Mirror and Triplet Energy Differences within Density Functional Theory

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Nucleon-nucleon (NN) interaction

$$V_{nn} \stackrel{?}{=} V_{pp} \stackrel{?}{=} V_{pn}$$

electromagnetic

Coulomb

$\Uparrow$

different charge

neutron	$q = 0$
proton	$q = +1$

strong

from scattering experiments:

$a_{nn} \neq a_{pp} \neq a_{pn}$

$\Uparrow$

different quark composition

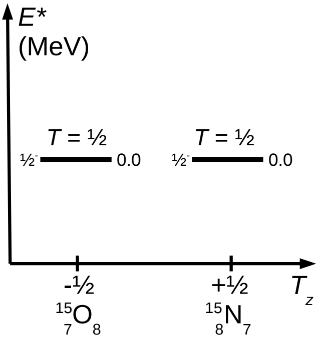
(different mass and charge for u and d)

neutron	*udd*
proton	*uud*

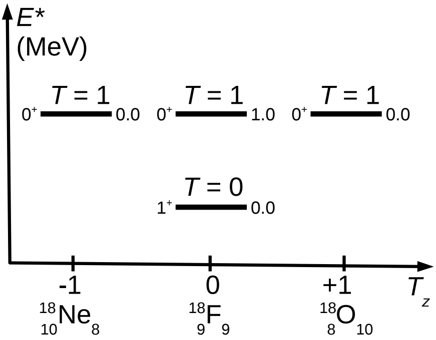
- What are the consequences in atomic nuclei?
- Can we built a successful theoretical description?

Isobaric analog states (IAS)

isospin doublet $\mathbf{T = \frac{1}{2}}$



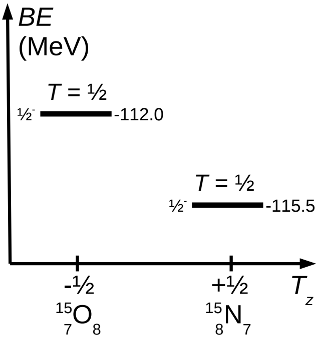
isospin triplet $\mathbf{T = 1}$



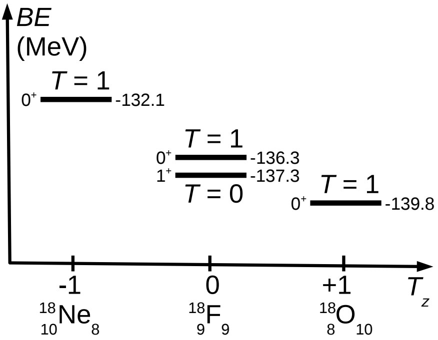
without Coulomb

Isobaric analog states (IAS)

isospin doublet $\mathbf{T = \frac{1}{2}}$



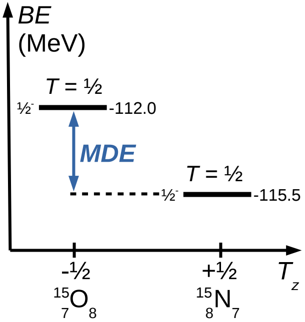
isospin triplet $\mathbf{T = 1}$



with Coulomb

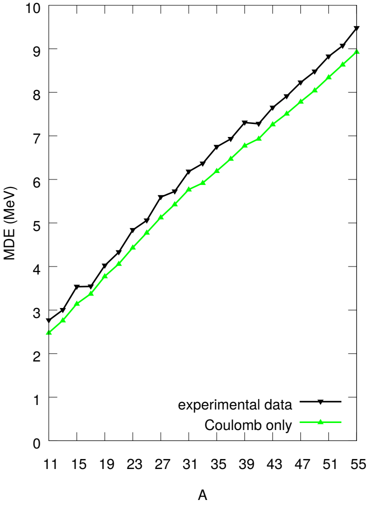
Mirror Displacement Energy (MDE)

$$V_{nn} \neq V_{pp}$$



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

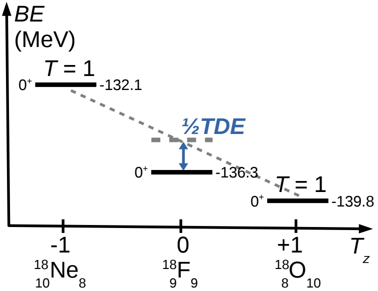
$T = \frac{1}{2}$ mirrors



Nolen-Schiffer anomaly (1969)

