Proton-neutron mixed density functional calculation with strong-force isospin symmetry breaking

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- Introduction
- Method
- Results with isoscalar p-n mixed HF
- Results with isospin-breaking nuclear interaction
- Summary

Energy-density-functional calculation with proton-neutron mixing

superposition of protons and neutrons

Isospin symmetry

$$|n\rangle = |\tau = +1/2\rangle = \binom{1}{0}$$

$$|p\rangle = |\tau = -1/2\rangle = \binom{0}{1}$$

Protons and neutrons can be regarded as identical particles (nucleons) with different quantum numbers

In general, a nucleon state is written as $|N\rangle = \binom{\phi_1}{\phi_2}$

- Proton-neutron mixing:

  Single-particles are mixtures of protons and neutrons

  EDF with an arbitrary mixing between protons and neutrons

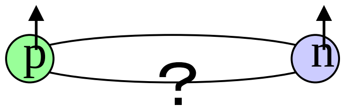
$$\rho_\tau(\alpha,\beta) = \langle \Psi | c^+_{\beta,\tau} c_{\alpha,\tau} | \Psi \rangle \quad \tau = p,n \longrightarrow \rho_{\tau\tau'}(\alpha,\beta) = \langle \Psi | c^+_{\beta,\tau'} c_{\alpha,\tau} | \Psi \rangle \quad \tau,\tau' = p,n$$

⇨ more general EDFs & rigorous treatment of isospin

⇨ A first step toward nuclear DFT for proton-neutron pairing and its application

Pairing between protons and neutrons (isoscalar T=0 and isovector T=1)

Goodman, Adv. Nucl. Phys.11, (1979) 293.
Perlinska et al, PRC 69 , 014316(2004)



Basic idea of p-n mixing

Let's consider two p-n mixed s.p. wave functions

$$\begin{aligned}\phi_1(\boldsymbol{r}) &= \phi_1(\boldsymbol{r},n)+\phi_1(\boldsymbol{r},p),\\ \phi_2(\boldsymbol{r}) &= \phi_2(\boldsymbol{r},n)+\phi_2(\boldsymbol{r},p),\end{aligned}$$

(spin indices omitted for simplicity)

$$\phi_1(\boldsymbol{r},p)=\phi_2(\boldsymbol{r},n)=0$$

→ standard unmixed neutron and proton w. f.

$\phi_1(r)=\phi_1(r,n)$
$\phi_2(r)=\phi_2(r,p)$

They contribute to the local density matrices as

$$\begin{aligned}\rho(\boldsymbol{r},nn) &= \phi_1(\boldsymbol{r},n)\phi_1^*(\boldsymbol{r},n)+\phi_2(\boldsymbol{r},n)\phi_2^*(\boldsymbol{r},n),\\ \rho(\boldsymbol{r},pp) &= \phi_1(\boldsymbol{r},p)\phi_1^*(\boldsymbol{r},p)+\phi_2(\boldsymbol{r},p)\phi_2^*(\boldsymbol{r},p),\end{aligned}$$

standard n and p densities

$$\begin{aligned}\rho(\boldsymbol{r},np) &= \phi_1(\boldsymbol{r},n)\phi_1^*(\boldsymbol{r},p)+\phi_2(\boldsymbol{r},n)\phi_2^*(\boldsymbol{r},p),\\ \rho(\boldsymbol{r},pn) &= \phi_1(\boldsymbol{r},p)\phi_1^*(\boldsymbol{r},n)+\phi_2(\boldsymbol{r},p)\phi_2^*(\boldsymbol{r},n).\end{aligned}$$

p-n mixed densities

→ Here, we consider p-n mixing at the Hartree-Fock level (w/o pairing)

Hartree-Fock calculation including proton-neutron mixing (pnHF)

- Extension of the single-particle states

$$\left|\psi_{i,n}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle$$
$$\left|\psi_{j,p}\right\rangle = \sum_{\alpha} a_{j,\alpha}^{(p)} \left|\alpha, p\right\rangle$$
$$\longrightarrow \quad \left|\psi_{i}\right\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} \left|\alpha, n\right\rangle + \sum_{\beta} a_{i,\beta}^{(p)} \left|\beta, p\right\rangle$$

i=1,…,A

- Extension of the density functional

$$E^{Skyrme}[\rho_n, \rho_p] \longrightarrow E^{Skyrme'}[\rho_0, \vec{\rho}\ ]$$

isoscalar isovector

Invariant under rotation in isospin space

Perlinska et al, PRC 69 , 014316(2004)

can be written in terms of ρ_0, ρ_3
not invariant under rotation in isospin space

pnHF

isoscalar	isovector
$\rho_0 = \rho_n + \rho_p$	$\rho_1 = \rho_{np} + \rho_{pn}$
Standard HF	$\rho_2 = -i\rho_{np} + i\rho_{pn}$
	$\rho_3 = \rho_n - \rho_p$

Energy density functionals are extended such that they are invariant under rotation in isospin space

2 implementations of p-n mixed HF:

HFODD

KS et al, PRC 88(2013) 061301(R).

http://www.fuw.edu.pl/~dobaczew/hfodd/hfodd.html

J. Dobaczewski, et al., Comp. Phys. Comm. 183 (2012) 166.

- Skyrme energy density functional
- Hartree-Fock or Hartree-Fock-Bogoliubov
- Harmonic-oscillator basis
- No spatial & time-reversal symmetry restriction (3D cartetian basis)

HFBTHO

Sheikh, et al, PRC 89(2014) 054317.

Axially symmetric shape assumed（Cylindrical basis）

Good agreement in benchmark comparison

Isocranking calculation

$$\hat{h}' = \hat{h} - \vec{\lambda} \cdot \hat{\vec{t}},$$ Isocranking term

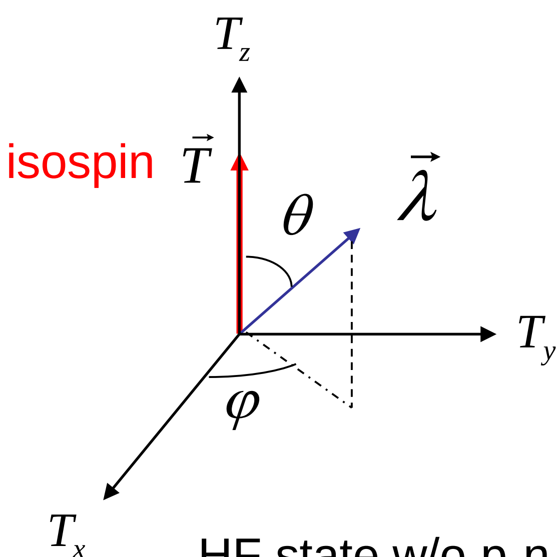
Analog with the TAC for high- spin states

$\vec{\lambda}$: Input to control the isospin of the system

How to obtain isobaric analog states

w/ p-n mixing and no Coulomb

Initial state: HF solution w/o p-n mixing (e.g. ^{48}Ca (Tz=4,T=4))

