Mead-field calculation including proton-neutron mixing —toward proton-neutron pairing—

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Nuclear DFT for proton-neutron pairing and its application

(e.g. GT transition strength)

- Proton-neutron pairing: Goodman, Adv. Nucl. Phys.11, (1979) 293.

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

- Proton-neutron mixing:

  Quasiparticles are mixtures of protons and neutrons

  EDF with an arbitrary mixing between protons and neutrons

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

$$\tau = p, n$$

Related (?) physics:

Wigner energy, β decays and, in particular, superallowed β decays, interplay between $T = 0$ and $T = 1$ states in $N = Z$ nuclei, isospin mixing and mirror symmetry breaking, α decay and α clustering, moments of inertia, deformation properties, etc.

Perlinska et al, PRC 69 , 014316(2004)

For a review on *p-n* pairing, see A. Afanasjev, arXiv:1205.2134

As a first step, we consider p-n mixing on the Hartree-Fock level without pairing.

Mean-field calculation including proton-neutron mixing

- 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 Skyrme density functional

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

Invariant under rotation in isospace

isoscalor isovector

Perlinska et al, PRC 69 , 014316(2004)

$$\rho_0 = \rho_n + \rho_p$$

$$\rho_1 = \rho_{np} + \rho_{pn}$$
$$\rho_2 = -i\rho_{np} + i\rho_{pn}$$
$$\rho_3 = \rho_n - \rho_p$$

Mean-field calculation including proton-neutron mixing

- 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 Skyrme density functional

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

Invariant under rotation in isospace

isoscalar isovector

Perlinska et al, PRC 69 , 014316(2004)

- p-n mixed Hartree-Fock Hamiltonian :

$$h_n,\ h_p \longrightarrow h_{mixed} = \begin{pmatrix} \text{n-n} & \text{n-p} \\ \text{p-n} & \text{p-p} \end{pmatrix}$$

It is a hard task to develop a code from scratch …

→ Use of a existing HFB code

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 restricted
- Harmonic-oscillator basis
- Multi-function (CHFB, Cranking, angular mom. projection, isospin projection, finite temperature,….)

Road map

HFODD (Skyrme-HF(B) code)

↓

Proton-neutron mixing at HF level ⇨ **Test calc. for A=14 and 48 nuclei**

We are here!

↓

Isospin projection with p-n mixing

↓

Proton-neutron pairing (T=1 & T=0)

↓

QRPA with FAM, Isospin projection w/ p-n pairing, etc.

e.g. calc. of GT strengths

↓

Application to large-amplitude collective motion(?)

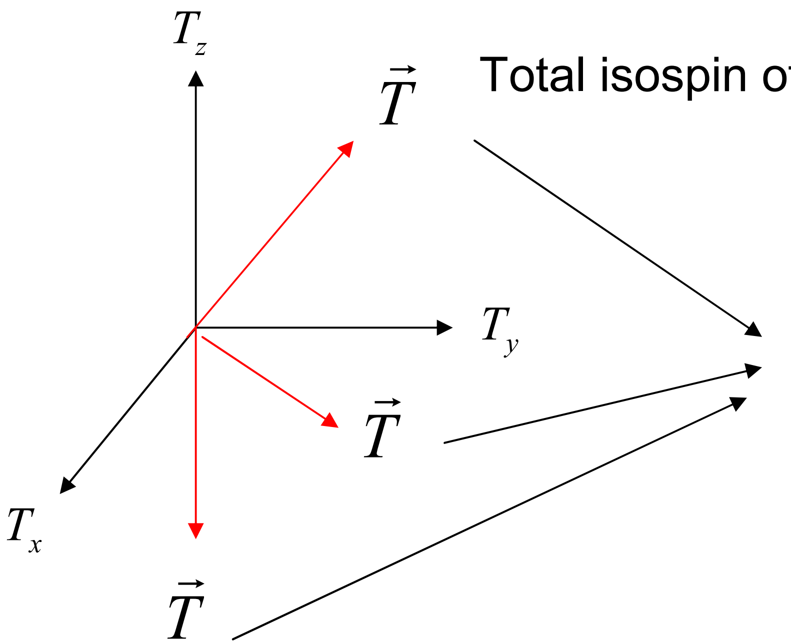
We have developed a code for *Hartree-Fock calculation with proton-neutron mixing* *and performed some test calculations.*

<u>*Test calculation*</u>

p-n mixing for EDF is correctly implemented?

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



Rotational invariance in isospace

Total energy should be independent of the orientation of T.

Check of the code

How to control the isospin direction ?

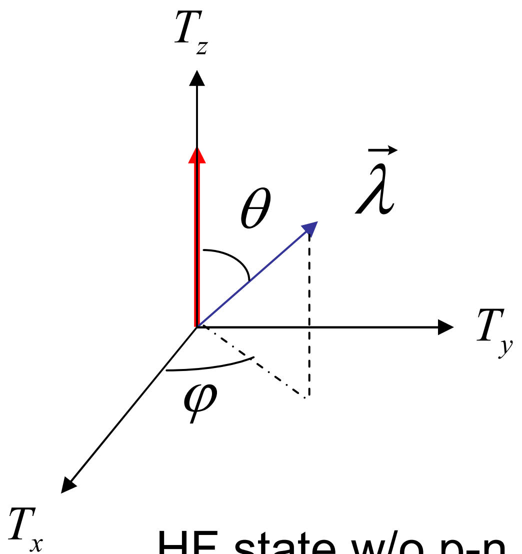
Isocranking calculation $\hat{H}' = \hat{H} - \vec{\lambda} \cdot \vec{T}$ Isocranking term

controlls the isospin of the system

HF eq. solved by iterative diagnalizaion of MF Hamiltonian.

w/ p-n mixing and no Coulomb

Initial state: HF solution w/o p-n mixing (e.g. ^{14}C(Tz=1,T~1))



