On the way to symmetry-unrestricted HFB calculations in coordinate space

Wouter Ryssens

IPN Lyon

February 2017

Université Claude Bernard Lyon 1

1 Introduction: symmetries and MOCCa

2 HFB without symmetries
- HFB equations
- Two-basis method
- Selecting the correct vacuum
- A toy model
- Thouless solver
- Fission of an odd nucleus?

3 Conclusion

Symmetry groups

There are many relevant symmetry operators

$$\mathcal{D}_{2h}^{T} = \left\{ \hat{1}, \hat{\mathcal{P}}, \check{\mathcal{T}}, \check{\mathcal{P}}^{T}, \hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T} \right\} ,$$

$$\mathcal{D}_{2h}^{TD} = \left\{ \hat{1}, -\hat{1}, \hat{\mathcal{P}}, -\hat{\mathcal{P}}, \check{\mathcal{T}}, -\check{\mathcal{T}}, \hat{\mathcal{R}}_{\mu}, -\hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, -\check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, -\hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T}, -\check{\mathcal{S}}_{\mu}^{T}, \check{\mathcal{P}}^{T}, -\check{\mathcal{P}}^{T} \right\} .$$

Symmetry groups

There are many relevant symmetry operators

$$\mathcal{D}_{2h}^{T} = \left\{ \hat{1}, \hat{\mathcal{P}}, \check{\mathcal{T}}, \check{\mathcal{P}}^{T}, \hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T} \right\} ,$$

$$\mathcal{D}_{2h}^{TD} = \Big\{ \hat{1}, -\hat{1}, \hat{\mathcal{P}}, -\hat{\mathcal{P}}, \check{\mathcal{T}}, -\check{\mathcal{T}}, \hat{\mathcal{R}}_{\mu}, -\hat{\mathcal{R}}_{\mu}, \check{\mathcal{R}}_{\mu}^{T}, -\check{\mathcal{R}}_{\mu}^{T}, \hat{\mathcal{S}}_{\mu}, -\hat{\mathcal{S}}_{\mu}, \check{\mathcal{S}}_{\mu}^{T}, -\check{\mathcal{S}}_{\mu}^{T}, \check{\mathcal{P}}^{T}, -\check{\mathcal{P}}^{T} \Big\} .$$

Very large amount of possible symmetry options

MOCCa

MOdular **C**ranking **C**ode

```
     ;  ,
     ) ;( (
    ( (  ) ;
    ,_"""_.
 ,-|`-...-'|
((_|       |
 `-\       /
    `.___.'
```

MOCCa

```
     ;  ,
     ) ;( (
    ( (  ) ;
    ,_"""_.
 ,-|`-...-'|
((_|       |
 `-\       /
    `.___.'
```

MOdular **C**ranking **C**ode

- Based on EV8, CR8 and EV4

MOCCa

```
      ;  ,
      ) ;( (
     ( (  ) ;
     ,_"""_.
  ,-|`-...-'|
 ((_|       |
  `-\      /
     `.___.'
```

MOdular **C**ranking **C**ode

- Based on EV8, CR8 and EV4
- Easier to use

MOCCa

```
     ;  ,
     ) ;( (
    ( (  ) ;
    ,_"""_.
 ,-|`-...-'|
((_|       |
 `-\      /
    `.___.'
```

MOdular **C**ranking **C**ode

- Based on EV8, CR8 and EV4
- Easier to use
- Independently choose $\hat{\mathcal{P}}, \check{\mathcal{T}}, \hat{\mathcal{R}}_z, \check{\mathcal{S}}_y^T$

MOCCa

```
      ;  ,
      ) ;( (
     ( (   ) ;
     ,-"""-.
  ,-|`-...-'|
 ((_|       |
  `-\       /
     `.___.'
```

MOdular **C**ranking **C**ode

- Based on EV8, CR8 and EV4
- Easier to use
- Independently choose $\hat{\mathcal{P}}, \check{\mathcal{T}}, \hat{\mathcal{R}}_z, \check{\mathcal{S}}^T_y$
- 16 different symmetry combinations