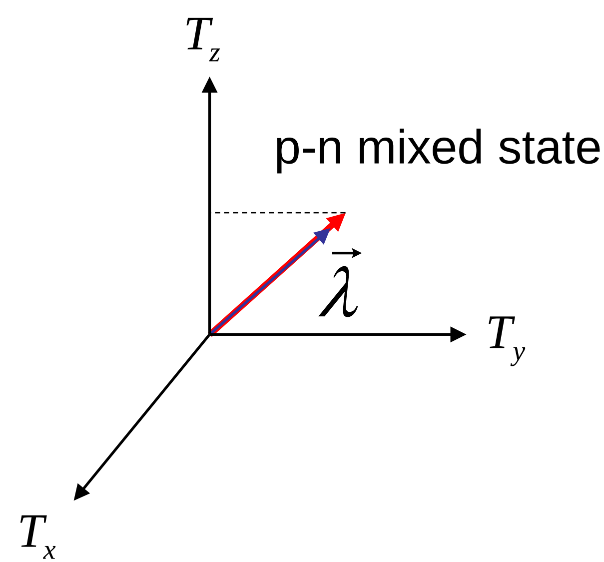


HF state w/o p-n mixing

$$-\vec{\lambda} \cdot \vec{T}$$

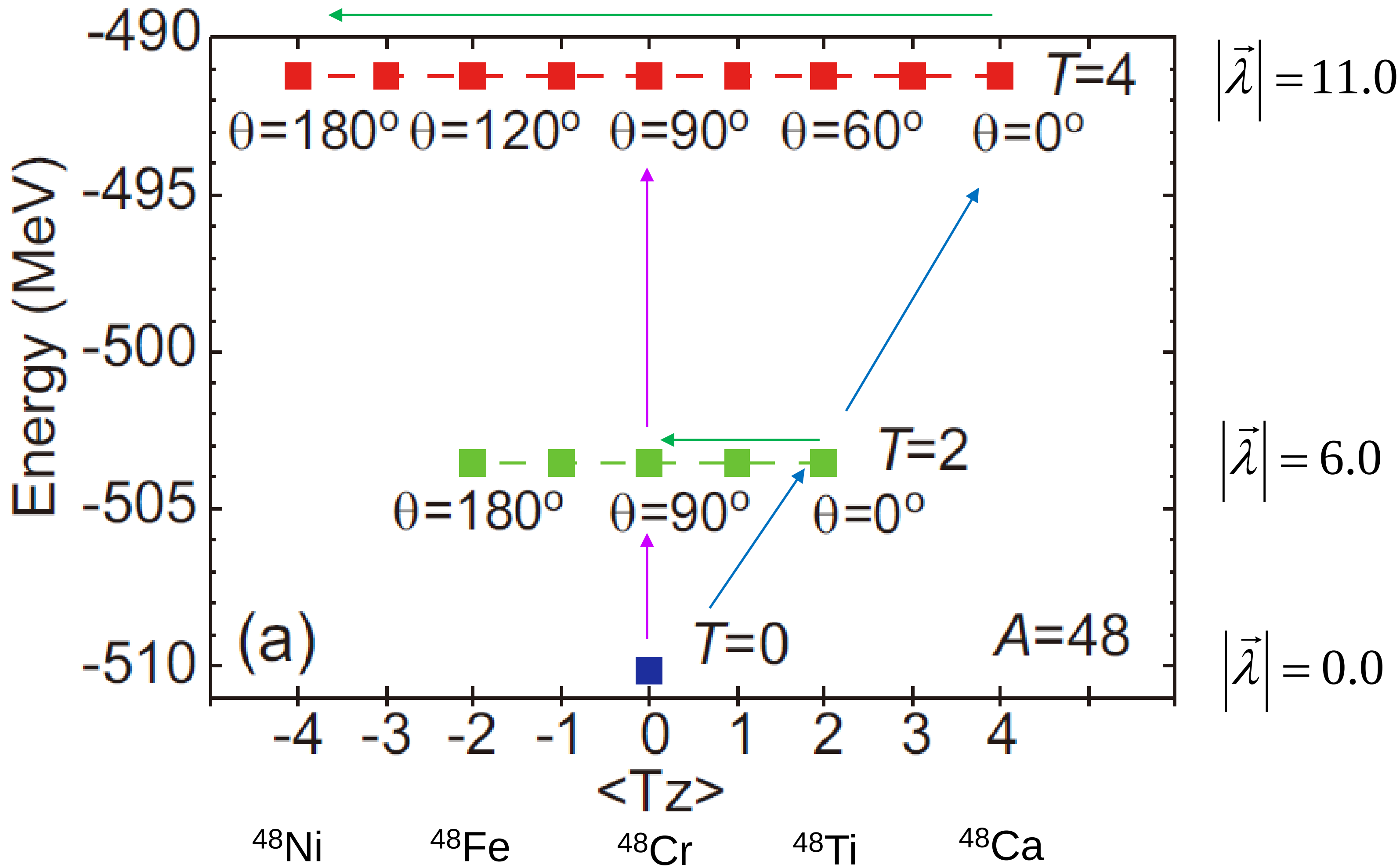
Iteration

Final state



By varying the titling angle,
we can obtain isobaric analog states

Calculation for A=48 nuclei w/ isoscalar EDF & no Coulomb

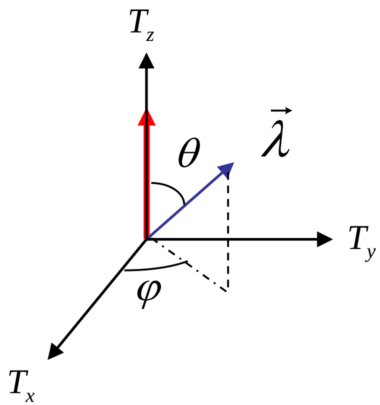


$|T_z| \neq T$ states can be obtained by isocranking the initial $|T_z| = T$ state

Non-zero T states can be obtained by isocranking the initial T=0 state along Tx axis

|Tz|=T states can be obtained by isocranking the initial T=0 state along Tz axis

Isocranking calculation for T~8 IASs in A=40 isobars w/ isospin-invariant functional



$\varphi = 0$

$$\vec{\lambda} = (\lambda \sin\theta, 0, \lambda\cos\theta) = (\lambda' \sin\theta', 0, \lambda'\cos\theta' + \lambda_{\rm off})$$

