China-Japan collaborative workshop

Nuclear mass and life for unravelling mysteries of r-process

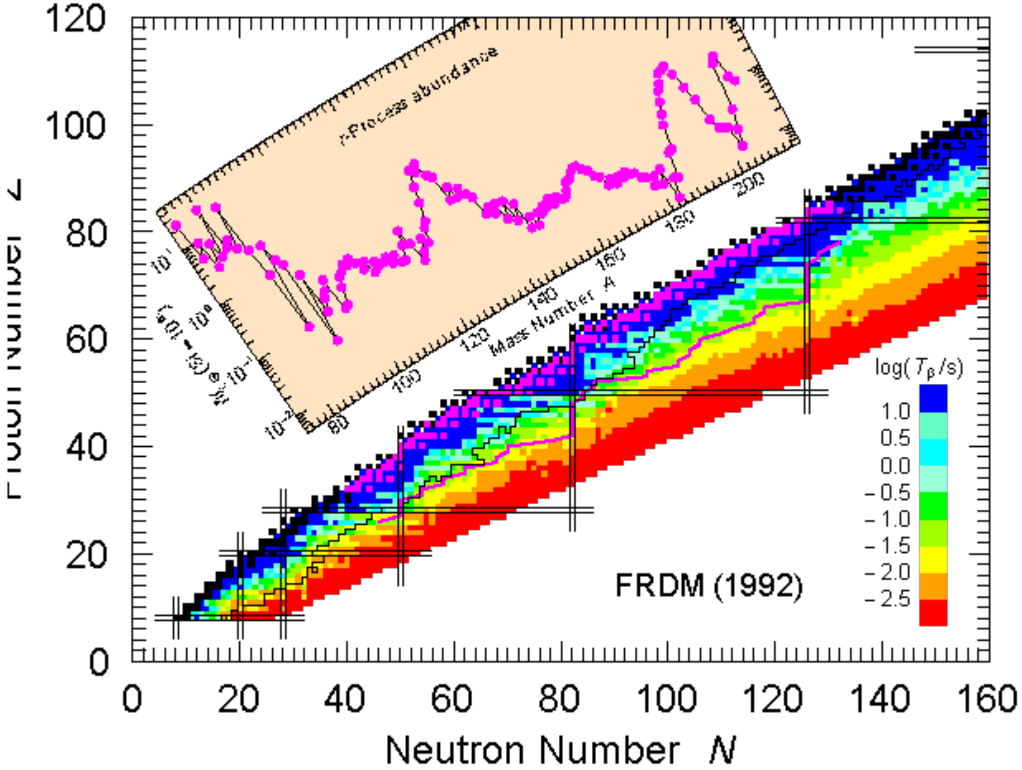
June 26-28, 2017

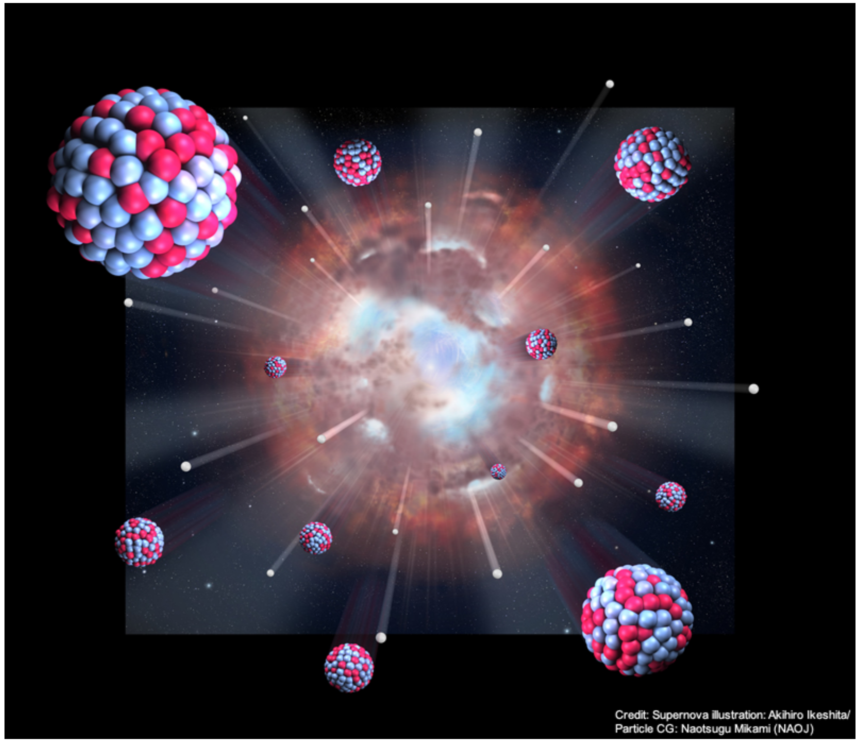
Takashi Nakatsukasa (University of Tsukuba)

- Bilateral Program
- City of Tsukuba
- Isospin-symmetry-breaking effect on nuclear mass

China-Japan Bilateral Program

- Microscopic information for r-process
  - Nuclear mass
  - Nuclear life time





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Blue: Theory
Red: Experiment

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Mt.Tsukuba（筑波山）

筑波山（紫峰）

Isospin symmetry preserving energy density functional and its breaking effect on nuclear mass

Sato et al. PRC 88, 061301(R) (2013)
Sheikh et al. PRC 89, 054317 (2014)
Baczyk et al. arXiv: 1701.04628.

Isoscalar and isovector densities

Isospin

$$|n\rangle = \left|\tau = \frac{1}{2}, \tau_3 = \frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|p\rangle = \left|\tau = \frac{1}{2}, \tau_3 = -\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Nucleon in general

$$|N\rangle = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

One-body isoscalar and isovector density operators

$$\hat{\rho}_i \equiv \left(c_n^+, c_p^+\right)\tau_i \begin{pmatrix} c_n \\ c_p \end{pmatrix}, \quad \tau_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \vec{\tau} = \left(\tau_1, \tau_2, \tau_3\right) \text{:Pauli matrix}$$

$$= \left(c_n^+ c_n + c_p^+ c_p, c_n^+ c_p + c_p^+ c_n, i(c_n^+ c_p - c_p^+ c_n), c_n^+ c_n - c_p^+ c_p\right)$$

$$\left(\hat{\rho}_0, \vec{\hat{\rho}}\right)$$

Energy density functionals of $\left(\rho_n, \rho_p\right)$ are not invariant under the rotation in the isospace.

Rotational invariance in isospace

Energy density functional (EDF) of $\left(\rho_n, \rho_p\right)$, or $\left(\rho_0, \rho_3\right)$

$$\rho_0^2 = \left(\rho_n + \rho_p\right)^2$$

$$\rho_3^2 = \left(\rho_n - \rho_p\right)^2$$

The Coulomb energy is anisotropic in the isospin space, but the rests are (almost) isotropic.