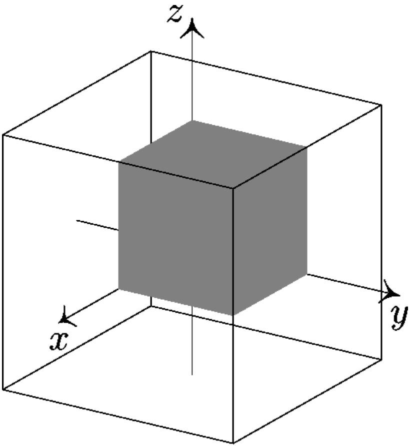
MOCCa

```
      ;  ,
      ) ;( (
     ( (  ) ;
     ,_"""_.
  ,-|`-...-'|
 ((_|       |
  `-\      /
     `.___.'
```

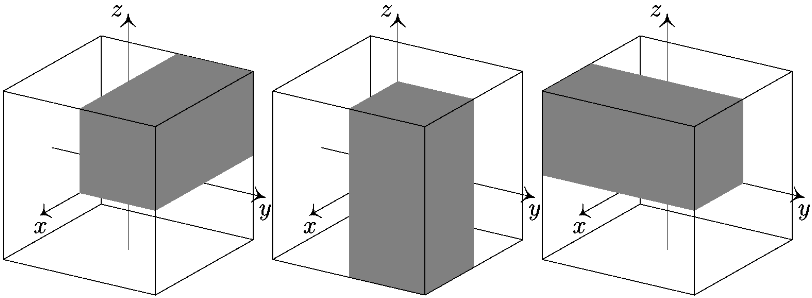
MOdular **C**ranking **C**ode

- Based on EV8, CR8 and EV4
- Easier to use
- Independently choose $\hat{\mathcal{P}}, \check{\mathcal{T}}, \hat{\mathcal{R}}_z, \check{\mathcal{S}}_y^T$
- 16 different symmetry combinations
- HF, HF+BCS or HFB

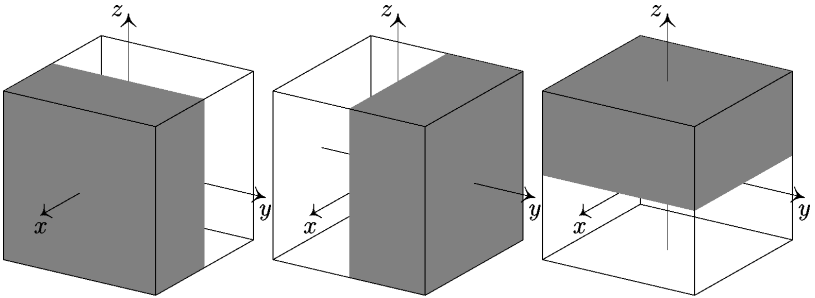
Possibilities



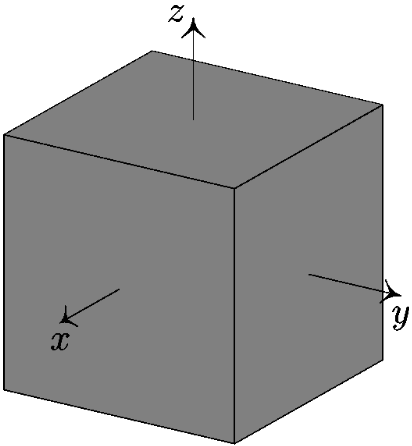
Possibilities



Possibilities



Possibilities



HFB equations

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

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

Two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$
2. Solve the HFB problem in this basis
3. Obtain canonical basis $|\Phi_l^{(i)}\rangle$
4. Calculate densities $\rho^{(i)}$ from $|\Phi_l^{(i)}\rangle$
5. Update Hartree-Fock basis $|\phi_l^{(i+1)}\rangle$ and restart