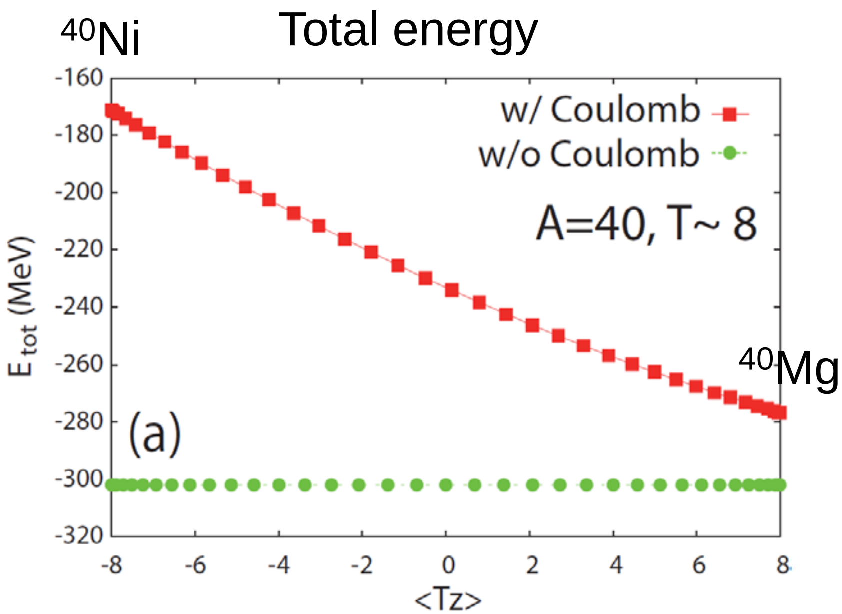
$$(\lambda_{\rm off}, \lambda') = \frac{1}{2}(\lambda_{np}^{T_z=T} + \lambda_{np}^{T_z=-T}, \lambda_{np}^{T_z=T} - \lambda_{np}^{T_z=-T})$$

$$\lambda_{np}^{T_z=\pm T} \equiv \lambda_n - \lambda_p$$

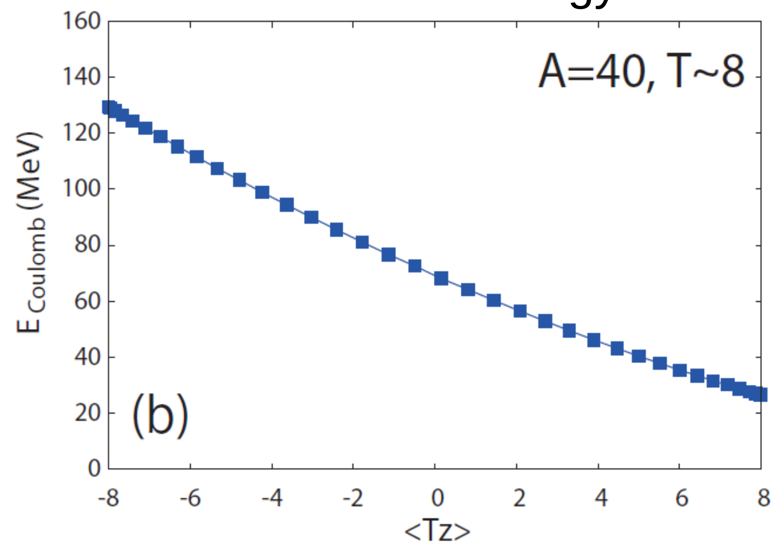
- Without Coulomb, total energy is independent of Tz
- With Coulomb, total energy behaves as

