The isospin- and angular-momentum-projected DFT and beyond: formalism and applications

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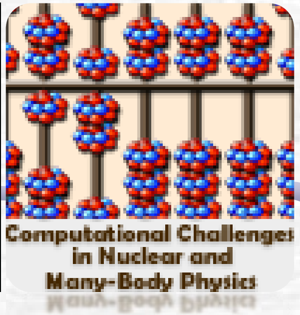
in collaboration with: J. Dobaczewski, W. Nazarewicz, M. Rafalski & M. Konieczka

- MR DFT: short presentation of main building blocks of our approach
  - → mean-field (or nuclear DFT)
  - → symmetry (rotational, isospin) breaking and restoration
    - → unphysical (spontaneous) symmetry violation isospin projection
    - → Coulomb rediagonalization (explicit symmetry violation)
  - isospin impurities
  - superallowed beta decay (sources of theoretical errors and limitations of the „static" MR DFT)
- **Extension:** → toward NO CORE shell model (CI) with basis cutoff dictated by the self-consistent p-h configurations
  - → examples: ^{32}Cl-^{32}S, ^{62}Zn-^{62}Ga, ^{38}Ca-^{38}K, ^{42}Sc
- **Summary & perspectives.**





The nuclear effective theory

is based on a simple and very intuitive assumption that low-energy nuclear theory is independent on high-energy dynamics

ultraviolet cut-off →

$$v_S(q^2) \approx v_S(0) + v_S^{(1)}(0)q^2 + v_S^{(2)}(0)q^4 \dots ,$$

Fourier

regularized

$$v_{eff}(\boldsymbol{r}) \approx v_{long}(\boldsymbol{r})$$
$$+ ca^2\delta_a(\boldsymbol{r})$$
$$+ d_1a^4\boldsymbol{\nabla}^2\delta_a(\boldsymbol{r}) + d_2a^4\boldsymbol{\nabla}\delta_a(\boldsymbol{r})\boldsymbol{\nabla}$$
$$+ \dots$$
$$+ g_1a^{n+2}\boldsymbol{\nabla}^n\delta_a(\boldsymbol{r}) + \dots ,$$

correcting pseudopotential

$\delta_a(\boldsymbol{r})$ denotes an arbitrary Dirac-delta model

Skyrme interaction: $\lim_{a\to 0}\delta_a$

$$v(1,2) = t_0(1 + x_0\hat{P}_\sigma)\delta(\boldsymbol{r}_{12})$$ **LO**

$$+ \frac{1}{2}t_1(1 + x_1\hat{P}_\sigma)\left(\hat{\boldsymbol{k}}'^2\delta(\boldsymbol{r}_{12}) + \delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}^2\right)$$
$$+ t_2(1 + x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}'\delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}$$ **NLO**

$$+ \frac{1}{6}t_3(1 + x_3\hat{P}_\sigma)\rho_0^\gamma(\boldsymbol{R})\delta(\boldsymbol{r}_{12})$$ ← density dependence

$$+ iW_0(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)\left(\hat{\boldsymbol{k}}' \times \delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}\right) ,$$ ← spin-orbit

SV

$\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$; $\boldsymbol{R} = (\boldsymbol{r}_1 + \boldsymbol{r}_2)/2$; $\hat{\boldsymbol{k}} = \frac{1}{2i}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)$ $\hat{\boldsymbol{k}}' = -\frac{1}{2i}(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)$ relative momenta

$\hat{P}_\sigma = \frac{1}{2}(1 + \boldsymbol{\sigma}_1\boldsymbol{\sigma}_2)$ spin exchange

Skyrme local energy density functional

Skyrme (hadronic) interaction conserves such symmetries like:

→ rotational (spherical) symmetry

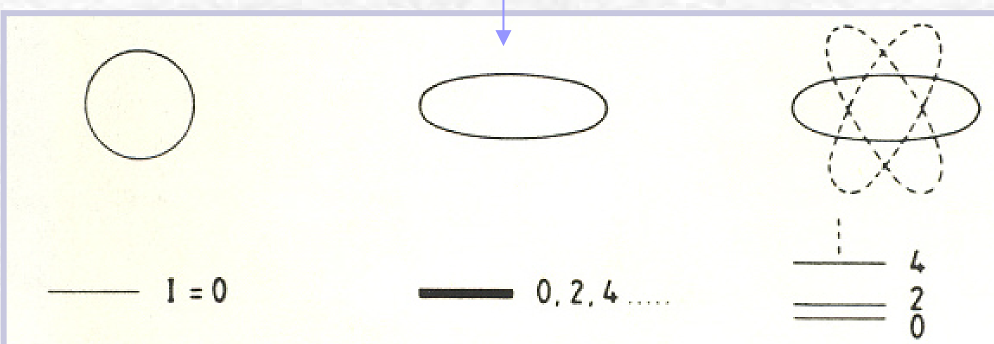
→ isospin symmetry: $V^{LS}_{nn} = V^{LS}_{pp} = V^{LS}_{np}$ (in reality approximate)

→ parity…

Self-consistent solutions (Slater dets) break these symmetries (are deformed) spontaneously

$$\hat{R}(\boldsymbol{Q})|\varphi(\boldsymbol{Q}_0)\rangle = |\varphi(\boldsymbol{Q}')\rangle$$

$$\langle\varphi|\hat{H}|\varphi\rangle = \langle\varphi|\hat{R}^{\dagger}(\boldsymbol{Q})\hat{H}\hat{R}(\boldsymbol{Q})|\varphi\rangle$$



advantages:
builts in correlations into single Slater determinant

disadvantages:
symmetry must be restored to compare theory to data

Restoration → beyond mean-field → multi-reference density functional theory

Isospin symmetry restoration

There are two sources of the isospin symmetry breaking:
- **unphysical**, caused solely by the HF approximation → Engelbrecht & Lemmer, PRL24, (1970) 607
- **physical**, caused mostly by Coulomb interaction
(also, but to much lesser extent, by the strong force isospin non-invariance)

- Find self-consistent HF solution (including Coulomb) → deformed Slater determinant |HF>:

$$|\mathrm{HF}\rangle = \sum_{T\geq|T_z|} b_{T,T_z}|\alpha;T,T_z\rangle$$

See: Caurier, Poves & Zucker, PL 96B, (1980) 11; 15

- Apply the isospin projector:

$$\hat{P}^T_{T_zT_z} = \frac{2T+1}{2}\int_0^\pi d\beta \sin\beta d^{T*}_{T_zT_z}(\beta)\hat{R}(\beta)$$

in order to create good isospin „basis”:

$$|\alpha;T,T_z\rangle = \frac{1}{b_{T,T_z}}\hat{P}^T_{T_zT_z}|\mathrm{HF}\rangle$$

- Diagonalize total Hamiltonian in „good isospin basis” $|\alpha,T,T_z\rangle$ → takes physical isospin mixing

$$\sum_{T'\geq|T_z|}\langle\alpha;T,T_z|\hat{H}|\alpha;T',T_z\rangle a^n_{T',T_z} = E^{\mathrm{AR}}_{n,T_z} a^n_{T,T_z}$$

$$|\alpha;n,T_z\rangle = \sum_{T\geq|T_z|} a^n_{T,T_z}|\alpha;T,T_z\rangle,$$

$$\alpha_C^{\mathrm{AR}} = 1 - |a^{n=1}_{T=T_z}|^2$$

Isospin-projection is non-singular:

W.Satuła, J.Dobaczewski, W.Nazarewicz, M.Rafalski, PRC81 (2010) 054310

$$\tilde{O}(\beta) = \begin{pmatrix} \cos\frac{\beta}{2} I_N & -\sin\frac{\beta}{2} O \\ \sin\frac{\beta}{2} O^\dagger & \cos\frac{\beta}{2} I_Z \end{pmatrix}$$

SVD →

$$O = W D V^\dagger$$

SVD eigenvalues (diagonal matrix)

$$\tilde{O}(\beta)^{-1} = \begin{pmatrix} \tilde{W}\frac{\cos\frac{\beta}{2}}{\cos^2\frac{\beta}{2} I_N + \sin^2\frac{\beta}{2}\tilde{D}^2}\tilde{W}^\dagger & \tilde{W}\frac{\sin\frac{\beta}{2}}{\cos^2\frac{\beta}{2} I_N + \sin^2\frac{\beta}{2}\tilde{D}^2}\tilde{D}\tilde{V}^\dagger \\ V\frac{-\sin\frac{\beta}{2}}{\cos^2\frac{\beta}{2} I_Z + \sin^2\frac{\beta}{2} D^2} D W^\dagger & V\frac{\cos\frac{\beta}{2}}{\cos^2\frac{\beta}{2} I_Z + \sin^2\frac{\beta}{2} D^2} V^\dagger \end{pmatrix}$$

→ $$\tilde{O}(\beta)^{-1}_{ij} \sim \frac{1}{\cos\frac{\beta}{2}}$$

singularity (if any) at $\beta=\pi$ is inherited by a transition density $\tilde{\rho}$

$$\tilde{\rho} = \sum_{ij} \psi_i^* \, \tilde{O}^{-1}_{ij} \, \varphi_j$$

- **Power [cos(β/2)] counting:**

$$\mathcal{H}(\beta) \sim \tilde{\rho}^{\eta}(\beta)\, \mathrm{Det}\tilde{O}(\beta)$$

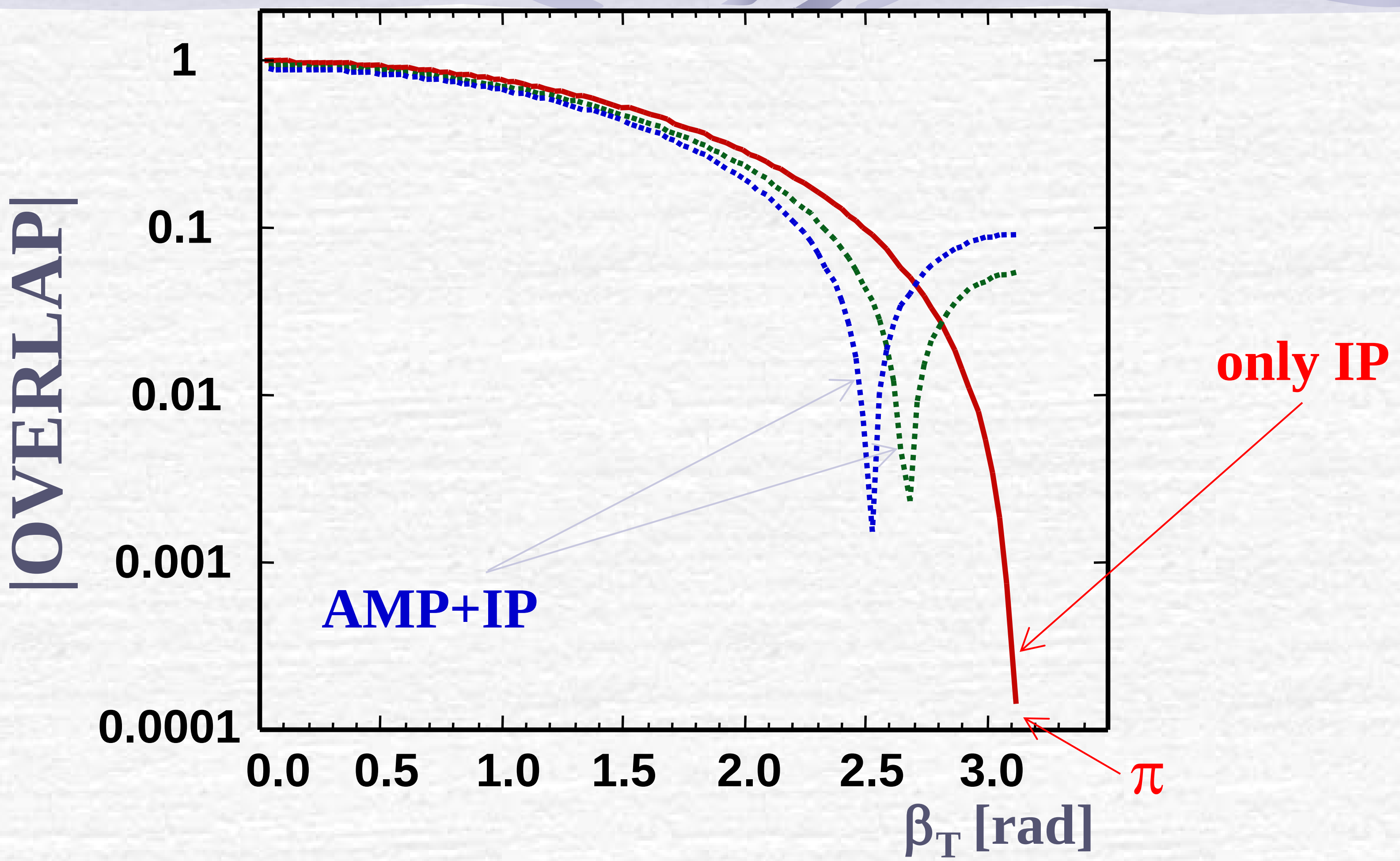
$$\int d\beta \sin\beta \; d^T_{T_z T_z}(\beta)\; \tilde{\rho}^{\eta}(\beta)\; \mathrm{Det}\tilde{O}(\beta) \propto \int d\beta \cos^{\xi}\frac{\beta}{2}$$

