Nuclear density functional calculations with proton-neutron mixing

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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

$$|n\rangle = \left|\tau = +1/2\right\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$

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

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

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

- Proton-neutron mixing:

  Single-particles are mixtures of protons and neutrons

  EDF with an arbitrary mixing between protons and neutrons

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

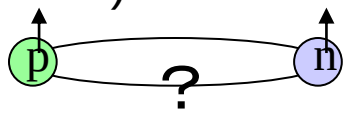
$$\tau = p,n \qquad \tau,\tau' = p,n$$

➡ Extension of the EDF approach with rigorous treatment of the isospin d. o. f.

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

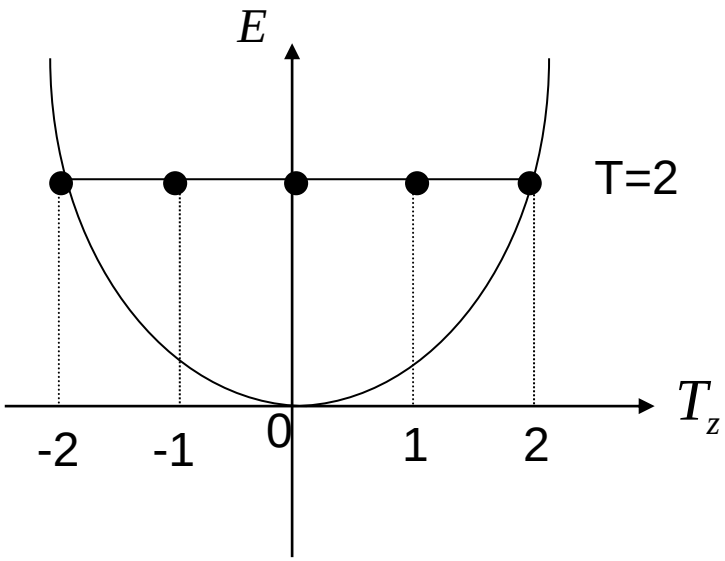
Pairing between protons and neutrons (isoscalar T=0 and isovector T=1)

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



Isobaric analog states (IASs) : isospin multiplets

Isobaric symmetry



If Hamiltonian is invariant under rotation in isospin space, T is a good quantum numbe

$$T_z = (N - Z)/2$$

Bohr & Mottelson, "Nuclear Structure" vol.1

T=1 states in A=14 isobars

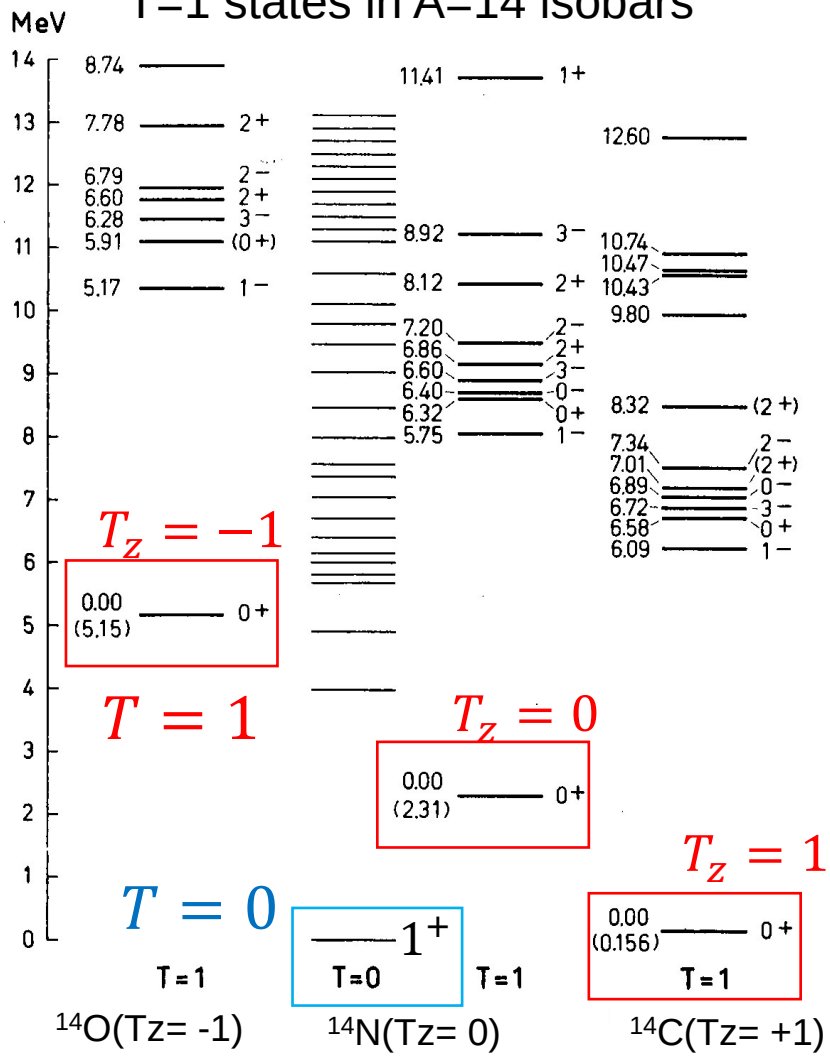


Figure 1-7 The level schemes for the nuclei with $A = 14$ are based on the compilation by F. Ajzenberg-Selove and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959), on the results given by D. E. Alburger, A. Gallmann, J. B. Nelson, J. T. Sample, and E. K. Warburton, *Phys. Rev.* **148**, 1050 (1966), and on a private communication by G. Ball and J. Cerny (August, 1966). The relative energies represent atomic masses.

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

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

standard n and p densities

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

$$|\psi_{i,n}\rangle = \sum_{\alpha} a_{i,\alpha}^{(n)} |\alpha, n\rangle$$
$$|\psi_{j,p}\rangle = \sum_{\alpha} a_{j,\alpha}^{(p)} |\alpha, p\rangle$$

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

i=1,…,A

- Extension of the density functional

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

Invariant under rotation in isospin space

isoscalar isovector

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

Two implementations of p-n mixed Hartree-Fock (pnHF)

HFODD

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

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

N. Schunck, et al., Comp. Phys. Comm. 216 (2017) 145.
J Dobaczewski et al, J. Phys. G: Nucl. Part. Phys. **48** (2021)102001.

- 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.

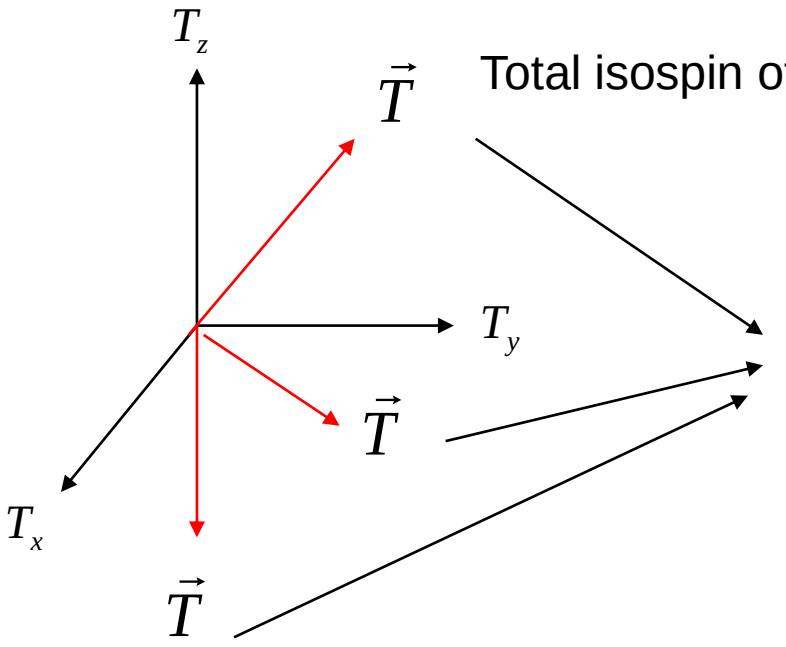
Axially symmetric shape assumed（Cylindrical basis）

Good agreement in benchmark comparison

p-n mixing calculation w/o Coulomb

w/o Coulomb force (and w/ equal proton and neutron masses)

$\mathcal{H} = \mathcal{H}_{\mathrm{kin}} + \mathcal{H}_{\mathrm{Skyrme}}$:invariant under rotation in isospin space



Total isospin of the system

Rotational invariance in isospace

Total energy should be independent of the orientation of T.

All the isobaric analog states should give exactly the same energy

"Isobaric analog states"

How to control the isospin direction ?

Isocranking calculation

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

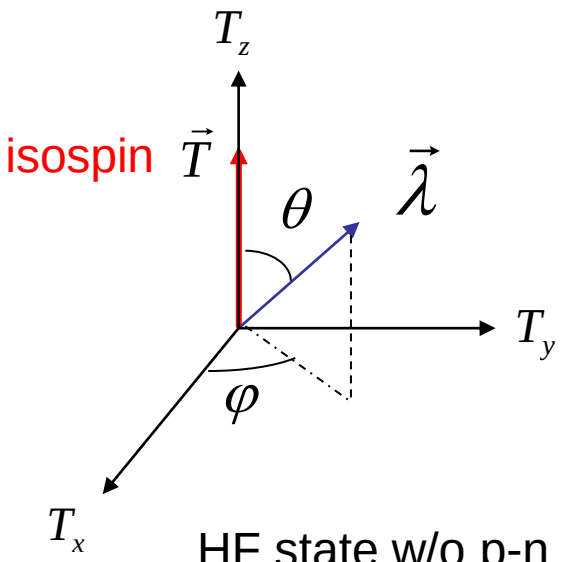
Analog with the tilted axis cranking for high-spin states

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

HF eq. solved by iterative diagonalization of MF Hamiltonian.

w/ p-n mixing and no Coulomb

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

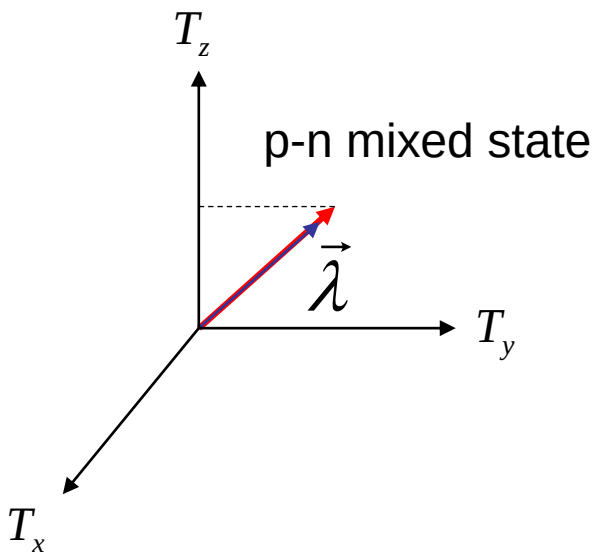


HF state w/o p-n mixing

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

iteration

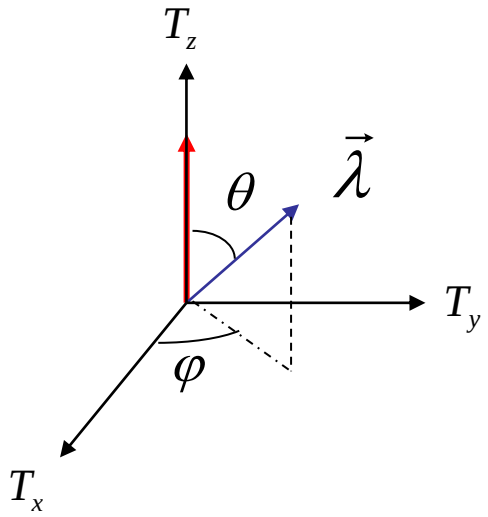
Final state



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

Even with the Coulomb interaction, the Hamiltonian is invariant under the isorotation about Tz axis.

H depends on only $\hat{\tau}_z$ in the form of $\frac{(1-\hat{\tau}_z)}{2}$



We set the azimuthal angle φ=0.

Isocranking calculations in the Tx-Tz plane.

This choice has an advantage of avoiding the time-reversal symmetry breaking inherent to the isorotation about the Ty axis.

time-reversal op.

