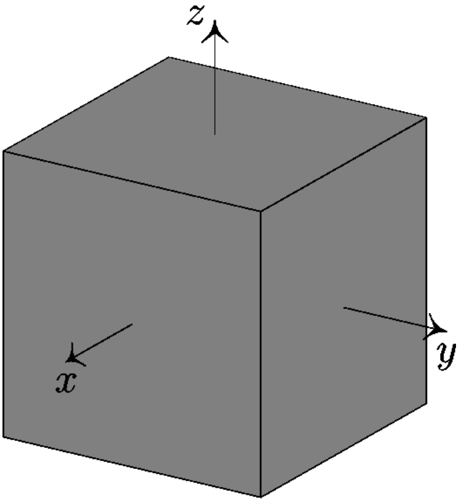
MOCCa's implementation



MOCCa's implementation



MOCCa's implementation



Symmetries of selected densities

Symmetries of the densities in this talk are not simple reflection symmetries

Many-body $(\hat{\mathcal{J}}_x, \hat{\mathcal{J}}_y, \hat{\mathcal{J}}_z)$ and single-particle $(\hat{j}_x, \hat{j}_y, \hat{j}_z)$.

Single-particle

Even-even

Even-odd

Methods, or how to block qps.

Reminder: two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$

Add figures/equations for every step

Reminder: two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$
2. Solve the HFB problem in this basis

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Reminder: two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$
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3. Obtain canonical basis $|\Phi_l^{(i)}\rangle$

Add figures/equations for every step

Reminder: two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$
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5. Update Hartree-Fock basis $|\phi_l^{(i+1)}\rangle$

Add figures/equations for every step

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3. Obtain canonical basis $|\Phi_l^{(i)}\rangle$
4. Calculate densities $\rho^{(i)}$ from $|\Phi_l^{(i)}\rangle$
5. Update Hartree-Fock basis $|\phi_l^{(i+1)}\rangle$
6. Restart

Add figures/equations for every step

HFB equations in the HF basis

Assume

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

Bogoliubov transformation from particles to quasiparticles

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

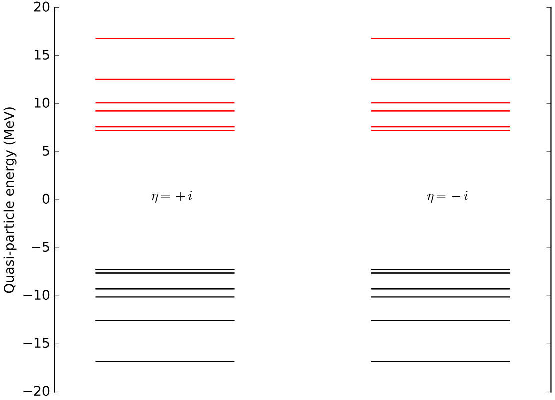
Where the U, V matrices are determined by

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

Inherent HFB symmetry: multiple vacua

Inherent symmetry:

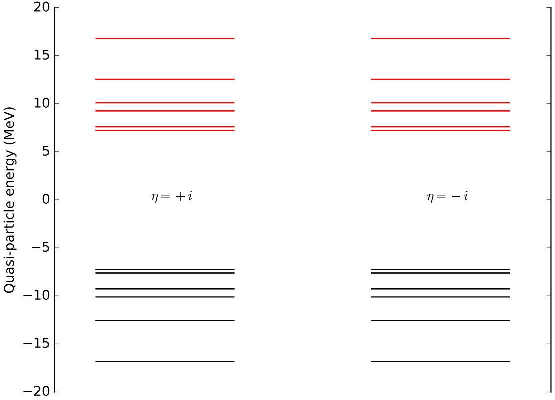
$$U_l \leftrightarrow V_l^*$$
$$V_l \leftrightarrow U_l^*$$
$$E_l^{qp} \leftrightarrow -E_l^{qp}$$
$$\hat{\beta}_l \leftrightarrow \hat{\beta}_l^\dagger$$