$1 + |N\text{-}Z| - \eta + |N\text{-}Z| + 2k$

in the worst case i.e. for N=Z and k=1 → $\eta > 3$ to get a singularity

k is a multiplicity of zero singular values

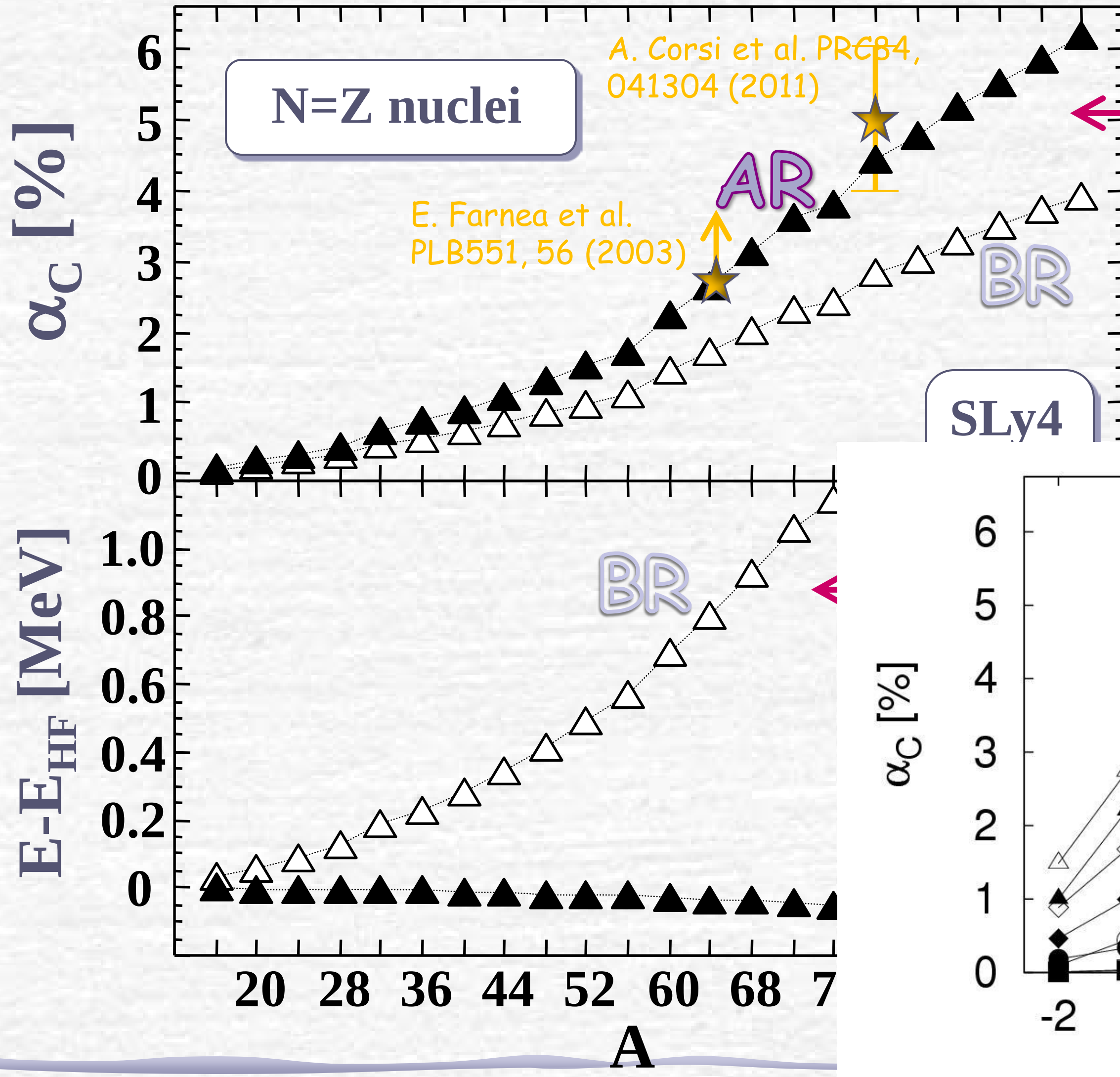
$$|\mathrm{Det}\tilde{O}(\beta)| = |\cos\frac{\beta}{2}|^{N-Z} \prod_{i=1}^{Z} \left(\cos^2\frac{\beta}{2} + \sin^2\frac{\beta}{2} D_i^2\right)$$



Coupled AMP+IP projection is singular forcing us to use the Skyrme interaction SV

(or density-independent interaction)

Isospin mixing & energy in the ground states of e-e N=Z nuclei:

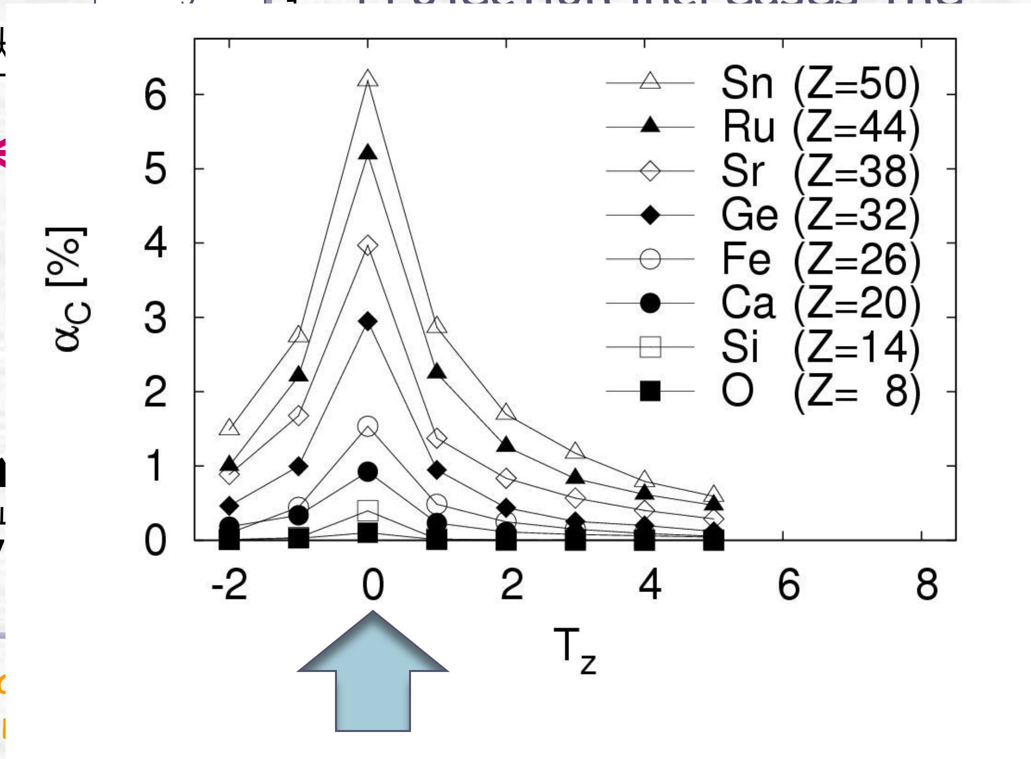


HF tries to reduce the isospin mixing by:

$\Delta\alpha_C$ ~30%

in order to minimize the total energy

Projection increases the

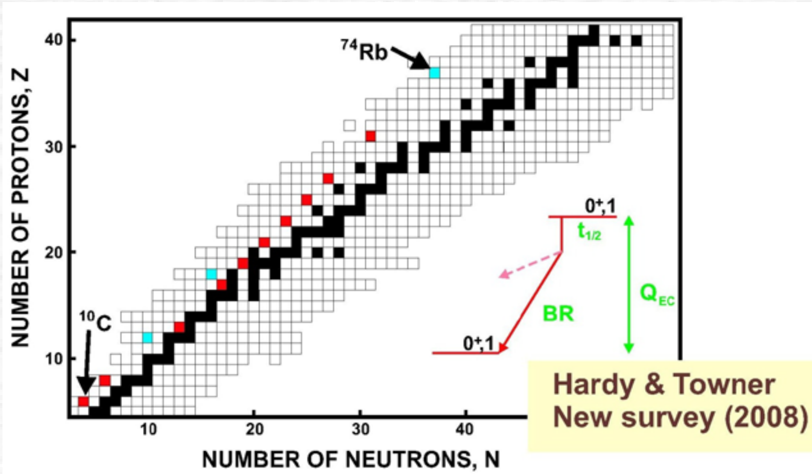


This is not a single Sl

There are no constraints o

Superallowed $0^+ \to 0^+$ Fermi beta decays (testing the Standard Model)

adopted from J.Hardy's, ENAM'08 presentation



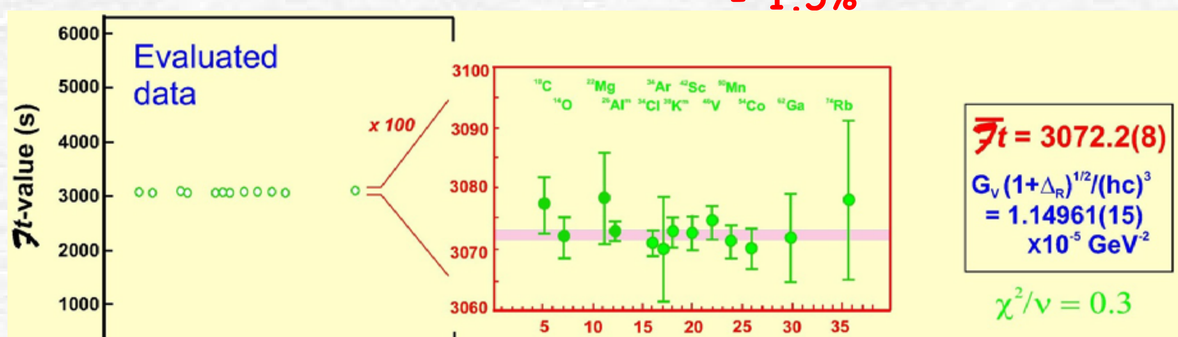
10 cases measured with accuracy *ft* ~0.1%
3 cases measured with accuracy *ft* ~0.3%

