DFT rooted NCCI approach and its applications to N~Z nuclei

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In colaboration with: Jacek Dobaczewski, Paweł Bączyk, Maciek Konieczka

- Frontiers in nuclear structure theory:
  - golden decade of ab initio methods
  - spectacular developments in (SR) DFT, TD-DFT or MR-DFT-rooted approaches
    - new developments (in particular the DFT-rooted NCCI) and the physics highlights (personal selection)
  - vivid activity and spectacular progress in large-scale calculations using shell-model, RPA, collective models…
- Final remarks and perspectives

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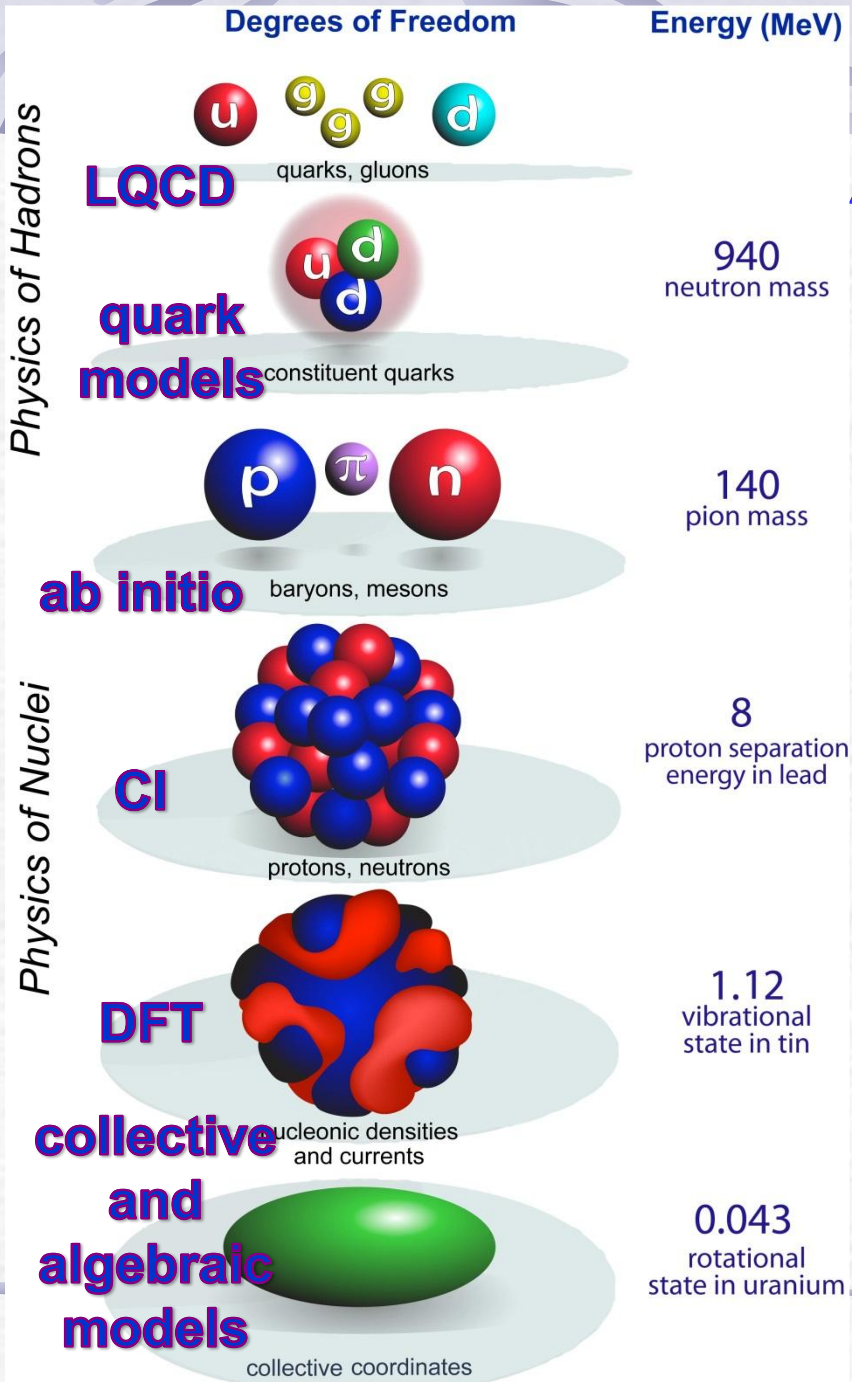
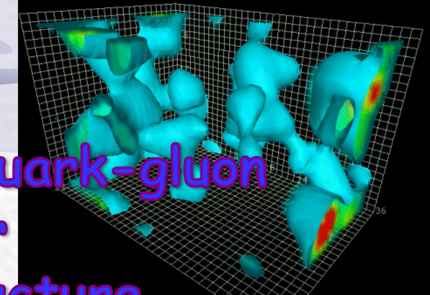