Two-basis method

1. Hartree-Fock basis $|\phi_l^{(i)}\rangle$
2. Solve the HFB problem in this basis $\rightarrow$ **Hard!**
3. Obtain canonical basis $|\Phi_l^{(i)}\rangle$
4. Calculate densities $\rho^{(i)}$ from $|\Phi_l^{(i)}\rangle$
5. Update Hartree-Fock basis $|\phi_l^{(i+1)}\rangle$ and restart

Selecting the correct vacuum

Problem in general:

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

Selecting the correct vacuum

Problem in general:

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

- 2^N possible vacua related through qp excitations

Selecting the correct vacuum

Problem in general:

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

- 2^N possible vacua related through qp excitations
- Traditional answer: take positive E_{qp}

Selecting the correct vacuum

Problem in general:

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

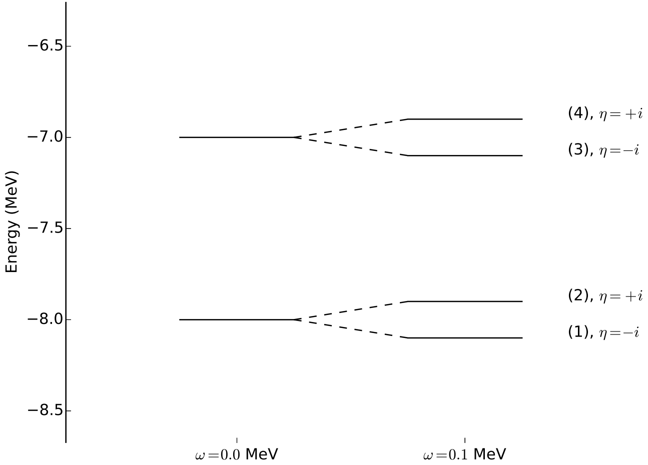
- 2^N possible vacua related through qp excitations
- Traditional answer: take positive E_{qp}
- More practical: use an antihermitian s.p. operator $\hat{R}_z$ to discern between states

A toy model

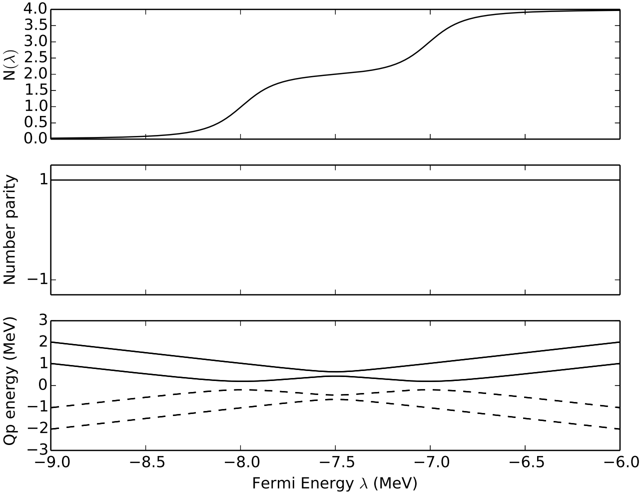
$$\hat{\mathcal{H}}^{\mathsf{Toy}}_{\mathsf{HFB}} = \begin{pmatrix} h-\omega & 0 & \Delta_{\mathsf{sig}} & \Delta \\ 0 & h+\omega & -\Delta & \Delta_{\mathsf{sig}} \\ -\Delta_{\mathsf{sig}} & \Delta & -h+\omega & 0 \\ -\Delta & -\Delta_{\mathsf{sig}} & 0 & -h-\omega \end{pmatrix},$$

$$h = \begin{pmatrix} -8 & 0 \\ 0 & -7 \end{pmatrix}, \Delta = \begin{pmatrix} 2\alpha & \alpha \\ \alpha & 2\alpha \end{pmatrix}, \quad \Delta_{\mathsf{sig}} = \begin{pmatrix} 0 & \gamma \\ -\gamma & 0 \end{pmatrix}.$$