Inherent HFB symmetry: multiple vacua

Inherent symmetry:

$$
\begin{array}{ccc}
U_l & \leftrightarrow & V_l^* \\
V_l & \leftrightarrow & U_l^* \\
E_l^{qp} & \leftrightarrow & -E_l^{qp} \\
\hat{\beta}_l & \leftrightarrow & \hat{\beta}_l^\dagger \\
\eta & \leftrightarrow & -\eta
\end{array}
$$

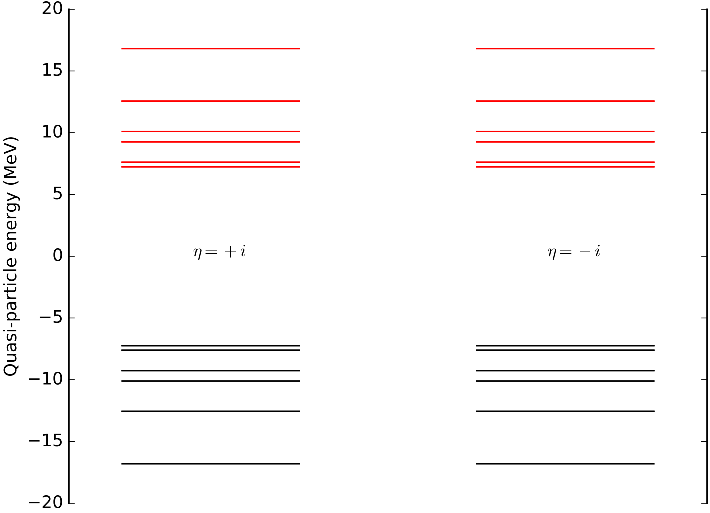


Antilinear, hermitian symmetries come to the rescue.

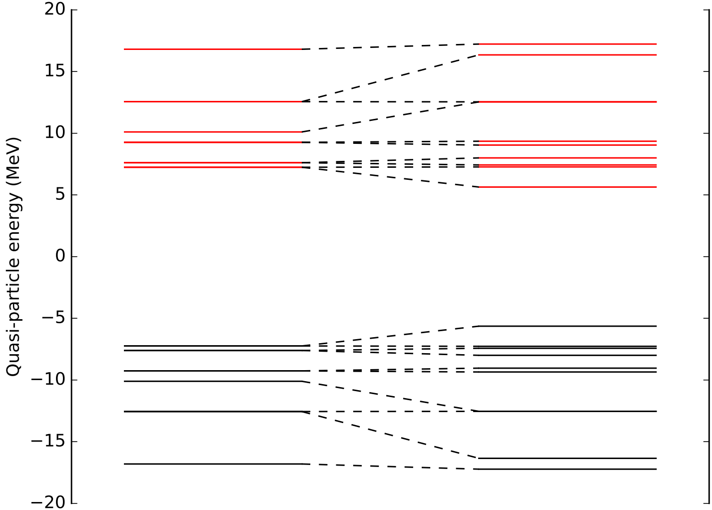
$$\hat{\mathcal{R}}_{x/y/z}, \hat{\mathcal{S}}_{x/y/z}$$