Effective (field) theories → Resolution



Hot and dense quark-gluon matter
Hadron structure

Hadron-Nuclear interface

Nuclear structure & reactions

Third Law of Progress in Theoretical Physics by Weinberg:

"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Effective or low-energy (low-resolution) theory explores separation of scales. Its formulation requires:

in coordinate space:

→**define** R **to separate short- and long-distance physics**

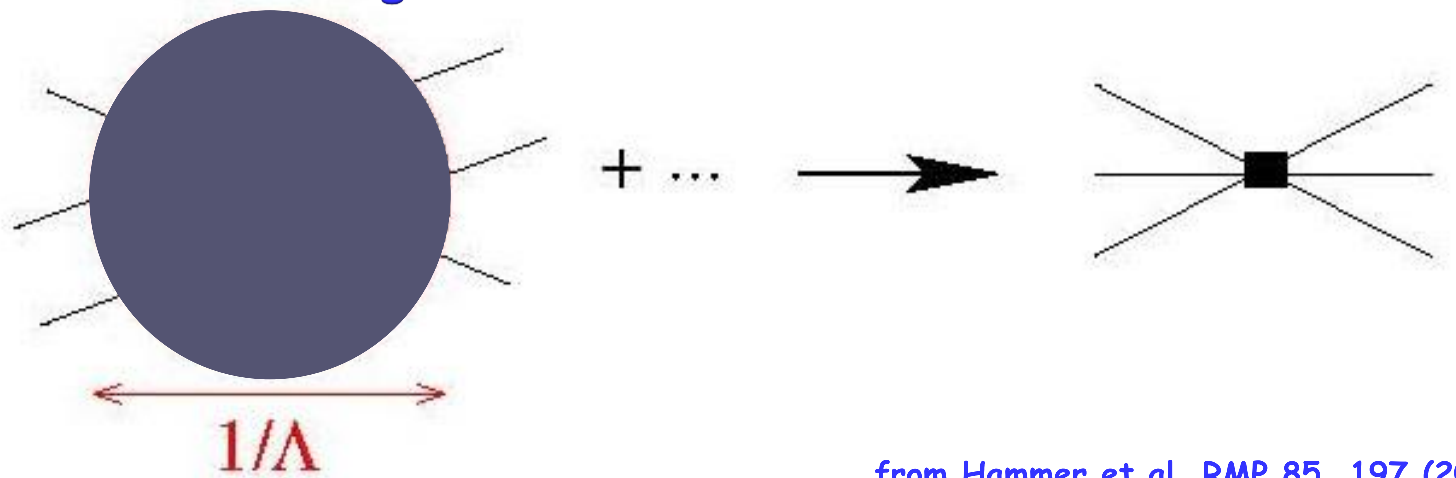
or, in momentum space:

→**define** Λ **(1/R) to separate low and high momenta**

replace (complicated and, in nuclear physics, unknown) short distance (or high momentum) physics by a LCP (local correcting potential)

(there is a lot of freedom how this is done concerning both the scale and form but physics is (should be!) independent on the scheme!!!)

emergence of 3NF due to finite resolution



from Hammer et al. RMP 85, 197 (2013)

Nuclear effective theory for EDF (nuclear DFT)