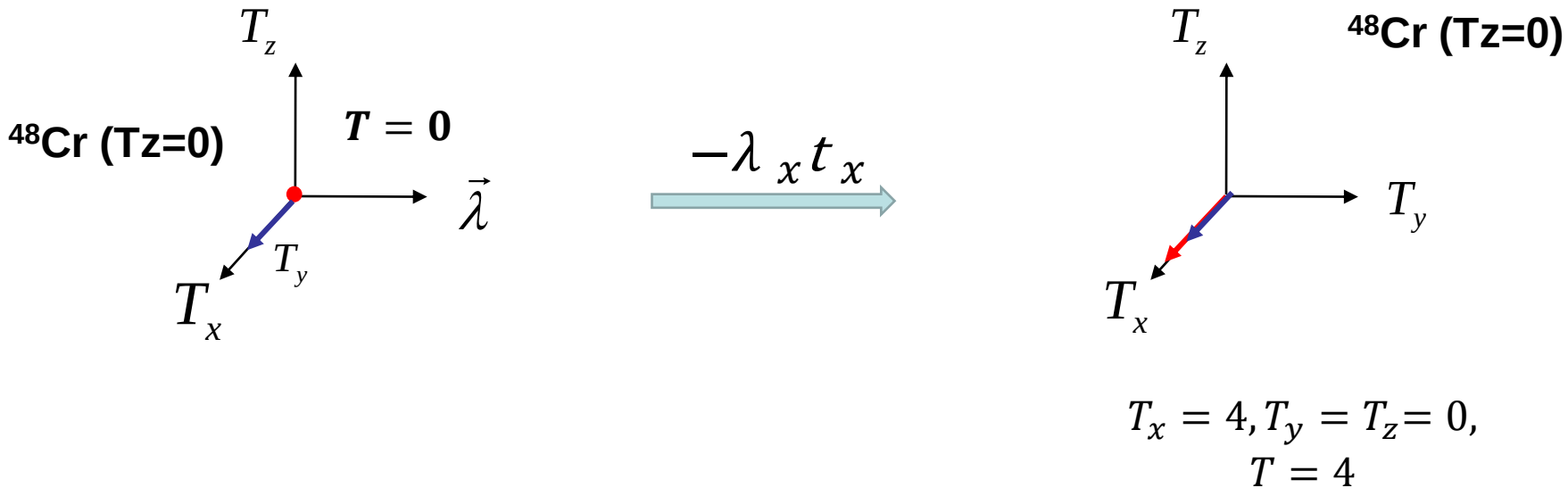
$$\hat{T} \equiv \bigotimes_{n=1}^{A} (-i\hat{\sigma}_y^{(n)})\hat{K}$$

$$\tau_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$: imaginary

$$\tau_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$: real

Assume we want to obtain the T=4 & Tz=0 IAS in 48Cr (w/o Coulomb)

(a) Starting with the T=0 state

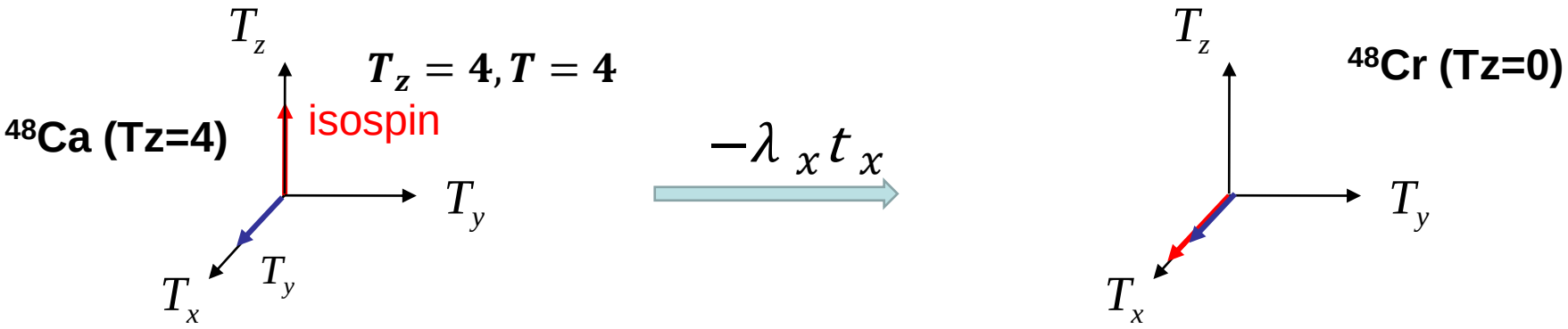


48Cr (Tz=0)

48Cr (Tz=0)

$T_x = 4, T_y = T_z = 0,$
$T = 4$

(b) Starting with the highest weight state.

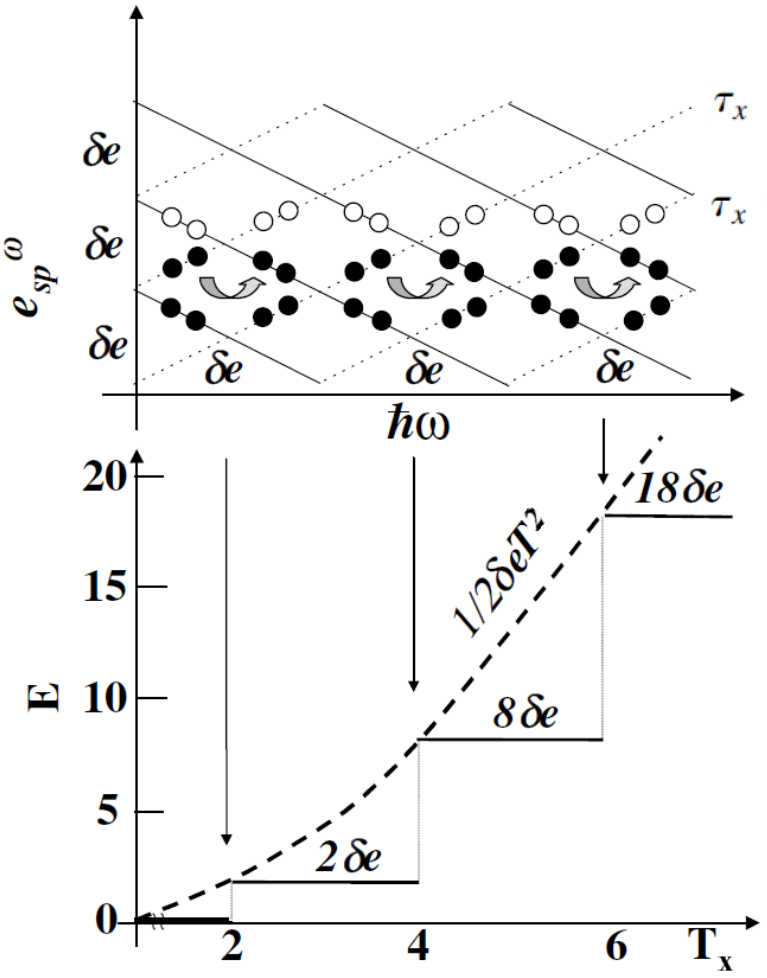


48Ca (Tz=4)

48Cr (Tz=0)

(a) Starting with the T=0 state

Illustration with a simple model W. Satuła & R. Wyss, PRL 86, 4488 (2001).



$$\hat{H}^{\omega} = \hat{H}_{sp} - \hbar\omega\hat{t}_x$$

equidistant $[e_i = i\delta e]$

Four-fold degeneracy at ω=0
(isospin & time-reversal)

At each crossing freq., $\Delta T_x = 2$

$T_z = T_y \equiv 0$, i.e., $\Delta T_x \equiv \Delta T$

To get T=1,3, ･･ states,
we make a 1p1h excitation

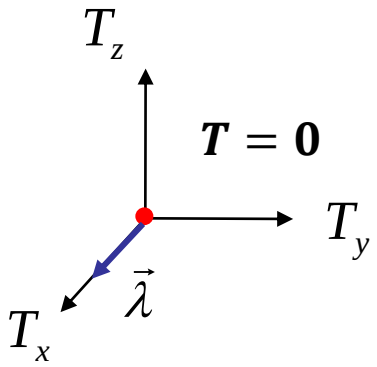
In this study, we use the Hamiltonian based on the EDF with p-n mixed densities.

Assume we want to obtain the T=4 & Tz=0 IAS in 48Cr (w/o Coulomb)

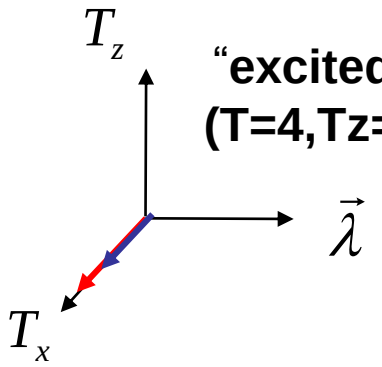
N=Z=24

(a) Starting with the T=0 state

^{48}Cr (g. s.)
(T=Tz=0)



$-\lambda_x t_x$



"excited ^{48}Cr"
(T=4,Tz=0)

Increase T w/o changing Tz

$T_x = 4, T_y = T_z = 0,$
$T = 4$

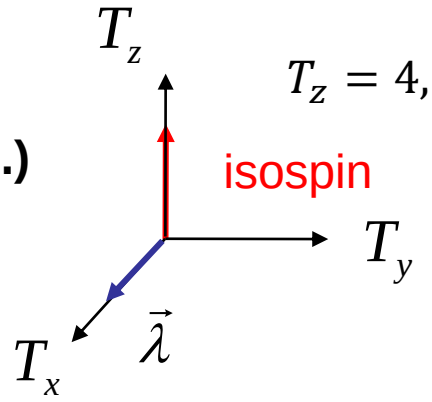
Actually, the state with $T_z = 0$ obtained here is not a pure "^{48}Cr", but a mixture of states with different T_z values, whose expectation value of T_z, $\langle T_z \rangle$ is equal to 0.

The state on the right is a state with good T_x , but $\hat{T}_x$and $\hat{T}_z$ do not commute. Therefore, it is not an eigenstate of $\hat{T}_z$.

Another way to obtain the T=4 & Tz=0 IAS in 48Cr

$T_x = 4, T_y = T_z = 0,$
$T = 4$

(b) Starting with the highest weight state.



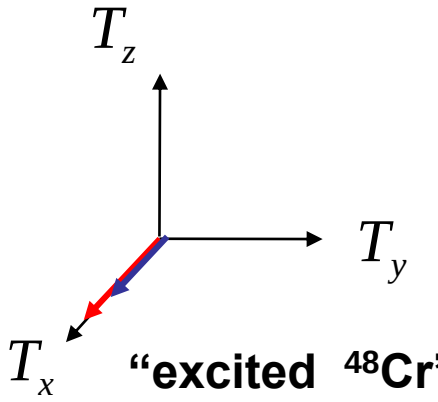
$T_z = 4, T = 4$

^{48}Ca (g. s.)
(T=Tz=4)

isospin

$-\lambda_x t_x$

change the orientation of $\vec{T}$



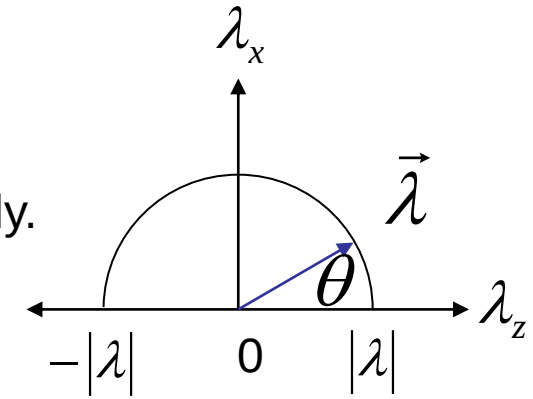
"excited ^{48}Cr"
(T=4,Tz=0)

We employ this way of obtaining the state with $\langle T_z \rangle$ =0.

