(Preparations for)
Symmetry unrestricted Skyrme mean-field study of heavy nuclei

Wouter Ryssens

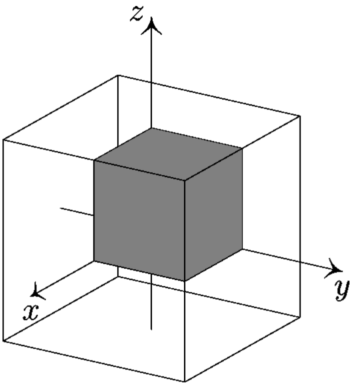
26th of June, Warsaw

Summary

Symmetries

$\hat{P}, \hat{R}_z, \check{T}, \check{S}_y^T$

- Parity
- Signature
- Time Simplex
- Time Reversal



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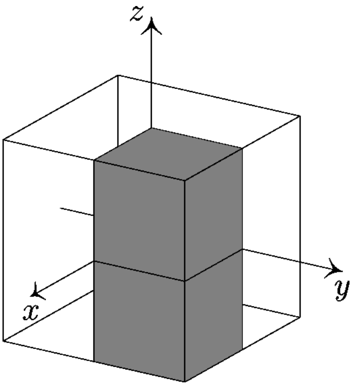

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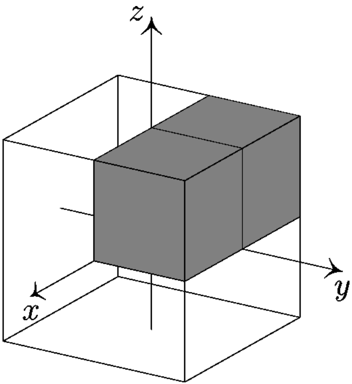

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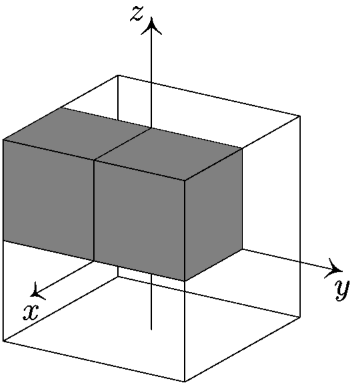

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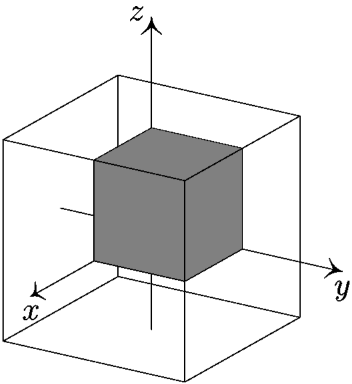

MOCCa


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MOCCa = **Mo**dular **C**ranking **C**ode

MOCCa: status

Done:

1. (Almost) all interactions
2. Hartree-Fock in any combination of symmetries
3. BCS in any spatial symmetry combination you wish
4. HFB in any spatial (!) symmetry you wish

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Problem:

1. HFB for time-reversal breaking configurations

Breaking symmetries: extra degrees of freedom

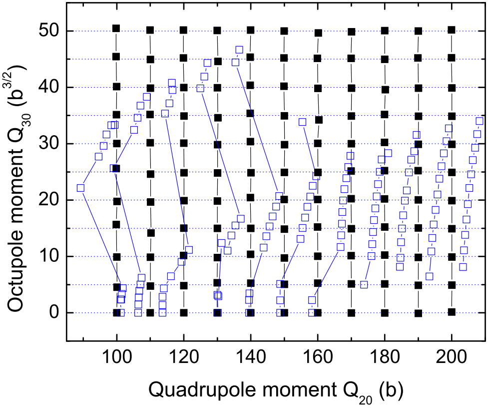
Broken symmetries	Physical	Non-physical
$\hat{P}$	Re $\hat{Q}_{30}$, Re $\hat{Q}_{32}$, ...	Re $\hat{Q}_{10}$
$\check{S}^T_y$	Im $\hat{Q}_{20}$, Im $\hat{Q}_{42}$, ...	Im $\hat{Q}_{22}$
$\hat{R}_z$	Re $\hat{Q}_{41}$, Re $\hat{Q}_{43}$, ...	Re $\hat{Q}_{21}$
$\hat{R}_z$,$\hat{P}$	Re $\hat{Q}_{31}$, Re $\hat{Q}_{33}$, ...	Re $\hat{Q}_{11}$
$\check{S}^T_y$,$\hat{P}$	Im $\hat{Q}_{32}$, ...	Im $\hat{Q}_{11}$
$\check{T}$	$\hat{J}_z$	
$\check{T}$, $\hat{R}_z$	$\hat{J}_x$	
$\check{T}$, $\check{S}^T_y$	$\hat{J}_y$	