Choosing a vacuum

Time-reversal invariant

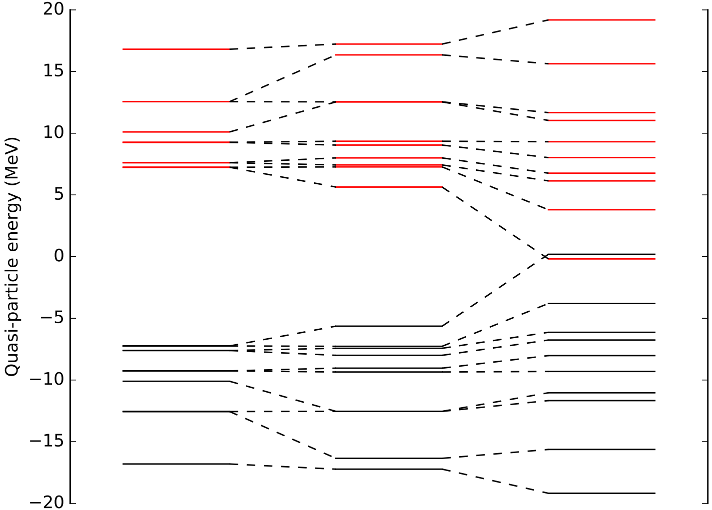


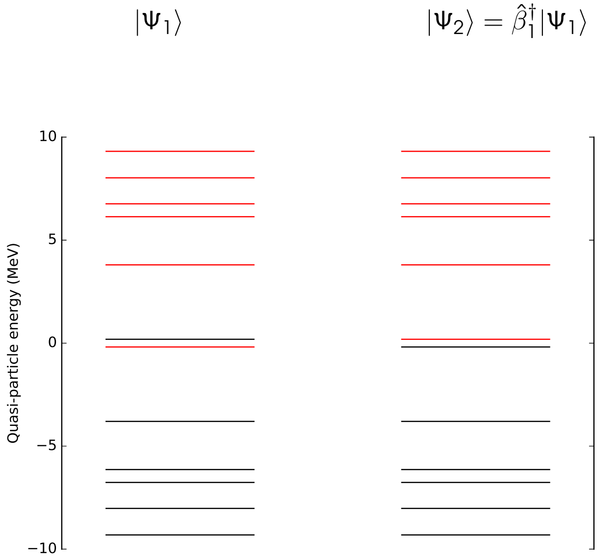
Lifting the degeneracy



Choosing a vacuum

Crossings




$|\Psi_1\rangle$
$|\Psi_2\rangle = \hat{\beta}_1^\dagger|\Psi_1\rangle$
10
5
0
−5
−10
Quasi-particle energy (MeV)

Consequences of choosing wrong

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

Disaster for any numerical solver.

Signature broken HFB

Problem: Choosing is impossible without antihermitian symmetry.

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Solution: Avoid making a choice.

Signature broken HFB

Problem: Choosing is impossible without antihermitian symmetry.
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$$|\Psi(Z)\rangle = \left[-\frac{1}{2}\sum_{ij} Z_{ij}\beta_i^\dagger\beta_j^\dagger\right]|\Psi_{\mathrm{sym}}\rangle \,. \qquad E(Z,\Psi_0) = \frac{\langle\Psi(Z)|\hat{\mathcal{H}}_{\mathrm{HFB}}|\Psi(Z)\rangle}{\langle\Psi(Z)|\Psi(Z)\rangle} \,.$$

Problem: Choosing is impossible without antihermitian symmetry.
Solution: Avoid making a choice.

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

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

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

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
Ping-pong	Yes	Much more

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(MeV)	^{25}Mg	^{65}Ge	^{223}Th	^{178}Lu
Remark	$K = 3/2^+$	Triaxial	No parity	Odd-Odd
Thouless	-202.3515**38**	-548.14**8448**	-1695.2403721525038	-1423.092**1**
Direct	-202.3515**40**	-548.14**7910**	-1695.31253	-1423.092**0**

Equivalence

(MeV)	^{25}Mg	^{65}Ge	^{223}Th	^{178}Lu
Remark	$K = 3/2^{+}$	Triaxial	No parity	Odd-Odd
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Direct	-202.3515**40**	-548.14**7910**	-1695.31253	-1423.092**0**

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

Symmetries in blocking

Orientations of the nucleus

Add 6 different ellipses

Add full (β, γ) plane for ^{64}Ge with crosses

Orientations

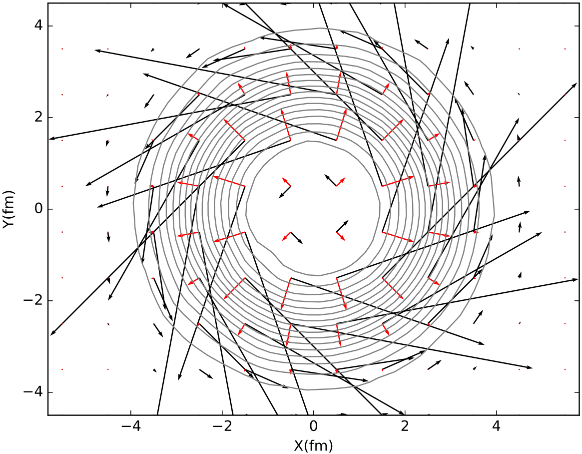
Orientation	Energy (MeV)	q (fm^2)	$\gamma(^\circ)$
	^{24}Mg		
$(X > Y = Z)$	-196.81520837	67.9338575	0.0242
$(Y > X = Z)$	-196.81520837	67.9338575	0.0241
$(Z > X = Y)$	-196.81520838	67.9338578	0.0241