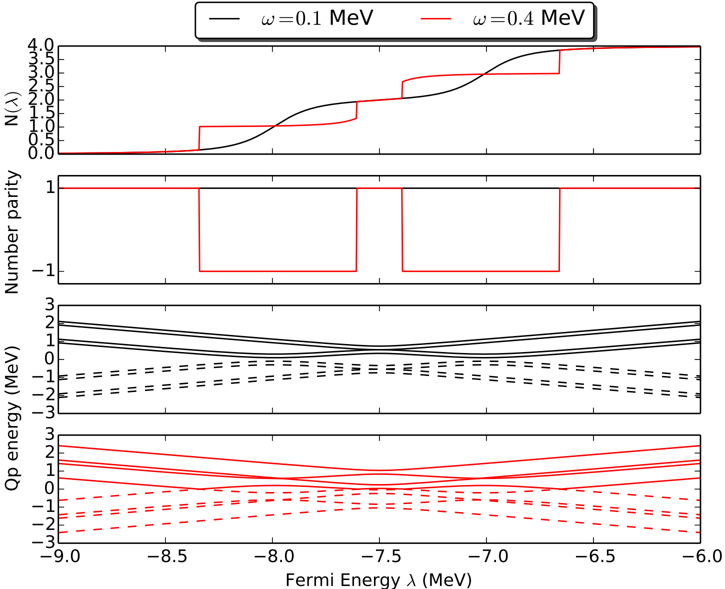
A toy model


Energy (MeV)
−6.5
−7.0
−7.5
−8.0
−8.5
(4), $\eta = +i$
(3), $\eta = -i$
(2), $\eta = +i$
(1), $\eta = -i$
$\omega = 0.0$ MeV
$\omega = 0.1$ MeV

Time-reversal conserved

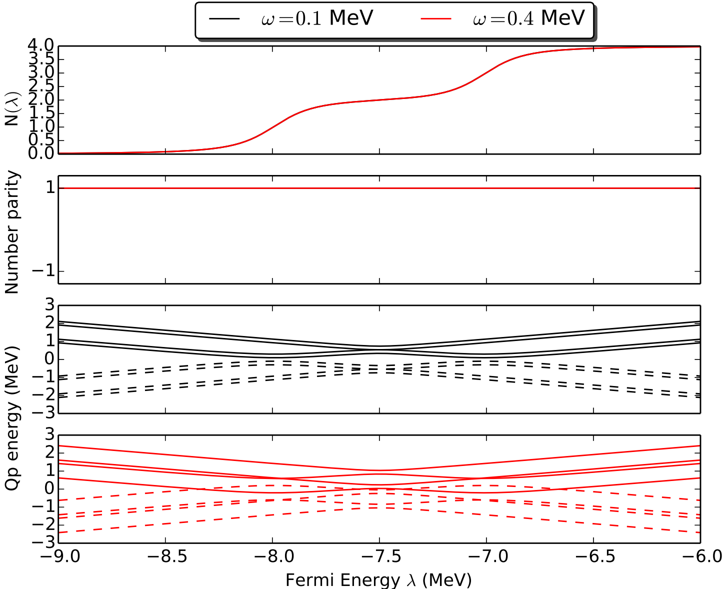


Cranked

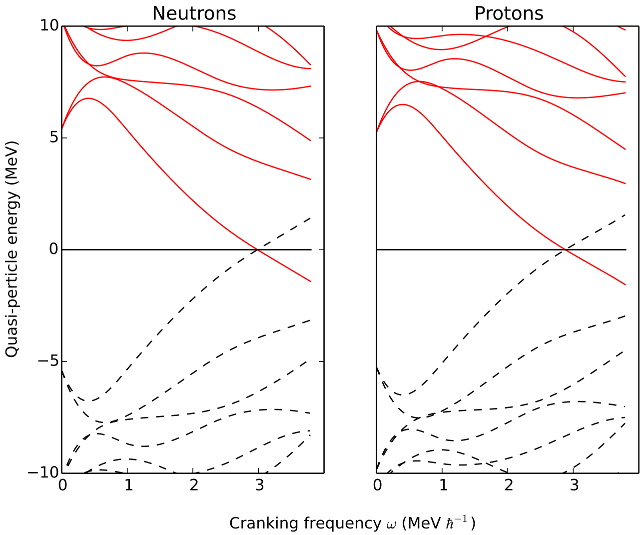


$\omega = 0.1$ MeV
$\omega = 0.4$ MeV
N(λ)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
Number parity
1
−1
Qp energy (MeV)
3
2
1
0
−1
−2
−3
−9.0
−8.5
−8.0
−7.5
−7.0
−6.5
−6.0
Fermi Energy λ (MeV)

