# Class II and III Interactions within DFT

**P. Bączyk**[1] J. Dobaczewski[1,2,3]
M. Konieczka[1] W. Satuła[1,2]

[1]**Faculty of Physics, University of Warsaw, PL 02-093 Warszawa, Poland**
[2]Helsinki Institute of Physics, P.O. Box 64, FI-00014 University of Helsinki, Finland
[3]Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland

The future of multireference DFT
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## Plan of the presentation

1. Classification of ISB interactions
2. Implementation in HFODD code
3. First results and outlook

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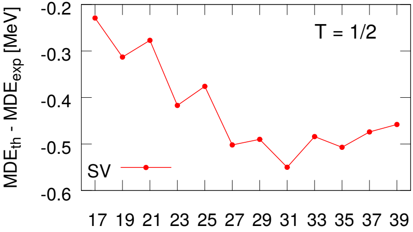
# Do we need additional ISB terms?

## Mirror displacement energy (MDE)

$$\mathrm{MDE} = \mathrm{BE}\,(T, T_z = -T) - \mathrm{BE}\,(T, T_z = +T)$$

Nolen-Schiffer anomaly
J.A. Nolen, Jr. and J.P. Shiffer,
Annu. Rev. Nucl. Phys. **19**, 471 (1969)

charge symmetry breaking
CSB
$V_{pp} \neq V_{nn}$



# Do we need additional ISB terms?

**Triplet displacement energy (TDE)**

$$\mathrm{TDE} = \mathrm{BE}\,(T=1,\, T_z=-1) + \mathrm{BE}\,(T=1,\, T_z=+1) - 2\mathrm{BE}\,(T=1,\, T_z=0)$$

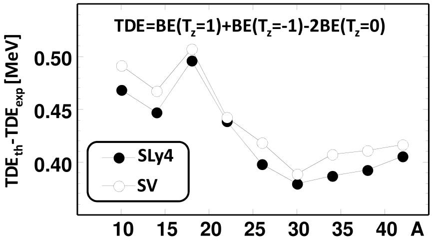
$T = 1$ triplets curvature

W. Satuła, J. Dobaczewski, M. Konieczka, W. Nazarewicz, Acta Phys. Pol. B **45**, 167 (2014)

charge independence breaking

CIB

$V_{np} \neq (V_{nn} + V_{pp})/2$



# Classification of Henley and Miller

- class I – isospin independent

$$V_I^{NN}(i,j) = a + b\vec{\tau}(i)\cdot\vec{\tau}(j)$$

- class II – introduces CIB

$$V_{II}^{NN}(i,j) = c\left[\tau_3(i)\tau_3(j) - \frac{1}{3}\vec{\tau}(i)\cdot\vec{\tau}(j)\right]$$

- class III – introduces CSB

$$V_{III}^{NN}(i,j) = d\left[\tau_3(i) + \tau_3(j)\right]$$

- class IV – mix isospin already at two-body level

$$\begin{aligned} V_{IV}^{NN}(i,j) = {} & e\left[\vec{\sigma}(i) - \vec{\sigma}(j)\right]\cdot\vec{L}\left[\tau_3(i) + \tau_3(j)\right] \\ & + f\left[\vec{\sigma}(i)\times\vec{\sigma}(j)\right]\cdot\vec{L}\left[\vec{\tau}(i)\times\vec{\tau}(j)\right]_3 \end{aligned}$$

E.M. Henley, and G.A. Miller, in *Mesons in Nuclei* (North Holland, Amsterdam, 1979), p. 405

- only **class II** and **class III** considered so far
- new terms implemented as **effective zero-range corrections** to conventional Skyrme modifying **central part**

$$V^{ISB}(i,j) = V^{Skyrme}(i,j) + V^{II}(i,j) + V^{III}(i,j)$$

$$V^{II}(i,j) = \frac{1}{2} t_0^{II} \, \delta\left(\vec{r}_i - \vec{r}_j\right) \left(1 - x_0^{II} \, \hat{P}_{ij}^{\sigma}\right) \left[3\tau_3(i)\tau_3(j) - \vec{\tau}(i) \cdot \vec{\tau}(j)\right]$$

$$V^{III}(i,j) = \frac{1}{2} t_0^{III} \, \delta\left(\vec{r}_i - \vec{r}_j\right) \left(1 - x_0^{III} \, \hat{P}_{ij}^{\sigma}\right) \left[\tau_3(i) + \tau_3(j)\right]$$