→ test of the CVC hypothesis
(Conserved Vector Current)

INCLUDING RADIATIVE CORRECTIONS

$$\mathcal{F}t = ft\,(1 + \delta'_R)[1 - (\delta_C - \delta_{NS})] = \frac{K}{2G_V^2\,(1 + \Delta_R)}$$

1.5%   0.3% - 1.5%   ~2.4%



Towner & Hardy
Phys. Rev. C77, 025501 (2008)

$|V_{ud}| = 0.97418 \pm 0.00026$

→ test of unitarity of the CKM matrix

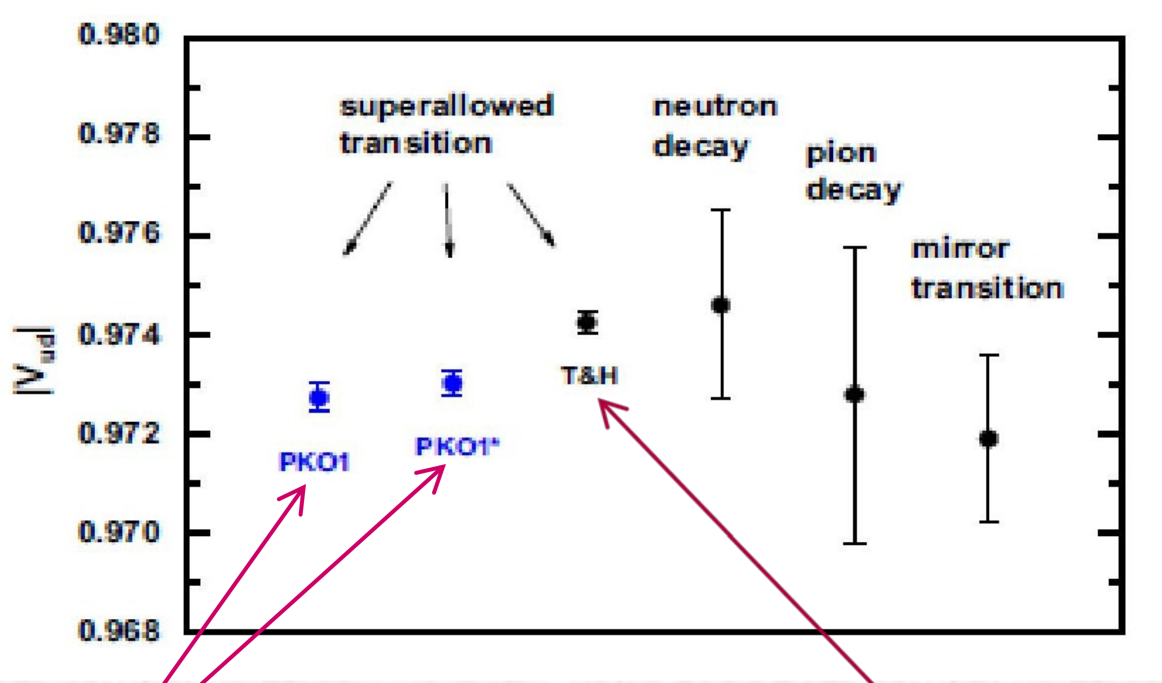
$$|V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 = 0.9997(6)$$

0.9490(4)   0.0507(4)   <0.0001

$$\begin{pmatrix} d' \\ s' \\ b' \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} d \\ s \\ b \end{pmatrix}$$

weak eigenstates   **CKM** Cabibbo-Kobayashi-Maskawa   mass eigenstates

model dependence & model limitations



Liang & Giai & Meng
Phys. Rev. C79, 064316 (2009)

spherical RPA
Coulomb exchange treated in the Slater approximation

Hardy & Towner
Phys. Rev. C77, 025501 (2008)

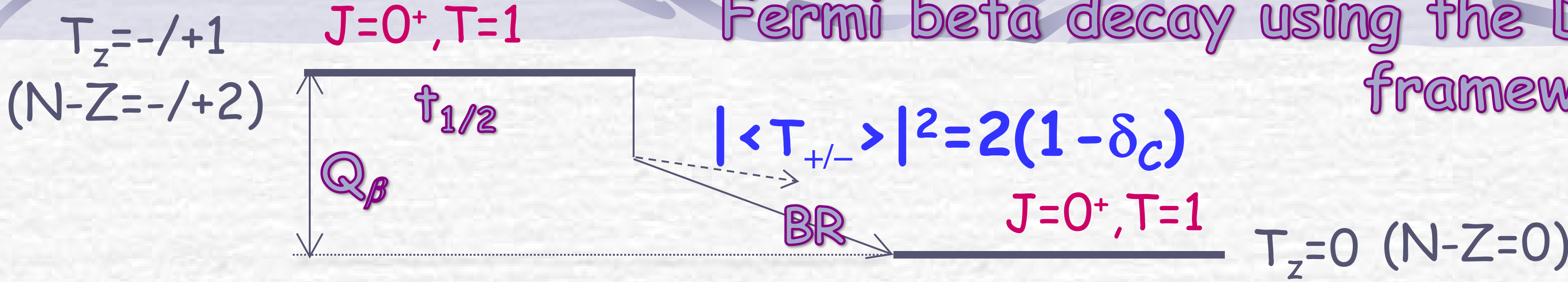
$$\delta_C = \delta_{C1} + \delta_{C2}$$

mean field
radial mismatch of the wave functions

shell model
configuration mixing

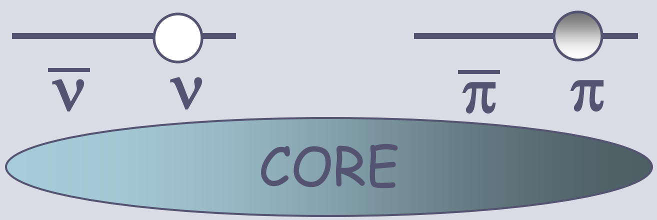
Miller & Schwenk
Phys. Rev. C78 (2008) 035501;C80 (2009) 064319

How to calculate the superallowed Fermi beta decay using the DFT framework?



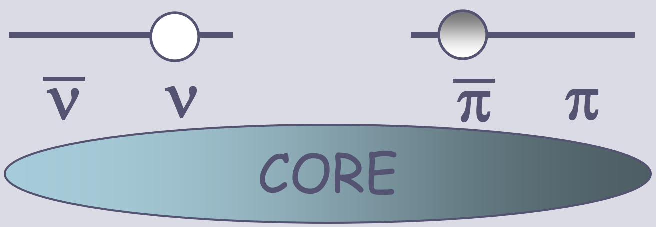
$$|\langle T_{+/-}\rangle|^2=2(1-\delta_C)$$

MEAN FIELD



aligned configurations

$\nu \otimes \pi$ or $\bar{\nu} \otimes \bar{\pi}$



anti-aligned configurations

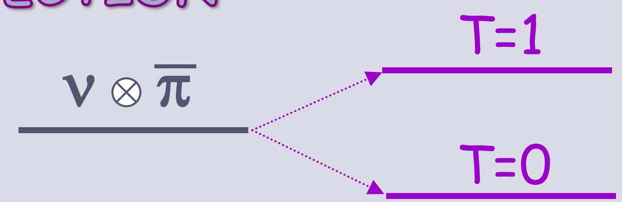
$\nu \otimes \bar{\pi}$ or $\bar{\nu} \otimes \pi$

ISOSPIN PROJECTION

Mean-field can differentiate between

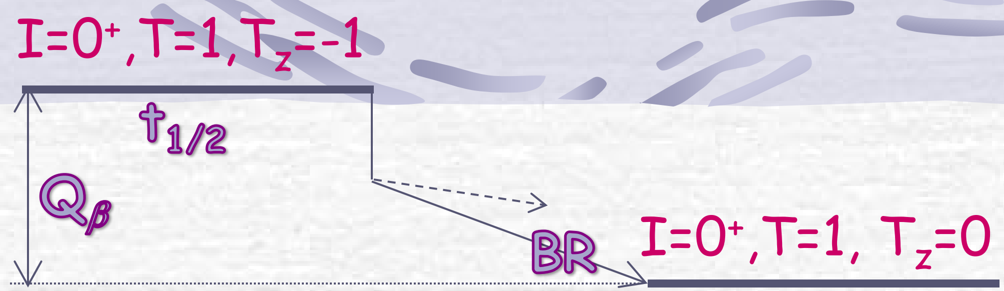
$\nu \otimes \pi$ and $\nu \otimes \bar{\pi}$

only through time-odd polarizations!



T=1 state

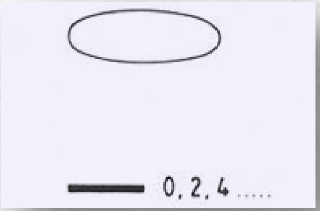
is beyond mean-field!

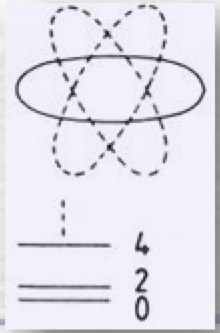


Skyrme-Hartree-Fock
DF

ground state
in N-Z=+/-2 (e-e) nucleus

Project on good isospin (T=1) and angular momentum (I=0)
(and perform Coulomb rediagonalization)





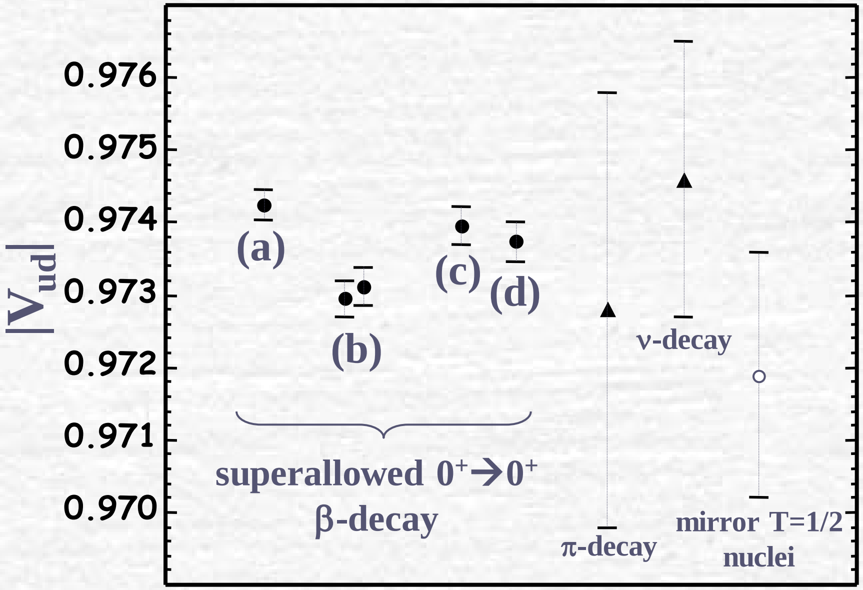
antialigned state
in N=Z (o-o) nucleus

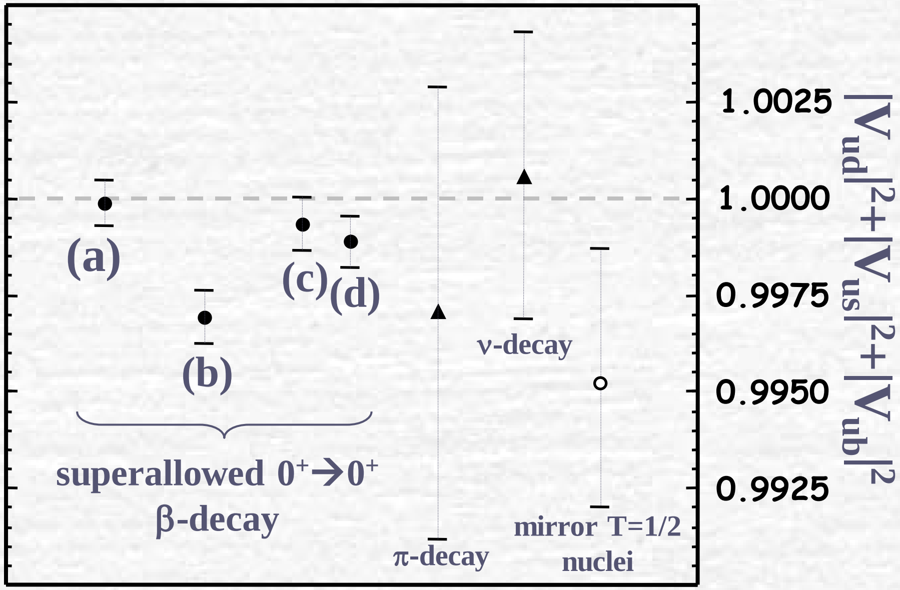
Project on good isospin (T=1) and angular momentum (I=0)
(and perform Coulomb rediagonalization)