Selecting according to signature



All of this does happen in real systems: ^{24}Mg



Thouless solver

Thouless operator

$$
\begin{aligned}
|\Psi_{\mathsf{HFB}}\rangle &= \hat{\Theta}(Z)|\Psi_0\rangle \\
&= \exp\left[\sum_{i,j} Z_{ij}\hat{\beta}^\dagger_i\hat{\beta}^\dagger_j\right]|\Psi_0\rangle \\
&\approx |\Psi_0\rangle + \sum_{i,j} Z_{ij}\hat{\beta}^\dagger_i\hat{\beta}^\dagger_j|\Psi_0\rangle
\end{aligned}
$$

Thouless solver

Thouless operator

$$
\begin{aligned}
|\Psi_{\mathsf{HFB}}\rangle &= \hat{\Theta}(Z)|\Psi_0\rangle \\
&= \exp\left[\sum_{i,j} Z_{ij}\hat{\beta}_i^\dagger\hat{\beta}_j^\dagger\right]|\Psi_0\rangle \\
&\approx |\Psi_0\rangle + \sum_{i,j} Z_{ij}\hat{\beta}_i^\dagger\hat{\beta}_j^\dagger|\Psi_0\rangle
\end{aligned}
$$

One varies the following, for fixed initial Ψ_0

$$
\langle\Psi_0|\hat{\Theta}(Z)^\dagger\hat{\mathcal{H}}\hat{\Theta}(Z)|\Psi_0\rangle
$$

Thouless solver

Thouless operator

$$
\begin{aligned}
|\Psi_{\text{HFB}}\rangle &= \hat{\Theta}(Z)|\Psi_0\rangle \\
&= \exp\left[\sum_{i,j} Z_{ij}\hat{\beta}^\dagger_i\hat{\beta}^\dagger_j\right]|\Psi_0\rangle \\
&\approx |\Psi_0\rangle + \sum_{i,j} Z_{ij}\hat{\beta}^\dagger_i\hat{\beta}^\dagger_j|\Psi_0\rangle
\end{aligned}
$$

One varies the following, for fixed initial Ψ_0

$$
\langle\Psi_0|\hat{\Theta}(Z)^\dagger\hat{\mathcal{H}}\hat{\Theta}(Z)|\Psi_0\rangle
$$

- Pro: Cannot change the quantum numbers

Thouless solver

Thouless operator

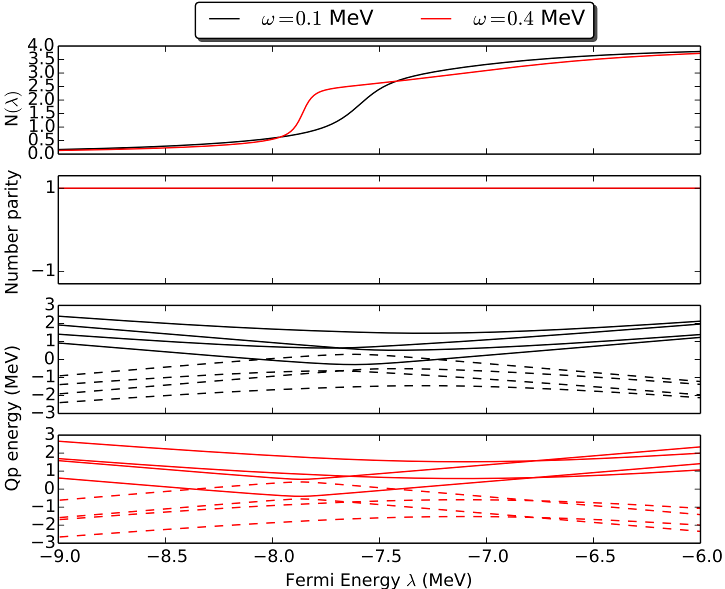
$$\begin{aligned} |\Psi_{\mathsf{HFB}}\rangle &= \hat{\Theta}(Z)|\Psi_0\rangle \\ &= \exp\left[\sum_{i,j} Z_{ij}\hat{\beta}_i^\dagger\hat{\beta}_j^\dagger\right]|\Psi_0\rangle \\ &\approx |\Psi_0\rangle + \sum_{i,j} Z_{ij}\hat{\beta}_i^\dagger\hat{\beta}_j^\dagger|\Psi_0\rangle \end{aligned}$$