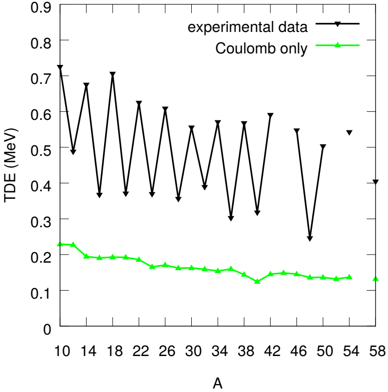
Triplet Displacement Energy (TDE)

$$V_{pn} \neq \frac{V_{nn}+V_{pp}}{2}$$



$$TDE = BE\left(T=1, T_z=-1\right) + BE\left(T=1, T_z=+1\right) - 2BE\left(T=1, T_z=0\right)$$

$T = 1$ triplets



$A = 4n,\ 4n+2$ staggering

Status of isospin-symmetry-breaking (ISB) forces

The need of ISB nucleon-nucleon interaction is well established:

- Hartree-Fock calculations,
- *ab initio* calculations,
- Shell Model calculations.

How can our approach contribute?

- implementation within a robust model based on **DFT**
- **full non-perturbative** Coulomb force
- **transparent** way of treating CSB and CIB
- applicability to **any nucleus** (including odd-odd systems)
- a lot of ISB effects in one model

Density Functional Theory (DFT)

Hohenberg-Kohn theorem

A-body wave-function of the nuclear ground-state is
an unambiguously defined functional of a single-particle density.

DFT strategy

- the existence of an exact functional leading to exact many-body solution is proven, but the way of finding it is unknown
- constructing the nuclear density functional explores formal similarity between the DFT method, in particular in the Kohn-Sham formulation, and the HF approximation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + v_{eff}(\mathbf{r})\right)\phi_i(\mathbf{r}) = \epsilon_i \phi_i(\mathbf{r})$$

Skyrme interaction

$$
\begin{aligned}
\hat{V}_{Sk}(\vec{r}_1, \vec{r}_2) &= t_0(1 + x_0\hat{P}_\sigma)\delta(\vec{r}_1 - \vec{r}_2) \\
&+ \frac{1}{2}t_1(1 + x_1\hat{P}_\sigma)\left(\delta(\vec{r}_1 - \vec{r}_2)\vec{k}^2 + \vec{k}'^2\delta(\vec{r}_1 - \vec{r}_2)\right) \\
&+ t_2(1 + x_2\hat{P}_\sigma)\vec{k}'\delta(\vec{r}_1 - \vec{r}_2)\vec{k} \\
&+ \frac{1}{6}t_3(1 + x_3\hat{P}_\sigma)\rho_0^\alpha\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)\delta(\vec{r}_1 - \vec{r}_2) \\
&+ iW_0(\vec{\sigma}_1 + \vec{\sigma}_2)\vec{k}' \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k}
\end{aligned}
$$

Short characteristics

- low-momentum transfer **expansion**
- composed of various terms: central, spin-orbit, density dependent...
- successful description of bulk properties in **broad** range of masses
- only 10 parameters

Parametrisations used in our work:

- SV: Hamiltonian-derived interaction (no density-dependent term), well-suited for projections and No-Core Configuration Interaction (NCCI) method
- SkM*: describing well properties of nuclei, fitted in particular to fission barriers
- SLy4: well-established and widely-used parametrization

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

New terms implemented as **effective zero-range corrections** to conventional Skyrme modifying **central part**.

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

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

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

Skyrme parametrizations used: SV, SKM*, SLy4

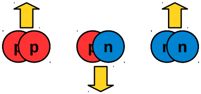
$$\mathcal{H}^{II} = \frac{1}{2} t_0^{II} \Big[\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \vec{S_n}^2 - \vec{S_p}^2 + 2\vec{S_n}\cdot\vec{S_p} + 2\vec{S_{np}}\cdot\vec{S_{pn}} \Big]$$

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

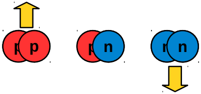
$$\mathcal{H}^{II} = \frac{1}{2} t_0^{II} \Big[\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \vec{S_n}^{\,2} - \vec{S_p}^{\,2} + 2\vec{S_n}\cdot\vec{S_p} + 2\vec{S_{np}}\cdot\vec{S_{pn}} \Big]$$

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

- class II:

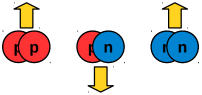
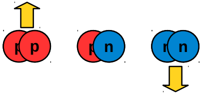


- class III: (with $t_0^{III} < 0$)



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

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

- class II: 
- class III: (with $t_0^{III} < 0$) 