EDF of $\left(\rho_0, \vec{\rho}\,\right)$

$$\rho_0^2 = \left(\rho_n + \rho_p\right)^2$$

$$\vec{\rho}^{\,2} = \rho_1^2 + \rho_2^2 + \rho_3^2$$

$$= \left(\rho_{np} + \rho_{pn}\right)^2 + \left(-i\rho_{pn} + i\rho_{np}\right)^2 + \left(\rho_n - \rho_p\right)^2$$

General EDF from: Perlinska et al, PRC 69, 014316(2004)

pn-mixed orbitals

p-n mixed s.p. wave functions

$\boxed{(p,n) \rightarrow (1,2)}$

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

$\phi_1(\boldsymbol{r},p) = \phi_2(\boldsymbol{r},n) = 0$ ⇨ Standard unmixed neutron and proton w. f. $\phi_1 = \phi_n, \phi_2 = \phi_p$

Hartree-Fock representation of density (Kohn-Sham)

$$\rho = \sum_{i:\mathrm{occ}} |\phi_i\rangle\langle\phi_i|$$

$$
\left.
\begin{aligned}
\rho(\boldsymbol{r},nn) &= \phi_1(\boldsymbol{r},n)\phi_1^*(\boldsymbol{r},n) + \phi_2(\boldsymbol{r},n)\phi_2^*(\boldsymbol{r},n), \\
\rho(\boldsymbol{r},pp) &= \phi_1(\boldsymbol{r},p)\phi_1^*(\boldsymbol{r},p) + \phi_2(\boldsymbol{r},p)\phi_2^*(\boldsymbol{r},p),
\end{aligned}
\right\} \text{Diagonal n and p densities}
$$

$$
\left.
\begin{aligned}
\rho(\boldsymbol{r},np) &= \phi_1(\boldsymbol{r},n)\phi_1^*(\boldsymbol{r},p) + \phi_2(\boldsymbol{r},n)\phi_2^*(\boldsymbol{r},p), \\
\rho(\boldsymbol{r},pn) &= \phi_1(\boldsymbol{r},p)\phi_1^*(\boldsymbol{r},n) + \phi_2(\boldsymbol{r},p)\phi_2^*(\boldsymbol{r},n).
\end{aligned}
\right\} \text{Off-diagonal p \& n densities}
$$

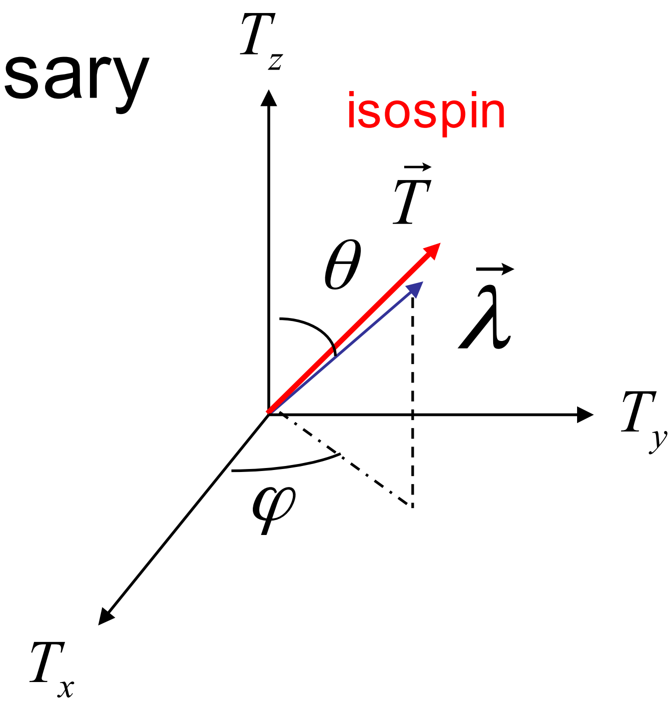
p-n mixing is required in the single-particle orbitals

Isocranking calculation

- Standard HF calculation
  - (N,Z) are specified.
- pn-mixed HF calculation
  - Only A=N+Z is specified.
  - Additional constraint is necessary
- Direction of isospin
  - Cranking terms

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

  - Eigenvalues: Routhians



Tilted cranking for IAS

- Standard HF calculation
  - Proton & neutron Fermi levels $\varepsilon_F^{(n)}, \varepsilon_F^{(p)}$
- pn-mixed HF calculation
  - Nucleon Fermi level only $\boxed{\varepsilon_F}$

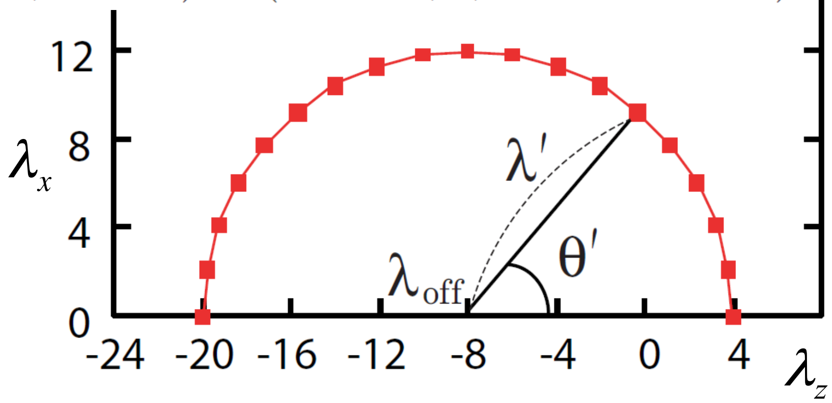
$$\hat{h}' = \hat{h} - \vec{\lambda} \cdot \hat{\vec{t}},$$

  - Cranking term $-\lambda_z T_z$ should lead to $\varepsilon_F^{(n)} \approx \varepsilon_F^{(p)} = \varepsilon_F$
  - Change the direction (tilted-axis) to obtain IAS with different T_z

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

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

$$\lambda_{np}^{T_z=\pm T} \equiv \varepsilon_F^{(n)} - \varepsilon_F^{(p)}$$



We have developed a code for pnHF by extending an HF(B) solver

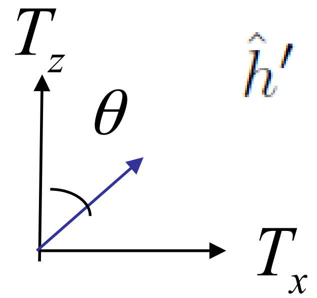
HFODD(1997-)

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

J. Dobaczewski, J. Dudek, Comp. Phys. Comm 102 (1997) 166.
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 102 (1997) 183.
J. Dobaczewski, J. Dudek, Comp. Phys. Comm. 131 (2000) 164.
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 158 (2004) 158.
J. Dobaczewski, P. Olbratowski, Comp. Phys. Comm. 167 (2005) 214.
J. Dobaczewski, et al., Comp. Phys. Comm. 180 (2009) 2391.
J. Dobaczewski, et al., Comp. Phys. Comm. 183 (2012) 166.

- Skyrme energy density functional
- Hartree-Fock or Hartree-Fock-Bogoliubov
- No spatial & time-reversal symmetry restriction
- Harmonic-oscillator basis
- Multi-function (constrained HFB, cranking, angular mom. projection, isospin projection, finite temperature….)