$$Z^2 = T_z^2 - AT_z + A^2/4$$

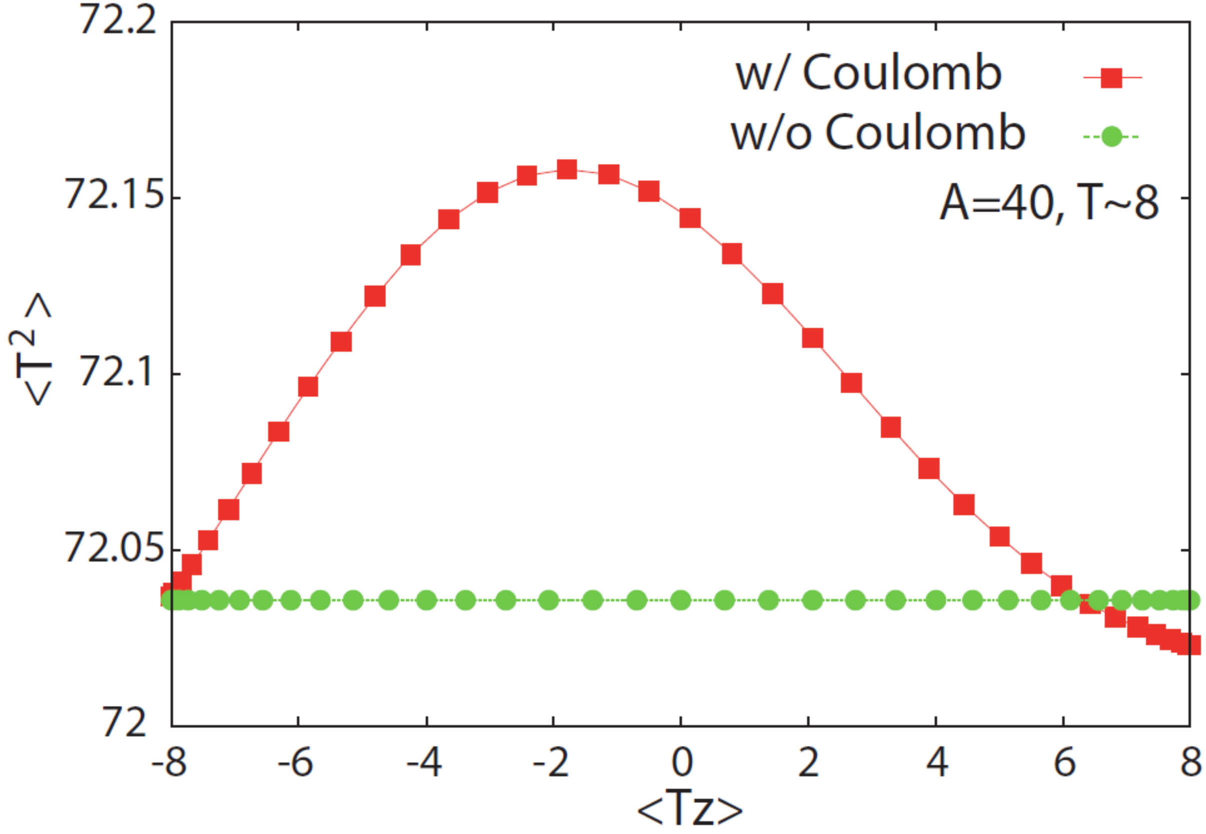
Total energy



Coulomb energy



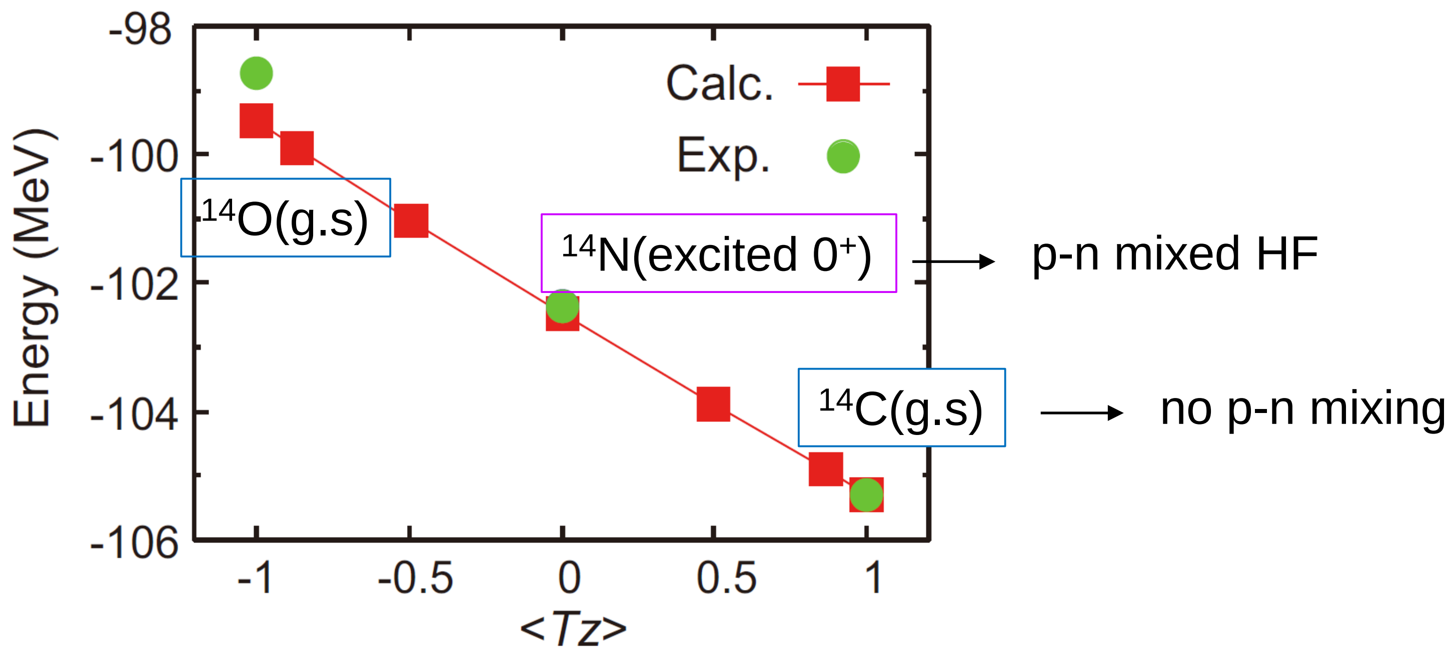
<T²> for T=8 IASs in A=40 isobars



Even without Coulomb, $\langle T^2 \rangle$ deviates from the exact value 72 due to the spurious isospin mixing within the mean-field approximation

⇨ Isospin projection needed

T=1 triplets in A=14 isobars



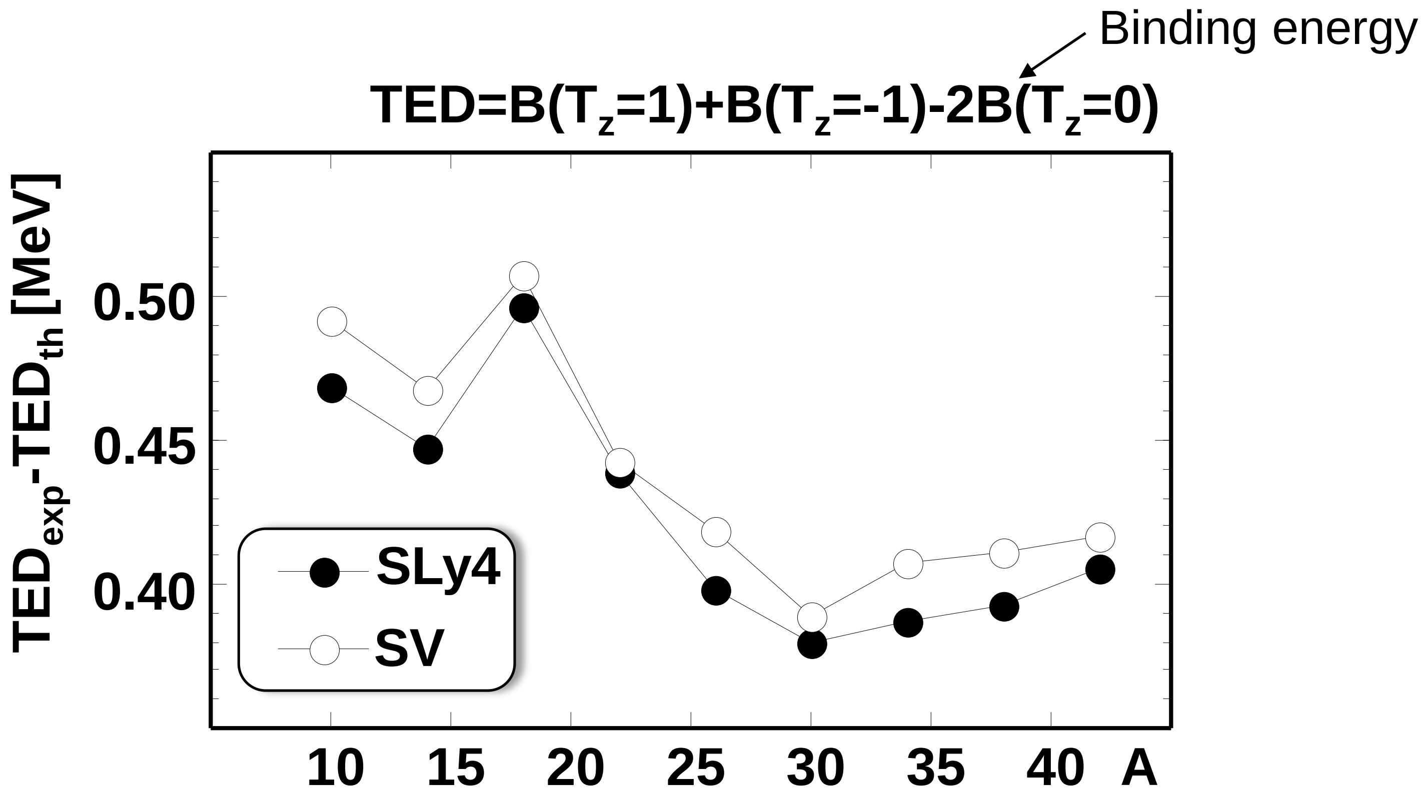
- Tz=0, T=1 states in odd-odd ^{14}N : Time-reversal symmetry conserved
- ^{14}N: p-n mixed , ^{14}C,O: p-n unmixed HF

Deviation from exp. ⟶ Need for further extension of EDF?