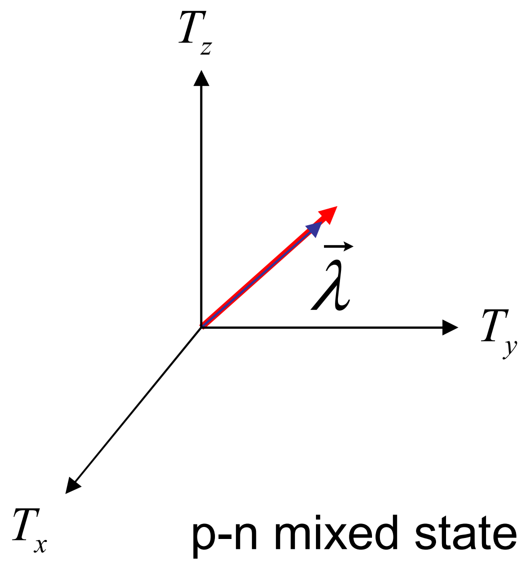
HF state w/o p-n mixing

Determine s. t. proton and neutron Fermi energies become equal

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

iteration

Final state



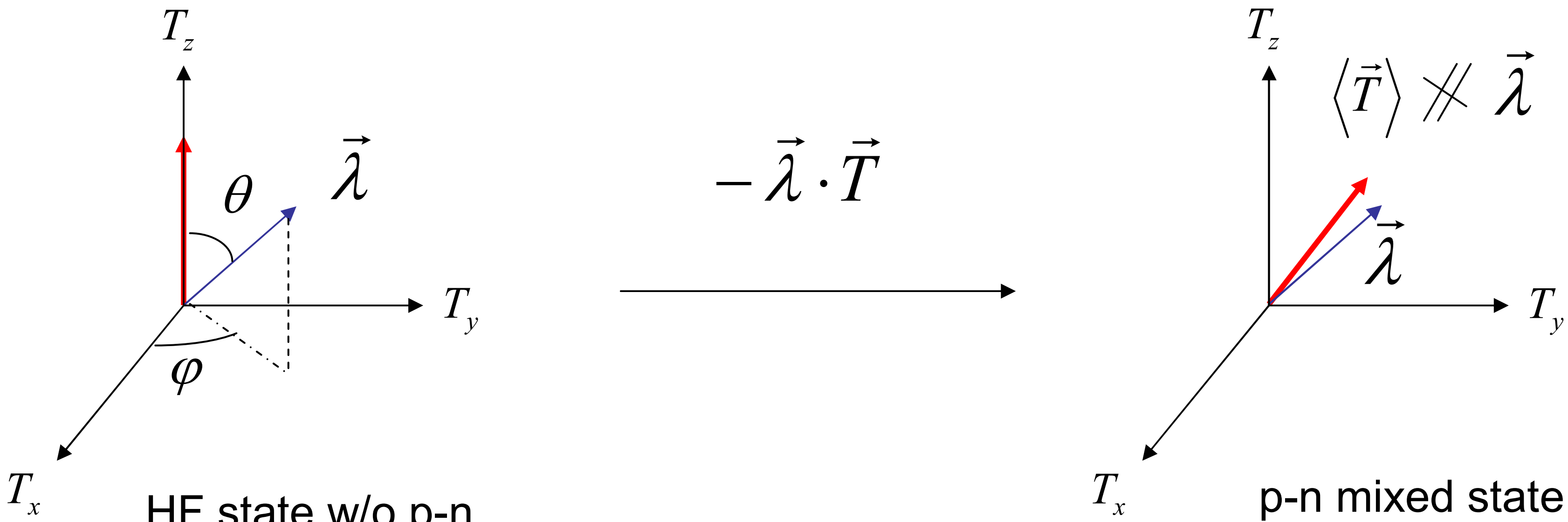
p-n mixed state

Isocranking calculation $\hat{H}' = \hat{H} - \vec{\lambda} \cdot \vec{T}$

With Coulomb interaction

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

Obtained state:



HF state w/o p-n mixing

p-n mixed state

With Coulomb, the system favors larger $\langle T_z \rangle$

Calculation for A=14 isobars

- w/ p-n mixing and no Coulomb
- w/ p-n mixing and Coulomb

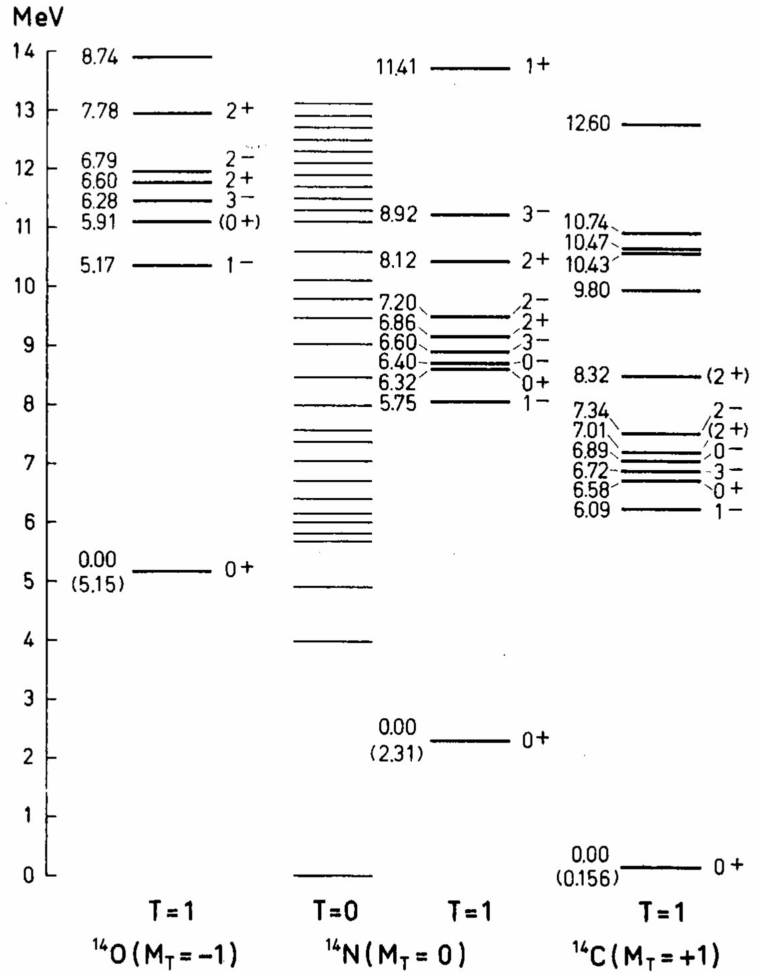
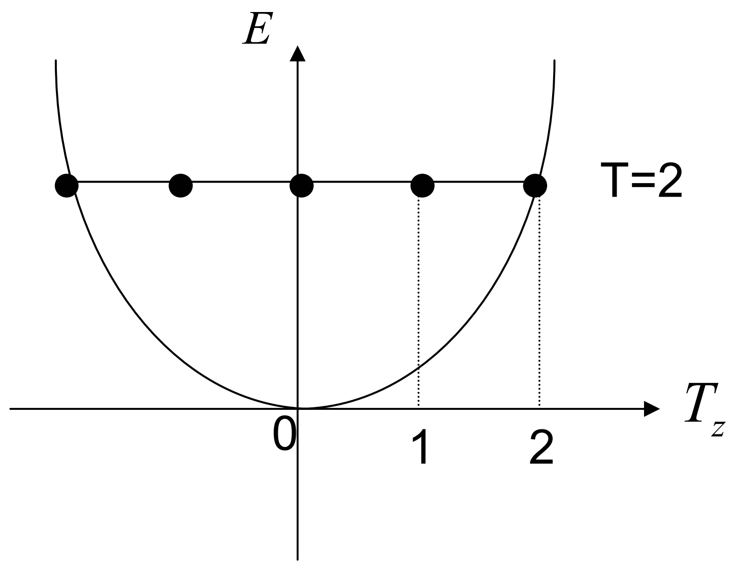


Figure 1-7 The level schemes for the nuclei with $A = 14$ are based on the compilation by F. Ajzenberg-Selove and T. Lauritsen, *Nuclear Phys.* **11**, 1 (1959), on the results given by D. E. Alburger, A. Gallmann, J. B. Nelson, J. T. Sample, and E. K. Warburton, *Phys. Rev.* **148**, 1050 (1966), and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