A=48 isobars w/o Coulomb



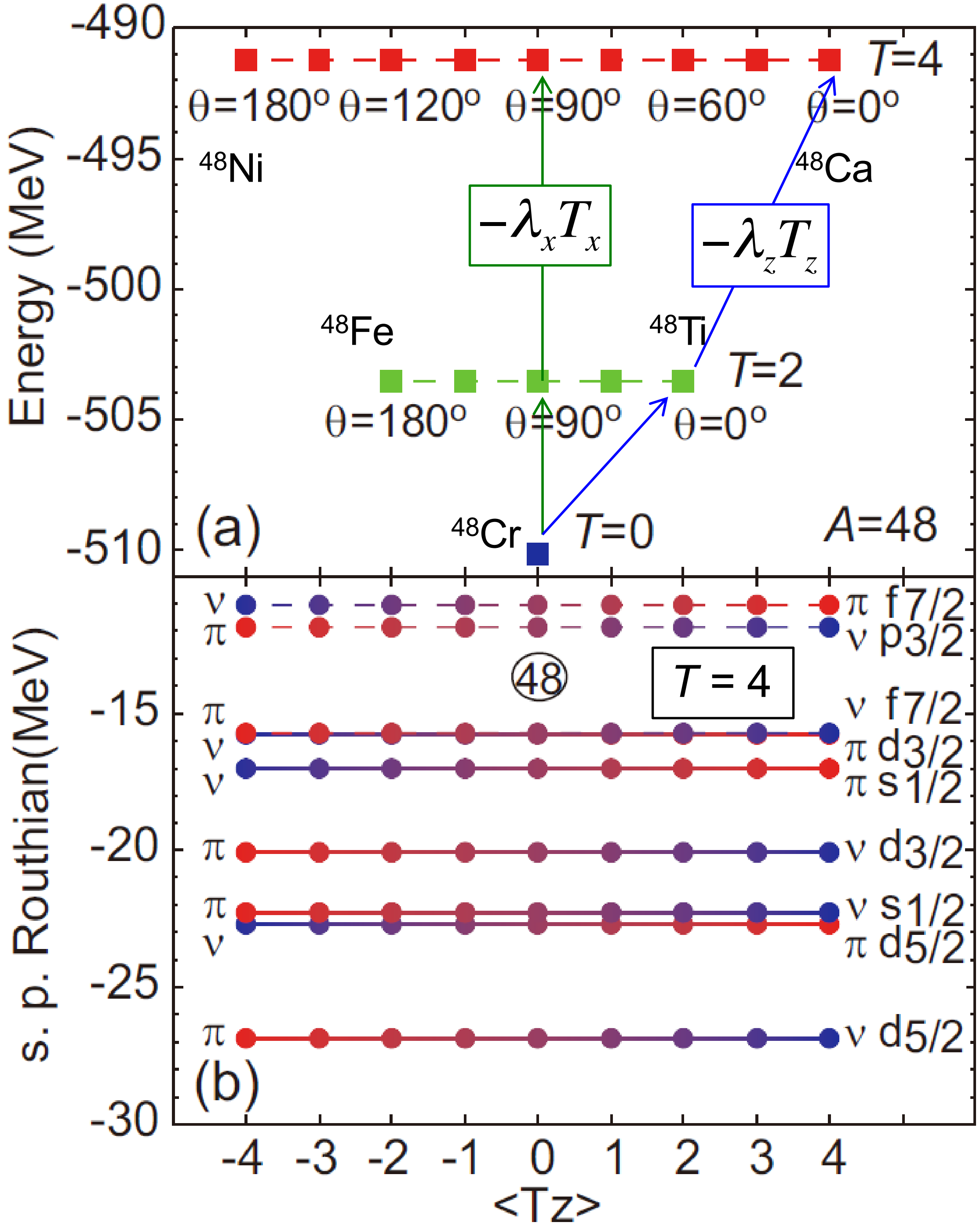
$$\hat{h}' = \hat{h} - \vec{\lambda} \cdot \vec{\hat{t}},$$

No p-n mixing at $|T_z|=T$

(T, T_z) are controlled by the "isocranking".

Energies are independent of T_z

In addition to the ground state, the IAS are described by HF states.



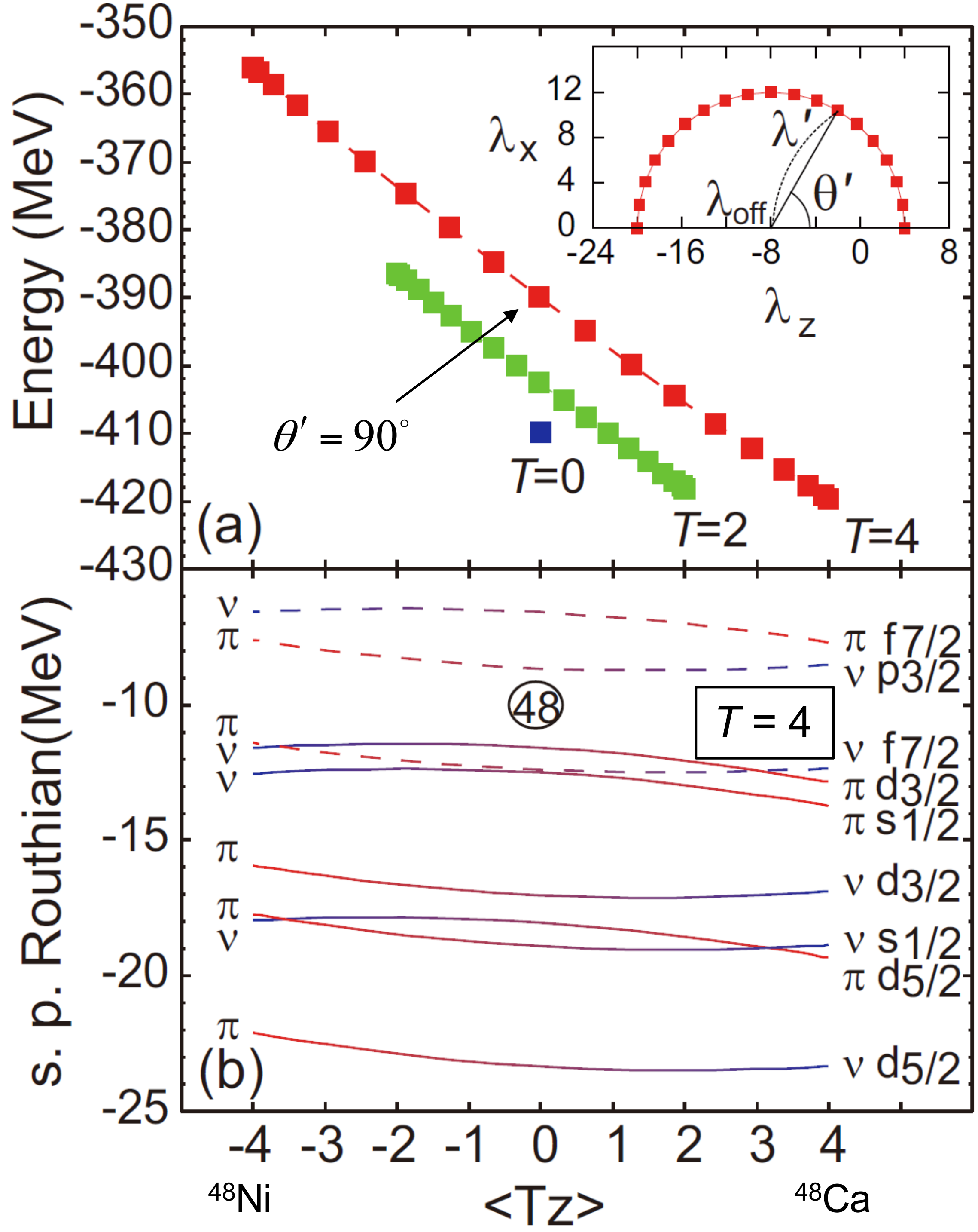
A=48 isobars with Coulomb

Energies now depend on T_z because of the Coulomb int.