(The origin of calc. BE is shifted by 3.2 MeV to correct the deficiency of SkM* functional in the left panel for A=14)

Triple Energy Differences in T=1 multiplets

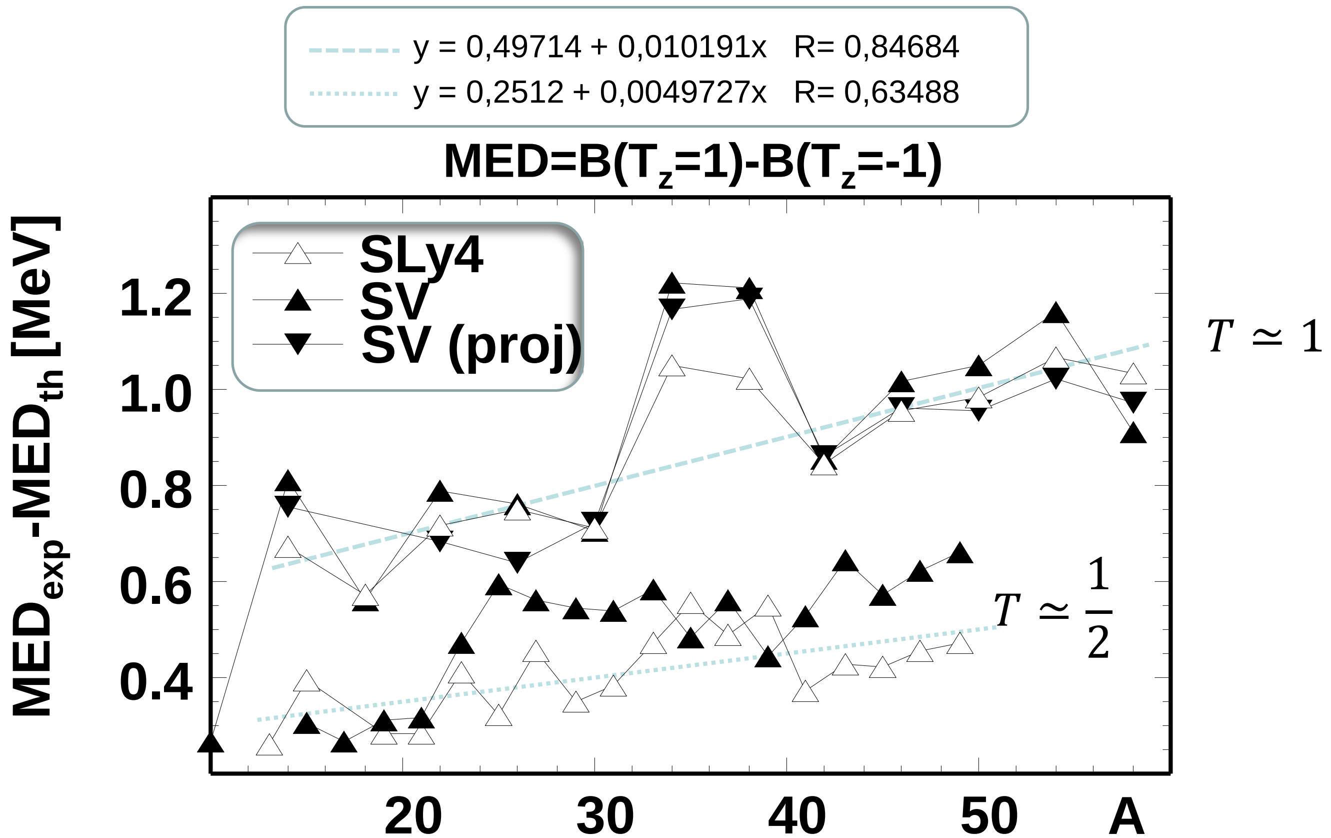
Probing a degree of the breaking of the charge independence



e.g.

B.E.(14C(g.s.)) + B.E.(14O(g.s.)) - 2 B.E.(^{14}N(excited 0^+))

Mirror Energy Differences in $T \simeq 1$ and $T \simeq \frac{1}{2}$ multiplets



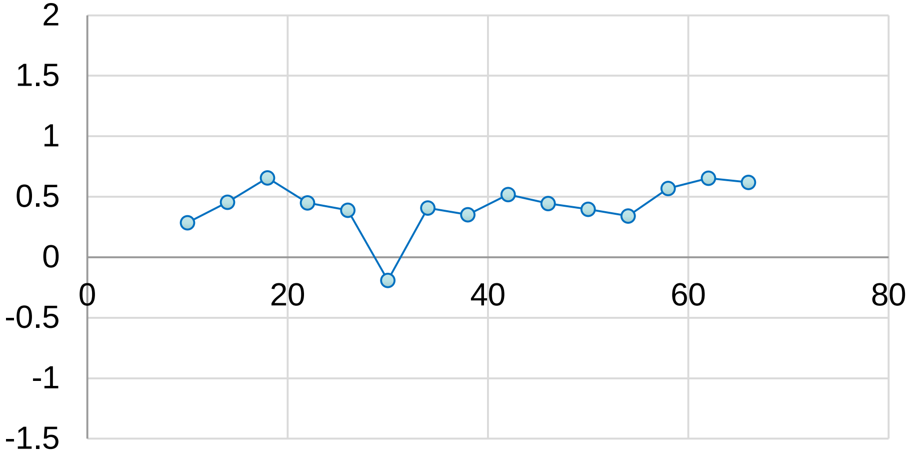
Coulomb itself is not strong enough to account for neither MED nor TED?

Need to include isospin-symmetry-breaking nuclear interaction?

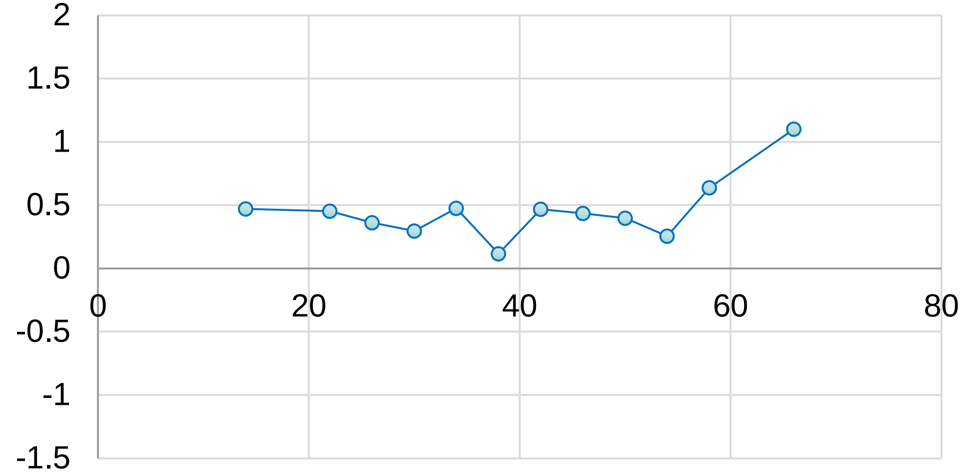
→ More systematic analysis required

Triple Energy Difference in T=1 triplets

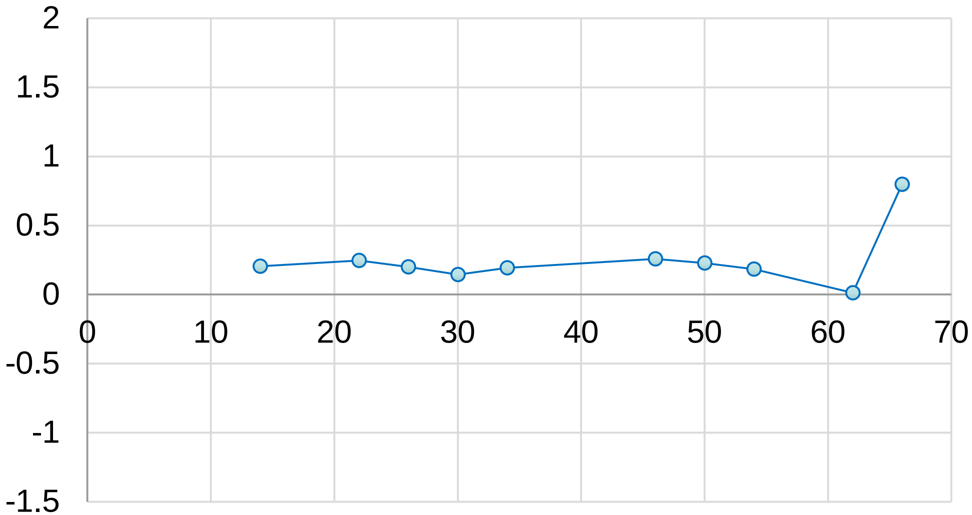
TED(exp)-TED(SIII)