Isobaric symmetry



Bohr & Mottelson, "Nuclear Structure" vol.1

A=14 without Coulomb

Calc. w/o Coulomb force and p-n mixing (Normal HF w/o Coulomb)

^{14}C Z=6, N=8

$$T_z = 1$$

Neutron single-particle energy:

NO)	ENERGY
1)	-32.919
2)	-32.919
3)	-16.520
4)	-16.520
5)	-16.446
6)	-16.446
7)	-9.6810
8)	-9.6810

Proton single-particle energy

NO)	ENERGY
1)	-38.207
2)	-38.207
3)	-21.447
4)	-21.447
5)	-21.402
6)	-21.402
7)	-14.541
8)	-14.541

Total energy: -114.611699

^{14}O Z=8, N=6

$$T_z = -1$$

Neutron single-particle energy

NO)	ENERGY
1)	-38.207
2)	-38.207
3)	-21.447
4)	-21.447
5)	-21.402
6)	-21.402
7)	-14.541
8)	-14.541

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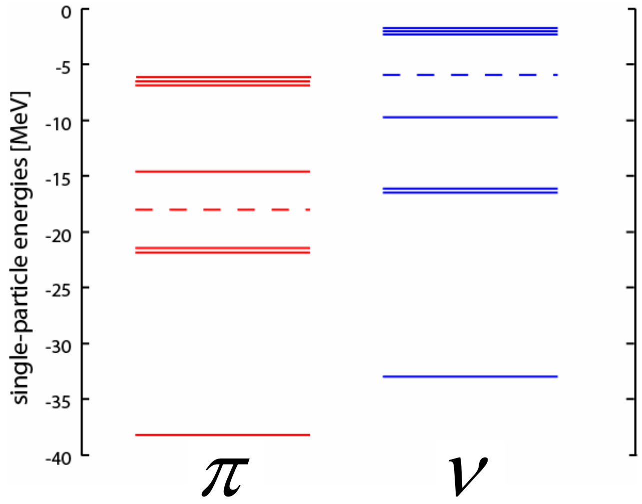
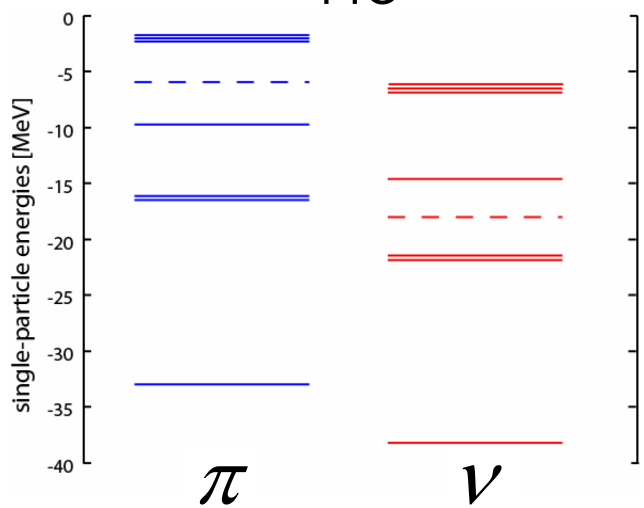
Total energy: -114.611699