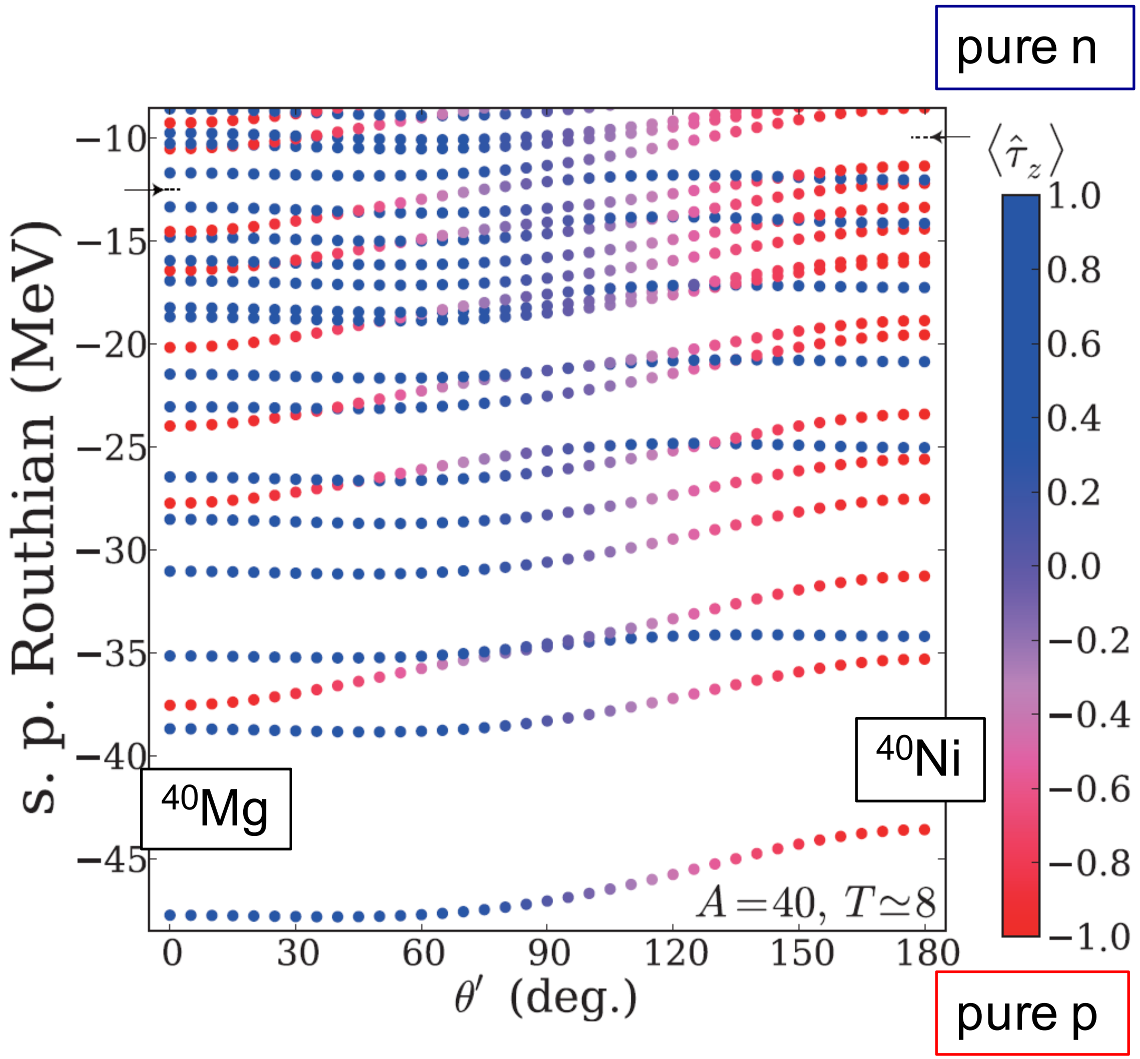
(almost linear dependence)

No p-n mixing at |Tz|=T

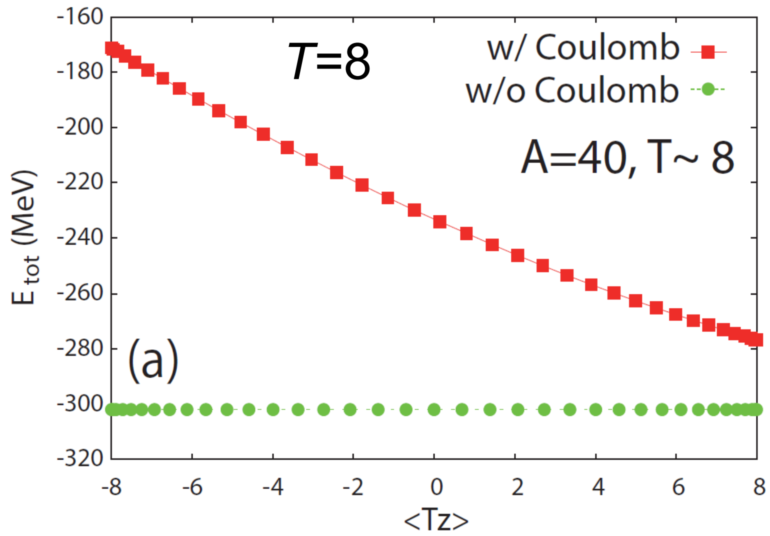
Single-particle routhians are roughly independent on the direction of T.