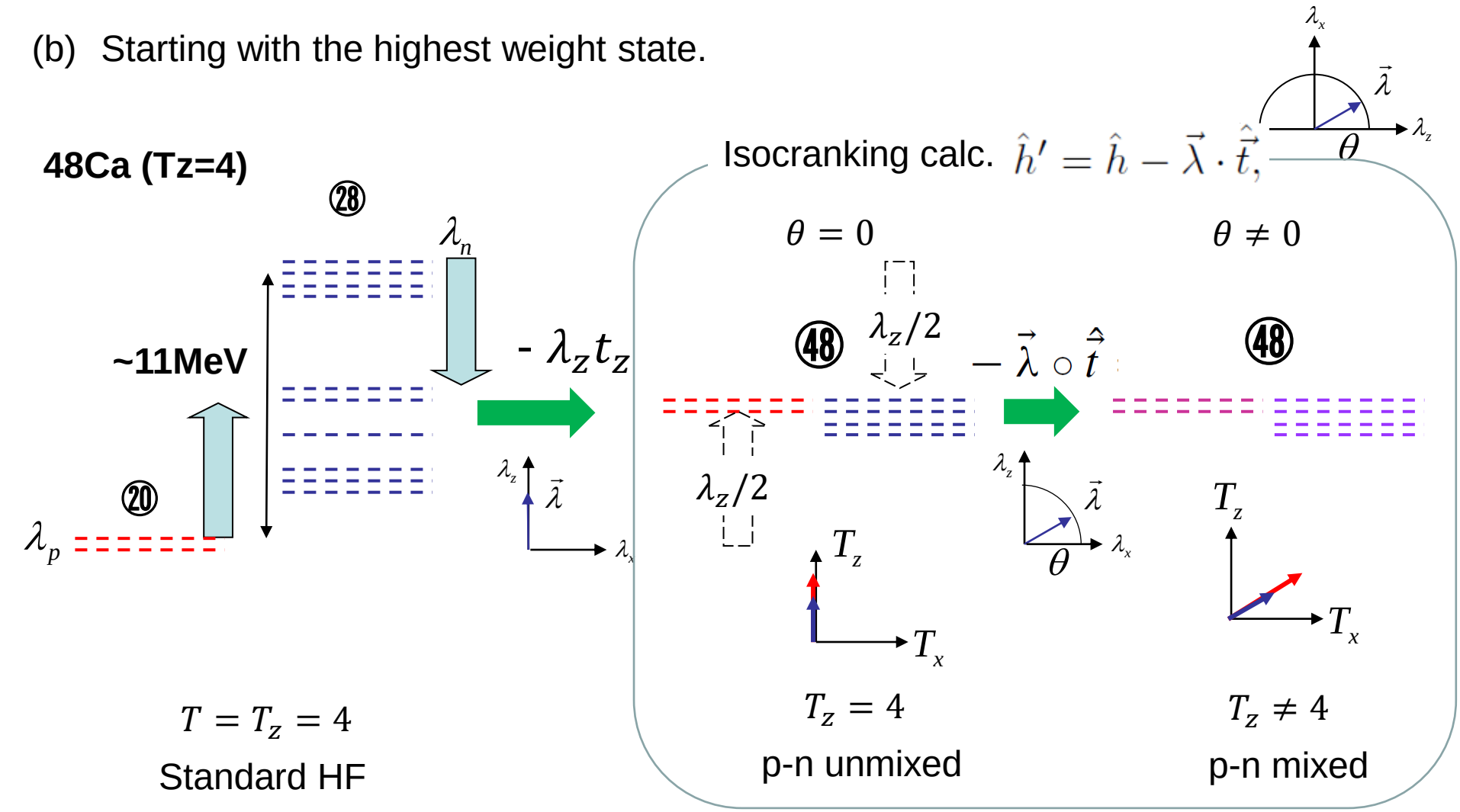
Reasons:

The states with $\langle T_z \rangle = 0, 1, 2, ..$ can be obtained straightforwardly.

It is easy to estimate the size of the Lagrange multiplier $|\vec{\lambda}|$.

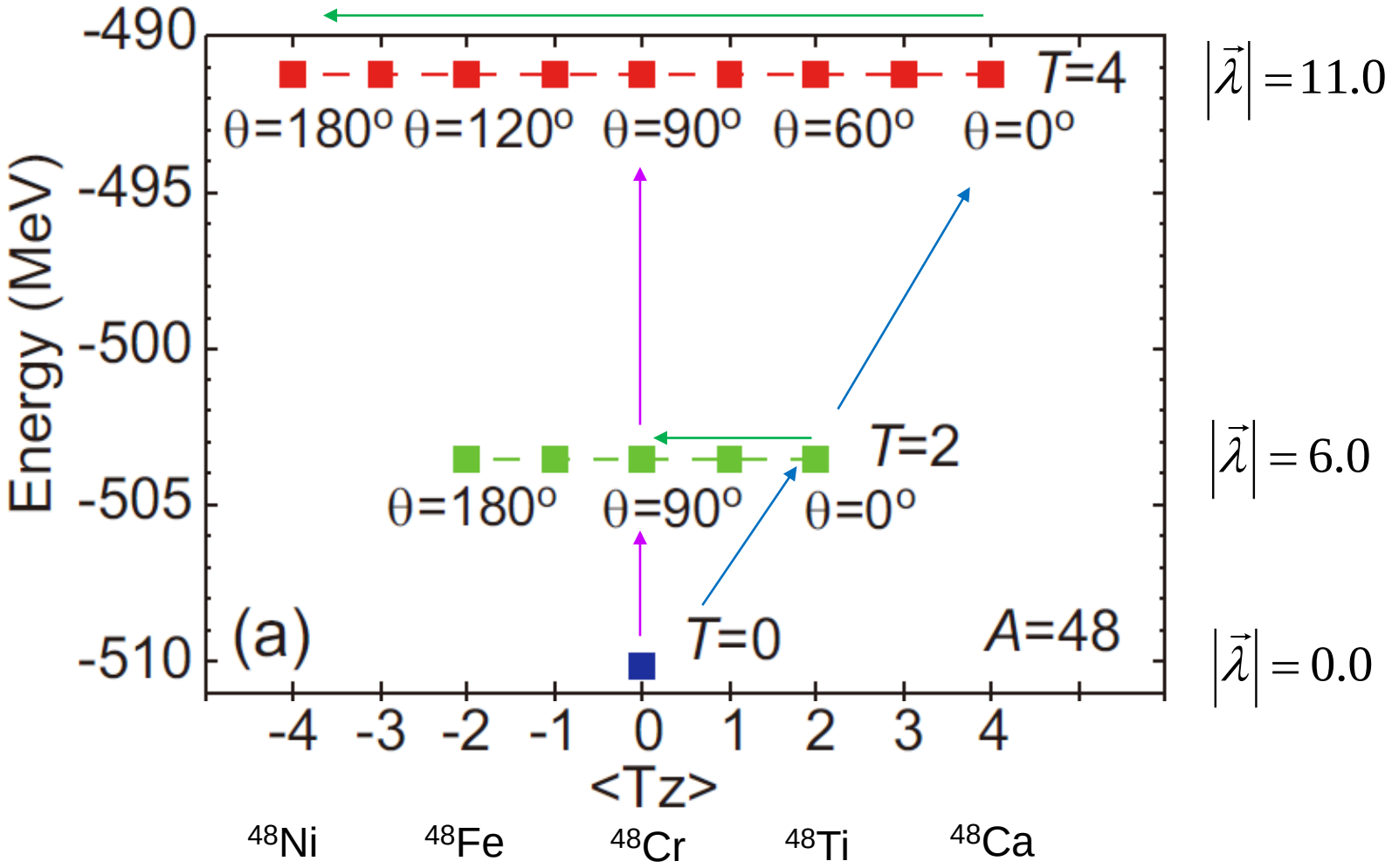


(b) Starting with the highest weight state.



The size of the isocranking frequency is determined from the difference of the proton and neutron Fermi energies in the $|T_z| = T$ states. $\left|\vec{\lambda}\right| = 11.0$

Calculation for A=48 nuclei w/o Coulomb



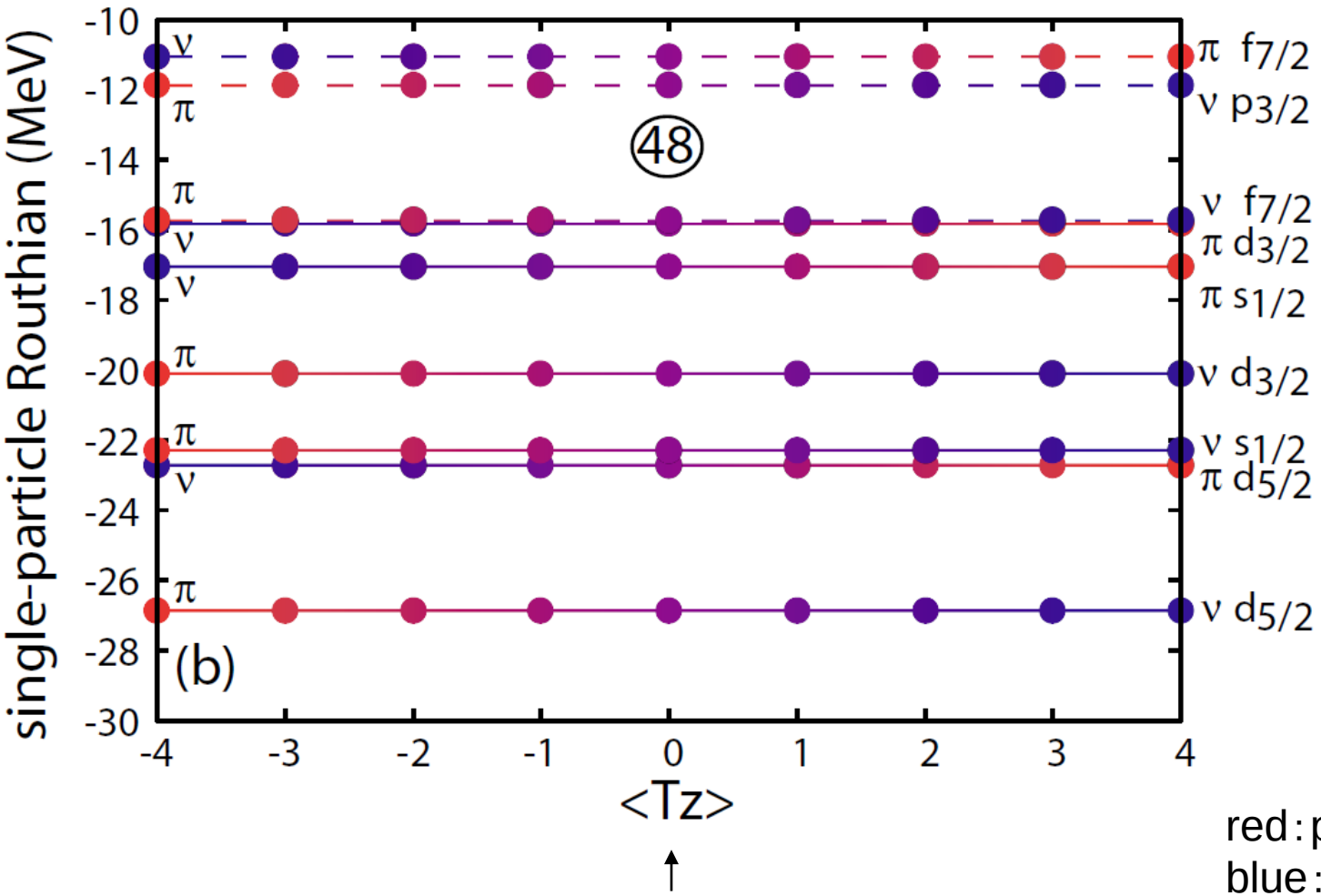
$|T_z| \neq T$ states can be obtained by isocranking the initial $|T_z| = T$ state

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

<Single-particle Routhian> for T=4 states（w/o Coulomb）

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



red : proton
blue : neutron

50% neutron & 50% proton

- s.p. energy is Tz-independent.
- No p-n mixing at |Tz|=T

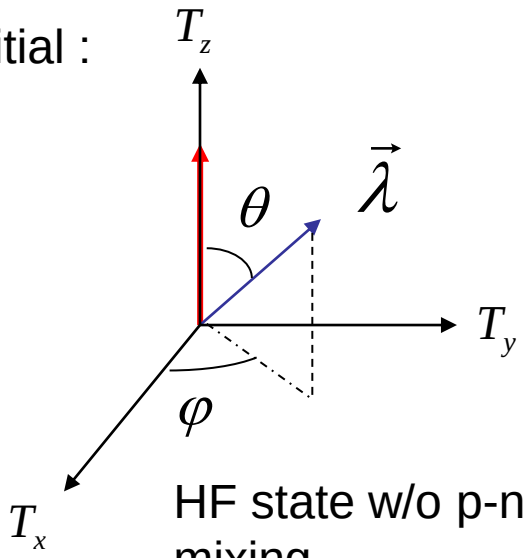
s. p. isospin is parallel or anti-parallel with $\vec{\lambda}$

With Coulomb interaction

$U^{Coulomb}(\tau_z)$:violates isospin symmetry

The total energy is now dependent on Tz but independent of azimuthal angle φ

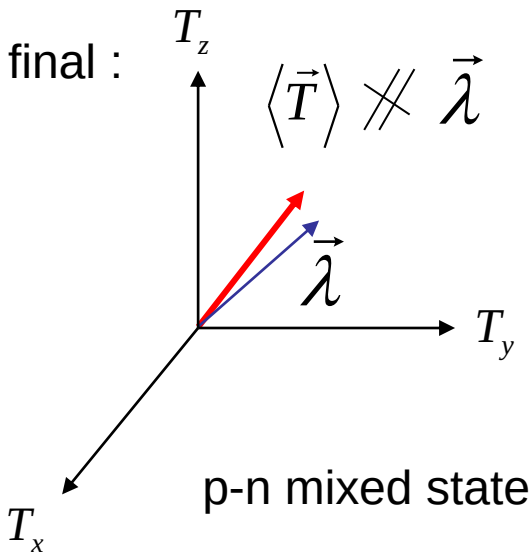
Initial :