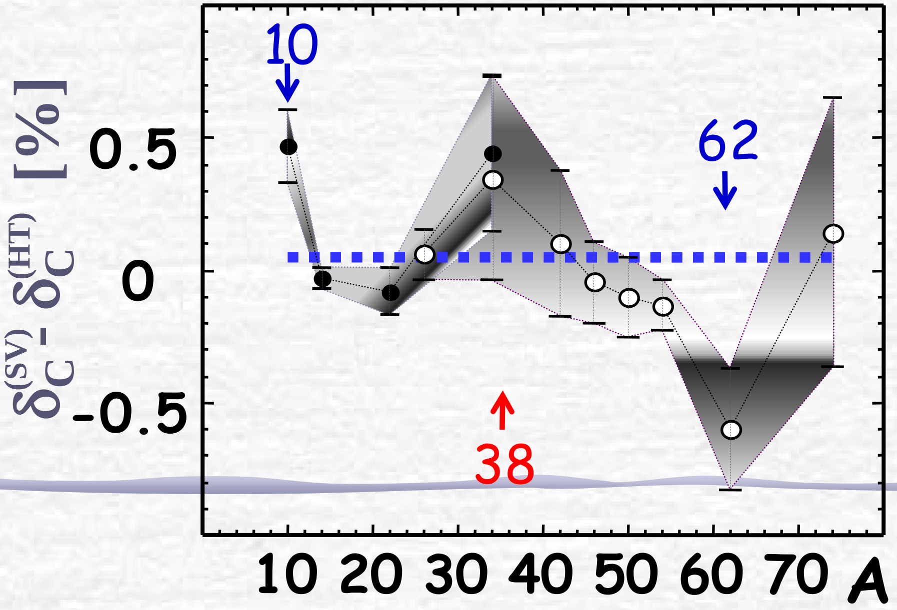
$$|\langle T\approx 1, T_z=+/-1, I=0|\, \mathbf{T_{+/-}}\, |I=0, T\approx 1, T_z=0\rangle|^2 = 2(1-\delta_C)$$

Tests of the weak-interaction flavor-mixing sector of the Standard Model of elementary particles

$|V_{ud}|$ & unitarity - world survey







(a) I.S. Towner and J. C. Hardy, Phys. Rev. C **77**, 025501(2008).

Ft=3071.4(8)+0.85(85); V_{ud}=0.97418(26)

(b) H. Liang, N. V. Giai, and J. Meng, Phys. Rev. C **79**,064316 (2009).

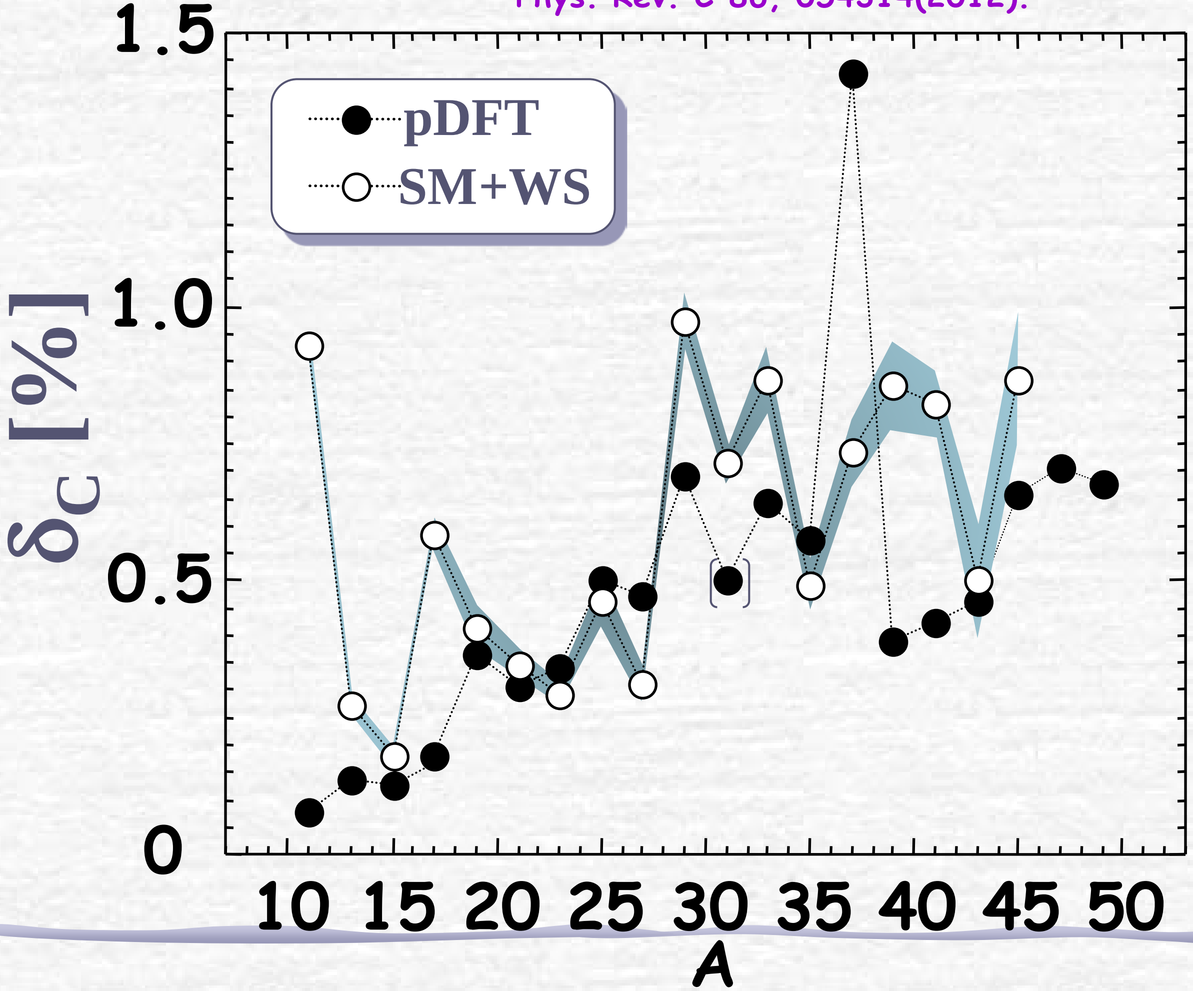
(c,d) W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski, Phys. Rev. Lett. 106, 132502 (2011); Phys. Rev. C **86**, 054314(2012).

Ft=3070.4(9); V_{ud}=0.97444(23) PRL

Ft=3073.6(12); V_{ud}=0.97397(27) PRC

ISB corrections to the Fermi transitions in T=1/2 mirrors

W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski
Phys. Rev. C 86, 054314(2012).

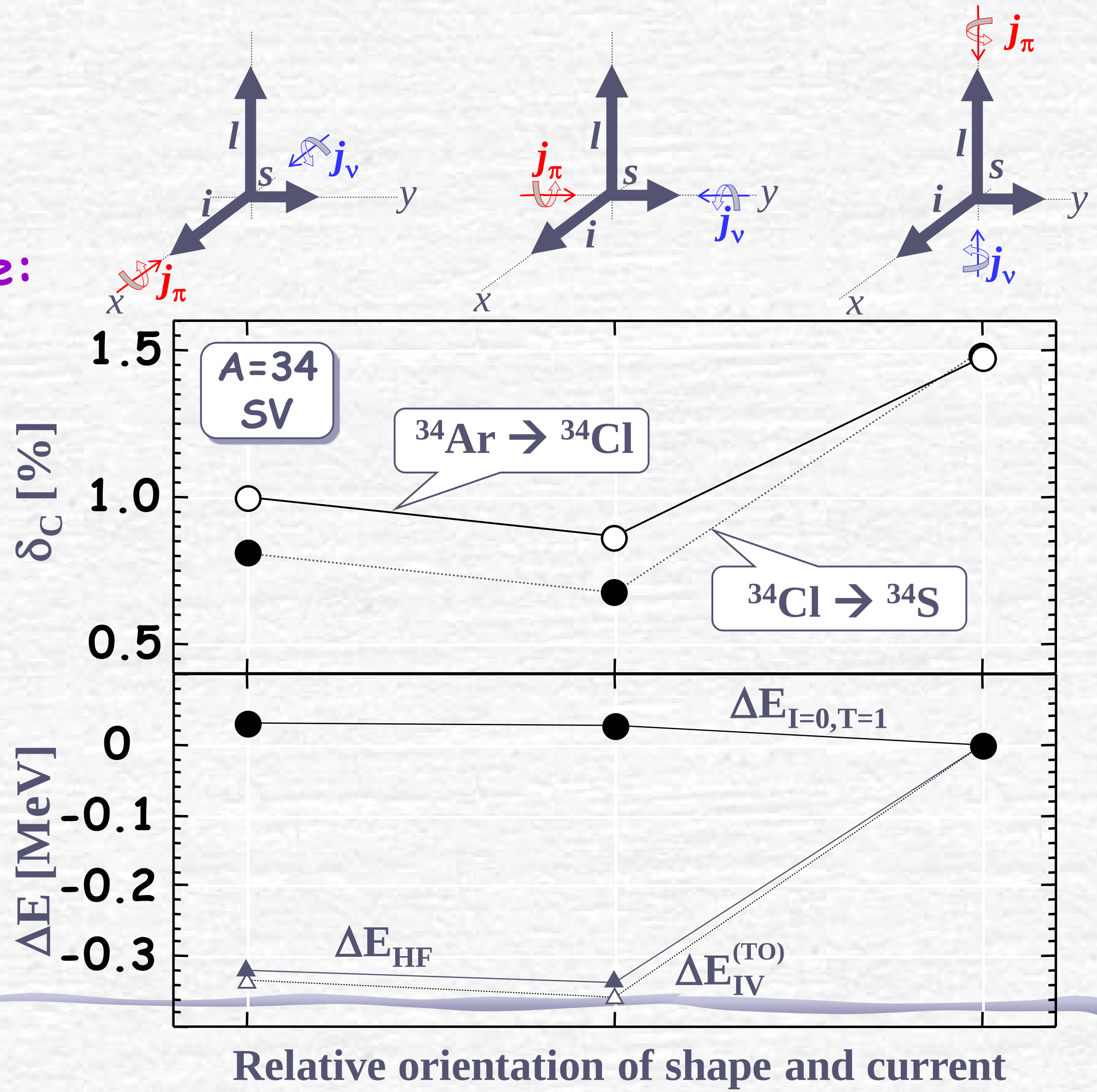


SM+WS results from:
N. Severijns, M. Tandecki,
T. Phalet, and I. S. Towner,
Phys. Rev. C **78**, 055501 (2008).