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

ultraviolet cut-off Λ →

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

regularization

Fourier

Coulomb

Long-range part of the NN interaction (must be treated exactly!!!)

hierarchy of scales: $v_{eff}(\boldsymbol{r}) \approx v_{long}(\boldsymbol{r})$

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

$\frac{2r_oA^{1/3}}{r_o}$ ~ $2A^{1/3}$ ~ 10

local correcting potential

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

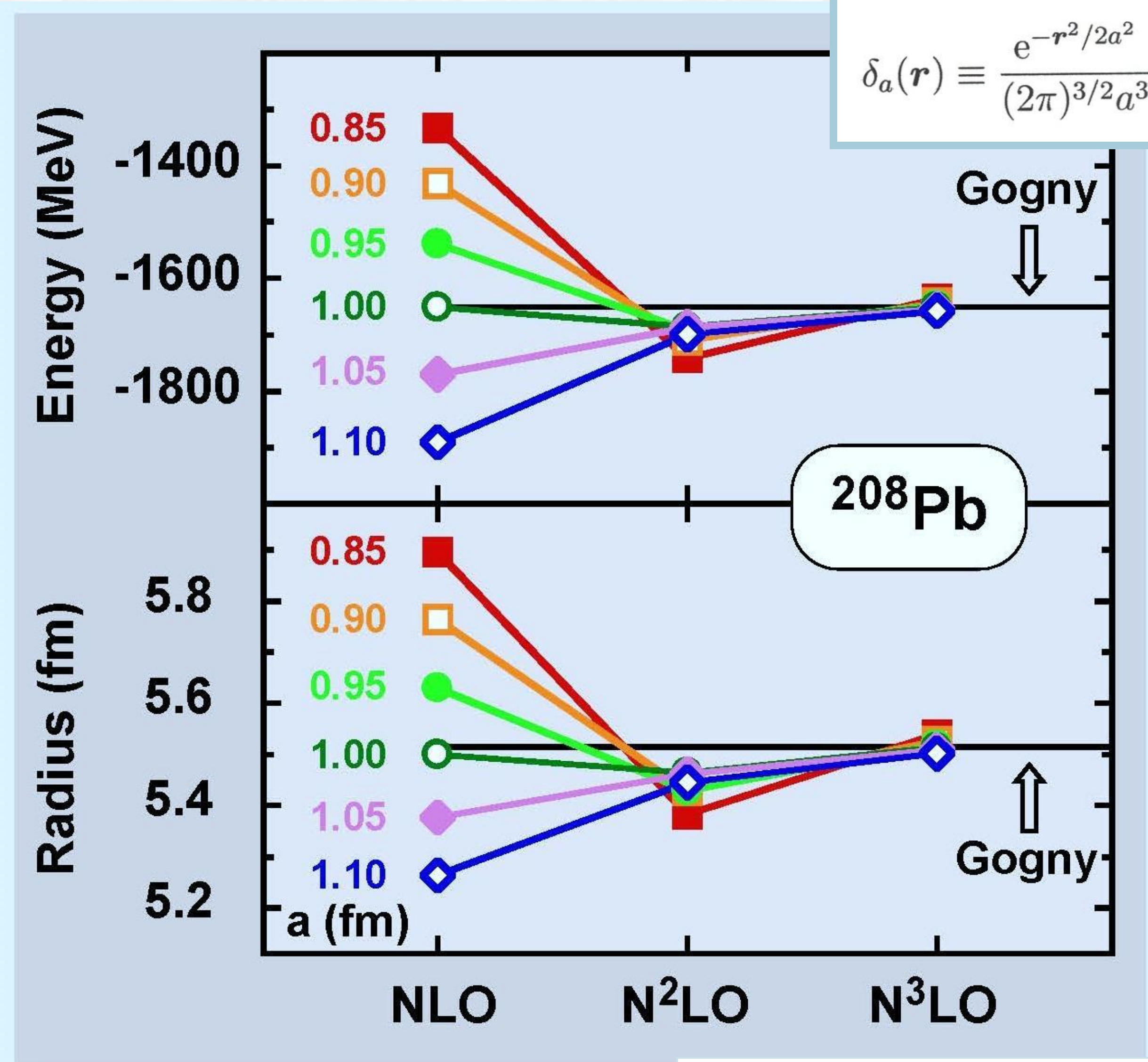
$$\delta_a(\boldsymbol{r}) \equiv \frac{e^{-\boldsymbol{r}^2/2a^2}}{(2\pi)^{3/2}a^3} .$$