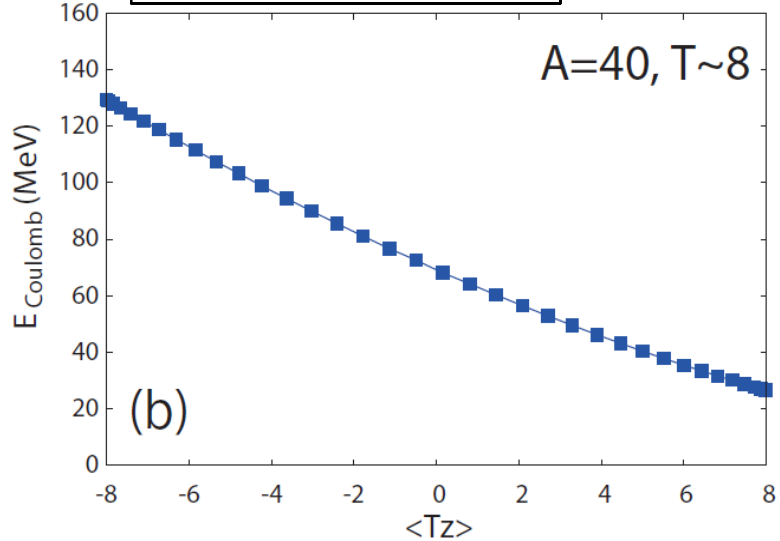
A=40 isobars for T=8 IAS's



Total energy



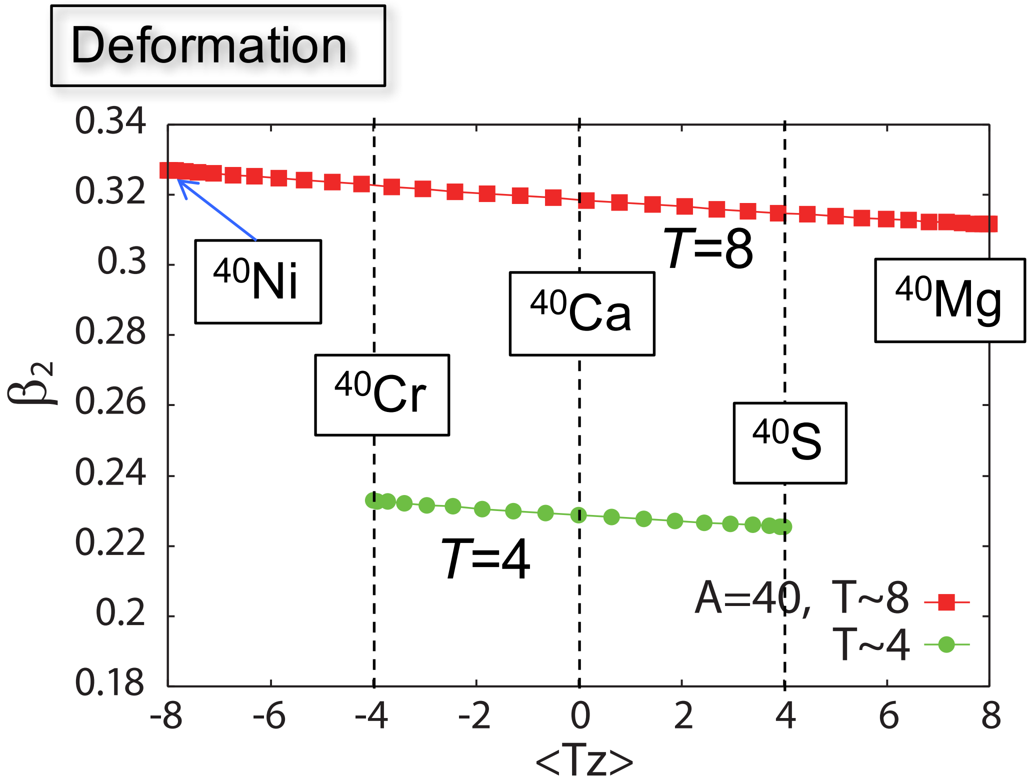
Coulomb energy

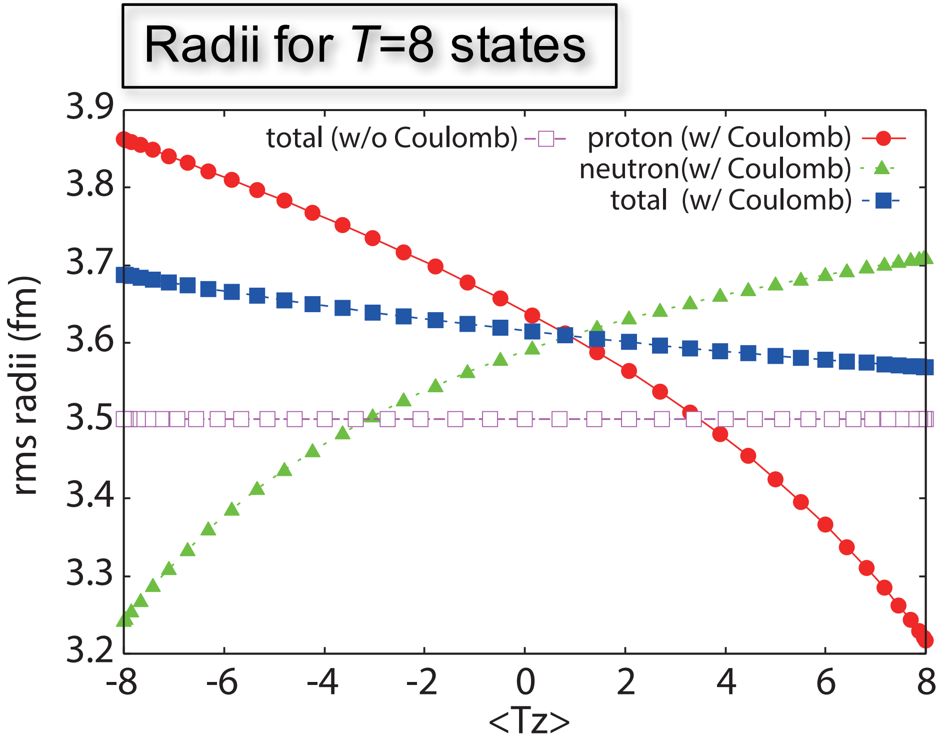


Energy difference mostly comes from the Coulomb energy difference.

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

IAS's in A=40 isobars





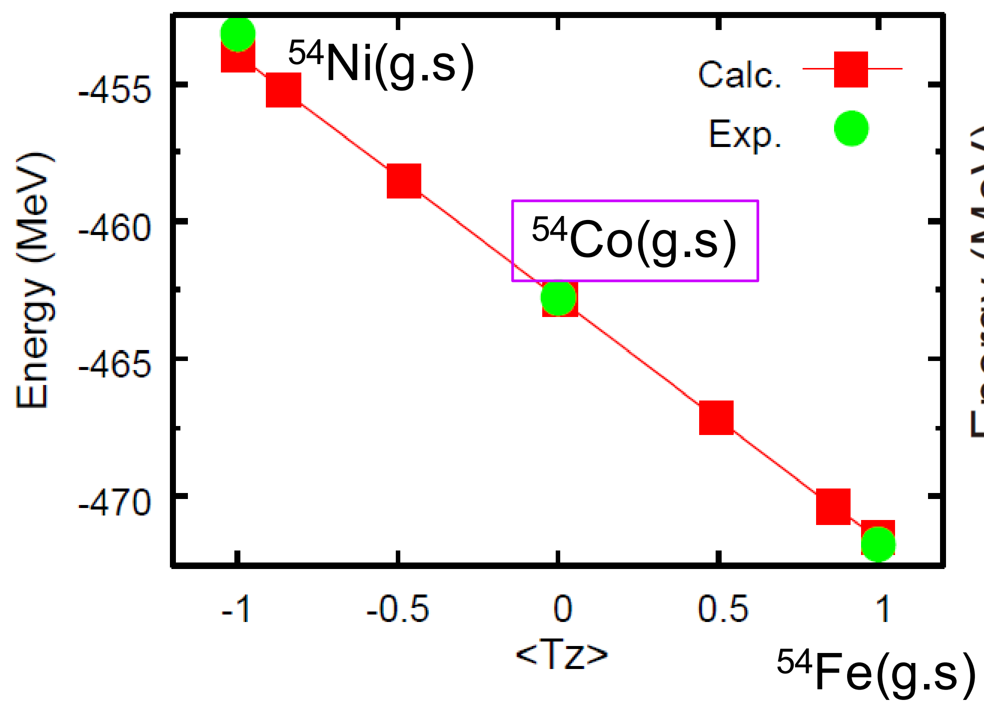
Deformation stays almost constant among IAS's.