HF state w/o p-n mixing

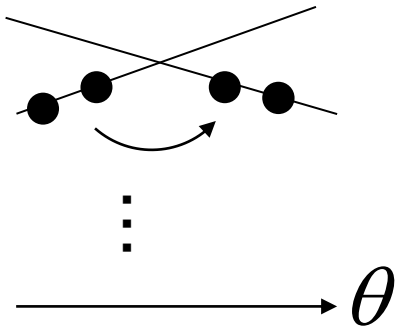
$-\vec{\lambda}\cdot\hat{\vec{T}}$

final :



p-n mixed state

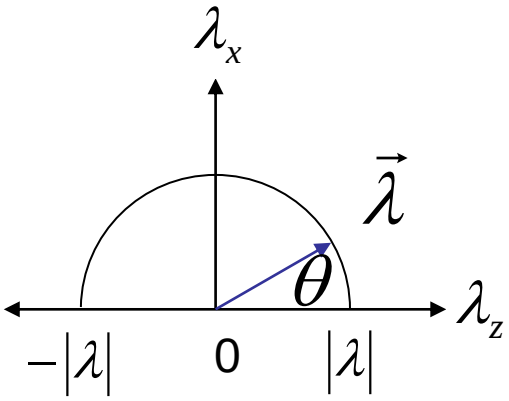
larger $<T_z>$ is favored



With Coulomb, the s. p. Routhians depend on the titling angle θ

w/o Coulomb

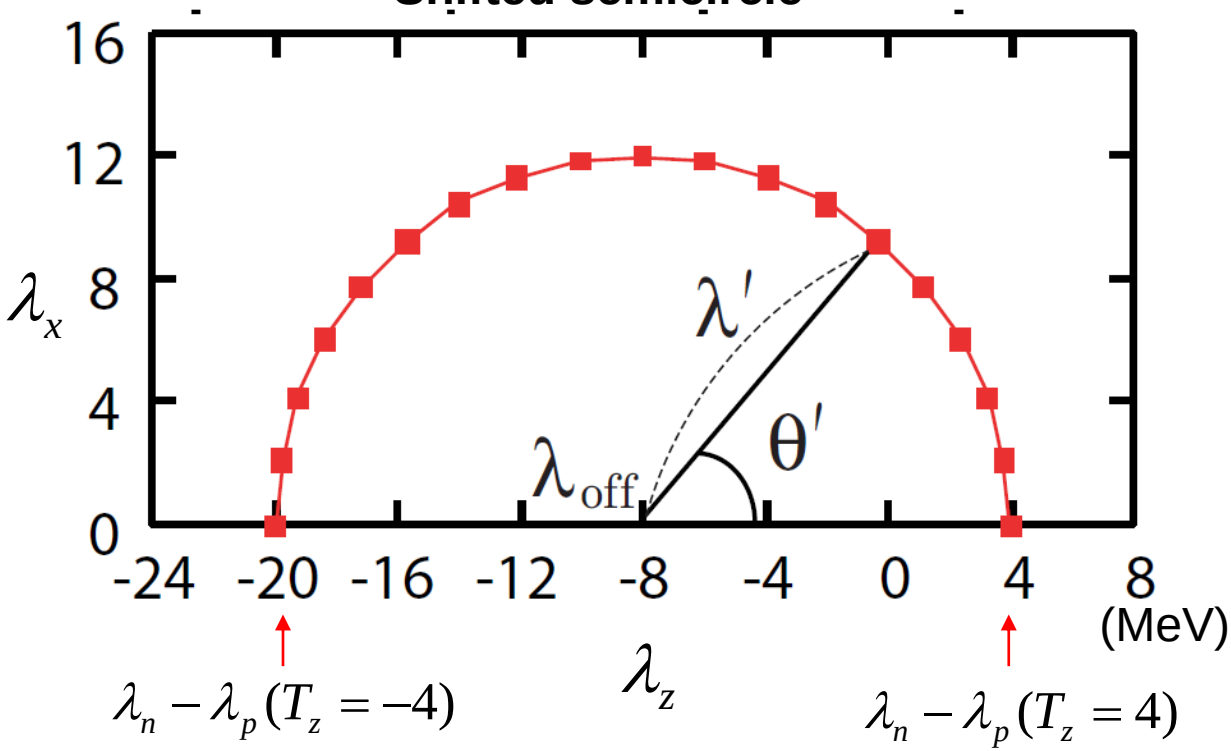
semicircle



$$|\lambda| = \lambda_n - \lambda_p(T_z = 4)$$
$$= \lambda_p - \lambda_n(T_z = -4)$$

w/ Coulomb

Shifted semicircle



Difference of p and n Fermi energies

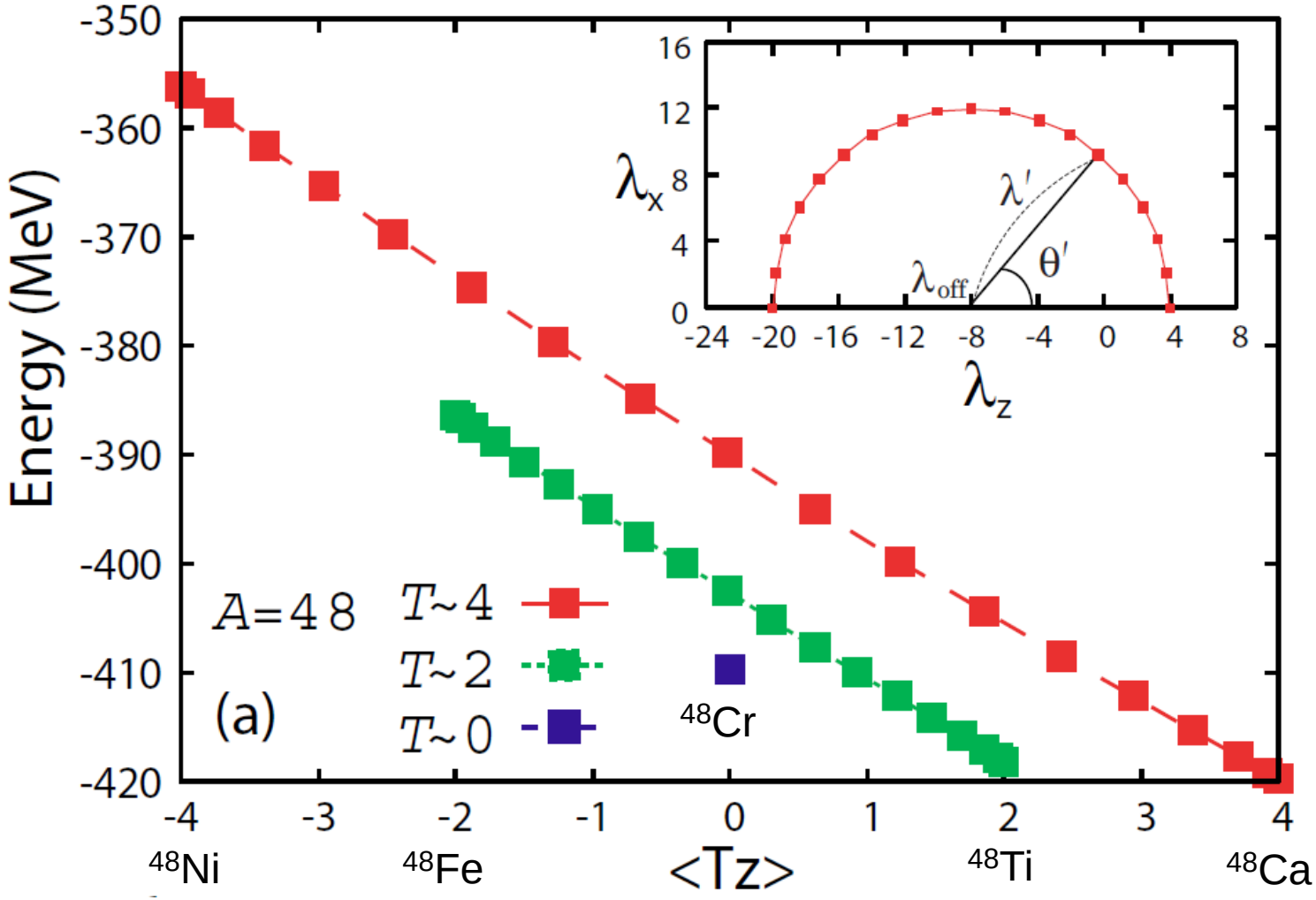
Coulomb gives additional isocranking freq. effectively $-\lambda_{off} \cdot t_z$

w/o Coulomb **w/ Coulomb**

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

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

Calculation for A=48 nuclei w/ Coulomb included



Almost linear dep. of energy ⇒ Coulomb behaves as

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

Two implementations of p-n mixed Hartree-Fock (pnHF)

HFODD

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

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

N. Schunck, et al., Comp. Phys. Comm. 216 (2017) 145.
J Dobaczewski et al, J. Phys. G: Nucl. Part. Phys. **48** (2021)102001.

- 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

Comparison with HFBTHO

- HFBTHO : Axial symmetry assumed (Cylindrical basis)

  Stoitsov et al.,Comp.Phys.Comm (2013)

- HFODD : No symmetry assumed (3D cartetian basis)

Functional: SkM*
Basis space : Nsh=10

$\left|\vec{\lambda}\right| = 11\mathrm{MeV}$ (w/o Coulomb)

$\left|\vec{\lambda}\right| = 8.0\mathrm{MeV}$ (w/ Coulomb)

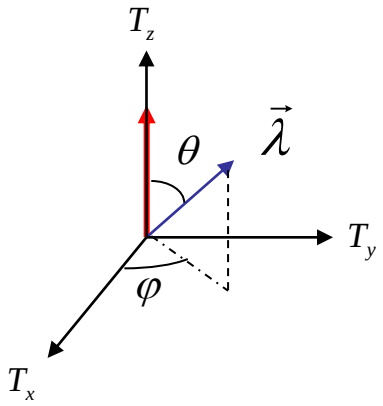
Very good agreement !

Results for T=4 Tz=0 state in A=48

$\theta' = 90$ (deg)	HFODD	HFBTHO
	Without Coulomb	
E_{tot} (MeV)	-491.243**706**	-491.243**724**
$E^{(\mathrm{n})}_{\mathrm{kin}}$ (MeV)	422.931**522**	422.931**576**
$E^{(\mathrm{p})}_{\mathrm{kin}}$ (MeV)	422.931**522**	422.931**426**
E_{Skyrme} (MeV)	-1337.106**749**	-1337.106**727**
E_{SO} (MeV)	-36.736**418**	-36.736**417**
$r^{(\mathrm{n})}_{\mathrm{rms}}$ (fm)	3.497**939**	3.497**940**
$r^{(\mathrm{p})}_{\mathrm{rms}}$ (fm)	3.497939	3.497939
T^2	20.03781**795**	20.037818
T_z	0.000000	0.000003
T_x	4.000000	4.000000
	With Coulomb	
E_{tot} (MeV)	-389.845**366**	-389.843**839**
$E^{(\mathrm{n})}_{\mathrm{kin}}$ (MeV)	415.**692439**	415.**707047**
$E^{(\mathrm{p})}_{\mathrm{kin}}$ (MeV)	404.67**2851**	404.67**9334**
E_{Skyrme} (MeV)	-1310.4**42289**	-1310.4**62779**
E_{SO} (MeV)	-34.12**1651**	-34.12**3978**
$E^{(\mathrm{dir})}_{\mathrm{Cou}}$ (MeV)	109.37**7390**	109.37**8116**
$E^{(\mathrm{exc})}_{\mathrm{Cou}}$ (MeV)	-9.145**757**	-9.145**814**
$r^{(\mathrm{n})}_{\mathrm{rms}}$ (fm)	3.526**332**	3.526**280**
$r^{(\mathrm{p})}_{\mathrm{rms}}$ (fm)	3.577**869**	3.577**844**
T^2	20.07**5675**	20.07**7079**
T_z	-0.012**676**	-0.012**663**
T_x	4.002**644**	4.002**778**

J.A. Sheikh, N. Hinohara, J. Dobaczewski,
T. Nakatsukasa, W. Nazarewicz, KS, PRC 89(2014) 054317