TED(exp)-TED(SkM*)



TED(exp)-TED(SKX)

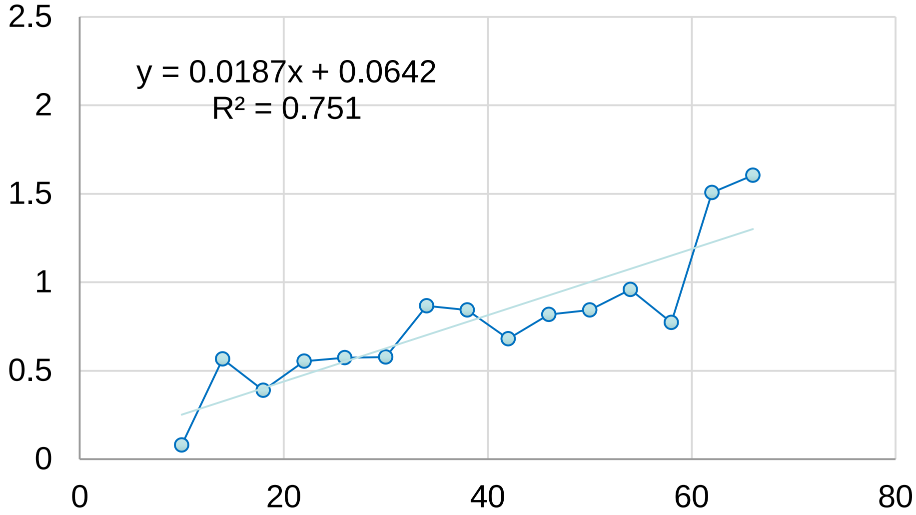


SKX：
Coulomb exchange int.
dropped

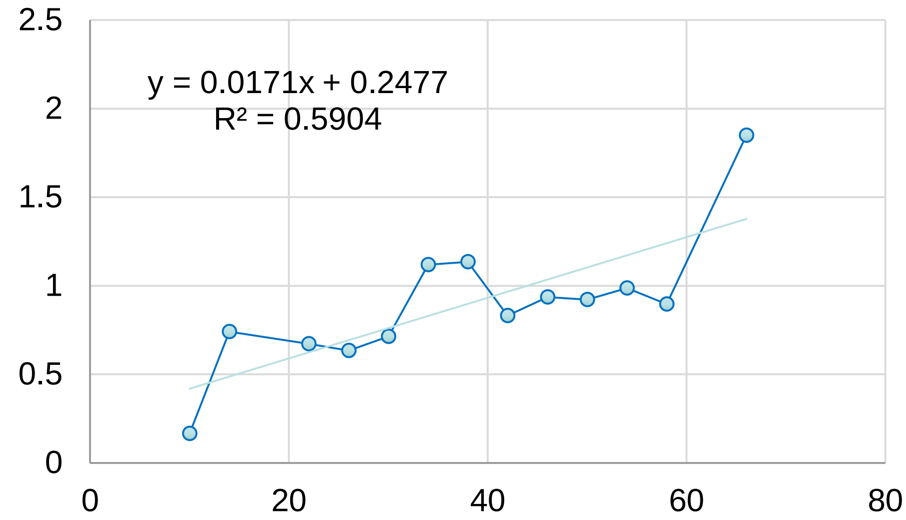
B.A. Brown et al., PLB483 (2000) 49.

Mirror Energy Difference in T=1 mirror nuclei

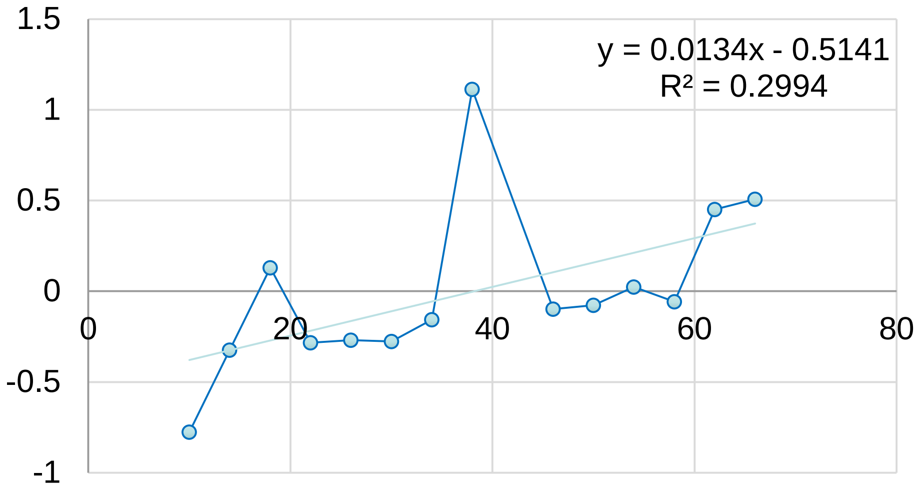
MED(exp)-MED(SIII)



MED(exp)-MED(SKM)



MED(exp)-MED(SKX)



Isoscalar EDFs lead to systematic deviation from experiment

Introduce nuclear isospin breaking terms

$$\mathcal{H}_{\mathrm{II}} = \frac{1}{2} t_0^{\mathrm{II}} (\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \boldsymbol{s}_n^2 - \boldsymbol{s}_p^2 + 2\boldsymbol{s}_n \cdot \boldsymbol{s}_p + 2\boldsymbol{s}_{np} \cdot \boldsymbol{s}_{pn}) \propto (3\rho_3^2 - \vec{\rho}^2 - 3\boldsymbol{s}_3^2 + \vec{\boldsymbol{s}}^2)$$

$$\mathcal{H}_{\mathrm{III}} = \frac{1}{2} t_0^{\mathrm{III}} \left(\rho_n^2 - \rho_p^2 - \boldsymbol{s}_n^2 + \boldsymbol{s}_p^2\right) \propto (\rho_0\rho_3 - \boldsymbol{s}_0\boldsymbol{s}_3)$$

Henly & Miller (1979)

Background of isospin symmetry breaking (other than Coulomb)