Proton and neutron radii changes, but the matter radius is roughly constant.

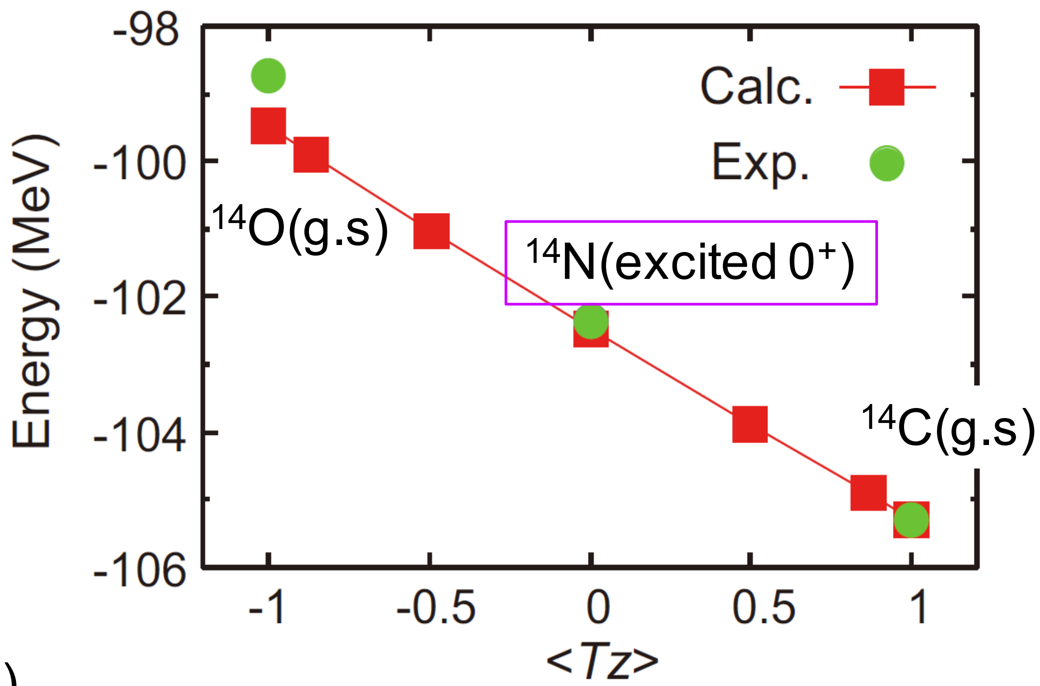
Comparison with experiments

- Energies of T=1 triplets (with SkM*)

A=54 isobars



A=14 isobars



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

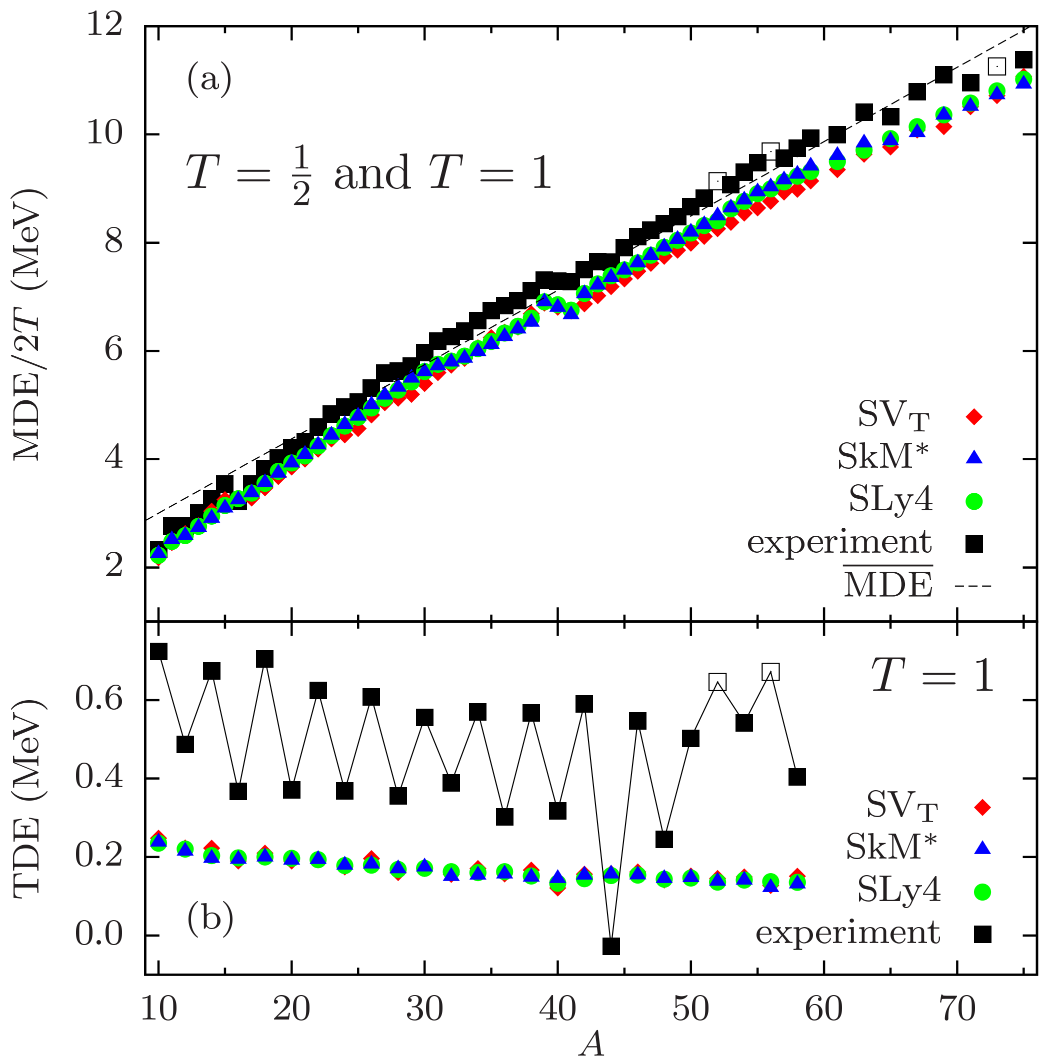
MDE & TDE

- Mirror Energy Displacement

$$MDE \equiv E(T, T_z = -T) - E(T, T_z = +T)$$

- Triple Energy Displacement

$$TDE \equiv E(T=1, T_z=-1) + E(T=1, T_z=+1) - 2E(T=1, T_z=0)$$



Extension of EDF

Standard EDF (SLy4 as an example)