How to constrain quantities in mean-field picture?

$$\hat{h}^{(i)} \rightarrow \hat{h}^{(i)} + \lambda^{(i)}_{\hat{O}} \hat{O} \text{ with } \langle \hat{O} \rangle = O_0$$

	Form
Constant	$\lambda^{(i)} = C$
Quadratic/Penalty function	$\lambda^{(i)} = C(\langle \hat{O} \rangle^{(i)} - O_0)$
Augmented Lagrangian	$\lambda^{(i)} = \lambda^{(i-1)} + C(\langle \hat{O} \rangle^{(i)} - O_0)$

Augmented Lagrangian is superior



Augmented lagrangian(black) versus quadratic(blue) constraints for ^{252}Fm using HFBTHO/HFODD.
Figure from A.Staszczak et al., Eur. Phys. A **46**, 85-90 (2010)

However, . . .

$$\lambda^{(i)} = \lambda^{(i-1)} + C_{\hat{O}}(\langle\hat{O}\rangle^{(i)} - O_0)$$

Optimal choice of $C_{\hat{O}}$ depends on:

- Initial mean-field configuration
- O_0
- $\hat{O}$
- the presence of other constraints!

However, . . .

^{20}Ne, $\mathrm{Re}\langle \hat{Q}_{10} \rangle = 0$ fm, $\mathrm{Re}\langle \hat{Q}_{20} \rangle = 10$ fm^2, $\mathrm{Re}\langle \hat{Q}_{30} \rangle = 10$ fm^3

$$\text{Deviation} = \sum_{l=1,2,3} r_{rms}^{-l} \left(\langle \hat{Q}_{l0} \rangle - Q_{l,desired} \right)^2$$

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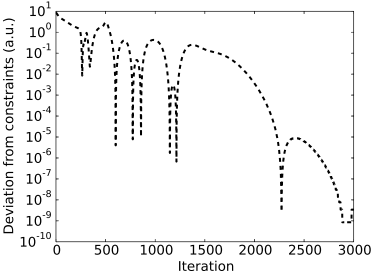

$C_{10} = 1, C_{20} = 0.08$

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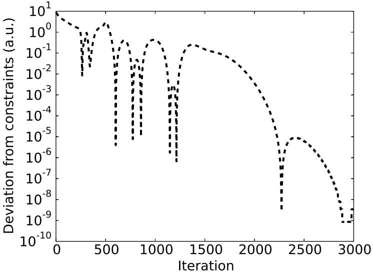

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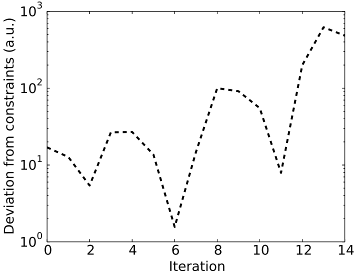

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Predictor-Corrector constraints

First description:

R.Y. Cusson et al., Z. Phys. A 320, 475-482 (1985)

More complete:

K. Rutz, PhD thesis, Ibidem-Verlag. Frankfurt (1998)

But the procedure described is not exactly the one K. Rutz used, nor the one I use!