Orientations

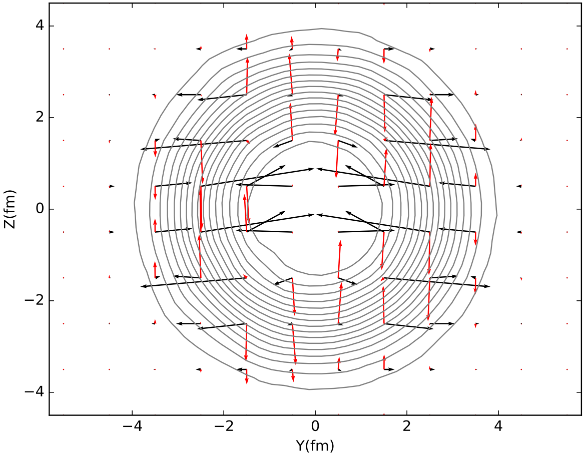
Orientation	Energy (MeV)	q (fm^2)	$\gamma(^\circ)$
	^{24}Mg		
$(X > Y = Z)$	-196.8152083**7**	67.933857**5**	0.024**2**
$(Y > X = Z)$	-196.8152083**7**	67.933857**5**	0.024**1**
$(Z > X = Y)$	-196.8152083**8**	67.933857**8**	0.024**1**

	^{25}Mg		
$(X > Y = Z)$	-202.351538**45**	85.845055**9**	0.71899**2**
$(Y > X = Z)$	-202.351538**39**	85.845055**8**	0.71899**3**
$(Z > X = Y)$	-202.295677	67.934	0.0240042

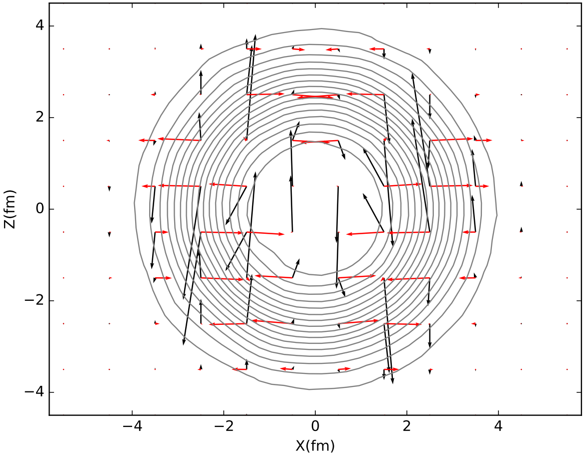
^{24}Mg, $(Z > X = Y)$ around the Z-axis, $\vec{j}$ and $\vec{s}$



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



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



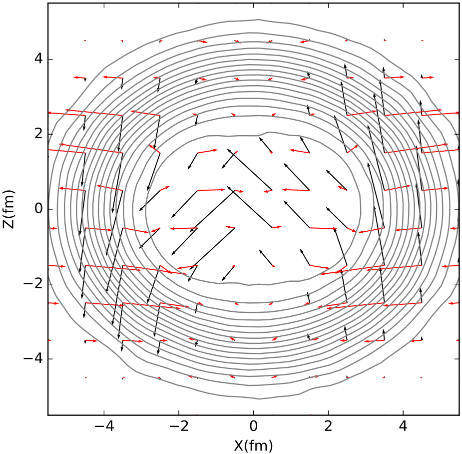
Orientation	Energy (MeV)	q (fm^2)	γ(°)
	^{64}Ge		
$(X > Y > Z)$	−543.0885988	269.2750	29.92727
$(Y > X > Z)$	−543.0885988	269.2749	29.92733
$(Z > X > Y)$	−543.0885972	269.2750	29.92774
$(X > Z > Y)$	−543.0885988	269.2750	29.92725
$(Y > Z > X)$	−543.0885986	269.2750	29.92724
$(Z > Y > X)$	−543.0885989	269.2751	29.92723