14C



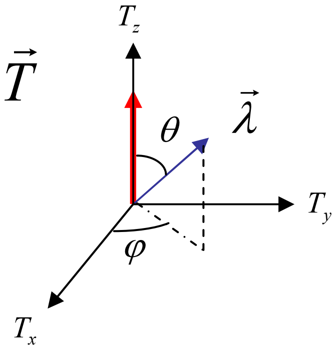
14O



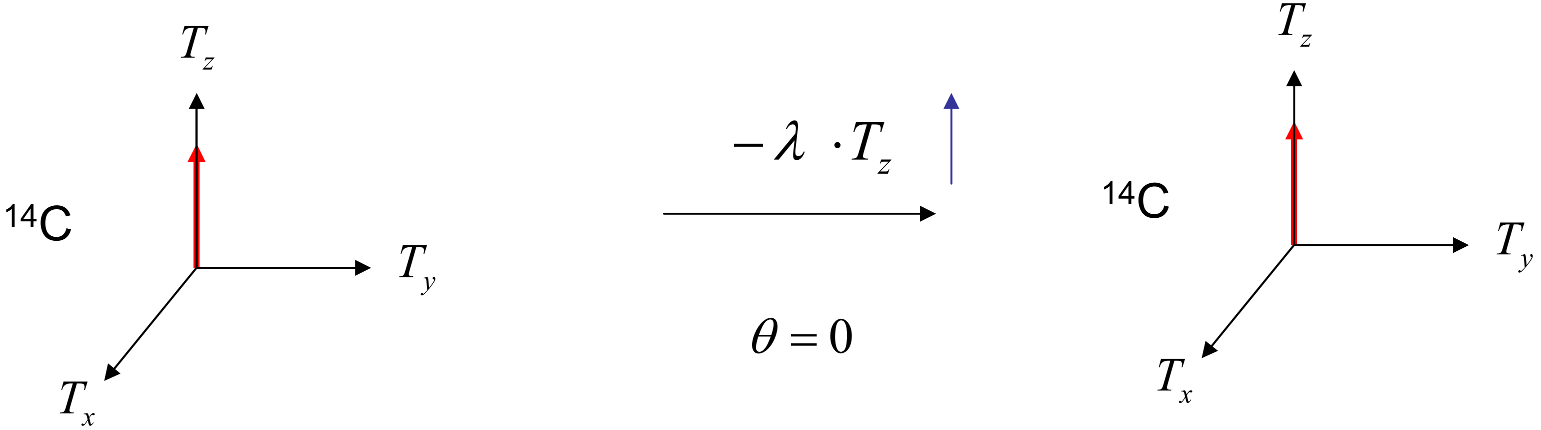
in MeV

Isocranking calculation w/o Coulomb

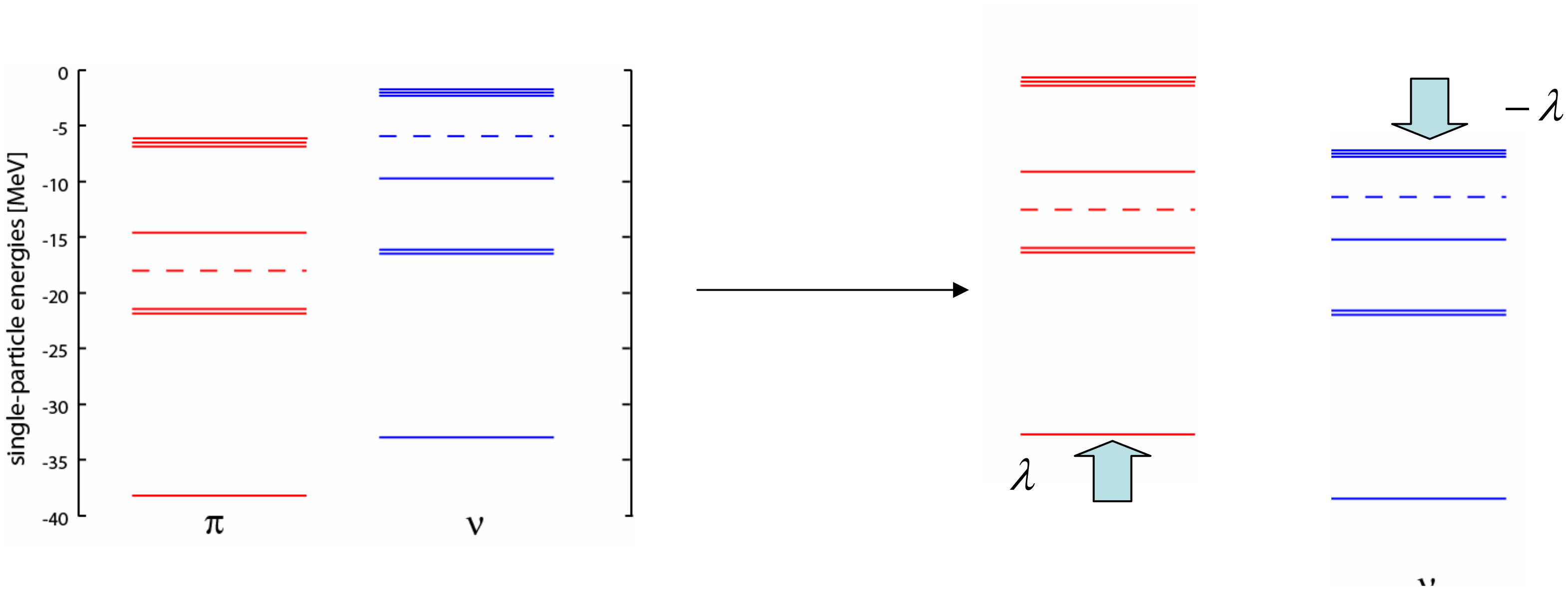
$$\hat{H}' = \hat{H} - \vec{\lambda} \cdot \vec{T}$$



The simplest case ($\theta = 0$)



If lambda is small enough, nothing happens



Result of the calculation with $|\vec{\lambda}| = 5.5 \quad \theta = 0$

Initial : ^{14}C

neutron sp energy:

NO)	ENERGY
1)	-32.919
2)	-32.919
3)	⋮
4)	
5)	
6)	
7)	
8)	

$-|\vec{\lambda}|$

$+|\vec{\lambda}|$

Proton sp energy:

NO)	ENERGY
1)	-38.207
2)	-38.207
3)	-21.447
4)	-21.447
5)	⋮
6)	
7)	
8)	

Total energy: -114.611699

$(\theta, \varphi) = (0,0)$

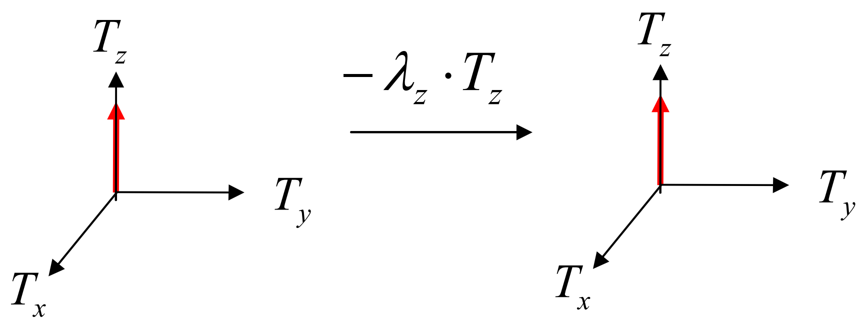
single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	100
2)	-38.419	100
3)	-32.707	-100
4)	-32.707	-100
5)		100
6)		100
7)	⋮	100
8)		100
9)		-100
10)		-100
11)		-100
12)		-100
13)		100
14)		100

pure neutron states

pure proton states

p-n not mixed



Total energy: -114.611699

$$\langle \hat{T}_z \rangle = 1$$

<T>=100(-100): pure n(p)

$$= \langle \tfrac{1}{2}\tau_z \rangle \times 200$$

w/ p-n mixing and no Coulomb

^{14}C

$|\vec{\lambda}| = 5.5$

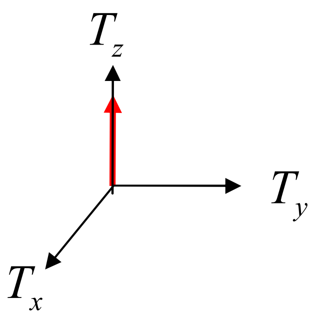
$(\theta,\varphi) = (0,0)$

single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	100
2)	-38.419	100
3)	-32.707	-100
4)	-32.707	-100
5)		
6)		
7)	⋮	
8)		
9)		
10)		
11)		
12)		
13)	-15.181	100
14)	-15.181	100

Total energy: -114.611699

$\langle \hat{T}_z \rangle = 1$



$(\theta,\varphi) = (90^\circ,0)$

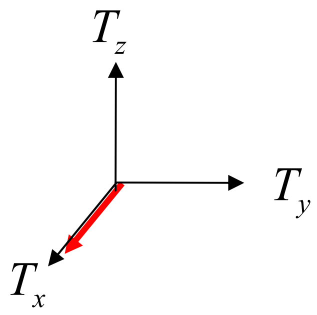
single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	0
2)	-38.419	0
3)	-32.707	0
4)	-32.707	0
5)	-	
6)	-	
7)	-	⋮
8)	-	
9)	-	
10)	-	
11)	-	
12)	-	
13)	-15.181	0
14)	-15.181	0

Total energy: -114.611699

$\langle \hat{T}_z \rangle = 0$

50% neutron &50% proton



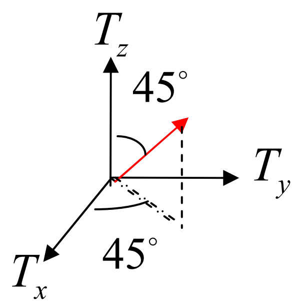
$(\theta,\varphi) = (45^\circ,45^\circ)$

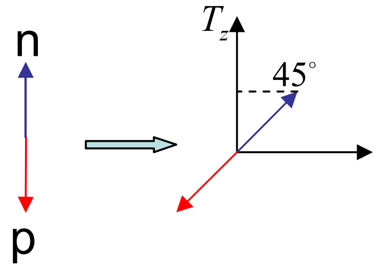
single-particle energy:

NO)	ENERGY	<T>
1)	-38.419	70.7
2)	-38.419	70.7
3)	32.707	-70.7
4)	-32.707	-70.7
5)		
6)		
7)	⋮	
8)		
9)		
10)		
11)		
12)		
13)	-15.181	70.7
14)	-15.181	70.7