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



$\varphi = 0$

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

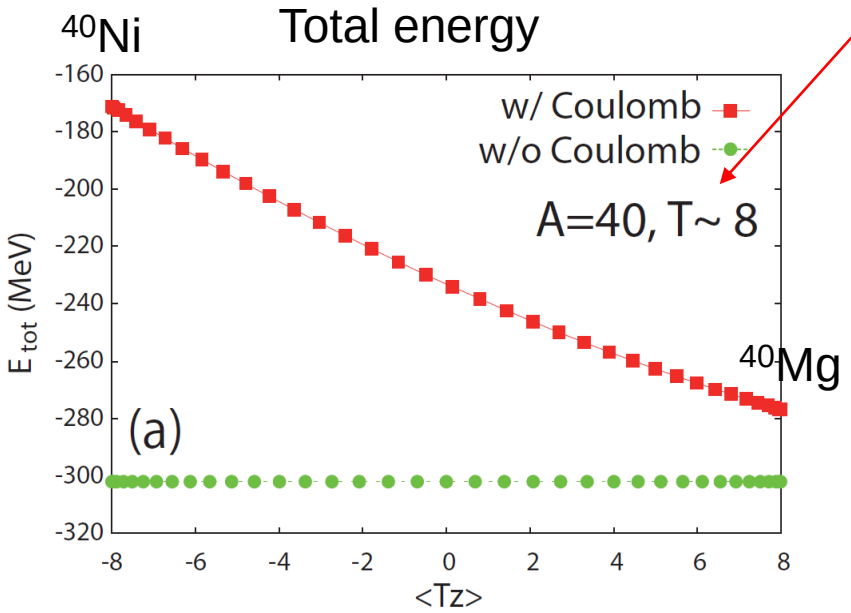
$$(\lambda_{\rm off}, \lambda') = \frac{1}{2}(\lambda_{np}^{T_z=T} + \lambda_{np}^{T_z=-T}, \lambda_{np}^{T_z=T} - \lambda_{np}^{T_z=-T})$$

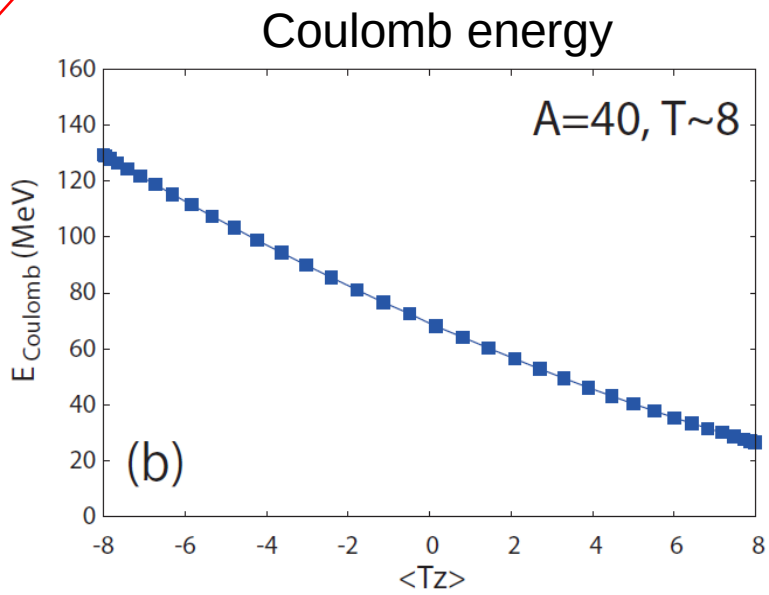
$$\lambda_{np}^{T_z=\pm T} \equiv \lambda_n - \lambda_p$$

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

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

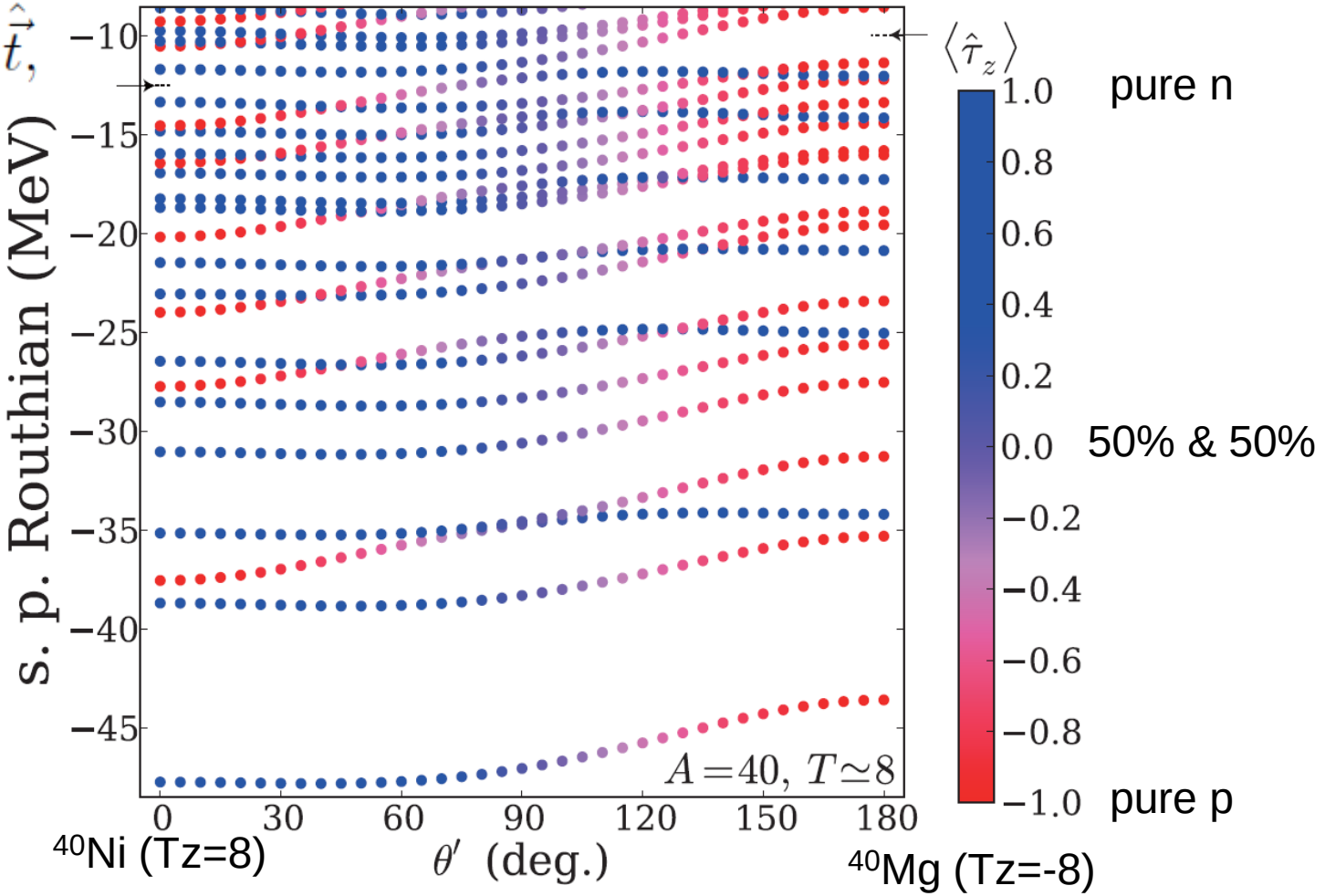
The T=8 component is dominant.





s. p. Routhian for T=8 IASs in A=40 isobars with Coulomb int.

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



- No p-n mixing at |Tz|=T ($\theta' = 0$ & 180°)

  The highest and lowest weight states are standard HF states

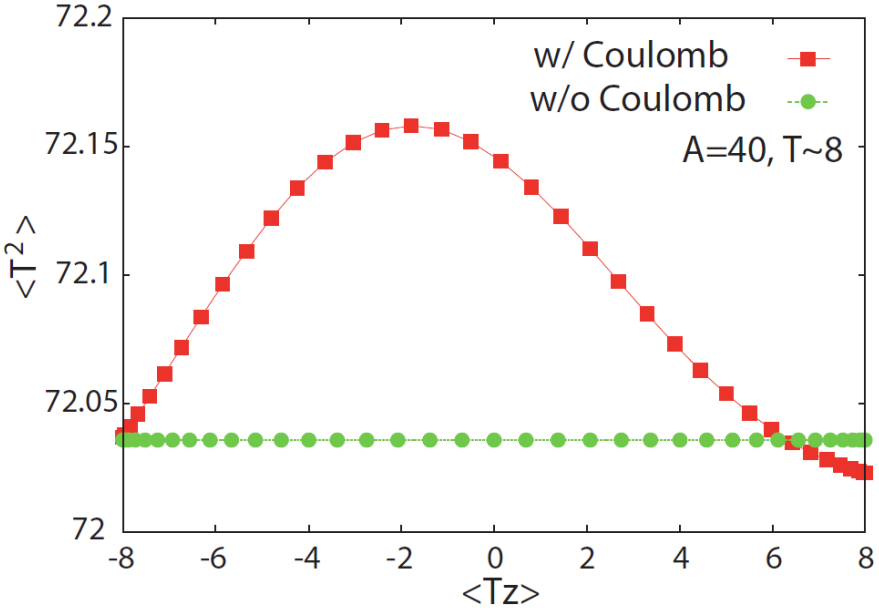
- Proton and neutron components almost equally mixed mixing at Tz=0

In reality, the isospin symmetry is slightly broken.

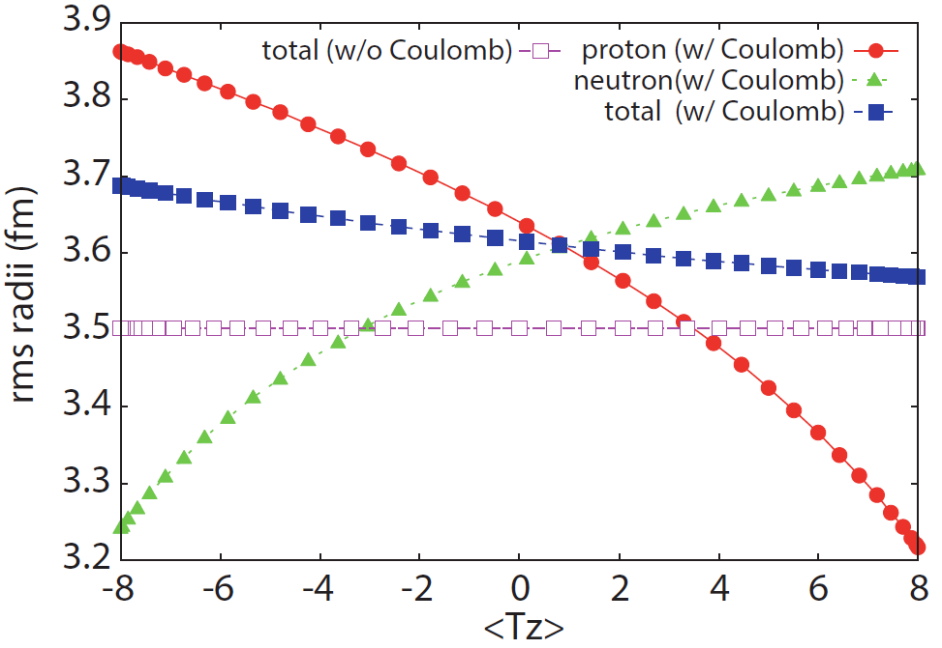
⇨ The total isospin T is not a good quantum number.

Isospin mixing

<T^2> for T=8 IASs in A=40 isobars



rms radii for T=8 IASs in A=40 isobars



Even without Coulomb, <T^2> deviates from the exact value 72 due to the spurious isospin mixing within the mean-field approximation

With decreasing <Tz> total rms radius increases.

Without Coulomb, total rms radius stays constant.

⇨ Isospin projection

Isospin mixing & Isospin projection

Why isospin projection needed?

There is spurious isospin mixing inherent to MF approaches

In HFODD, the isospin projection for p-n separated HF has been implemented.