Symmetries and orientation

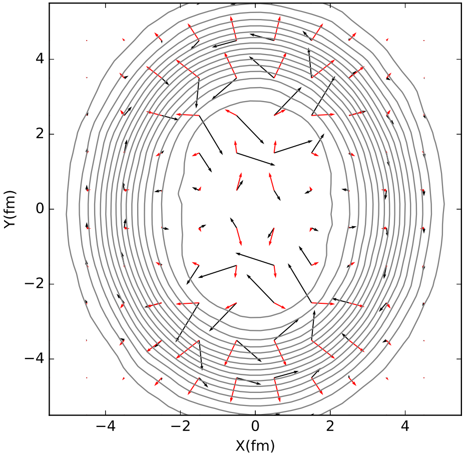
Orientation	Energy (MeV)	q (fm^2)	$\gamma(^\circ)$
	^{64}Ge		
$(X > Y > Z)$	-543.0885988	269.2750	29.92727
$(Y > X > Z)$	-543.0885988	269.2749	29.92733
$(Z > X > Y)$	-543.0885972	269.2750	29.92774
$(X > Z > Y)$	-543.0885988	269.2750	29.92725
$(Y > Z > X)$	-543.0885986	269.2750	29.92724
$(Z > Y > X)$	-543.0885989	269.2751	29.92723
	^{65}Ge		
$(X > Y > Z)$	-548.1544126	260.2480	38.51258
$(Y > X > Z)$	-548.1544108	260.2485	38.51364
$(Z > X > Y)$	-548.1274486	261.0480	37.73917
$(X > Z > Y)$	-548.1134288	260.4935	22.08575
$(Y > Z > X)$	-548.1134993	260.4933	22.08613
$(Z > Y > X)$	-548.1274993	261.0481	37.69863

Orientations and currents

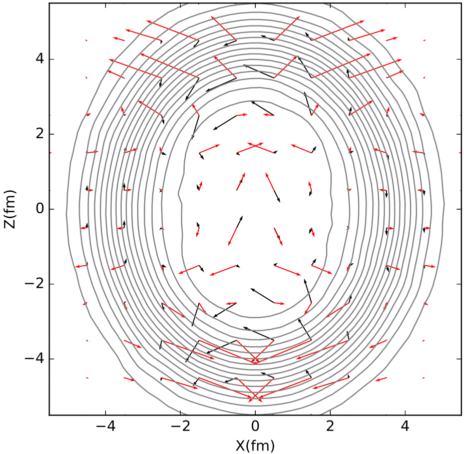
^{64}Ge, $(Y > Z > X)$ around the Y-axis, $\vec{j}$ and $\vec{s}$



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



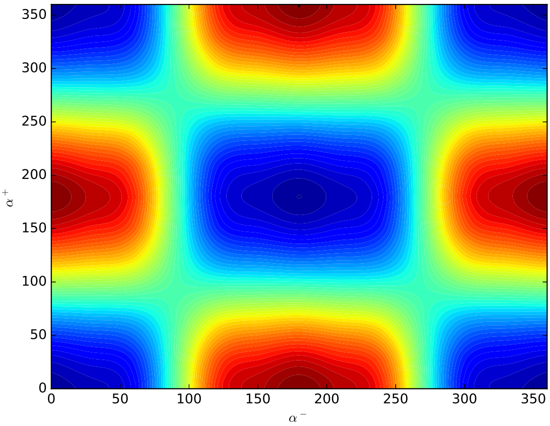
^{64}Mg, $(Y > X > Z)$ around the Y-axis, $\vec{j}$ and $\vec{s}$



Alispin theory

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

$$|\psi'\rangle = \cos(\alpha)|\psi\rangle + i\sin(\alpha)|\bar{\psi}\rangle$$



Cranked Skyrme-HFB

What I need in this section

- Introduction of 1D cranking
- Three possibilities of deriving it
- Link to experiment
- Show some successes
- Introduction to 2/3D cranking
- Discussion of Kerman-Onishi, demonstration of how that works
- Show a 2D minimum at constant omega
- Show a 3D minimum at constant omega
- Show a cranked 1qp that invalidates constant omega
- Compare to quadrupole constraints
- Introduce a new concept of J
- Show how it can be used

Optimize Routhian R instead of energy E

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

One-dimensional cranked-Skyrme HFB

Optimize Routhian R instead of energy E

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

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

1. Kamlah expansion to projection on angular momentum.

One-dimensional cranked-Skyrme HFB

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1. Kamlah expansion to projection on angular momentum.
2. Mean-field equations in the rotating frame.