Total energy: -114.611699

$\langle \hat{T}_z \rangle = 0.707$





A=14 with Coulomb

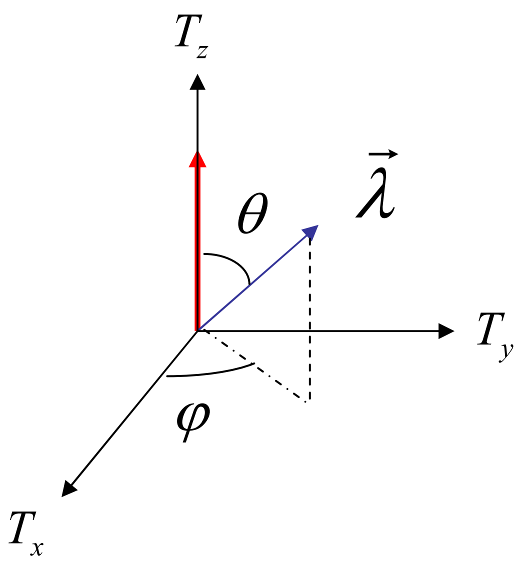
With Coulomb

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

The total energy is now dependent on Tz

but independent on Tx and Ty

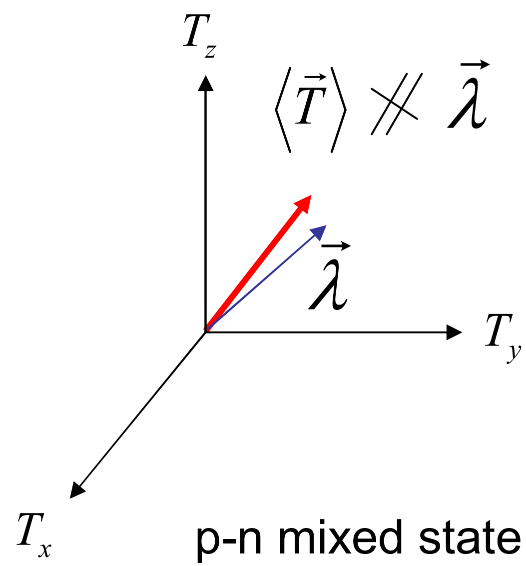
Initial state:



HF state w/o p-n mixing

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

final state:



p-n mixed state

With Coulomb, the system favors larger $\langle T_z \rangle$

w/ p-n mixing and Coulomb

angle of $\vec{\lambda}$

^{14}C ← $(\theta,\varphi)=(0,0)$

single-particle energy:

NO)	ENERGY	<T>
1)	-38.346	100
2)	-38.346	100
3)	-29.620	-100
4)	-29.620	-100
5)	-22.000	100
6)	-22.000	100
7)		
8)		
9)	⋮	
10)		
11)		
12)		
13)		
14)		

Total energy: -106.68

<Tz>=1

$(\theta,\varphi)=(45^\circ,0)$

Single-particle energy:

NO)	ENERGY	<T>
1)	-37.980	82.0
2)	-37.980	82.0
3)	-29.880	-82.0
4)	-29.880	-82.0
5)	-21.666	80.7
6)	-21.666	80.7
7)		
8)		
9)	⋮	
10)		
11)		
12)		
13)		
14)		

Total energy: -106.16

<Tz>=0.802

$(\theta,\varphi)=(180^\circ,0)$ → ^{14}O

single-particle energy:

NO)	ENERGY	<T>
1)	-34.362	-100
2)	-34.362	-100
3)	-32.527	100
4)	-32.527	100
5)	-18.41	-100
6)	-18.41	-100
7)		
8)		
9)	⋮	
10)		
11)		
12)		
13)		
14)		

Total energy: -100.70

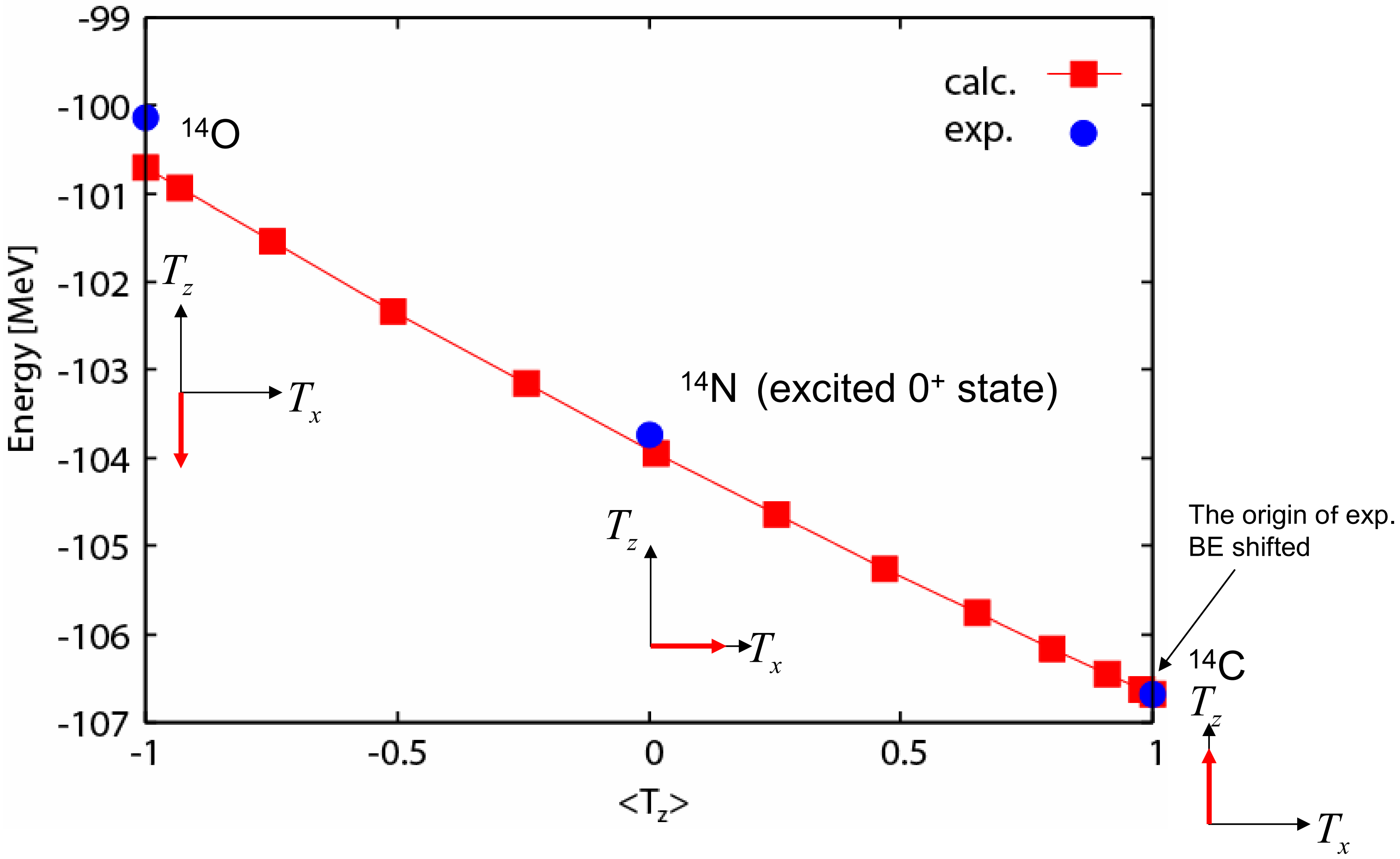
<Tz>=-1

The degree of p-n mixing depends of s.p. states

- Total and s. p. energies depend on Tz
- Total isospin and lambda are not parallel
- Protons and neutrons are not mixed for $\theta=0^\circ$ and $\theta=180^\circ$

(Neither Coulomb nor isocranking term contains Tx and Ty.)