PHYSICAL REVIEW C **81**, 054310 (2010)

Isospin-symmetry restoration within the nuclear density functional theory: Formalism and applications

W. Satuła,[1] J. Dobaczewski,[1,2] W. Nazarewicz,[1,3,4] and M. Rafalski[1]

Isospin symmetry of atomic nuclei is explicitly broken by the charge-dependent interactions, primarily the Coulomb force. Within the nuclear density functional theory, isospin is also broken spontaneously. We propose a projection scheme rooted in a Hartree-Fock theory that allows the consistent treatment of isospin breaking

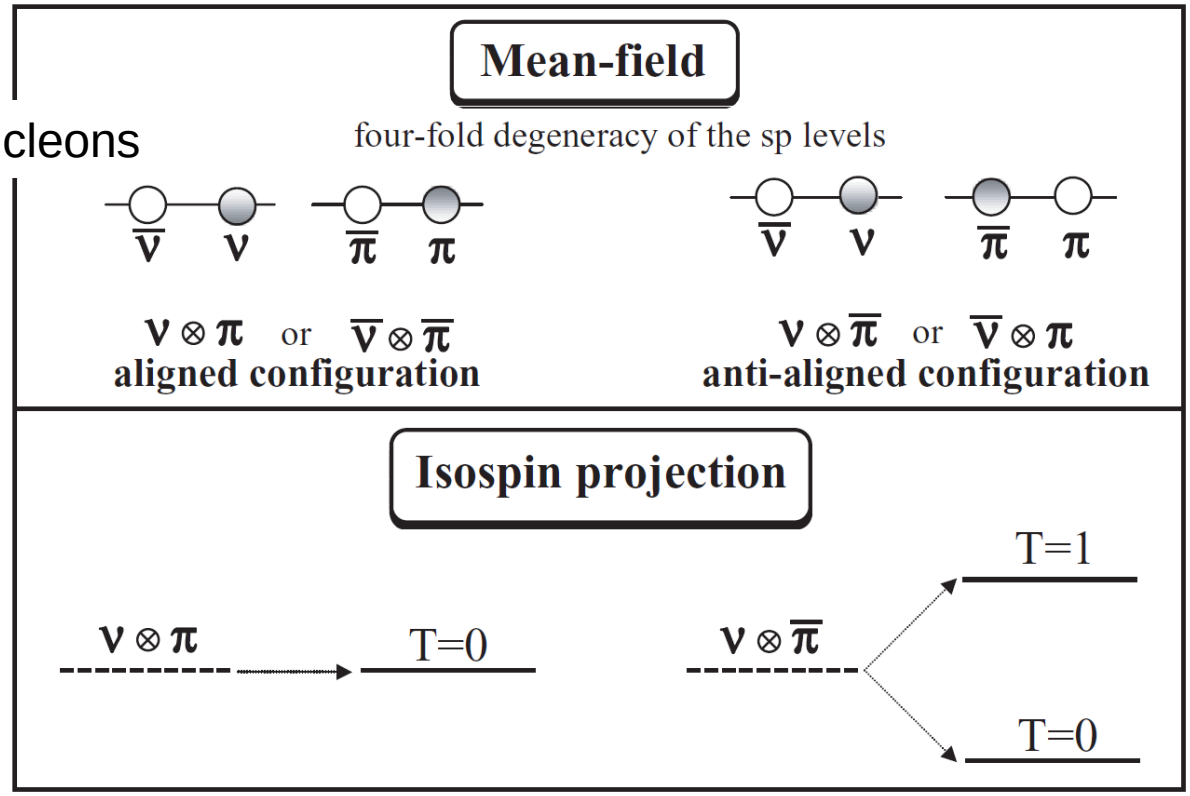
One typical example : g. s. of odd-odd N=Z nuclei

One typical example : g. s. of odd-odd N=Z nuclei

(Coulomb force & time-odd polarization neglected for simplicity)

(isospin & time-reversal symmetries)

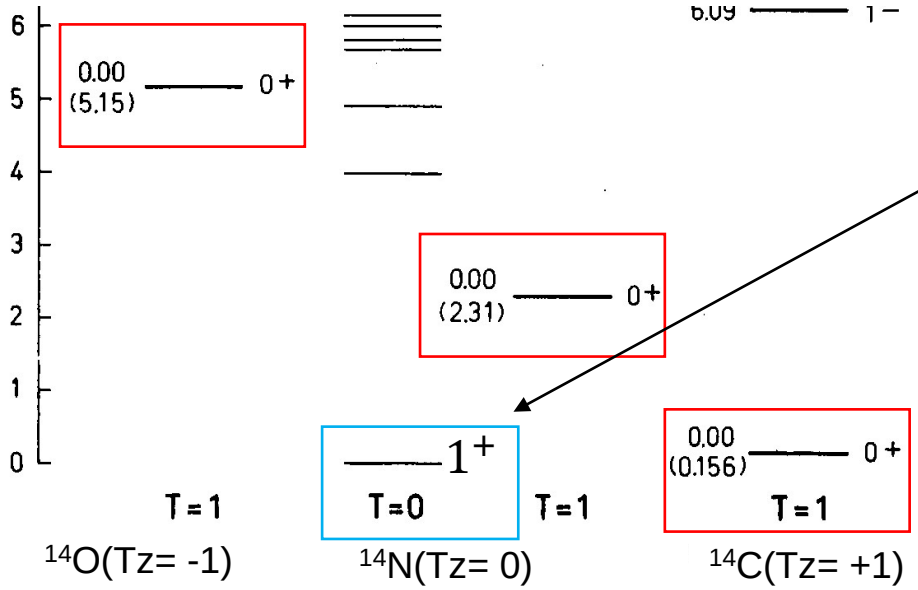
Valence nucleons



spatial w.f. : sym.
spin w.f. : sym. (S=1)
isospin w.f. : antisym. (T=0)

spatial w.f. : sym.
spin w.f. : $|\uparrow\rangle|\downarrow\rangle$ S=0 &S=1 mixed
isospin w.f. : T=0 &T=1 mixed

T=0 and T=1 states in 14N

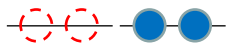


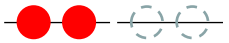
T=0 state -> time-reversal breaking

The conventional HF can describe.

T=1 state -> time-reversal conserving

Figure 1-7 The level schemes for the nuclei with $A = 14$ are based on the compilation by F. Ajzenberg-Selove and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959), on the results given by D. E. Alburger, A. Gallmann, J. B. Nelson, J. T. Sample, and E. K. Warburton, *Phys. Rev.* **148**, 1050 (1966), and on a private communication by G. Ball and J. Cerny (August, 1966). The relative energies represent atomic masses.

^{14}C 

^{14}O 

How can we describe the T=1 state in ^{14}N?

⇒ The p-n mixed EDF framework provides us with a natural way to describe time-even odd-odd IASs.

Bohr & Mottelson, “Nuclear Structure” vol.1

The isocranked states with $\langle \hat{T}_z \rangle = 0$ are not eigenstates of $\hat{T}_z$.

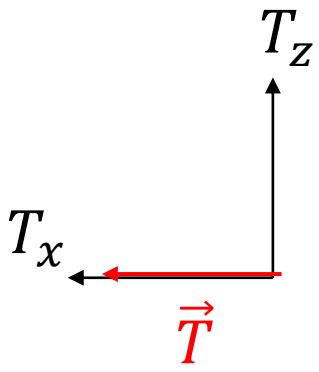
For simplicity, consider the case with isoscalar EDFs and no Coulomb int.

Let |0> be the isoscalar(T=0) core of A=4n nucleons.
The wave functions of the T=1 triplet with A=4n+2 are given by

$$|\Psi_{1,-1}\rangle = a^+_{p\uparrow} a^+_{p\downarrow} |0\rangle,$$

$$|\Psi_{1,0}\rangle = \frac{1}{\sqrt{2}} \left(a^+_{n\uparrow} a^+_{p\downarrow} + a^+_{p\uparrow} a^+_{n\downarrow} \right) |0\rangle,$$

$$|\Psi_{1,1}\rangle = a^+_{n\uparrow} a^+_{n\downarrow} |0\rangle,$$



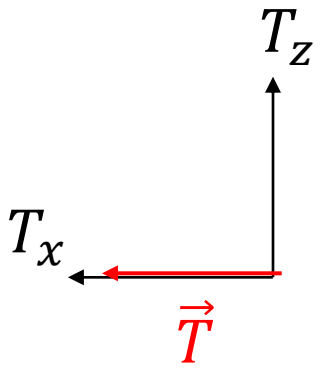
The x-isocranked state is

$$|\Psi_{++}\rangle = a^+_{+\uparrow} a^+_{+\downarrow} |0\rangle = \underline{\frac{1}{2}|\Psi_{1,-1}\rangle + \frac{1}{\sqrt{2}}|\Psi_{1,0}\rangle + \frac{1}{2}|\Psi_{1,1}\rangle},$$

Mixture of the $T_z = -1, 0, 1$ states

$$|+\uparrow\rangle = \frac{1}{\sqrt{2}}(|n\uparrow\rangle + |p\uparrow\rangle) \qquad |+\downarrow\rangle = \frac{1}{\sqrt{2}}(|n\downarrow\rangle + |p\downarrow\rangle)$$

Similarly to the T=1 case, other x-isocranked states for other T's (T=3, 4, 5,…) and $\langle \hat{T}_z \rangle = 0$ can be written as



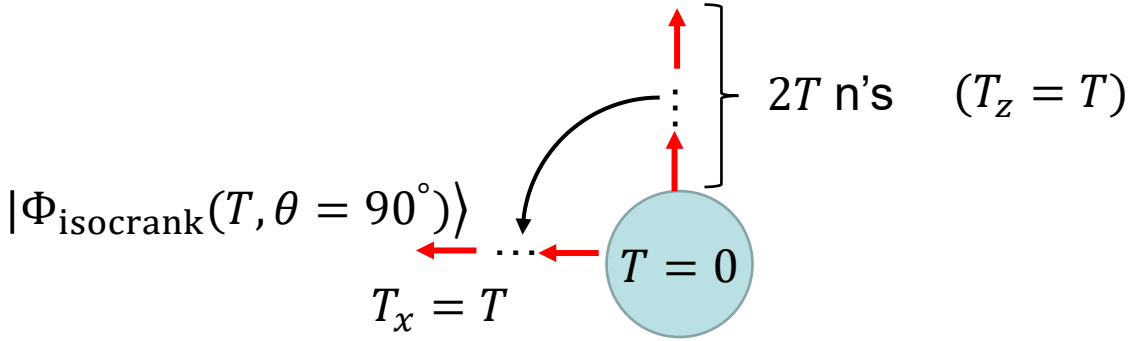
$$|\Phi_{\text{isocrank}}(T, \theta = 90^\circ)\rangle = \prod_{i=1}^{2T} \frac{1}{\sqrt{2}} (|n, i\rangle + |p, i\rangle)$$

$$= \sum_{T_z=-T}^{T} c_{T,T_z} \, |T, T_z\rangle$$

Superposition of states with different Tz values

(Here, we consider the isoscalar core + 2T valence nucleons. Only the valence part is shown.)

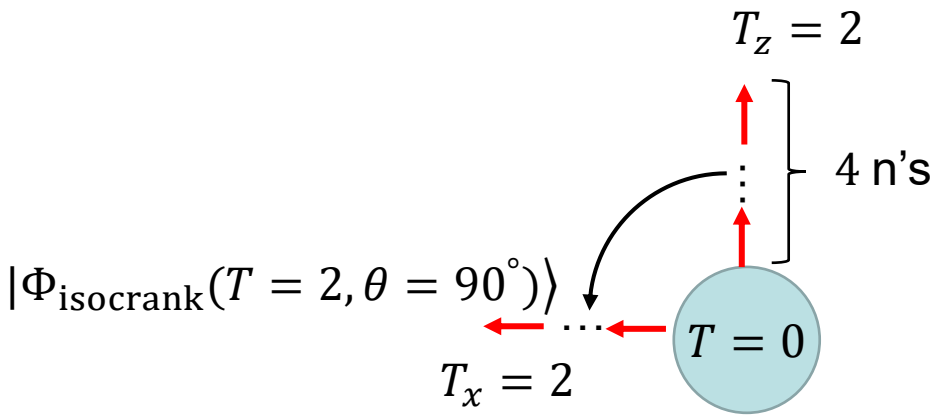
$$c_{T,T_z} = \frac{\sqrt{\binom{2T}{T - T_z}}}{2^T}$$



For example, the isocranked state with $T = 2, \theta = 90^\circ$ is given by

$$|\Phi_{\text{isocrank}}(T = 2, \theta = 90^\circ)\rangle$$

$$= \prod_{i=1}^{4} \frac{1}{\sqrt{2}} (|n, i\rangle + |p, i\rangle)$$



$$= \sum_{T_z=-2}^{2} c_{T,T_z} \, |T = 2, T_z\rangle$$

$$= \frac{1}{4} (|T = 2, T_z = 2\rangle + |T = 2, T_z = -2\rangle)$$

$$+ \frac{1}{2} (|T = 2, T_z = 1\rangle + |T = 2, T_z = -1\rangle) \quad + \frac{\sqrt{6}}{4} |T = 2, T_z = 0\rangle$$

The other isocranked states with $\langle T_z \rangle \neq T$ can be written as superpositions of $|T, T_z\rangle$'s.

How can we evaluate the energies for Tz=0 p-n mixed states?