Optimize Routhian R instead of energy E

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

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 collective coordinate, to be constrained.

Advantages of one-dimensional cranking

Main advantage is the link with experiment, either through

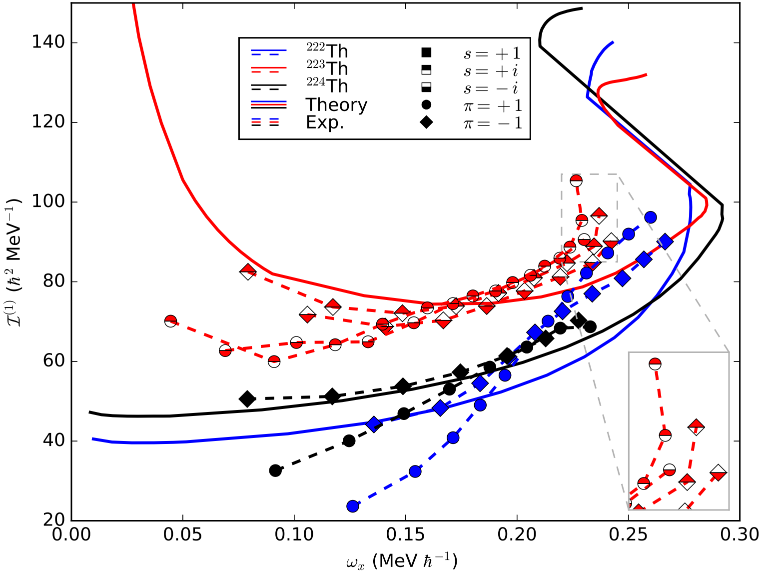
$$\hat{\mathcal{I}}^{(1)} = \frac{I}{\omega} \qquad \qquad \hat{\mathcal{I}}^{(2)} =$$

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

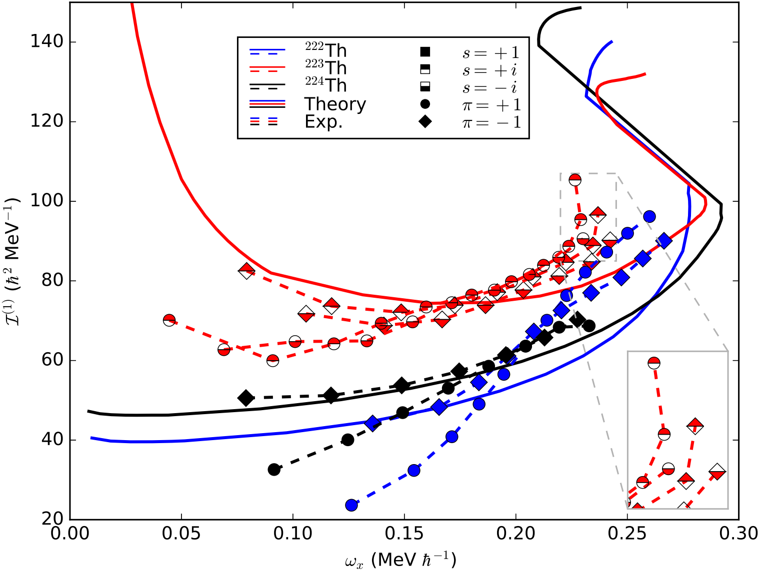
$$\omega = \qquad \qquad \hat{\mathcal{I}}^{(1)} = \frac{I}{\omega} \qquad \qquad \hat{\mathcal{I}}^{(2)} = \ .$$

Examples

Strongly coupled band in ^{177}Au



Octupole shape transition in ^{222}Th



Tilted axis cranking: 2D and 3D cranked Skyrme-HFB

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

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

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

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.