# Implementation
## Energy densities

$$\mathcal{H}^{II} = \frac{1}{2} t_0^{II} \left(1 - x_0^{II}\right) \Big[ \rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \vec{S_n}^{\,2} - \vec{S_p}^{\,2} + 2\vec{S_n}\cdot\vec{S_p} + 2\vec{S_{np}}\cdot\vec{S_{pn}} \Big]$$

$$\mathcal{H}^{III} = \frac{1}{2} t_0^{III} \left(1 - x_0^{III}\right) \left( \rho_n^2 - \rho_p^2 - \vec{S_n}^{\,2} + \vec{S_p}^{\,2} \right)$$

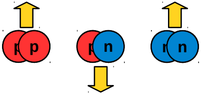
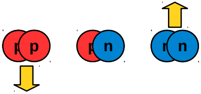
- $x_0^{II}$ and $x_0^{III}$ parameters are redundant
- *pn*-mixing is needed only in class II

# Implementation
## Energy densities

$$\mathcal{H}^{II} = \frac{1}{2} t_0^{II} \left(1 - x_0^{II}\right) \left[ \rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \vec{S_n}^2 - \vec{S_p}^2 + 2\vec{S_n}\cdot\vec{S_p} + 2\vec{S_{np}}\cdot\vec{S_{pn}} \right]$$

$$\mathcal{H}^{III} = \frac{1}{2} t_0^{III} \left(1 - x_0^{III}\right) \left( \rho_n^2 - \rho_p^2 - \vec{S_n}^2 + \vec{S_p}^2 \right)$$

- $x_0^{II}$ and $x_0^{III}$ parameters are redundant
- *pn*-mixing is needed only in class II

- class II CIB: 
- class III CSB: 

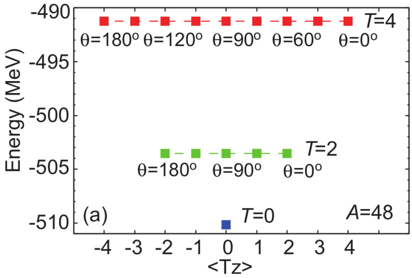
# Isocranking method

## Goal

building $|T = 1, T_z = 0 >$ state

## Difficulty

$T_z = 0$ state is almost a fifty-fifty mixture of $T = 0$ and $T = 1$ states




K. Sato, J. Dobaczewski, T. Nakatsukasa, and W. Satuła, Phys. Rev. C **88**, 061301(R) (2013)

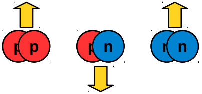
## Tool – isocranking

- approximate projection on isospin in *pn*-mixing formalism
- analogous to isocranking model
- description of $|T = 1, T_z = 0 >$ states by evolving $|T = 1, T_z = \pm 1 >$ solutions

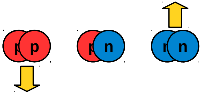
# First test for $A = 42$

## without Coulomb

only class II – CIB




only class III – CSB



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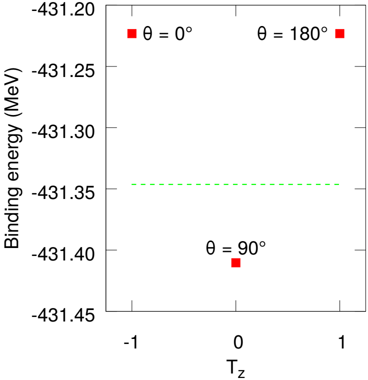
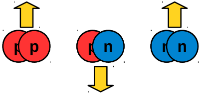
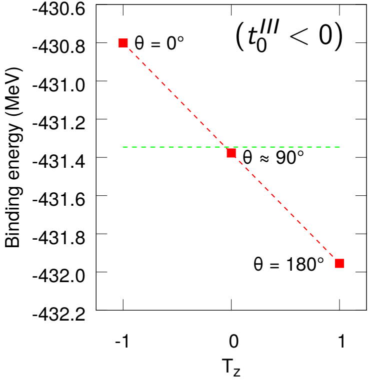
## without Coulomb

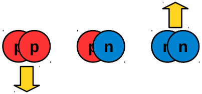



only class II – CIB




only class III – CSB



# First test for $A = 42$
## with Coulomb

| | | without Coulomb | | with Coulomb | |
|---|---|---|---|---|---|
| Parameters | | TDE [MeV] | MDE [MeV] | TDE [MeV] | MDE [MeV] |
| $t_0^{II}$ | $t_0^{III}$ | | | | |

Parameters $t_0^{II}$ and $t_0^{III}$ were chosen by hand.