One varies the following, for fixed initial Ψ_0

$$\langle\Psi_0|\hat{\Theta}(Z)^\dagger\hat{\mathcal{H}}\hat{\Theta}(Z)|\Psi_0\rangle$$

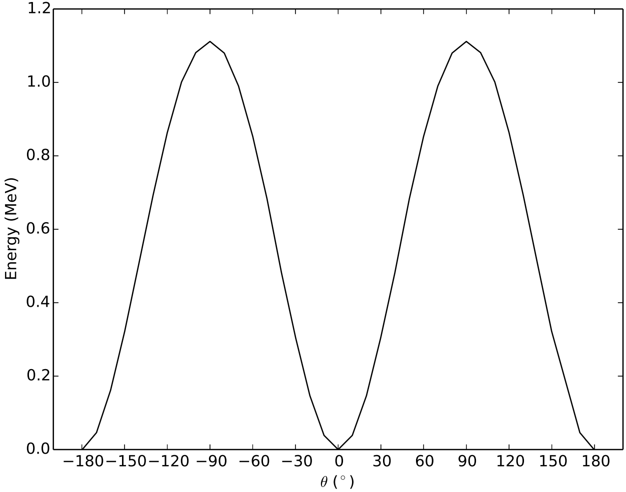
- Pro: Cannot change the quantum numbers
- Con: Cannot change the quantum numbers

What without signature?



Numerical test

^{64}Ge, fixed quadrupole deformation, $\langle \hat{J}_x \rangle^2 + \langle \hat{J}_z \rangle^2 = 16\hbar^2$



Odd nuclei

Direct diagonalisation

- Diagonalise $\hat{\mathcal{H}}$
- Choose even-even vacuum
- Choose a $\hat{\beta}_l$
- Construct odd state

Thouless strategy

Odd nuclei

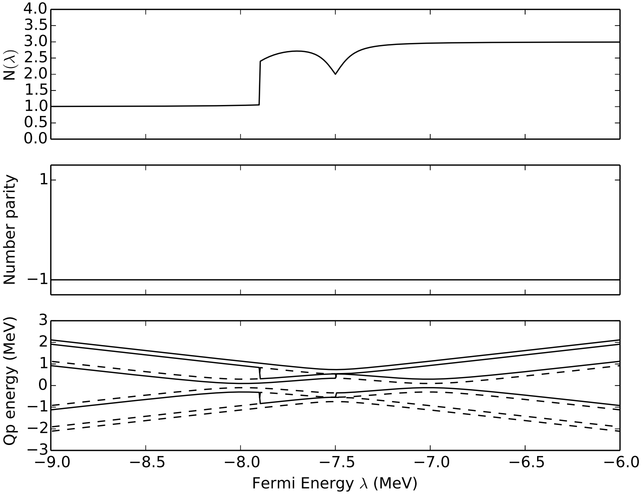
Direct diagonalisation

- Diagonalise $\hat{\mathcal{H}}$
- Choose even-even vacuum
- Choose a $\hat{\beta}_l$
- Construct odd state