Mass difference between protons & neutrons → Charge Symmetry Breaking

Pion mass splitting → Charge Independence Breaking

R. Machleidt, Phys. Rev. C 63, 024001 (2001).

Introduce isospin symmetry breaking terms

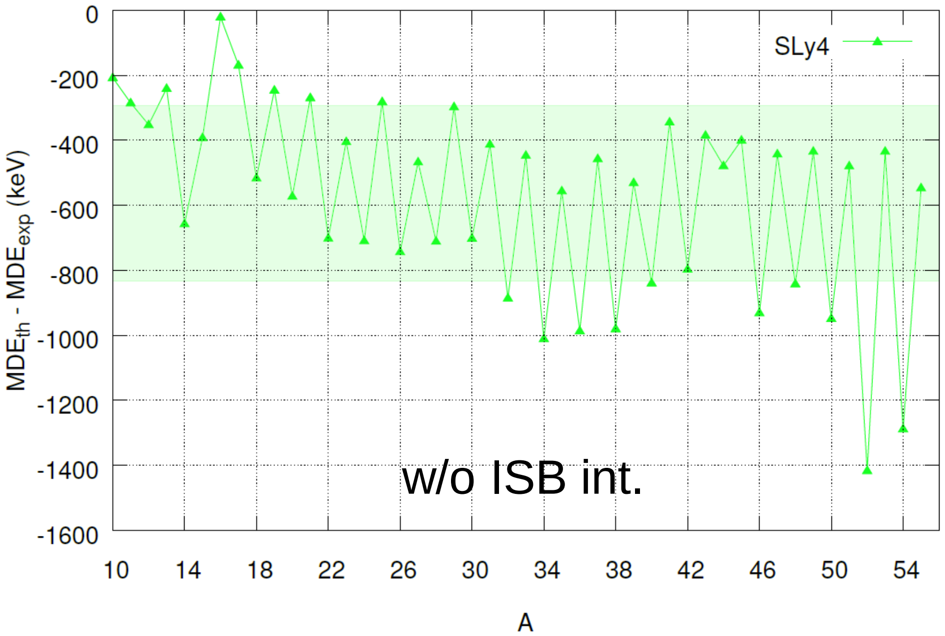
$$\mathcal{H}_{\rm II} = \frac{1}{2} t_0^{\rm II} (\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \boldsymbol{s}_n^2 - \boldsymbol{s}_p^2 + 2\boldsymbol{s}_n \cdot \boldsymbol{s}_p + 2\boldsymbol{s}_{np} \cdot \boldsymbol{s}_{pn})$$

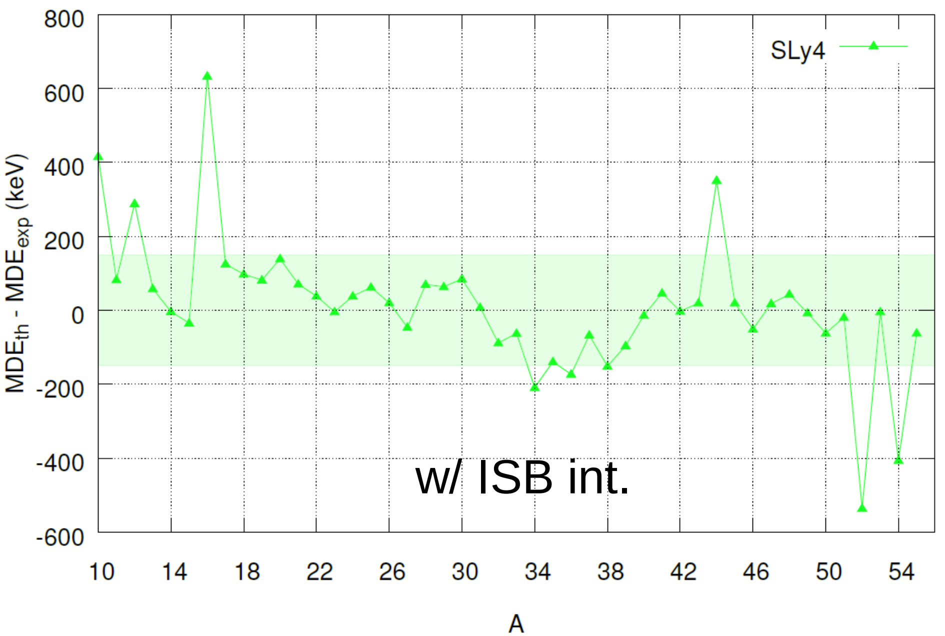
$$\mathcal{H}_{\rm III} = \frac{1}{2} t_0^{\rm III} \left(\rho_n^2 - \rho_p^2 - \boldsymbol{s}_n^2 + \boldsymbol{s}_p^2\right)$$