Gaussian regulator

There exist an „infinite" number of equivalent realizations of effective theories

J. Dobaczewski, K. Bennaceur, F. Raimondi, J. Phys. G 39, 125103 (2012)

Proof of principle of the regularization range (scale) independence for the gaussian-regularized density-independent EDFs



$$\delta_a(\boldsymbol{r}) \equiv \frac{e^{-\boldsymbol{r}^2/2a^2}}{(2\pi)^{3/2}a^3}\,.$$

J. Dobaczewski, K. Bennaceur, F. Raimondi,
J. Phys. G 39, 125103 (2012)

Having defined the generator, the nuclear EDF is built using mean-field (HF or Kohn-Sham) methodology

$$E[\rho(\vec{r}_1,\vec{r}_2)] = \iint d\vec{r}_1 d\vec{r}_2\, \mathcal{H}(\rho(\vec{r}_1,\vec{r}_2))$$

$$\mathcal{H}(\rho(\vec{r}_1,\vec{r}_2)) = V(\vec{r}_1-\vec{r}_2)\left[\rho(\vec{r}_1)\rho(\vec{r}_2) - \rho(\vec{r}_1,\vec{r}_2)\rho(\vec{r}_2,\vec{r}_1)\right]$$

direct term — exchange term

Skyrme interaction - specific (local) realization of the nuclear effective interaction: $\lim_{a\to 0} \delta_a$

$$\begin{aligned} v(1,2) = {} & t_0(1+x_0\hat{P}_\sigma)\delta(\boldsymbol{r}_{12}) && \text{LO} \\ & + \frac{1}{2}t_1(1+x_1\hat{P}_\sigma)\left(\hat{\boldsymbol{k}}'^2\delta(\boldsymbol{r}_{12})+\delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}^2\right) && \text{NLO} \\ & + t_2(1+x_2\hat{P}_\sigma)\hat{\boldsymbol{k}}'\delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}} && \text{NLO} \\ & + \frac{1}{6}t_3(1+x_3\hat{P}_\sigma)\rho_0^\gamma(\boldsymbol{R})\delta(\boldsymbol{r}_{12}) && \leftarrow \text{density dependence} \\ & + iW_0(\boldsymbol{\sigma}_1+\boldsymbol{\sigma}_2)\left(\hat{\boldsymbol{k}}'\times\delta(\boldsymbol{r}_{12})\hat{\boldsymbol{k}}\right), && \leftarrow \text{spin-orbit} \end{aligned}$$

10(11) parameters

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

- Skyrme EDF (for $N = Z$ and without pairing)

$$E[\rho,\tau,\mathbf{J}] = \int d\mathbf{r} \left\{ \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau + \frac{1}{64}(9t_1 - 5t_2)(\boldsymbol{\nabla}\rho)^2 - \frac{3}{4} W_0 \rho \boldsymbol{\nabla}\cdot\mathbf{J} + \frac{1}{16} t_3 \rho^{2+\alpha} + \cdots \right\}$$

where $\rho(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$, $\tau(\mathbf{r}) = \sum_i |\nabla\psi_i(\mathbf{r})|^2$, ...