- Isospin-symmetry-breaking interaction
  - Class II (CIB) and III (CSB)

$$\hat{V}^{\mathrm{II}}(i,j) = \frac{1}{2} t_0^{\mathrm{II}} \, \delta\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right) \left[3\hat{\tau}_3(i)\hat{\tau}_3(j) - \hat{\vec{\tau}}(i) \circ \hat{\vec{\tau}}(j) \right]$$

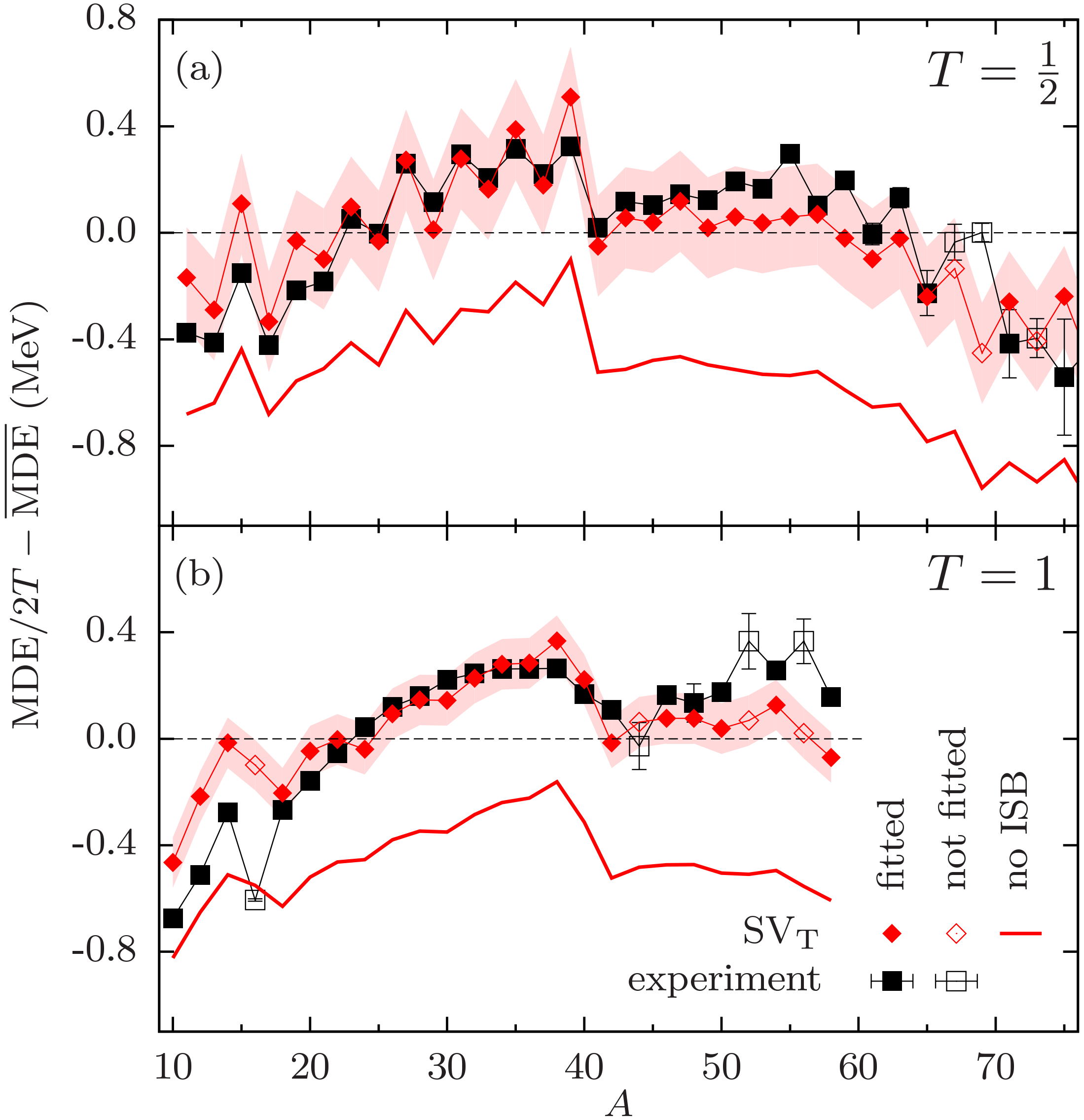
$$\hat{V}^{\mathrm{III}}(i,j) = \frac{1}{2} t_0^{\mathrm{III}} \, \delta\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right) \left[\hat{\tau}_3(i) + \hat{\tau}_3(j) \right].$$

  - Two parameters, t_0^{II} and t_0^{III}, are determined by fitting MDE and TDE.