THEORETICAL UNCERTAINITIES

- Basis-size dependence:
  ~5%

- Configuration dependence:

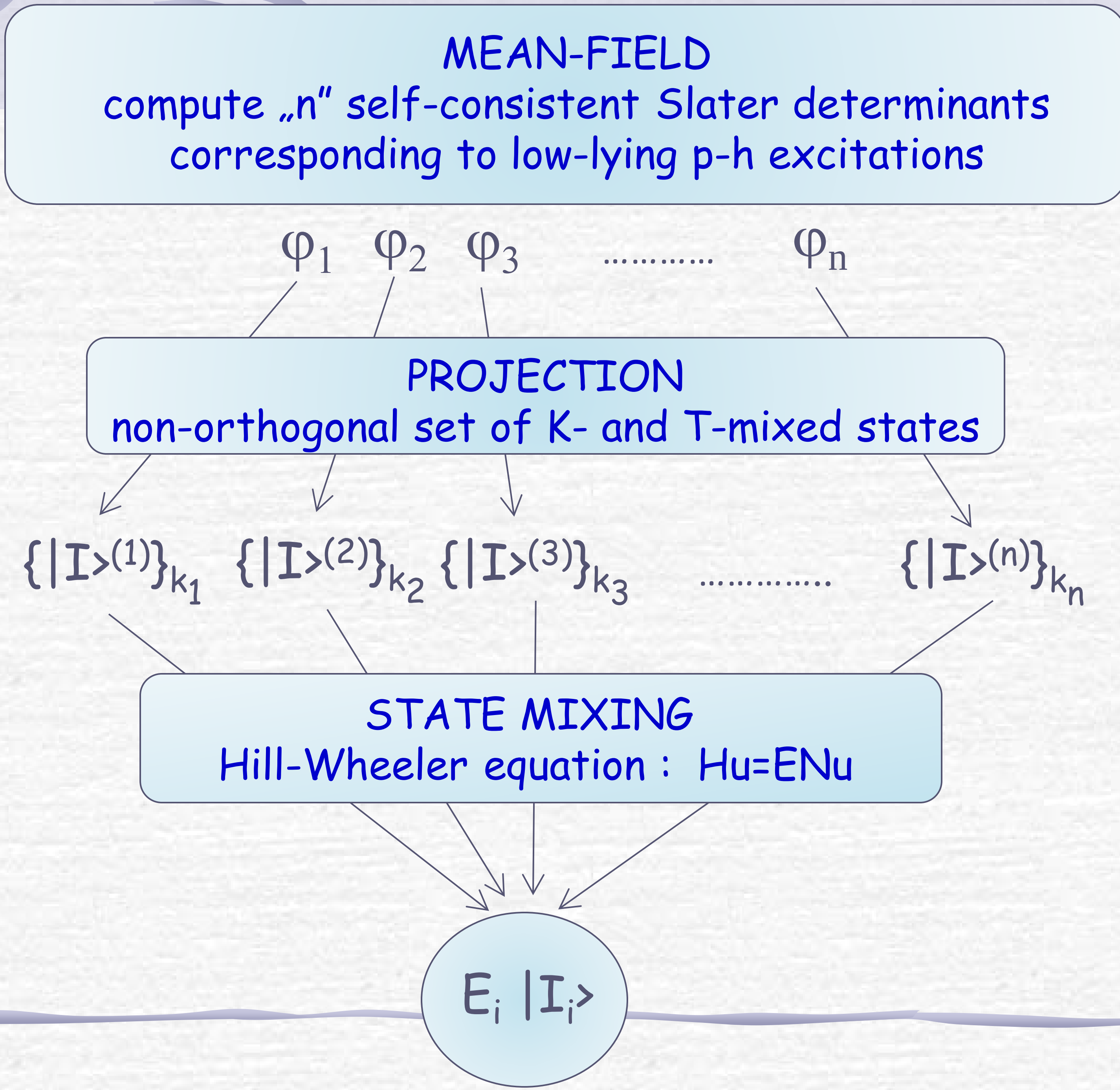


- Functional dependence:

SV: Ft=3073.6(12)
V_{ud}=0.97397(27)
$|V_{ud}|^2+|V_{us}|^2+|V_{ub}|^2=$
=0.99935(67)

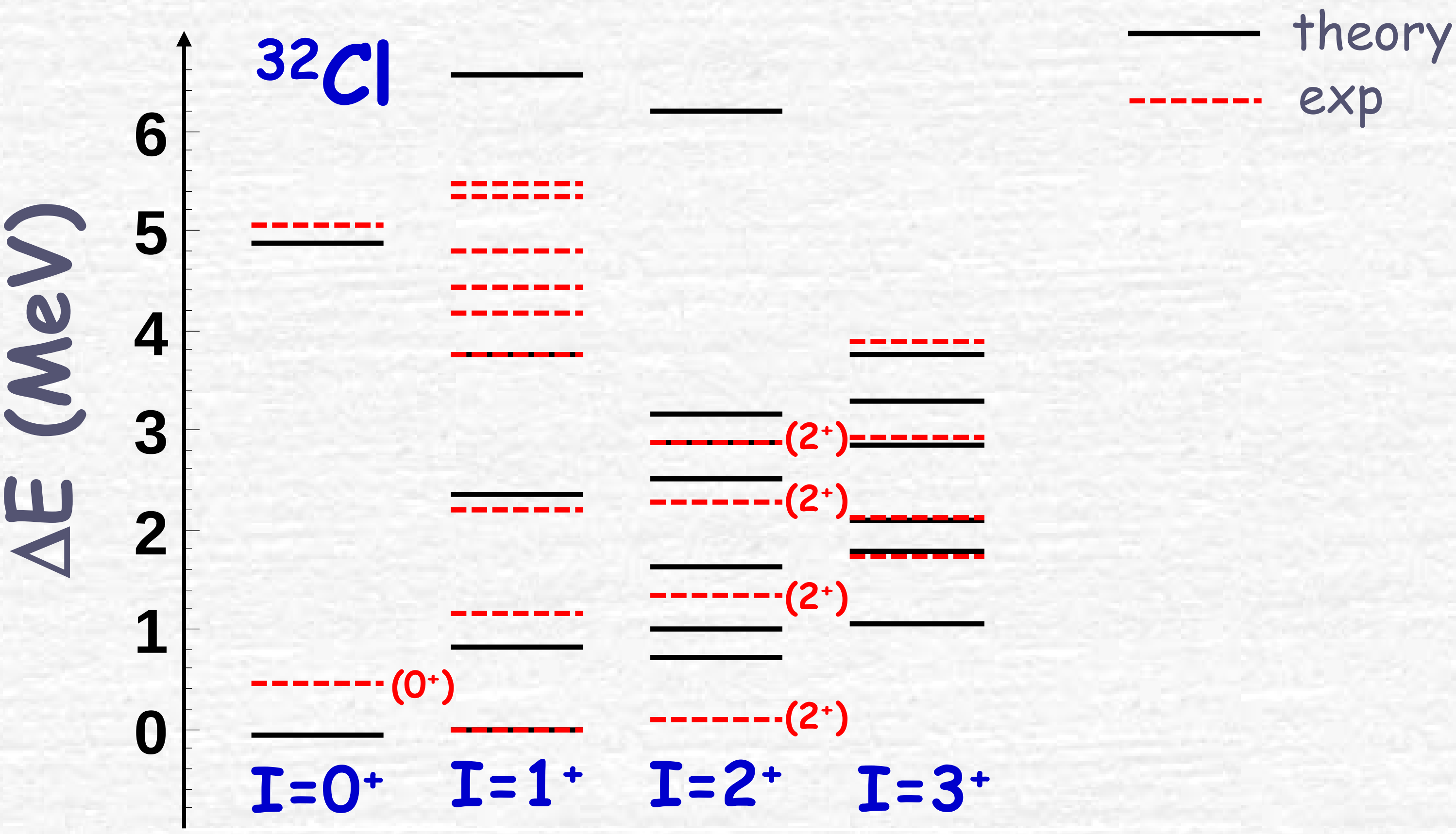
SHZ2: Ft=3075.0(12)
V_{ud}=0.97374(27)
$|V_{ud}|^2+|V_{us}|^2+|V_{ub}|^2=$
=0.99890(67)

a_{sym}=42.2MeV!!!



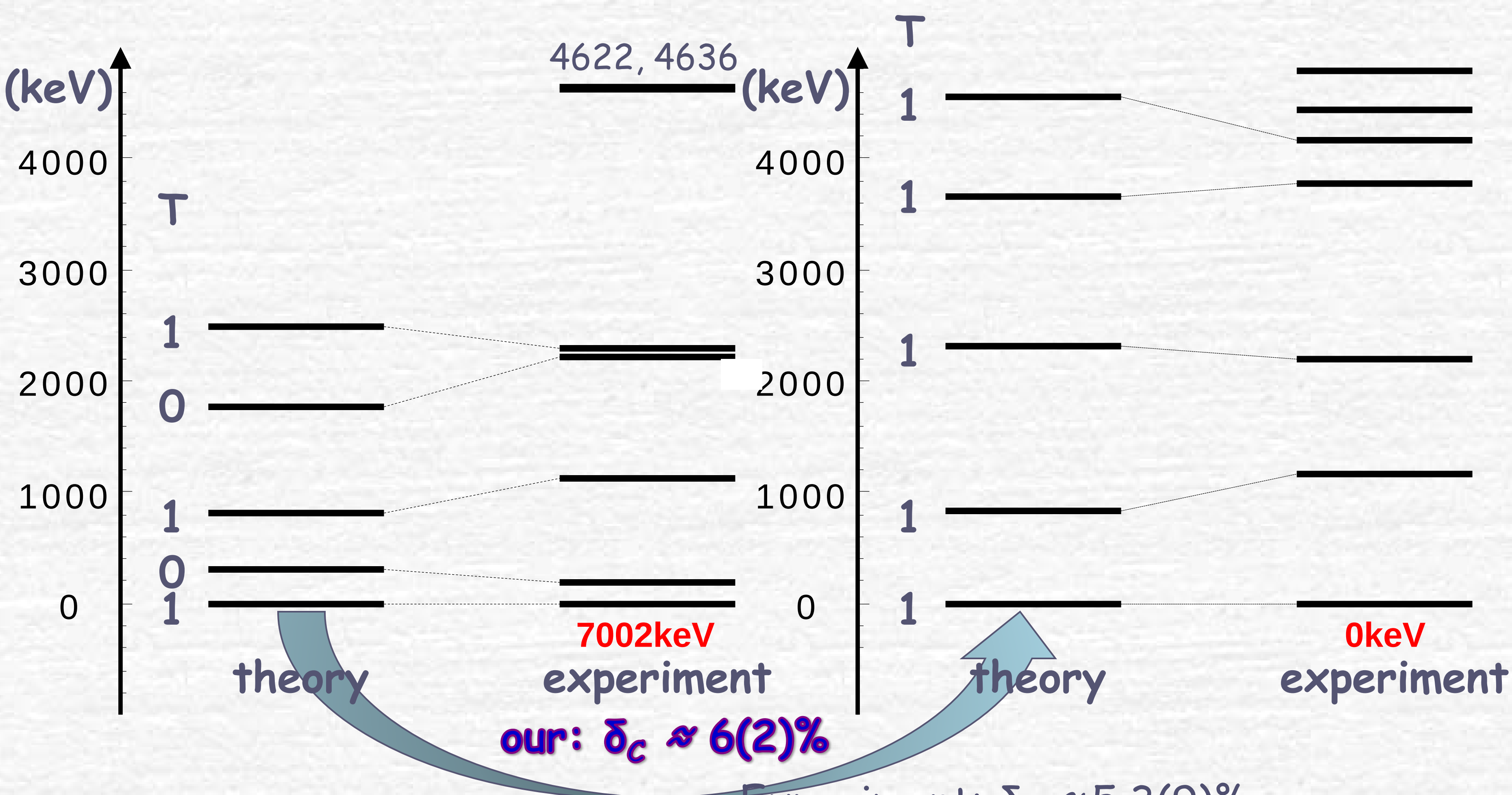
MEAN-FIELD
compute „n" self-consistent Slater determinants corresponding to low-lying p-h excitations
φ_1 φ_2 φ_3 .... φ_n
PROJECTION
non-orthogonal set of K- and T-mixed states
$\{|I>^{(1)}\}_{k_1}$ $\{|I>^{(2)}\}_{k_2}$ $\{|I>^{(3)}\}_{k_3}$ .... $\{|I>^{(n)}\}_{k_n}$
STATE MIXING
Hill-Wheeler equation : Hu=ENu
E_i $|I_i>$