We shall focus on T=1 triplets and calculated TDE's.

$$|\Psi_{++}\rangle = a^{+}_{+\uparrow} a^{+}_{+\downarrow} |0\rangle = \frac{1}{2}|\Psi_{1,-1}\rangle + \frac{1}{\sqrt{2}}|\Psi_{1,0}\rangle + \frac{1}{2}|\Psi_{1,1}\rangle,$$

$$BE_{++} = \frac{1}{4}BE(T_z = 1) + \frac{1}{2}BE(T_z = 0) + \frac{1}{4}BE(T_z = -1)$$

Triple displacement energy is given by

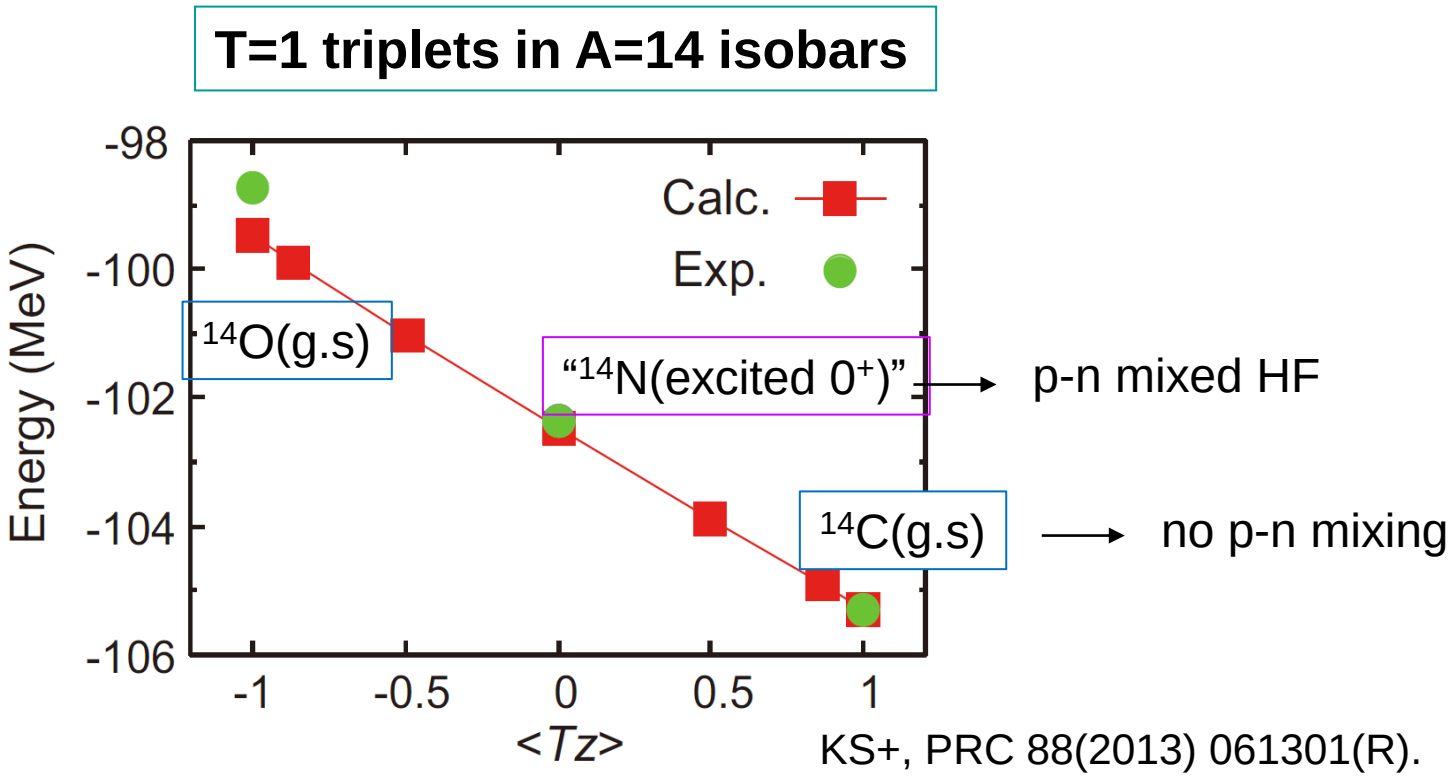
$$TDE = BE(T_z = 1) + BE(T_z = -1) - 2BE(T_z = 0)$$

[We define the binding energy with $BE(T_z) < 0$]

$$\mathrm{TDE} = 2\left[BE(T = 1, T_z = -1) + BE(T = 1, T_z = +1) - 2BE_{++}\right]$$

In the first paper on the p-n mixed EDFs[KS+, PRC88(2013)], we erroneously used that of the x-isocraked states for the energy of ^{14}N(excited 0^+).

(Before the correction)

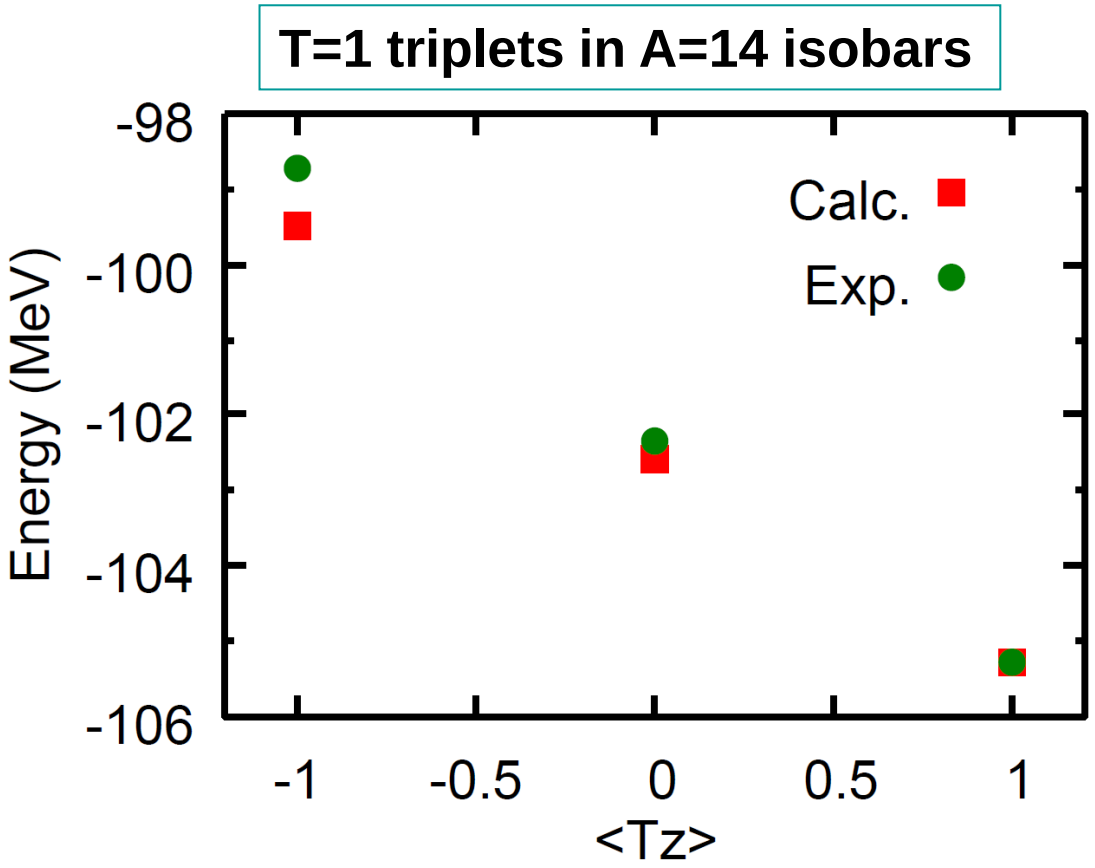


KS+, PRC 88(2013) 061301(R).

- Tz=0, T=1 states in odd-odd ^{14}N : Time-reversal symmetry conserved
  (cannot be described by conventional HF)

(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)

After the correction,



TDE(calc.) = 0.398 MeV, TDE(exp.) = 0.675 MeV

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

So far, we have considered the isoscalar nuclear EDFs.

Need for isospin symmetry breaking nuclear force?

Nuclear EDFs with isospin symmetry breaking

Charge symmetry breaking (CSB) and Charge independence breaking (CIB)

$$V_{nn}^{T=1} \cong V_{np}^{T=1} \cong V_{pp}^{T=1} \qquad (V_{np}^{T=1} \neq V_{np}^{T=0})$$

The nuclear force is almost isospin-symmetric.

Major cause

Charge symmetry breaking (CSB)
difference between nn and pp : "$V_{nn}^{T=1} - V_{pp}^{T=1}$" $m_n \neq m_p$

Charge independence breaking (CIB)
difference between np and the average of nn and pp : $m_{\pi^0} \neq m_{\pi^\pm}$

"$(V_{nn}^{T=1} + V_{pp}^{T=1})/2 - V_{np}^{T=1}$"

Manifestation of the CSBs and CIBs in nuclear mass :

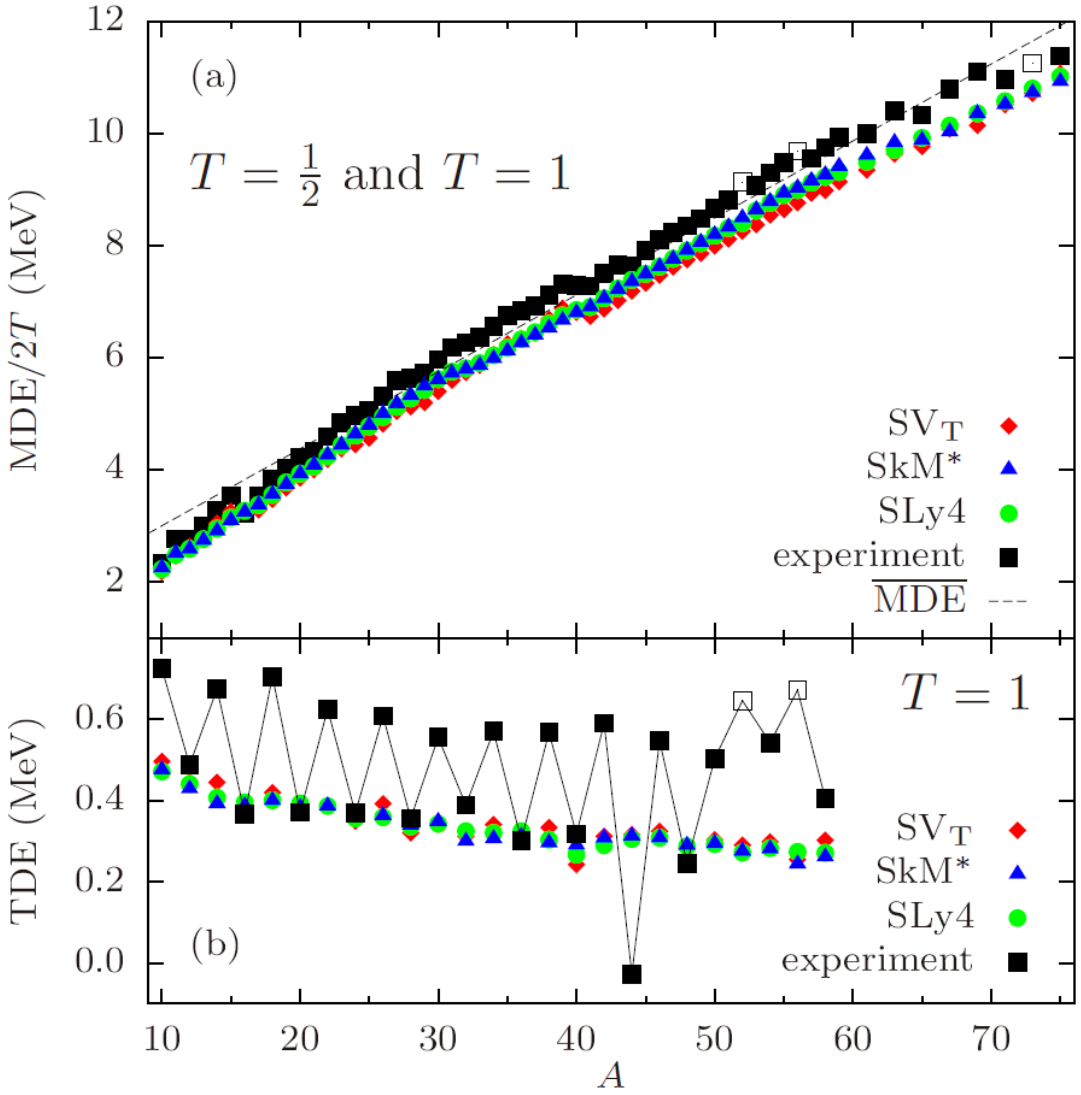
Mirror Displacement Energy = BE(T_z=T)-BE(T_z=-T)

Triplet Displacement Energy =BE(T_z=1)+BE(T_z=-1)-2BE(T_z=0)

(BE < 0)

Isoscalar nuclear force + Coulomb int.

can not reproduced the experimental data.



Mirror displacement energy:

MDEs systematically underrstimated.

(T=1 triplet)

Triple displacement energy:

BE(T_z) < 0

Baczyk, Dobaczewski, Konieczka, Satula, Nakatsukasa, KS, Phys. Lett. **B778** (2018) 178.

Introduce an isospin breaking nuclear force:

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

breaks CI but is invariant under a rotation by π w. r. t. the y-axis in isospace preserving CS.