MDE

- Mirror energy displacement
  - Can be well reproduced by

$t_0^{III} = -7.4$ MeV fm^3 for SV_T

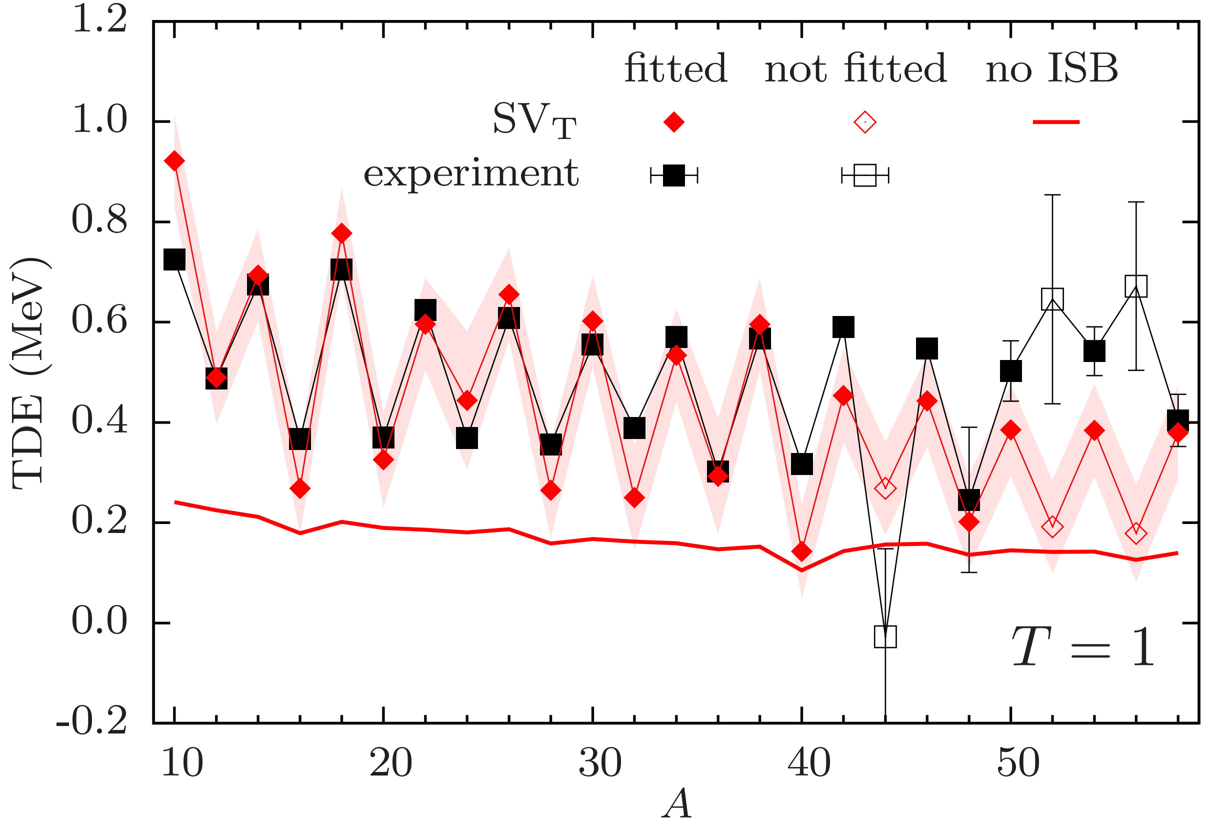


TDE

- Triple energy displacement
  - Can be well reproduced by

$$t_0^{II} = 17 \text{ MeV fm}^3$$

for SV_T



Relation to nuclear force

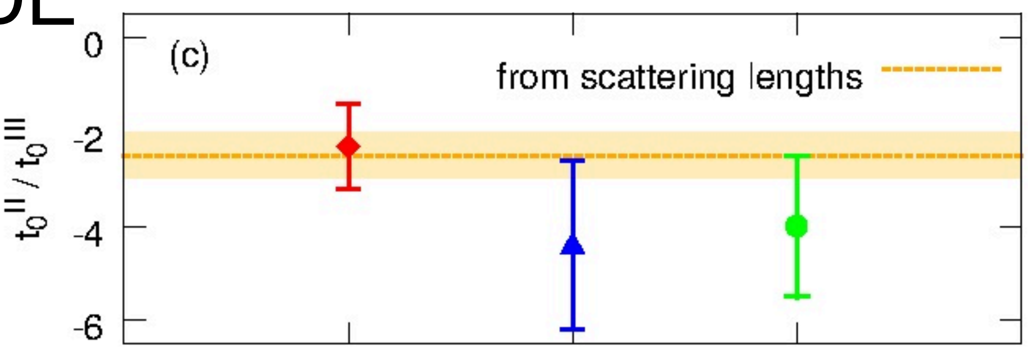
- Phase shift analysis
  - Charge symmetry breaking

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

  - Charge independence breaking

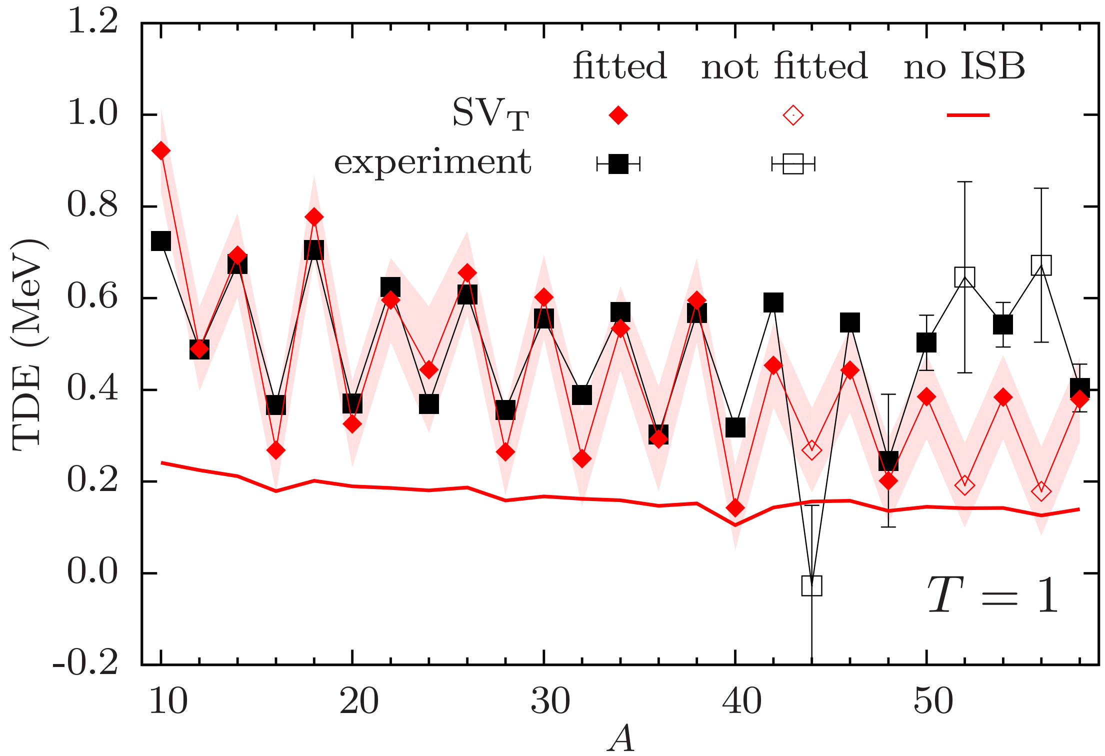
$$\Delta a_{CIB} \equiv \frac{1}{2}\left(a_{pp} + a_{nn}\right) - a_{np} = 5.7 \pm 0.3 \text{ fm}$$

- The present work
  - By fitting MDE & TDE
  - $\boxed{\dfrac{t_0^{II}}{t_0^{III}} = -\dfrac{2}{3}\dfrac{\Delta a_{CIB}}{\Delta a_{CSB}}}$



Error in experimental mass?

- Removing from fitting process
  - ^{52}Co, ^{56}Cu, ^{73}Rb
  - ^{44}V



Mass prediction

Nucleus	Mass excess (keV) This work	AME12 [22]
^{52}Co	−34450(50)	−33990(200)#
^{56}Cu	−38720(50)	−38240(200)#
^{73}Rb	−46100(80)	−46080(100)#
^{44}V	−23770(50)	−24120(180)

^{52}Co: −34361 MeV [Xu et al., PRL 117, 182503 (2016)]

Summary

- Energy density functional including the proton-neutron mixing in single-particle orbitals
- Natural description of isobaric analogue states in terms of “Slater determinants”
- Extension of the EDF: Isospin symmetry breaking terms
  - Good agreement with MDE and TDE
  - Discrepancy for specific nuclei: ^{52}Co, ^{56}Cu, ^{73}Rb, ^{44}V