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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!

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**

Kerman-Onishi for odd systems

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

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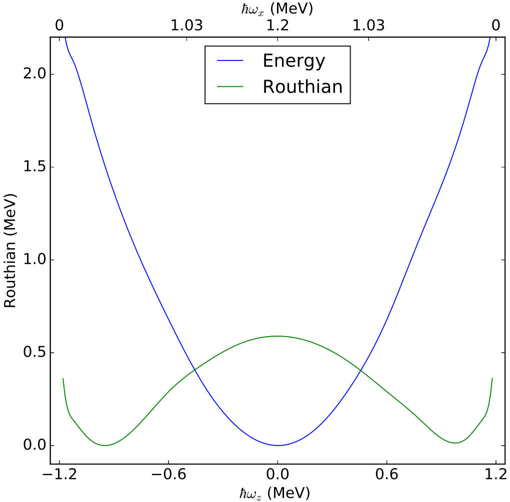


One can decompose $\langle \vec{\mathcal{J}} \rangle$

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

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 the Routhian is essentially

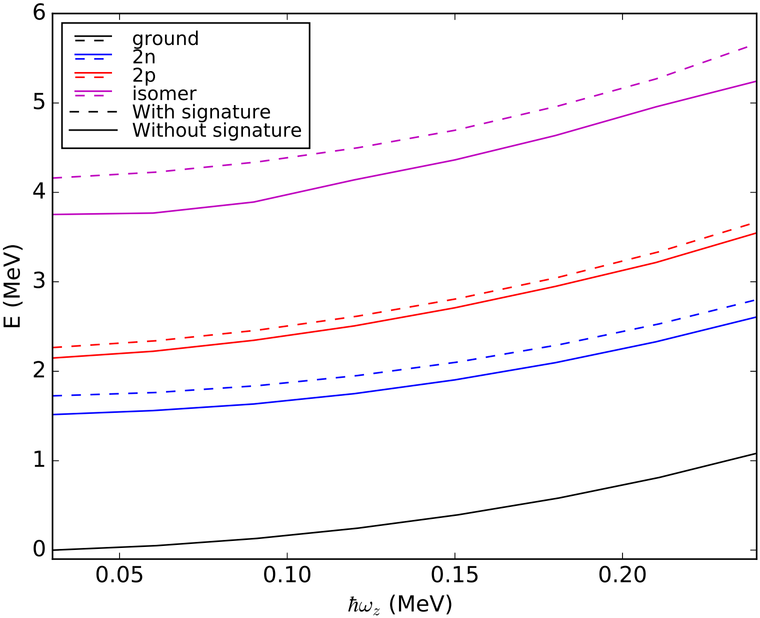
$$R = E - \vec{\omega} \cdot \langle \vec{\mathcal{J}} \rangle = E - \vec{\omega} \cdot \langle \vec{\mathcal{J}} \rangle_{\parallel} \,.$$

Now at the

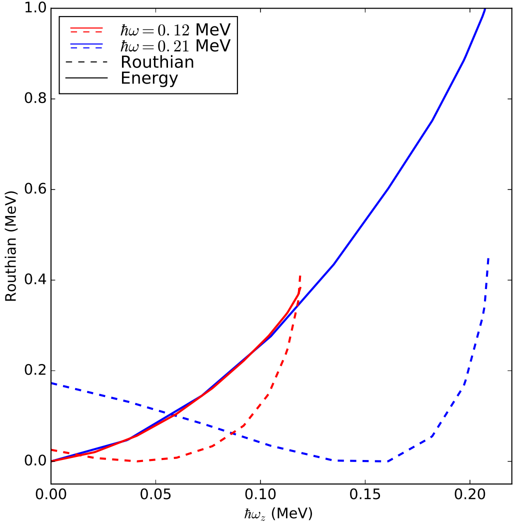
. . . to an end; (Multi-)quasi-particle rotational bands.

2-qp and 4-qp structures in ^{178}Hf and ^{178}Lu

Multi-qp bands in ^{178}Hf



Multi-qp bands in ^{178}Hf



Thank you

Collaborators

- M. Bender, CNRS
- P.-H. Heenen, ULB

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.