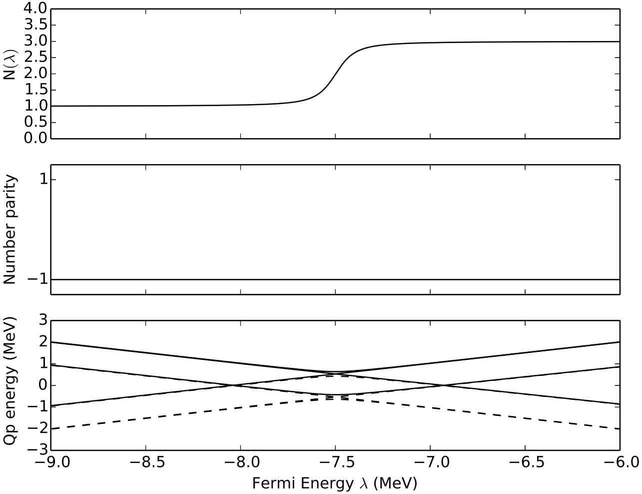
Thouless strategy

- Choose odd vacuum
- Transform the odd state using $\hat{\Theta}$
- $\hat{\beta}_l$ automatically selected
- No explicit choice

Blocking


N(λ)
Number parity
Qp energy (MeV)
Fermi Energy λ (MeV)
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
1
−1
3
2
1
0
−1
−2
−3
−9.0
−8.5
−8.0
−7.5
−7.0
−6.5
−6.0

Blocking with the gradient solver

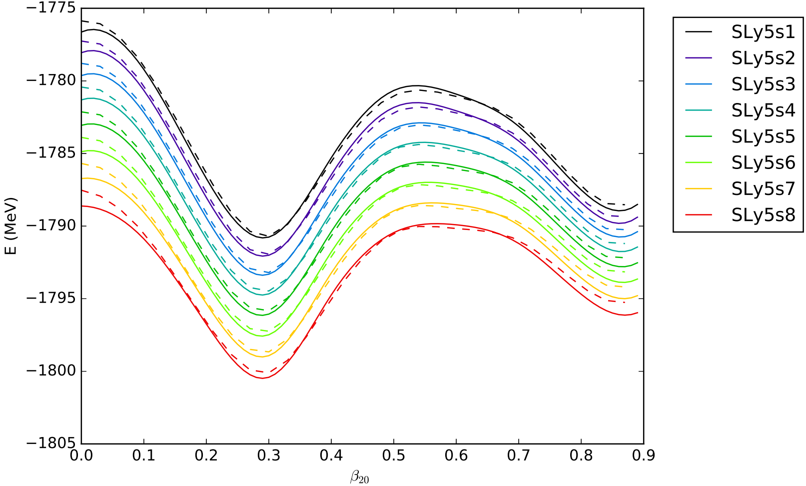


Blocking

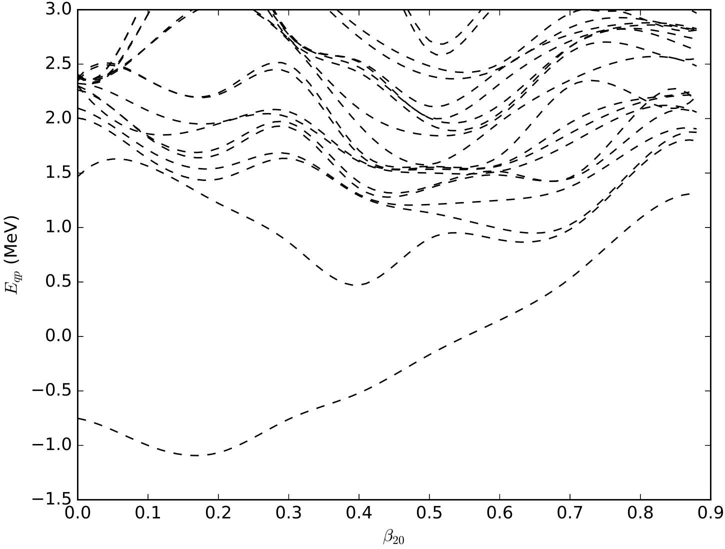
	Direct	Thouless (1)	Thouless (2)
E (MeV)	-1672.165	-1672.166	-1672.166
$\langle \hat{\mathcal{J}}_z \rangle (\hbar)$	0.056	0.000	-0.004
λ_p (MeV)	-2.710	-2.710	-2.710
ΔZ^2	5.724	5.724	5.725
$\lambda_{2,p}$ (MeV)	0.084	0.084	0.084
q_t (fm^2)	219.778	220.359	219.803
γ_t	-60.652	-60.493	-60.550