$t_0^{II} = 22.0$

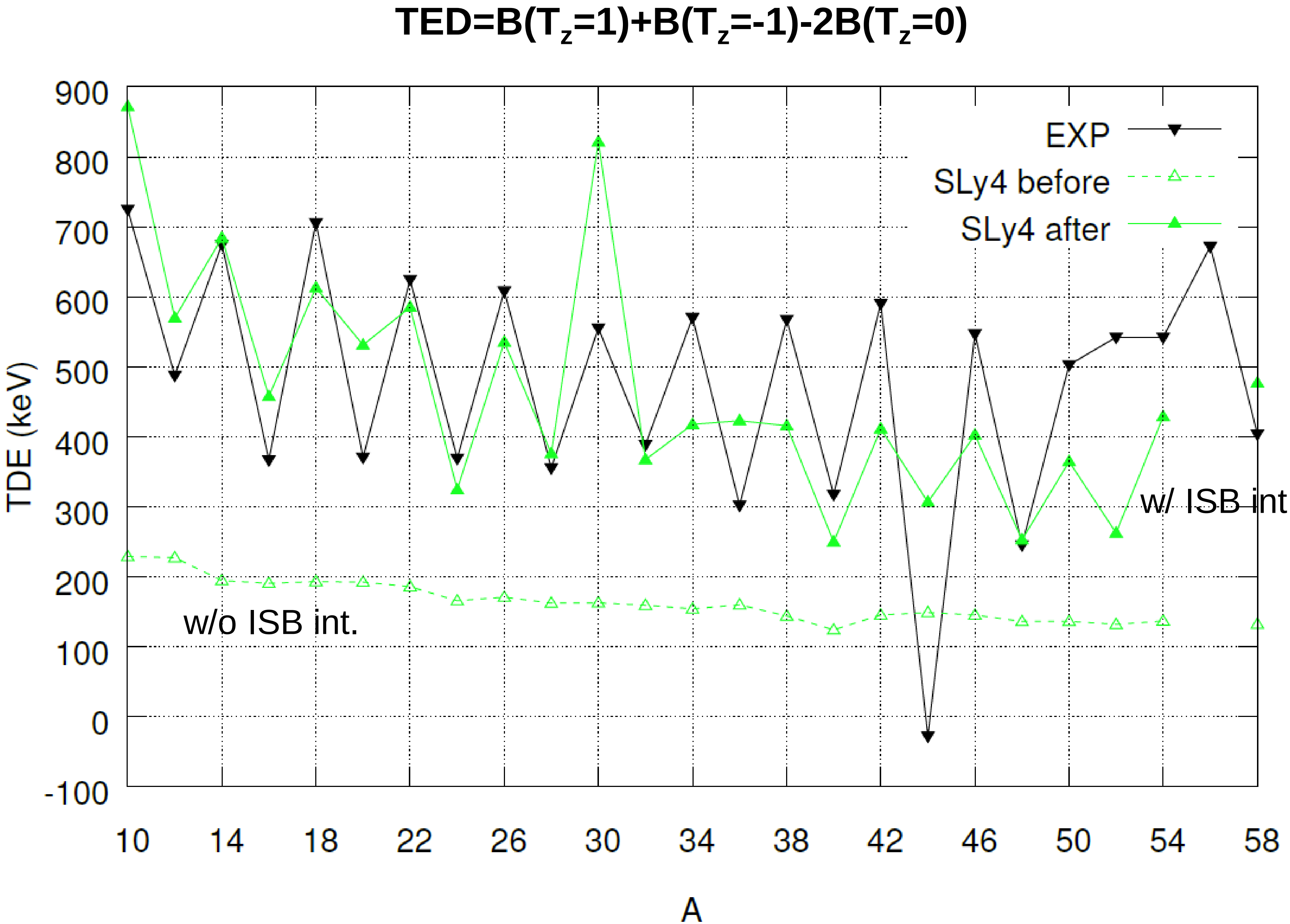
$t_0^{III} = -5.4$

MED(SLy4)-MED(exp) [keV] P. Bączyk et al, in preparation

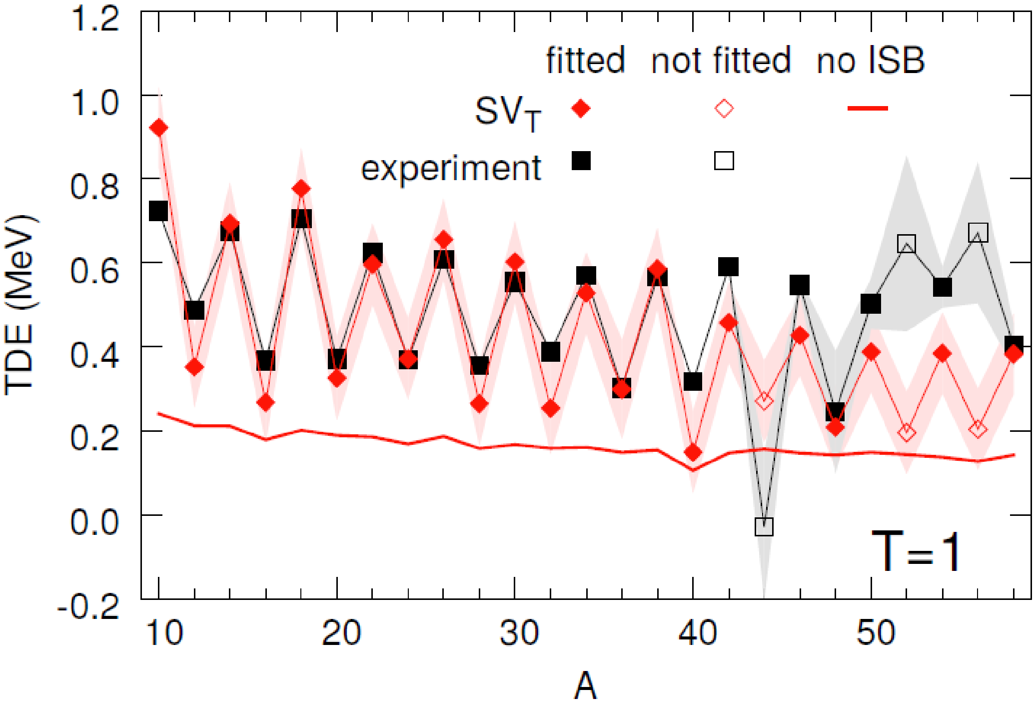


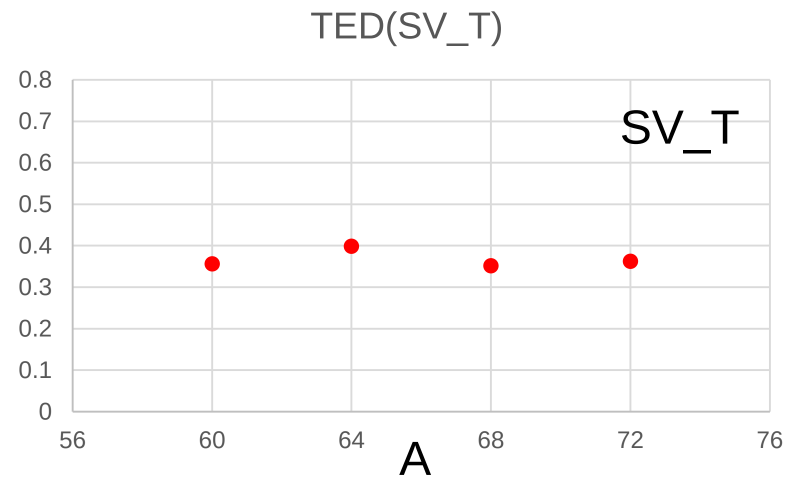


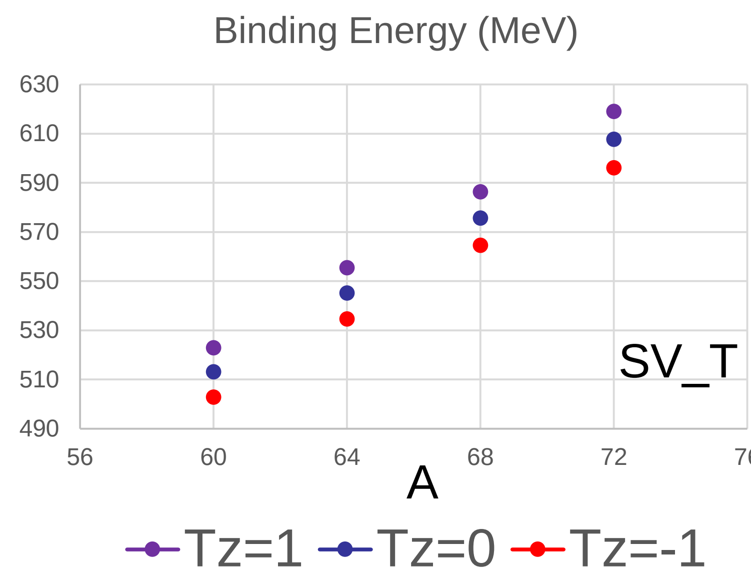
The region within standard deviation highlighted


TED=B(Tz=1)+B(Tz=-1)-2B(Tz=0)
EXP
SLy4 before
SLy4 after
w/ ISB int.
w/o ISB int.
TDE (keV)
A
900
800
700
600
500
400
300
200
100
0
-100
10
14
18
22
26
30
34
38
42
46
50
54
58

TED calculated with SV_T







$t_0^{II} = 16.7$

$t_0^{III} = -7.2$

Summary

- We have solved the Hartree-Fock equations based on the EDF including p-n mixing

- Isospin is controlled by using the isocranking model

- The p-n mixed single-reference EDF is capable of quantitatively describing the isobaric analog states

- For odd(even) A/2, odd(even)-T states can be obtained by isocranking e-e nuclei in their ground states with time-reversal symmetry.

- Possible extension of EDF including nuclear isospin breaking terms