Tz dep. of the total energy and comparison with data

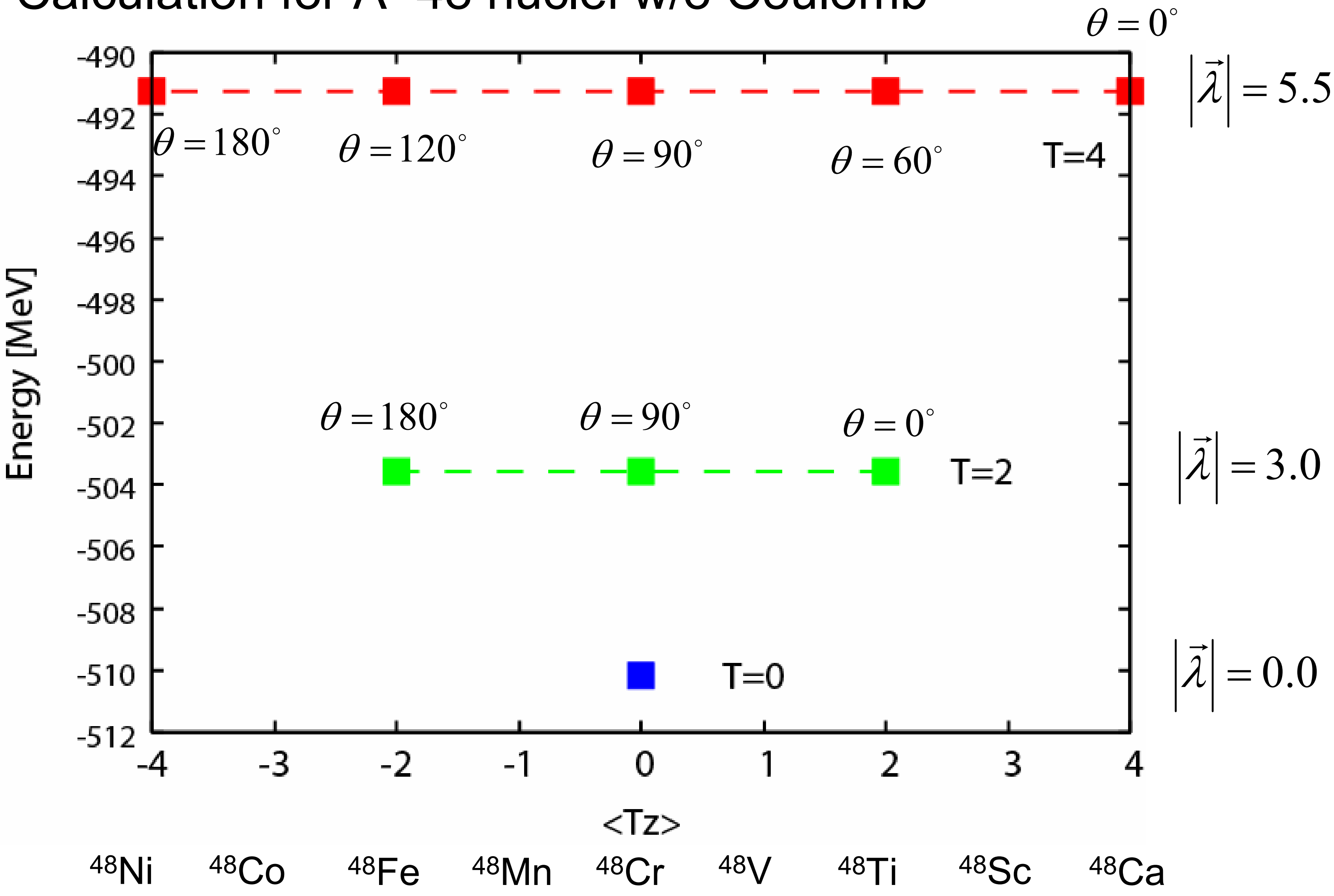


exp.: binding energy
(+excitation energy for 14N)

calc.: calculated for
every 15 deg. of θ bet. (0,180)

Results for A=48

Calculation for A=48 nuclei w/o Coulomb



Normal HF for 48Cr(Tz=0) → Higher isospin states

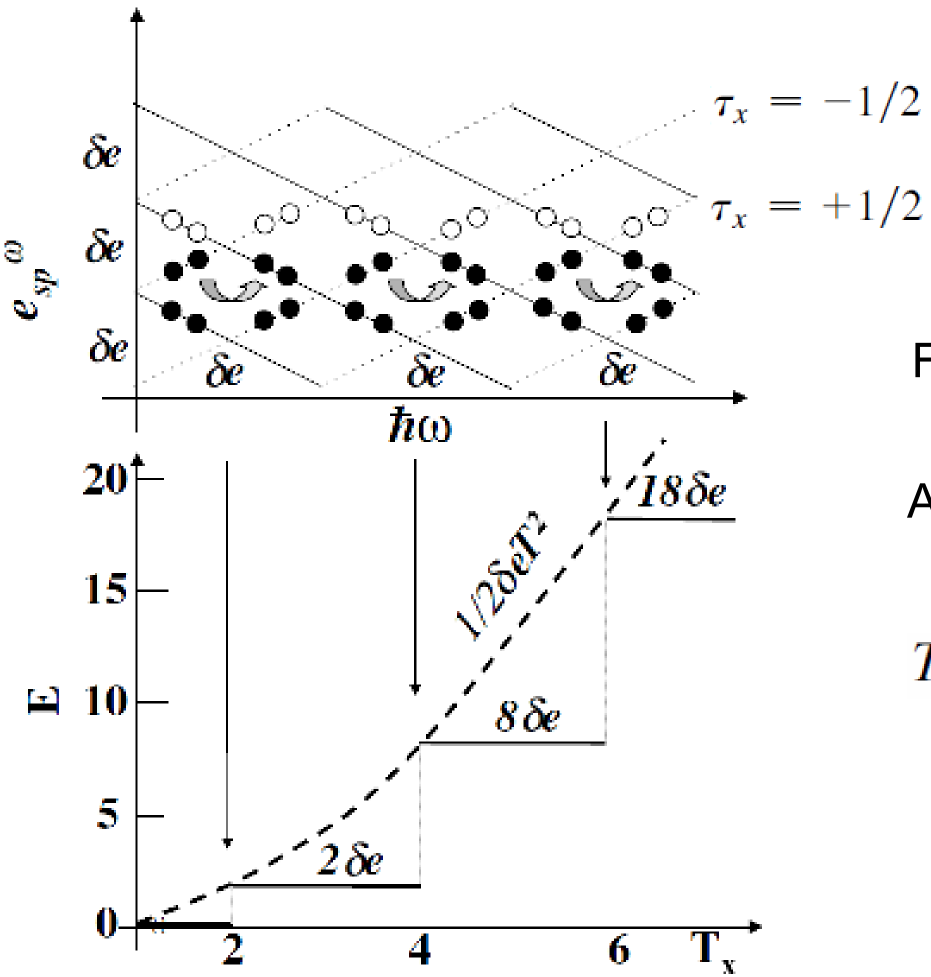
Add $-\vec{\lambda}\cdot\hat{\vec{T}}$

Can we make odd isospin states (T=1, 3, …) by isocranking ?