No-core configuration interaction (shell) model with basis cutoff dictated by the self-consistent p-h DFT states



W.Satula, J.Dobaczewski, M.Konieczka, W.Nazarewicz, Acta Phys. Polonica B45, 167 (2014)

^{32}S I=1^{+} ^{32}Cl I=1^{+}



Experiment: $\delta_C \approx 5.3(9)\%$

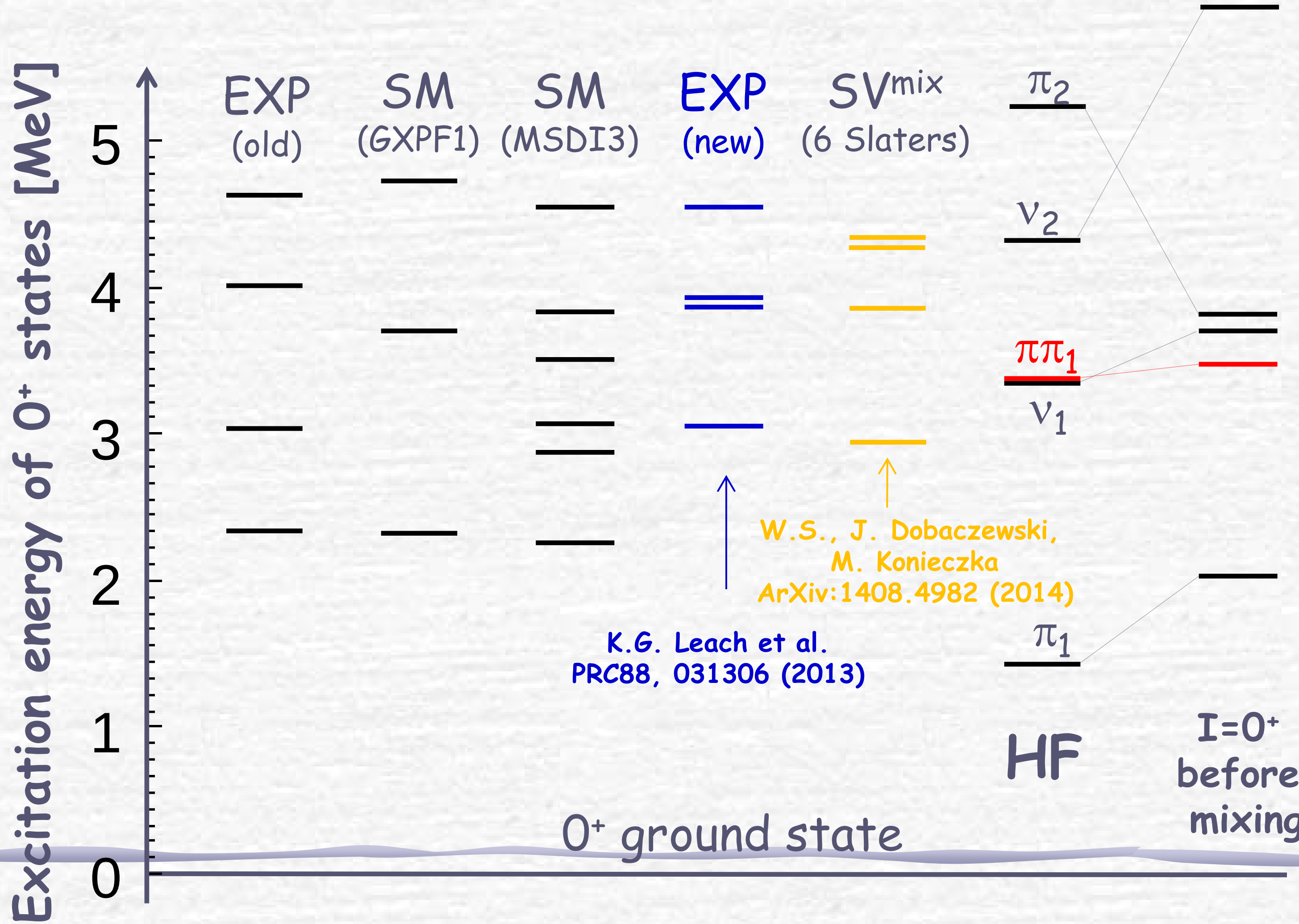
SM+WS calculations: $\delta_C \approx 4.6(5)\%$.

D. Melconian et al., Phys. Rev. Lett. **107**, 182301 (2011).

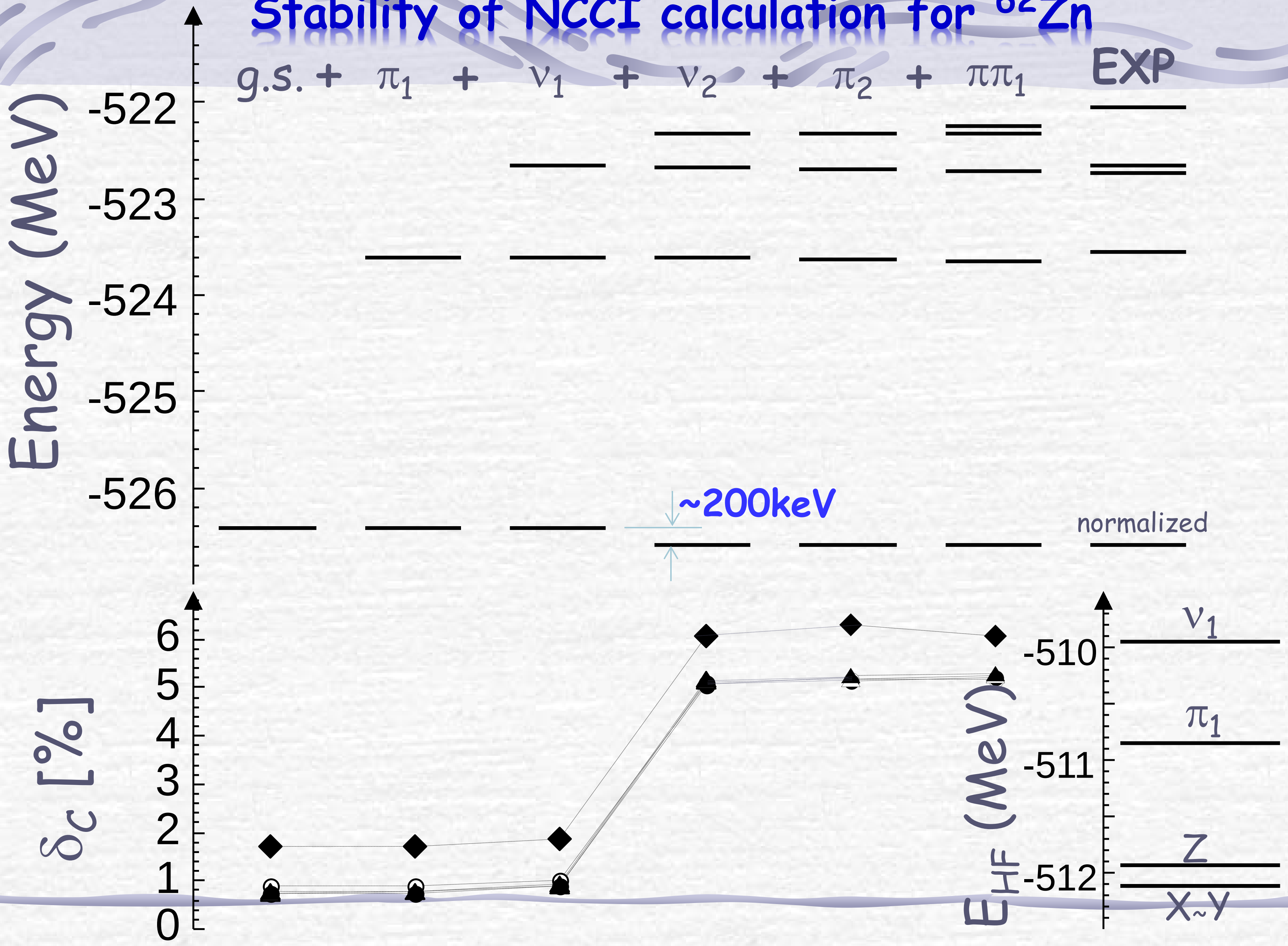
W.Satula, J.Dobaczewski, M.Konieczka, W.Nazarewicz, Acta Phys. Polonica B45, 167 (2014)

No-core configuration-interaction formalism based on the isospin and angular momentum projected DFT