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

breaks both CI and CS

The corresponding contributions to EDF read

$$\mathcal{H}_{\mathrm{II}} = \frac{1}{2}t_0^{\mathrm{II}}(\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} \longrightarrow$$

The p-n mixed EDF calc.

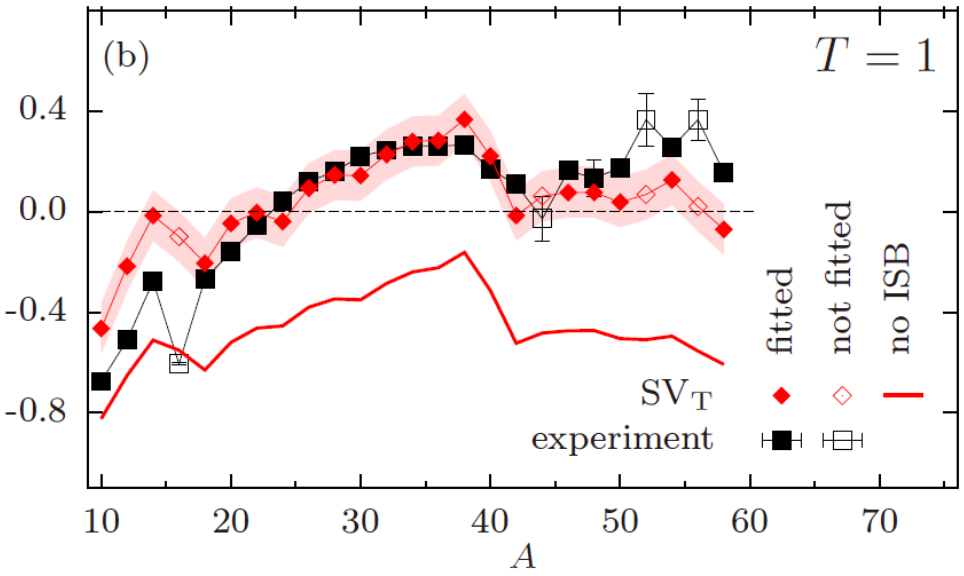
$$-\boldsymbol{s}_n^2 - \boldsymbol{s}_p^2 + 2\boldsymbol{s}_n\cdot\boldsymbol{s}_p + 2\boldsymbol{s}_{np}\cdot\boldsymbol{s}_{pn}),$$

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

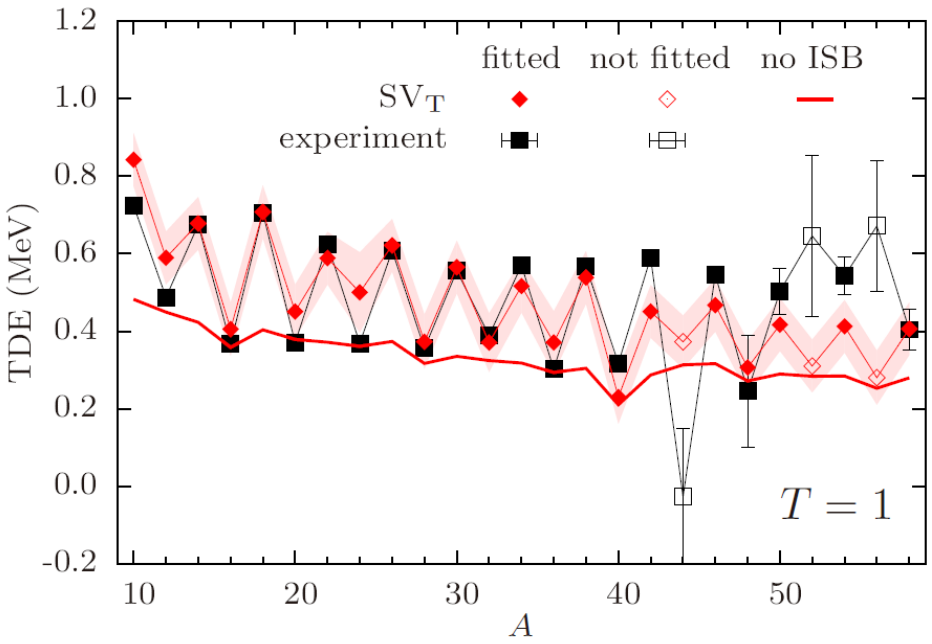
t_0^{II}, t_0^{III}: interaction strength to be determined from fitting to exp.

Henly, Miller, “Mesons in Nuclei ”, North Holland (1979)
Baczyk, Dobaczewski, Konieczka, Satula, Nakatsukasa, KS, Phys. Lett. B778 (2018) 178.

MDE



TDE



Results calculated with isospin symmetry breaking nuclear force

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

MDE=BE(T_z=T)-BE(T_z=-T)

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

TDE=BE(T_z=1)+BE(T_z=-1) -2BE(T_z=0)

	SV_T^{ISB}
t_0^{II} (MeV fm^3)	4.6 ± 1.6
t_0^{III} (MeV fm^3)	-7.4 ± 1.9
$t_0^{\mathrm{II}}/t_0^{\mathrm{III}}$	-0.6 ± 0.3

Further extension of EDFs including NLO terms

Baczyk et al., J. Phys. G: Nucl. Part. Phys. 46 (2019) 03LT01.

IOP Publishing Journal of Physics G: Nuclear and Particle Physics
J. Phys. G: Nucl. Part. Phys. 46 (2019) 03LT01 (11pp) https://doi.org/10.1088/1361-6471/aaffe4

Letter

Isobaric multiplet mass equation within nuclear density functional theory

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CrossMark

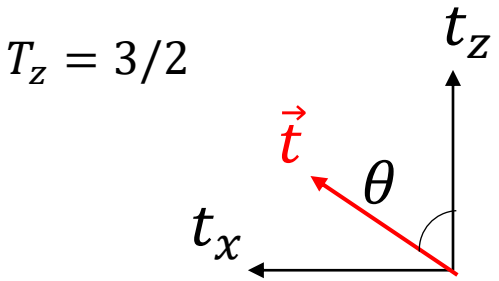
$$\hat{V}_1^{\mathrm{II}}(i,j) = \frac{1}{2}t_1^{\mathrm{II}}(\delta(\boldsymbol{r}_{ij})\boldsymbol{k}^2 + \boldsymbol{k}'^2\delta(\boldsymbol{r}_{ij}))\hat{T}^{(ij)}, \quad \hat{V}_1^{\mathrm{III}}(i,j) = \frac{1}{2}t_1^{\mathrm{III}}(\delta(\boldsymbol{r}_{ij})\boldsymbol{k}^2 + \boldsymbol{k}'^2\delta(\boldsymbol{r}_{ij}))\hat{T}_z^{(ij)},$$

$$\hat{V}_2^{\mathrm{II}}(i,j) = t_2^{\mathrm{II}}\boldsymbol{k}'\delta(\boldsymbol{r}_{ij})\boldsymbol{k}\hat{T}^{(ij)}, \qquad \hat{V}_2^{\mathrm{III}}(i,j) = t_2^{\mathrm{III}}\boldsymbol{k}'\delta(\boldsymbol{r}_{ij})\boldsymbol{k}\hat{T}_z^{(ij)},$$

The states with an odd # of the valence nucleon ($T = \frac{3}{2}, \frac{5}{2}, \ldots$) can be calculated as well.

$$|t_x = 1/2\sin\theta, t_y = 0, t_z = 1/2\cos\theta\rangle$$

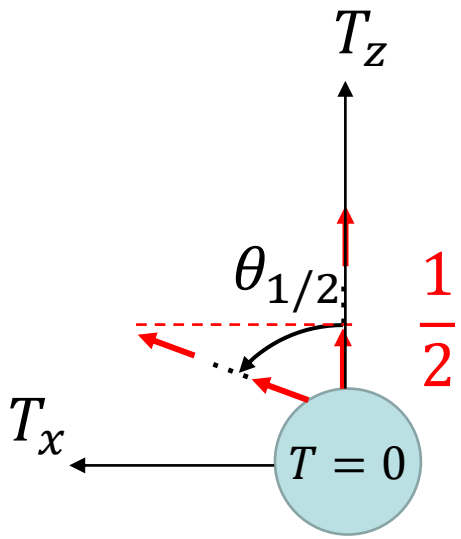
$$= \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix} = \cos\frac{\theta}{2}|n\rangle + \sin\frac{\theta}{2}|p\rangle$$



$$|\Phi_{\text{isocrank}}(T = 3/2, T_z = 1/2)\rangle$$

$$= \prod_{i=1}^{3} \left| t_x = \frac{1}{2}\sin\theta_{\frac{1}{2}}, t_z = \frac{1}{2}\cos\theta_{1/2}, i \right\rangle$$

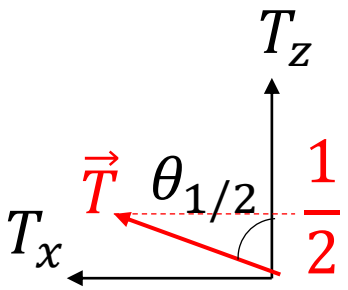
$$= \prod_{i=1}^{3} \left[\cos\frac{\theta_{1/2}}{2}|n, i\rangle + \sin\frac{\theta_{1/2}}{2}|p, i\rangle \right]$$



$$|\Phi_{\text{isocrank}}(T = 3/2, T_z = 1/2)\rangle$$

$$= \frac{2\sqrt{6}}{9}|T = 3/2, T_z = 3/2\rangle + \frac{2}{3}|T = 3/2, T_z = 1/2\rangle$$

$$+ \frac{\sqrt{2}}{3}|T = 3/2, T_z = -1/2\rangle + \frac{\sqrt{3}}{9}|T = 3/2, T_z = -3/2\rangle$$



Similarly,

$$|\Phi_{\text{isocrank}}(T = 3/2, T_z = -1/2)\rangle$$

$$= \frac{2\sqrt{6}}{9}|T = 3/2, T_z = -3/2\rangle + \frac{2}{3}|T = 3/2, T_z = -1/2\rangle$$

$$+ \frac{\sqrt{2}}{3}|T = 3/2, T_z = 1/2\rangle + \frac{\sqrt{3}}{9}|T = 3/2, T_z = 3/2\rangle$$

One can calculate the energies of $|T = 3/2, T_z = \pm 1/2\rangle$.

The p-n mixed EDFs may be useful to study the nuclear symmetry energy.

For example, the isocranked state with $T = 2, \theta = 90^\circ$ is given by

$$|\Phi_{\text{isocrank}}(T = 2, \theta = 90^\circ)\rangle = \prod_{i=1}^{4} \frac{1}{\sqrt{2}} (|n, i\rangle + |p, i\rangle)$$

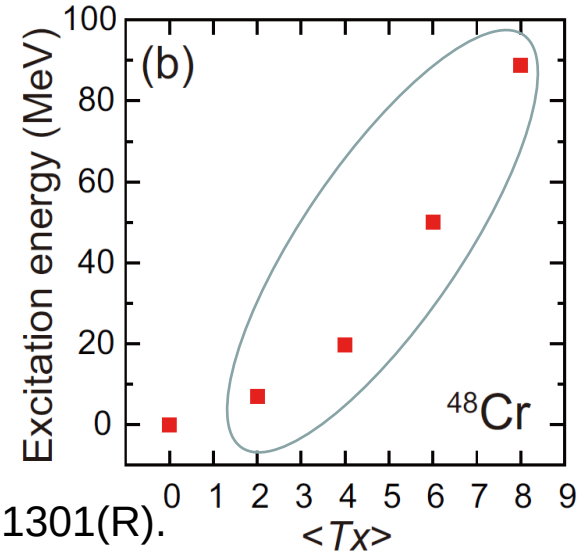
$$= \frac{1}{4}(|T = 2, T_z = 2\rangle + |T = 2, T_z = -2\rangle)$$

$$+ \frac{1}{2}(|T = 2, T_z = 1\rangle + |T = 2, T_z = -1\rangle) + \frac{\sqrt{6}}{4}|T = 2, T_z = 0\rangle$$

The isocranked states ≠ pure Tz=0 states

In the previous paper, for the excitation energies with different T's in Cr, we erroneously used the energies of the x-isocranked states.

By evaluating the energies as we did for TDEs, the p-n mixed EDFs can be used to study the nuclear symmetry energy.



KS+, PRC 88(2013) 061301(R).

Summary

- We have solved the Hartree-Fock equations based on the EDF including p-n mixing.
- Isospin is controlled by using the isocranking model.
- Although the isocranked states are not eigenstates of T_z except for $|T_z| = T$, the p-n mixed single-reference EDFs can provide us with a natural way to describe the isobaric analog states.
- For odd A/2, odd-T states can be obtained by isocranking e-e nuclei in their ground states with time-reversal symmetry.
- The extension of EDFs including the isospin breaking terms improves MDEs and TDEs, that are experimental manifestation of CSB and CIB, respectively
- The isospin projection for p-n mixed states is to be implemented.