Predictor-Corrector constraints

Augmented Lagrangian scheme:

1. Imaginary time step/gradient descent
$$\Psi^{(i)} = [1 - \epsilon(\hat{h}^{(i-1)} + \lambda^{(i-1)}\hat{O})]\Psi^{(i-1)}$$
2. Adapt
$$\lambda^{(i)} = \lambda^{(i-1)} + C(\langle\hat{O}\rangle^{(i)} - O_0)$$
3. construct $\hat{h}^{(i)}$
4. Repeat

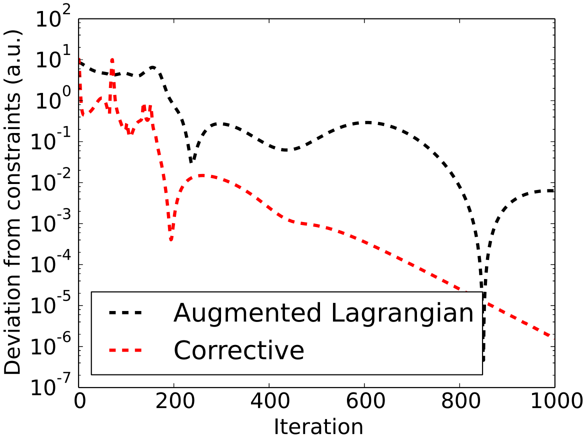
Predictor-Corrector constraints

Predictor-Corrector scheme with two constants $C = 7.0$ and $K = 0.7$:

1. Trial step
$$\chi^{(i)} = \left[1 - \epsilon(\hat{h}^{(i-1)} + \lambda\hat{O})\right] \Psi^{(i-1)}$$
2. Adapt
$$\lambda^{(i)} = \lambda^{(i-1)} + \frac{C}{A}\left(\langle\hat{O}\rangle^{(trial)} - \langle\hat{O}\rangle^{(i-1)}\right)$$
3. Do a corrective step
$$\Psi^{(i)} = \left[1 - \frac{K}{A}\left(\langle\hat{O}\rangle^{(trial)} - O_0\right)\hat{O}\right]\chi^{(i)}$$
4. construct $\hat{h}^{(i)}$
5. repeat

where $A = [\langle\hat{O}^2\rangle^{(trial)} + 0.00001]^{-1}$

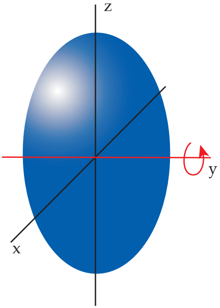
Predictor - Corrector constraints



Predictor-Corrector constraints for ^{20}Ne, constraints on $\hat{Q}_{10}$,$\hat{Q}_{20}$ and $\hat{Q}_{30}$.

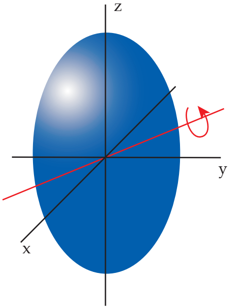
Tilted axis cranking

$$\hat{H}' = \hat{H} - \omega_z \hat{J}_z$$



Tilted axis cranking

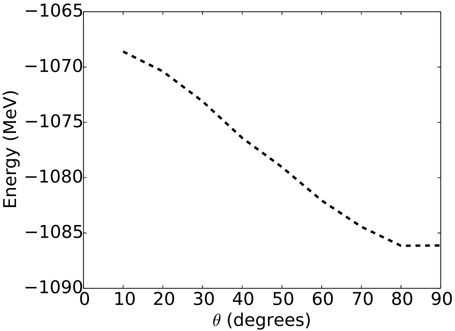
$$\hat{H}' = \hat{H} - \omega_x \hat{J}_x - \omega_y \hat{J}_y - \omega_z \hat{J}_z$$



^{158}Er

Y. Shi et al., Phys. Rev. Lett. **108** 092501 (2012)

- $\langle J_x \rangle = 70 \sin(\theta)\hbar$
- $\langle J_z \rangle = 70 \cos(\theta)\hbar$
- $\langle Q_{20} \rangle = 1900$ fm^2
- $\langle Q_{22} \rangle = 500$ fm^2
- $\langle Q_{21} \rangle = 0$ fm^2



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- Future: fix the remaining problems
- Future: implement the SLyMRX interactions