^{62}Zn, I=0$^+$ states below 5MeV

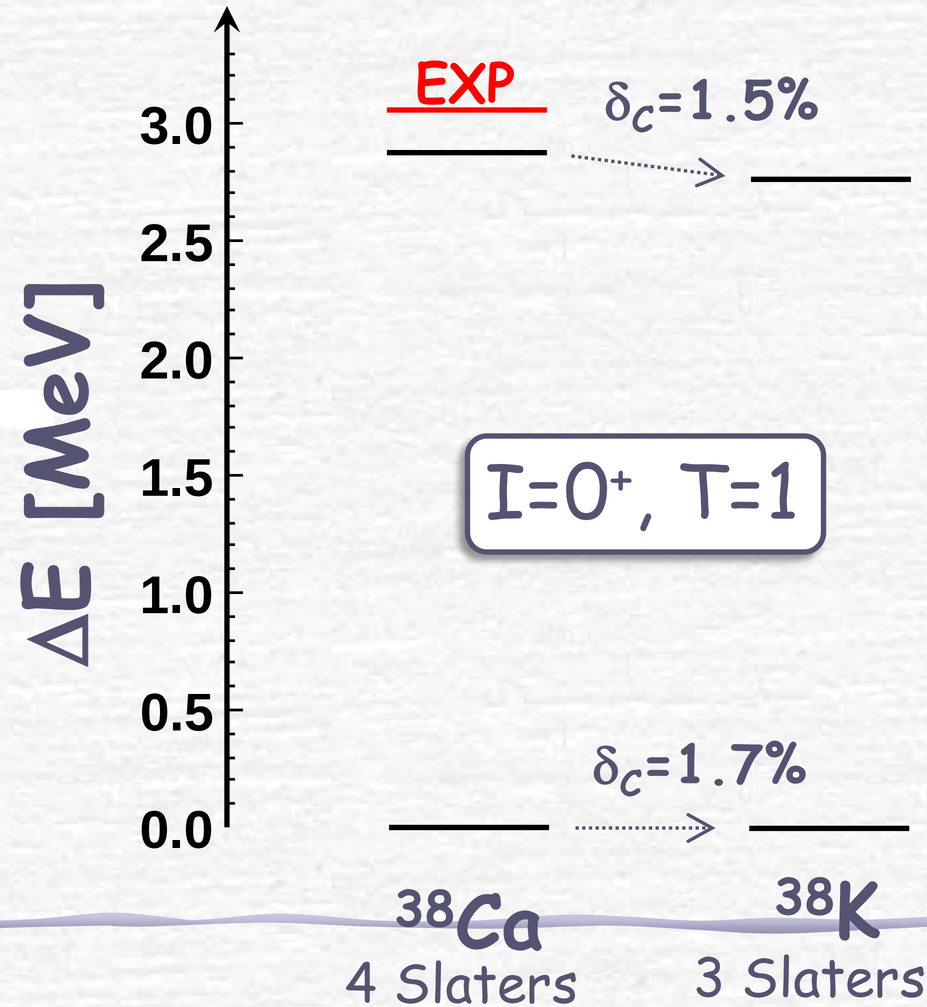


Stability of NCCI calculation for ^{62}Zn

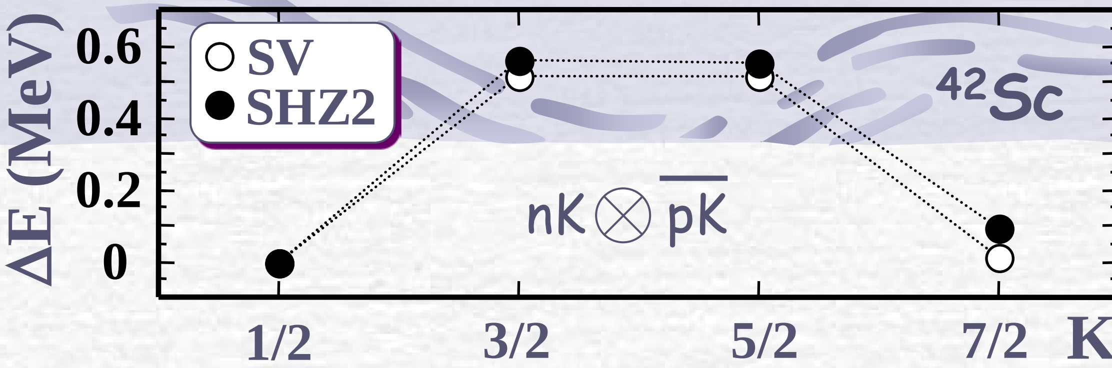


A case of A=38 ($^{38}Ca \rightarrow ^{38}K$)

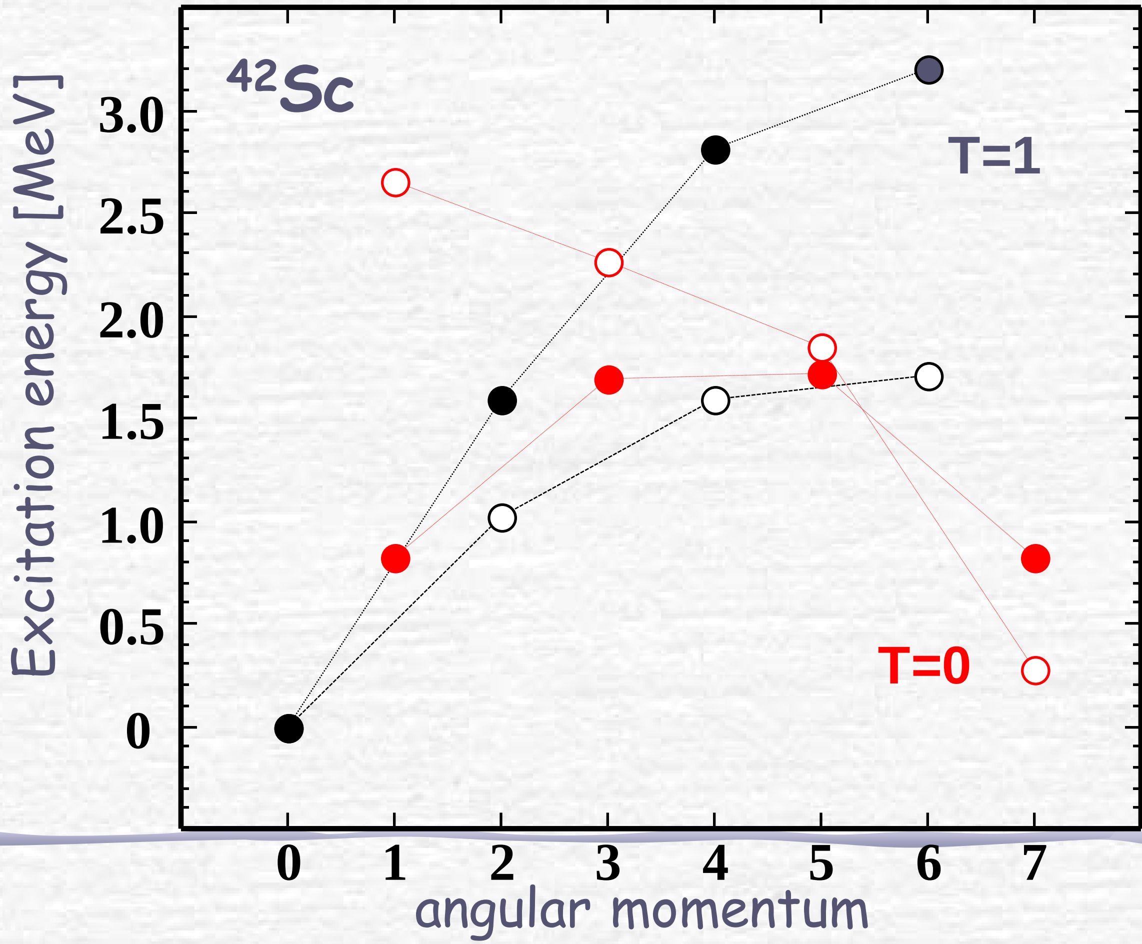
Static approach gives: δ_C=8.9%



W.Satuła, J.Dobaczewski & M.Konieczka, arXiv:1408.4982



Mixing of states projected from the antialigned configurations:



Summary

- Isospin symmetry breaking corrections from the „static" (single Slater based) double-projected DFT are in very good agreement with the Hardy–Towner results.

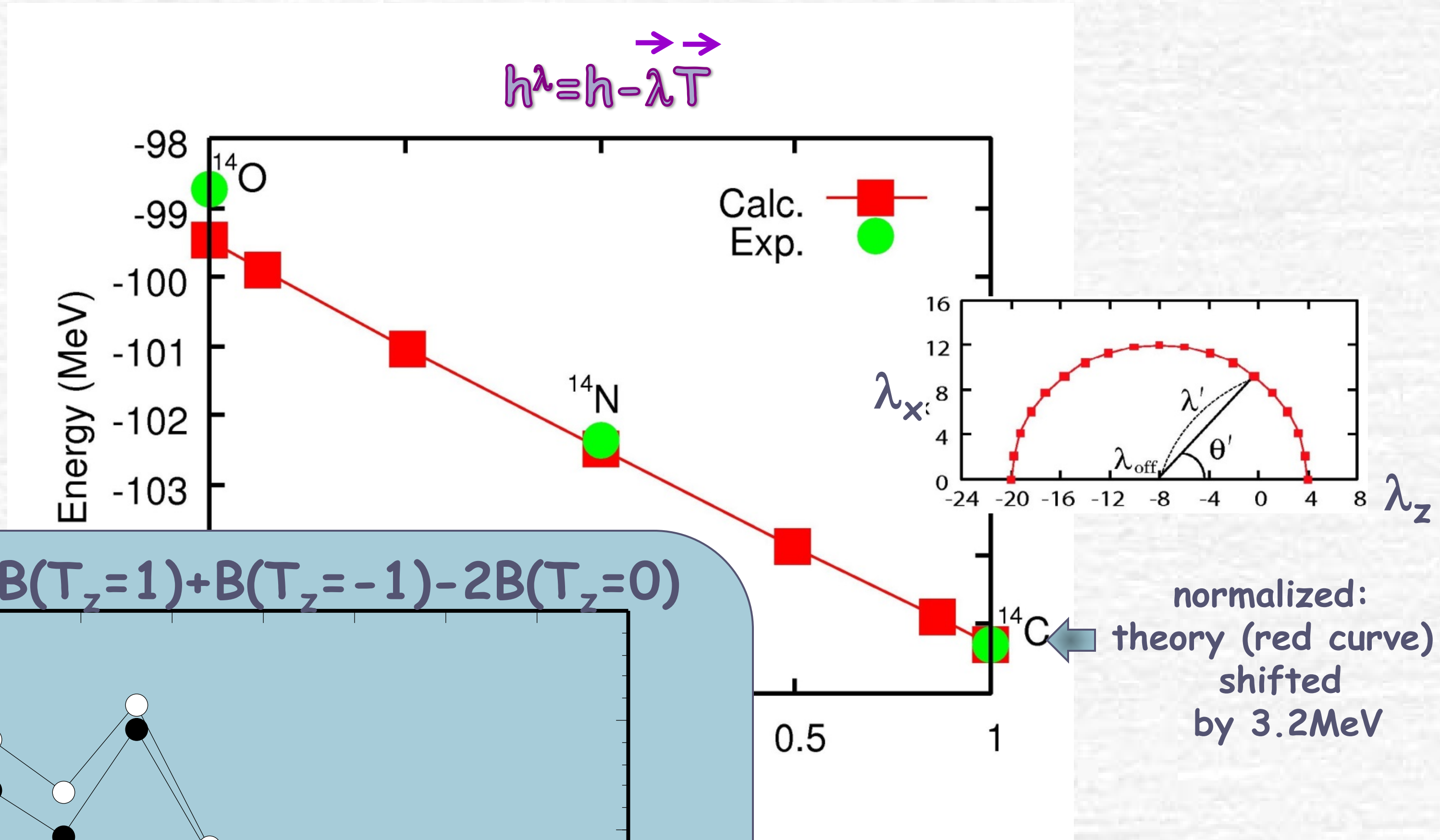
- **We have to go BEYOND „STATIC" MR-EDF in order to address high-quality spectroscopic data available today.**

First attempts are very encouraging at least concerning energy spectra!!!