Conclusion: *pn*-mixing is needed only in class II

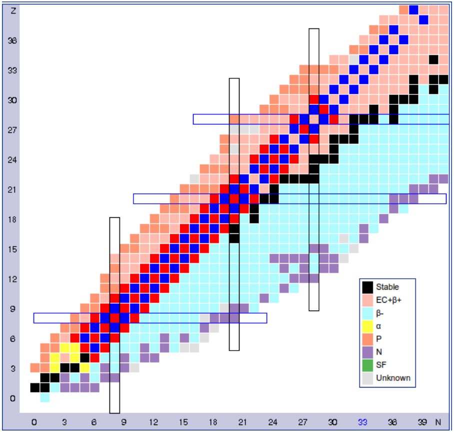
Data used for fitting

Calculations for:

- isospin doublets $T = \frac{1}{2}$ with $A = 11 - 75$ $\Rightarrow$ MDEs
- isospin triplets $T = 1$ with $A = 10 - 58$ $\Rightarrow$ MDEs, TDEs

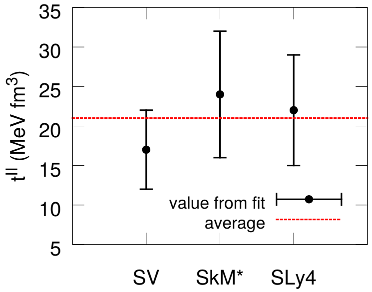
Experimental values of binding energies taken from AME2012

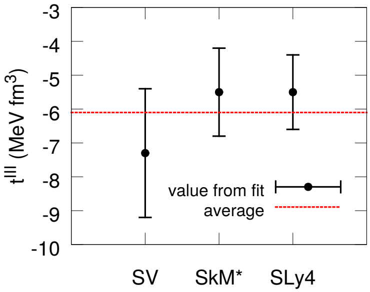
M. Wang *et al.*, CPC **36**, 1603 (2012)



Fit results:

Parametrization	SV	SkM*	SLy4
t_0^{II} (MeV fm^3)	17 ± 5	24 ± 8	22 ± 7
t_0^{III} (MeV fm^3)	-7.3 ± 1.9	-5.5 ± 1.3	-5.5 ± 1.1

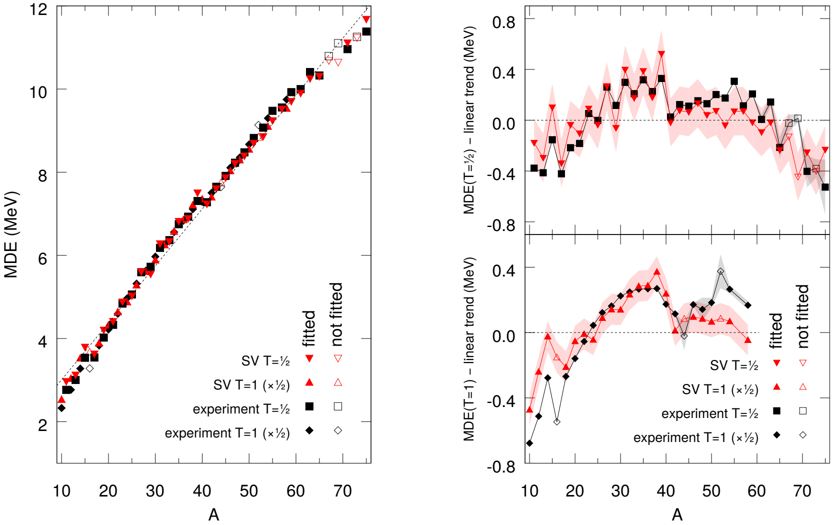




ISB part does not depend strongly on underlying parametrization!

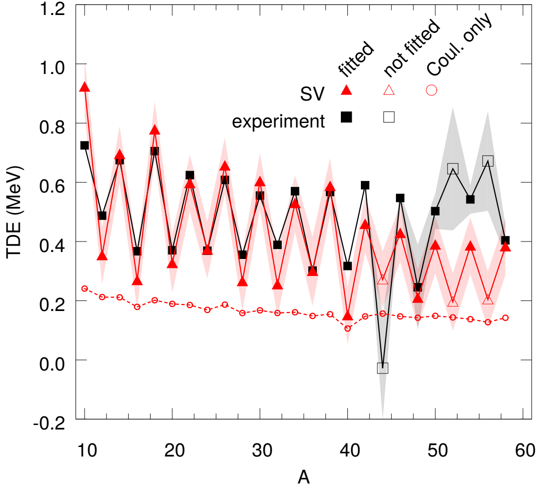
Results for MDE in doublets and triplets

SV parametrization



One parameter accounts for MDE in both doublets and triplets!

Results for TDE in triplets
SV parametrization



$A = 4n$ *versus* $A = 4n + 2$ staggering reproduced for the first time!