→ Yes, but we need a 1p1h configuration.

Illustration by a simple model

W. Satuła & R. Wyss, PRL 86, 4488 (2001).



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

equidistant $[e_i = i\,\delta e]$

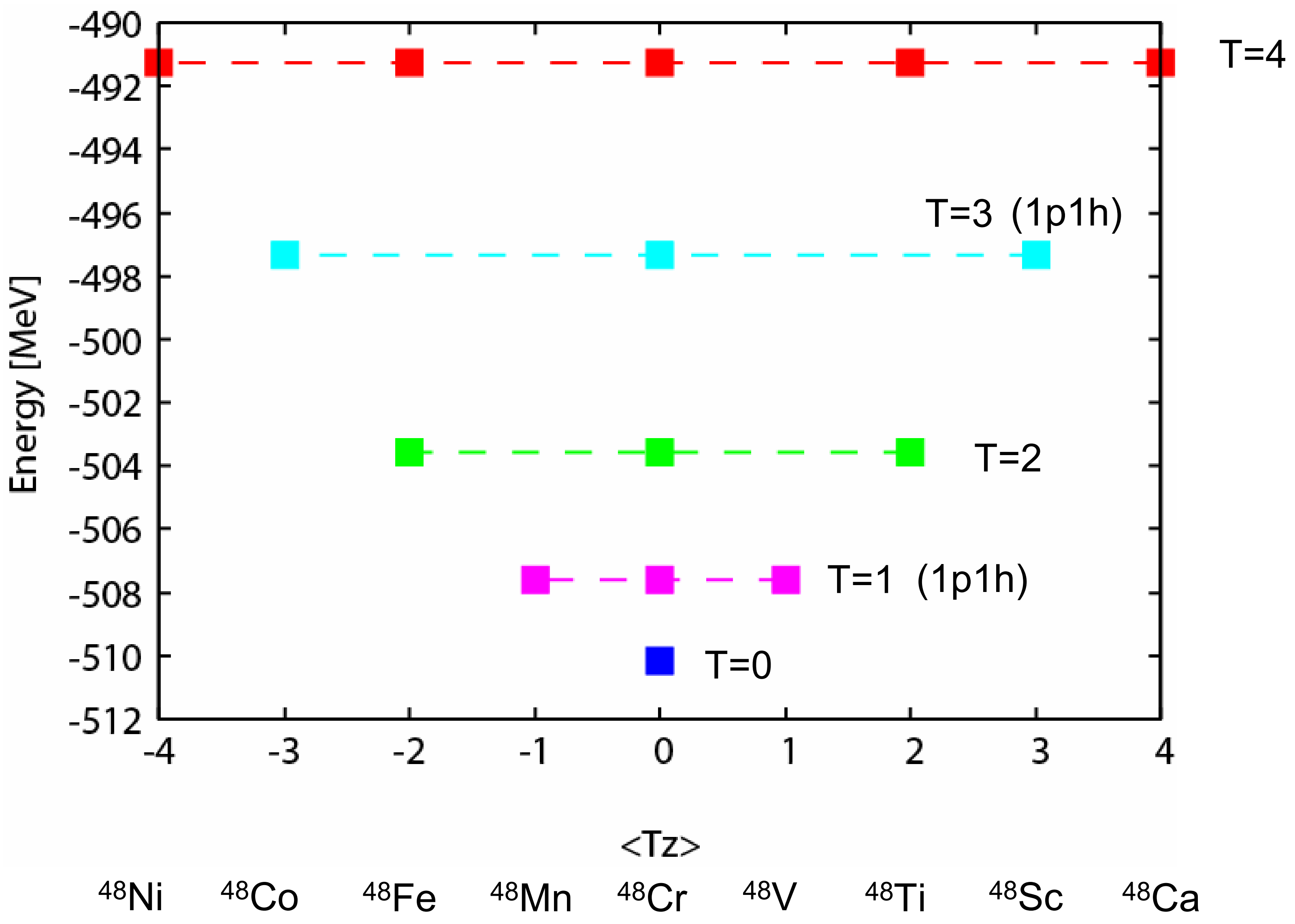
Four-fold degeneracy at ω=0

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

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

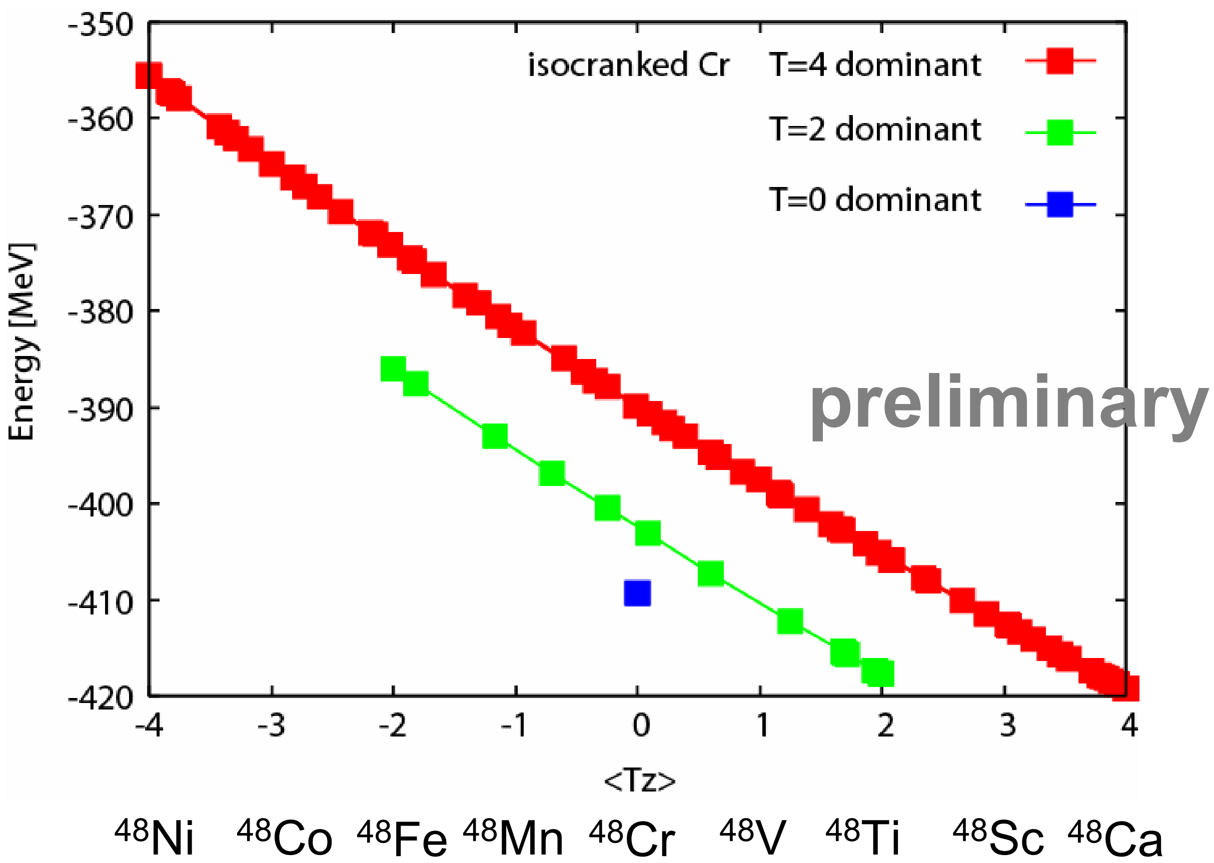
To get T=1,3, ･･ states,
we make a 1p1h excitation