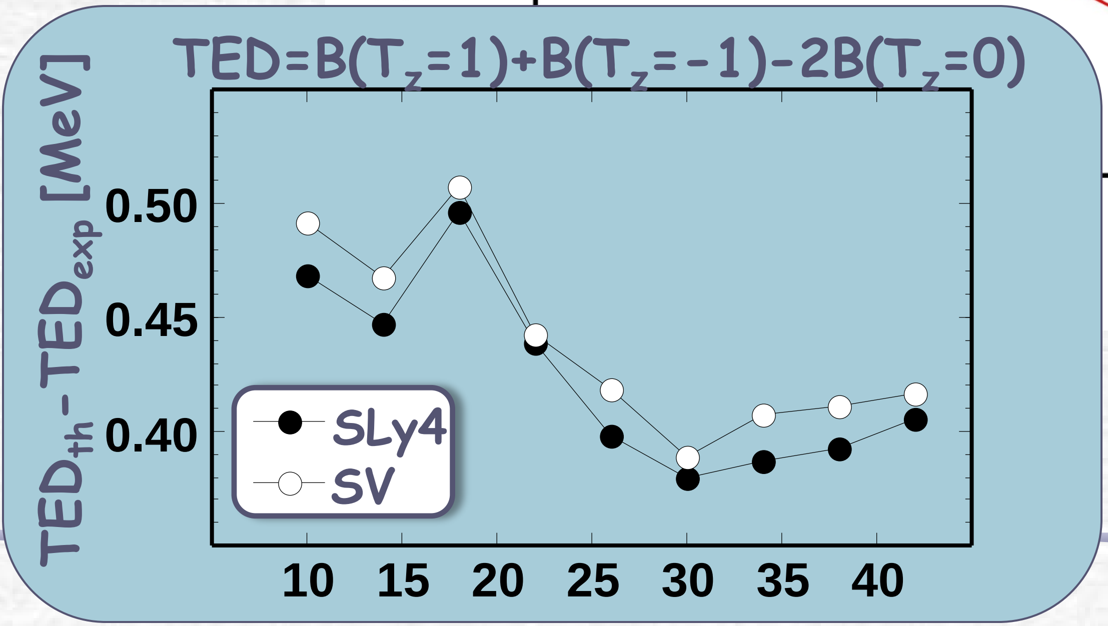
…… perspectives:

T=1, I=0⁺ isobaric analogue states from self-consistent 3D-isocranked HF: $h^{\lambda}=h-\vec{\lambda}\vec{T}$

K. Sato, J. Dobaczewski, T. Nakatsukasa, and W. Satuła, Phys. Rev. C88 (2013), 061301



normalized: theory (red curve) shifted by 3.2MeV



separable solution

bilinear in transition density matrix:

$$\frac{\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle}{\langle\Psi|\tilde{\Psi}\rangle} = \frac{1}{4}\sum_{ijkl}\bar{V}_{ijkl}\left[\tilde{\rho}\right]\ \left(\tilde{\rho}_{ki}\tilde{\rho}_{lj} - \tilde{\rho}_{li}\tilde{\rho}_{kj}\right)$$

$$V^{2\mathrm{B}}_{IMK} \equiv \langle\Psi|\hat{V}_{2\mathrm{B}}\hat{P}^{I}_{MK}|\Psi\rangle = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\,*}_{MK}(\Omega)\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle$$

$$\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle \sim \frac{1}{\langle\Psi|\tilde{\Psi}\rangle^{1+\eta}}$$

inherited from Skyrme

Regularization:

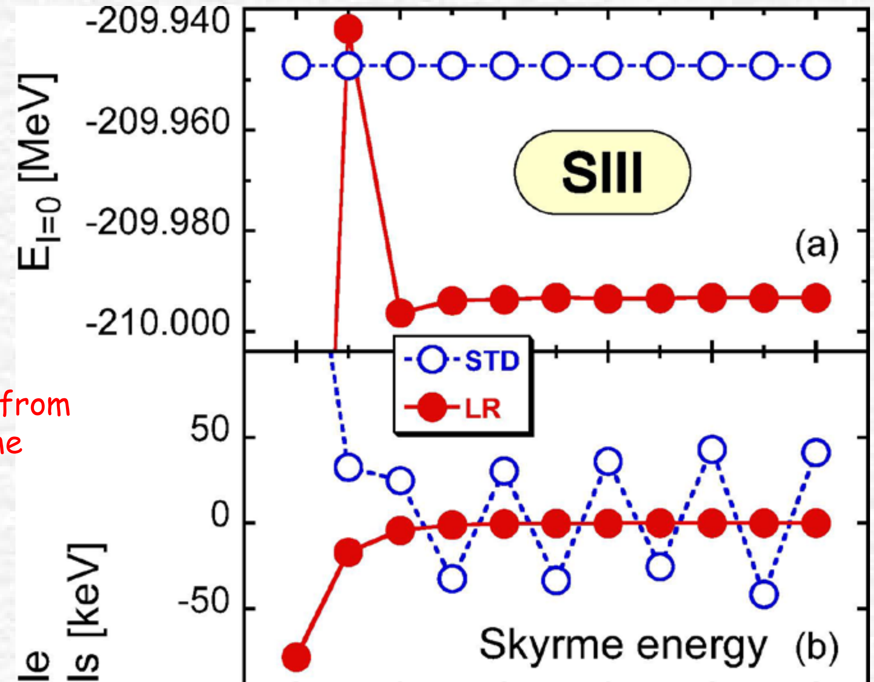
$$V^{2\mathrm{B,n}}_{IMK} = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\,*}_{MK}(\Omega)\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle\langle\Psi|\tilde{\Psi}\rangle^{n}$$

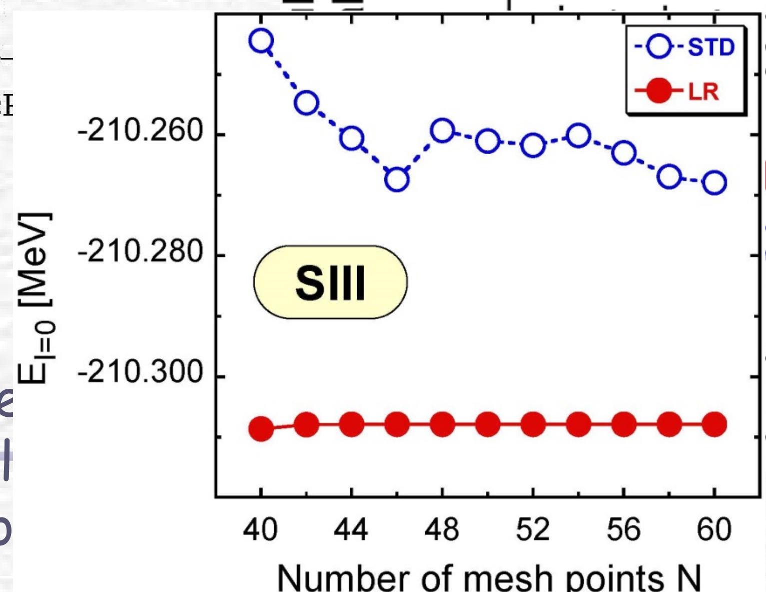
$$\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle \longrightarrow \widetilde{\langle\Psi|\hat{V}_{2\mathrm{B}}|\tilde{\Psi}\rangle}$$

$$\tilde{V}^{2\mathrm{B,n}}_{IMK} = \frac{2I+1}{8\pi^2}\int d\Omega\, D^{I\,*}_{MK}(\Omega)\langle\Psi|\hat{V}_{2\mathrm{I}}$$

$$V^{2\mathrm{B,n}}_{IMK} \equiv \tilde{V}^{2\mathrm{B,n}}_{IMK}$$

Regularized energie
can be calculated by sol
set of linear equatio

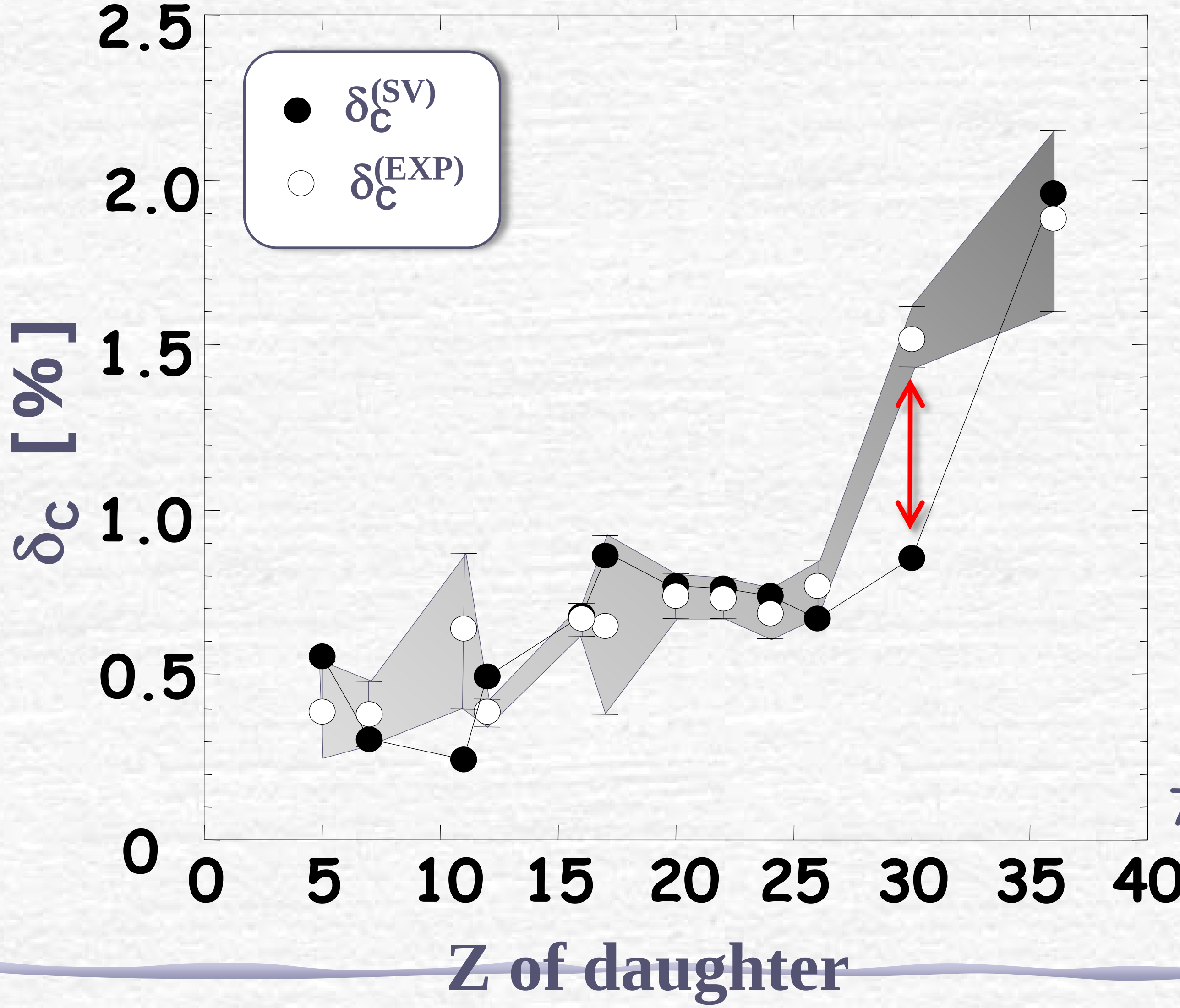




W.Satuła & J.Dobaczewski, arXiv:1407.0857

Confidence level test based on the CVC hypothesis

T&H PRC82, 065501 (2010)



$$\delta_C^{(EXP)} = 1+\delta_{NS} - \frac{\overline{\mathcal{F}t}}{ft(1+\delta_R')}$$

Minimize RMS deviation between the caluclated and experimental δ_C with respect to $\overline{\mathcal{F}t}$

χ^2/n_d=5.2
for Ft = 3070.0s
75% contribution to the χ^2 comes from A=62

From: W. Satuła, J. Dobaczewski, W. Nazarewicz, M. Rafalski Phys. Rev. Lett. 106, 132502 (2011).