Negative parity, positive signature quasiparticle ^{219}Ac state on top of axially deformed ^{218}Ac.

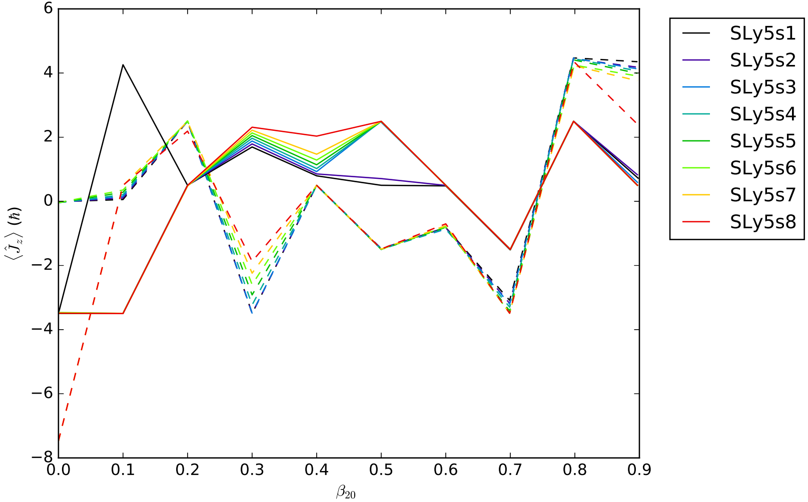
Fission of an odd nucleus?



Fission of an odd nucleus?



Fission of an odd nucleus?



Conclusion

Exploring the degrees of freedom we now have access to

- Cranking and blocking without signature
- Fission of an odd nucleus
- Tilted axis cranking

Conclusion

Exploring the degrees of freedom we now have access to

- Cranking and blocking without signature
- Fission of an odd nucleus
- Tilted axis cranking

Many questions are still left in practice

Conclusion

Exploring the degrees of freedom we now have access to

- Cranking and blocking without signature
- Fission of an odd nucleus
- Tilted axis cranking

Many questions are still left in practice

- Rotational bands for octupole deformed nuclei
- Systematics of the SLy5s1-8 functionals
- Special deformations: clusters, tetrahedrons, ...

Conclusion

Exploring the degrees of freedom we now have access to

- Cranking and blocking without signature
- Fission of an odd nucleus
- Tilted axis cranking

Many questions are still left in practice

- Rotational bands for octupole deformed nuclei
- Systematics of the SLy5s1-8 functionals
- Special deformations: clusters, tetrahedrons, ...

Conclusion: `MOCCa` is alive and kicking

Future

- A more developed framework for all symmetries in $\mathcal{D}_{2H}^{T(D)}$

Future

- A more developed framework for all symmetries in $\mathcal{D}_{2H}^{T(D)}$
- For more complicated functionals (e.g. SLyMR0)

Future

- A more developed framework for all symmetries in $\mathcal{D}_{2H}^{T(D)}$
- For more complicated functionals (e.g. SLyMR0)
- That includes (the first steps for) symmetry restoration

Future

- A more developed framework for all symmetries in $\mathcal{D}_{2H}^{T(D)}$
- For more complicated functionals (e.g. SLyMR0)
- That includes (the first steps for) symmetry restoration
- Always on the lookout for improvements to the algorithms to gain (human) time