Calculation for A=48 nuclei w/o Coulomb



Calculation for A=48 nuclei with Coulomb

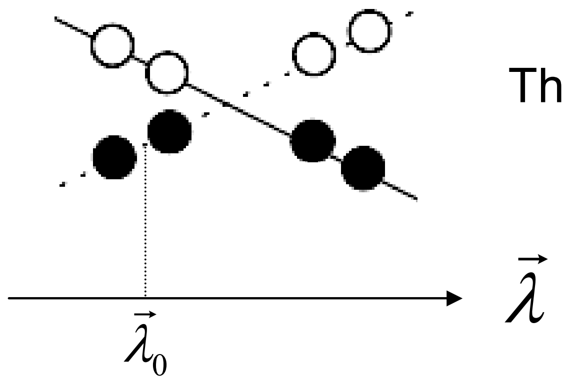
Isocranking for 48Cr(Tz=0)



With Coulomb, we have to adjust the isocranking frequency depending on the tilting angle. Otherwise, the calculation often diverges.

Near the crossing frequency, the “ping-pong” divergence often occurs.

The HF iteration procedure gives oscillating results in every second iteration.



The level ordering changes alternately.

A more efficient way

(✔) Diabatic blocking using isospin

Specify which player should take the ping-pong ball at each iteration.

(✔) Constraint on isospin with the augmented Lagrangian method.

Linear and quadrutic constraint terms

A. Staszczak, Eur. Phys. J. A **46**, 85–90 (2010)

Road map

HFODD (Skyrme-HF(B) code)

↓

Proton-neutron mixing at HF level

↓

ALM for isospin constraint
Diabatic blocking using isospin

Isospin projection with p-n mixing ← Next!

↓

Proton-neutron pairing (T=1 & T=0)

↓

QRPA with FAM, Isospin projection w/ p-n pairing, etc.

Application for GT strength

Isospin projection with p-n mixing

Why isospin projection needed?

There is unphysical isospin mixing inherent to MF approaches

For usual HF, the isospin projection 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]

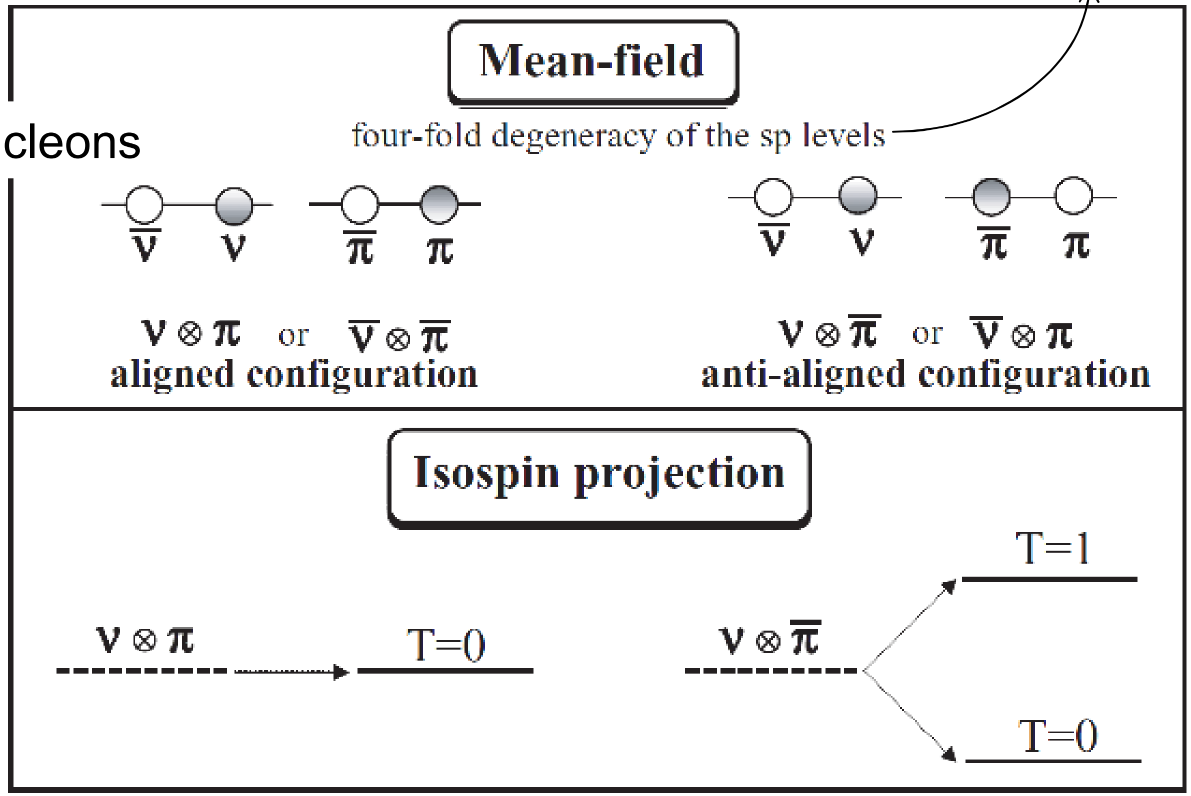
Isospin symmetry of atomic nuclei is explicitly broken by the charge-dependent interactions, primarily the Coulomb force. Within the nuclear density functional theory, isospin is also broken spontaneously. We propose a projection scheme rooted in a Hartree-Fock theory that allows the consistent treatment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

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

(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

Proton-neutron pairing

- Both T=0 and T=1 p-n pairings
- Formalism of DFT with p-n pairing correlations

Perlinska et al, PRC 69 , 014316(2004)

- Isospin restoration for HFB states
- Non-rotating and rotating nuclei (MoI, deformation properties, etc. ..)

QRPA calculation with Finite amplitude method (FAM)

Nakatsukasa, PRC **76**, 024318 (2007)

Avogadro & Nakatsukasa, PRC **84**, 014314 (2011)

Stoitsov et al., PRC **84**, 041305(R) (2011)

- An efficient method for QRPA calculations
- No need to evaluate A and B matrices

  Hot spot in conventional QRPA codes
- Simple modification to transform a HFB code to a QRPA code
- Successful applications (3D RPA, spherical QRPA, axial QRPA)

Summary

We have extended the Skyrme-Hatree-Fock code including the p-n mixing and performed test calculations for A=14 & A=48 isobars.

Ongoing

A=48 system (T=0 even-even nucleus and its isobars)

Tests for constrained HF on isospin and diabatic blocking

Future

Isospin projection

Proton-neutron pairing (T=0 & T=1)

Charge exchange reaction (QRPA calculation with FAM)

→ A very wide applicability expected