A link to scattering lengths

Assumption

proportionality between the strength of the interaction and the scattering length

Relation

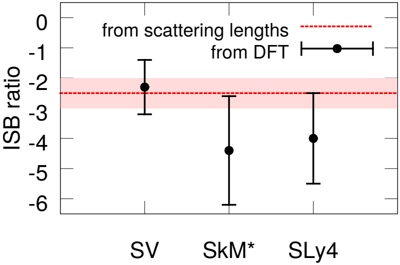
$$\frac{t_0^{\mathrm{II}}}{t_0^{\mathrm{III}}} = \frac{2}{3}\frac{\Delta a_{CIB}}{\Delta a_{CSB}} = -2.5 \pm 0.5$$

$$\Delta a_{CSB} = a_{nn} - a_{pp} = -1.5 \pm 0.3 \text{ fm}$$

$$\Delta a_{CIB} = \tfrac{1}{2}(a_{pp} + a_{nn}) - a_{pn} = 5.7 \pm 0.3 \text{ fm}$$

Results

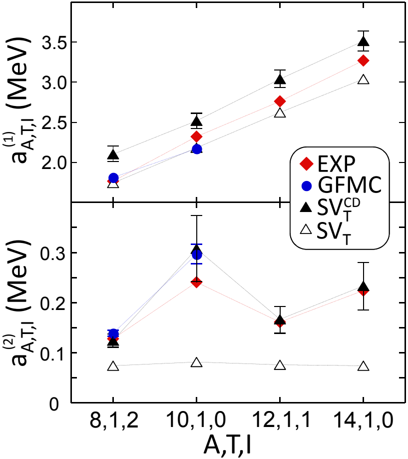
Parametrization	$t_0^{\mathrm{II}} \ / \ t_0^{\mathrm{III}}$
SV	-2.3 ± 0.9
SkM*	-4.0 ± 1.5
SLy4	-4.4 ± 1.8



Isobaric Multiplet Mass Equation (IMME)

$$\mathrm{BE}_{A,T,I}(T_z) = a + bT_z + cT_z^2 = \sum_{n\leq 2T} a^{(n)}_{A,T,I} Q_n(T, T_z)$$

$$Q_0 = 1,\ Q_1 = T_z,$$
$$Q_2 = \frac{1}{2}\left(3T_z^2 - T(T+1)\right)$$



Comparison of DFT and Green Function Monte Carlo (GFMC) calculations

- Both calculations reproduce empirical coefficients comparably well.
- **Staggering** of $a^{(2)}$ and TDE is attributed to **time-odd CIB** mean-field.

J. Carlson *et al.*, Rev. Mod. Phys. **87**, 1067 (2015)
P. Bączyk *et al.*, in preparation

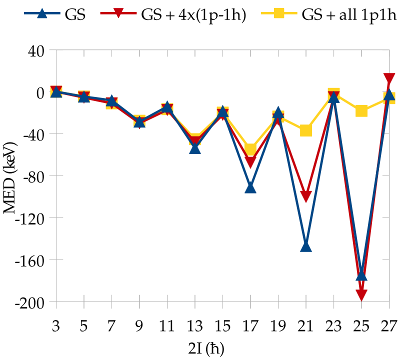
With IMME predictions of BE and S_p of heavy $N \approx Z$ nuclei are possible.

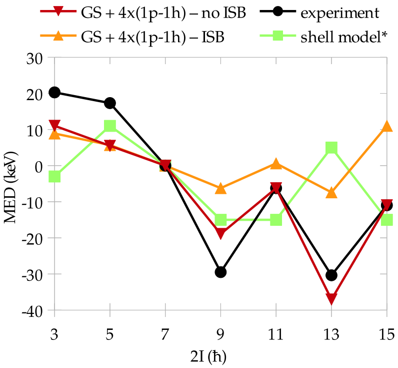
Mirror Energy Differences (MED) – Preliminary

$$\mathrm{MED}(I) = \mathrm{E}^*(I, T, T_z = -T) - \mathrm{E}^*(I, T, T_z = +T)$$

Calculations of **MED** in **^{45}Ti-^{45}V** isospin doublet done with:

- the **charge-symmetry-breaking** force of **class III**,
- recently developed DFT-rooted formalism: **No-Core Configuration-Interaction (NCCI)** W. Satuła *et al.*, *Phys. Rev. C* **94**, 024306 (2016).





*M.A. Bentley *et al.*, *Phys. Rev. C* **92**, 024310 (2015).

Summary and outlook

What has been done?

- successful implementation of ISB forces in the DFT formalism
- MDEs and TDEs reproduced with only two-parameters model
- new terms depend weakly on parametrization – a possibility to study fundamental aspects of ISB

What can be done?

- MED and TED for rotational bands
- influence of ISB forces on β decay
- E1 transition strengths in mirror nuclei