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## with Coulomb

| | | without Coulomb | | with Coulomb | |
|---|---|---|---|---|---|
| Parameters | | TDE [MeV] | MDE [MeV] | TDE [MeV] | MDE [MeV] |
| $t_0^{II}$ | $t_0^{III}$ | | | | |
| 0 | 0 | 0 | 0 | 0.159 | 13.789 |

Parameters $t_0^{II}$ and $t_0^{III}$ were chosen by hand.

# First test for $A = 42$
## with Coulomb

| Parameters $t_0^{II}$ | Parameters $t_0^{III}$ | without Coulomb TDE [MeV] | without Coulomb MDE [MeV] | with Coulomb TDE [MeV] | with Coulomb MDE [MeV] |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0.159 | 13.789 |
| 20 | 0 | 0.374 | 0 | 0.525 | 13.783 |

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| Parameters $t_0^{II}$ | Parameters $t_0^{III}$ | without Coulomb TDE [MeV] | without Coulomb MDE [MeV] | with Coulomb TDE [MeV] | with Coulomb MDE [MeV] |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0.159 | 13.789 |
| 20 | 0 | 0.374 | 0 | 0.525 | 13.783 |
| 0 | -8 | -0.002 | 1.153 | 0.145 | 14.899 |

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## with Coulomb

| Parameters $t_0^{II}$ | Parameters $t_0^{III}$ | without Coulomb TDE [MeV] | without Coulomb MDE [MeV] | with Coulomb TDE [MeV] | with Coulomb MDE [MeV] |
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| 0 | 0 | 0 | 0 | 0.159 | 13.789 |
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| 0 | -8 | -0.002 | 1.153 | 0.145 | 14.899 |
| 20 | -8 | 0.372 | 1.147 | 0.511 | 14.888 |

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| Parameters $t_0^{II}$ | Parameters $t_0^{III}$ | without Coulomb TDE [MeV] | without Coulomb MDE [MeV] | with Coulomb TDE [MeV] | with Coulomb MDE [MeV] |
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| 0 | 0 | 0 | 0 | 0.159 | 13.789 |
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The effect of class II is almost independent of class III and *vice versa*.

Parameters $t_0^{II}$ and $t_0^{III}$ were chosen by hand.

# First test for $A = 42$
## with Coulomb

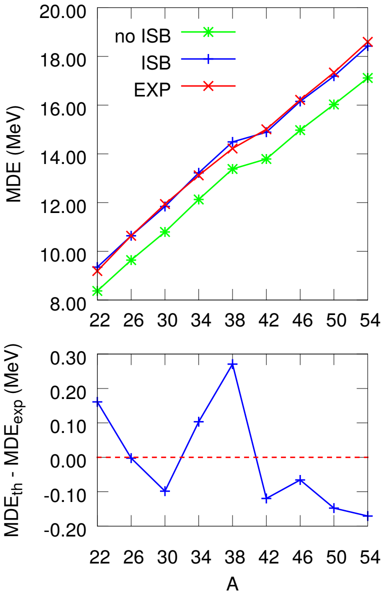
| Parameters $t_0^{II}$ | $t_0^{III}$ | without Coulomb TDE [MeV] | without Coulomb MDE [MeV] | with Coulomb TDE [MeV] | with Coulomb MDE [MeV] |
|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0.159 | 13.789 |
| 20 | 0 | 0.374 | 0 | 0.525 | 13.783 |
| 0 | -8 | -0.002 | 1.153 | 0.145 | 14.899 |
| 20 | -8 | 0.372 | 1.147 | 0.511 | 14.888 |

The effect of class II is almost independent of class III and *vice versa*.

Experiment: TDE = 0.590 MeV and MDE = 15.007 MeV

Parameters $t_0^{II}$ and $t_0^{III}$ were chosen by hand.

# Isovector triplets – MDE and TDE



# Outlook

- Fitting new parameters: $t_0^{II}$ and $t_0^{III}$
- Large scale calculations of MDE and TDE: $T = \frac{1}{2}$ and $T = 1$
- MED and TED in structure of rotational bands

$$\mathrm{MED}(J) = E(J, T, T_z = -T) - E(J, T, T_z = +T)$$
$$\mathrm{TED}(J) = E(J, T=1, T_z=-1) + E(J, T=1, T_z=+1) - 2E(J, T=1, T_z=0)$$

- Recalculating isospin corrections $\delta_C$ for $\beta$ decay
- Isospin-forbidden E1 $\gamma$ transitions
- Introducing class IV