- Pionless zero-range EFT $\Longrightarrow$ dilute LDA $\rho\tau\mathbf{J}$ EDF (with $V_{\mathrm{external}} = 0$)

$$E[\rho,\tau,\mathbf{J}] = \int d\mathbf{r} \left\{ \frac{\tau}{2M} + \frac{3}{8} C_0 \rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\boldsymbol{\nabla}\rho)^2 - \frac{3}{4} C_2'' \rho \boldsymbol{\nabla}\cdot\mathbf{J} + \frac{c_1}{2M} C_0^2 \rho^{7/3} + \frac{c_2}{2M} C_0^3 \rho^{8/3} + \frac{1}{16} D_0 \rho^3 + \cdots \right\}$$

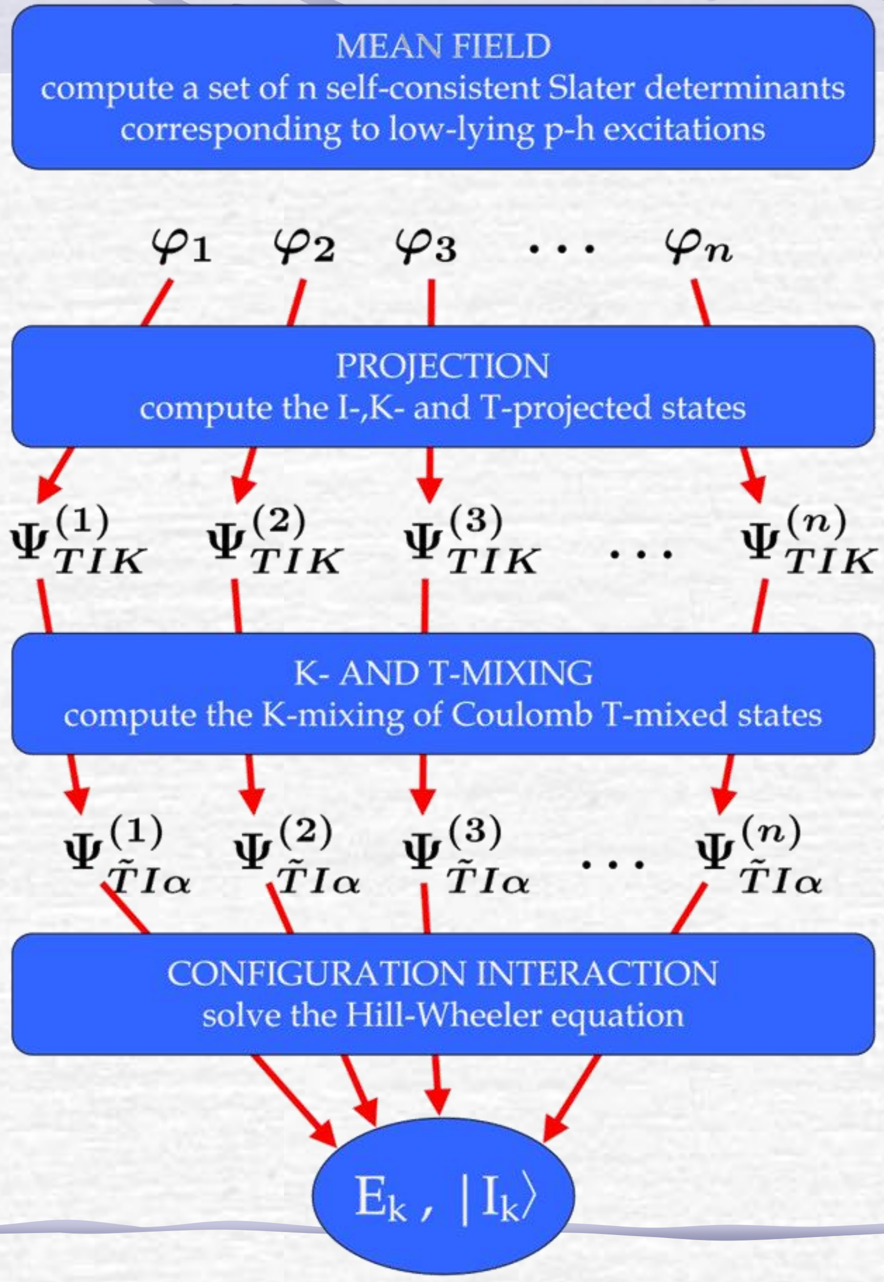
Look very similar except of „three-body" contributions!

Fractional powers of the density lead to singularities in extensions involving restoration of broken symmetries:

→ rotational (spherical) symmetry
→ isospin symmetry (approximate)
→ particle number...

and subsequent configuration mixing.

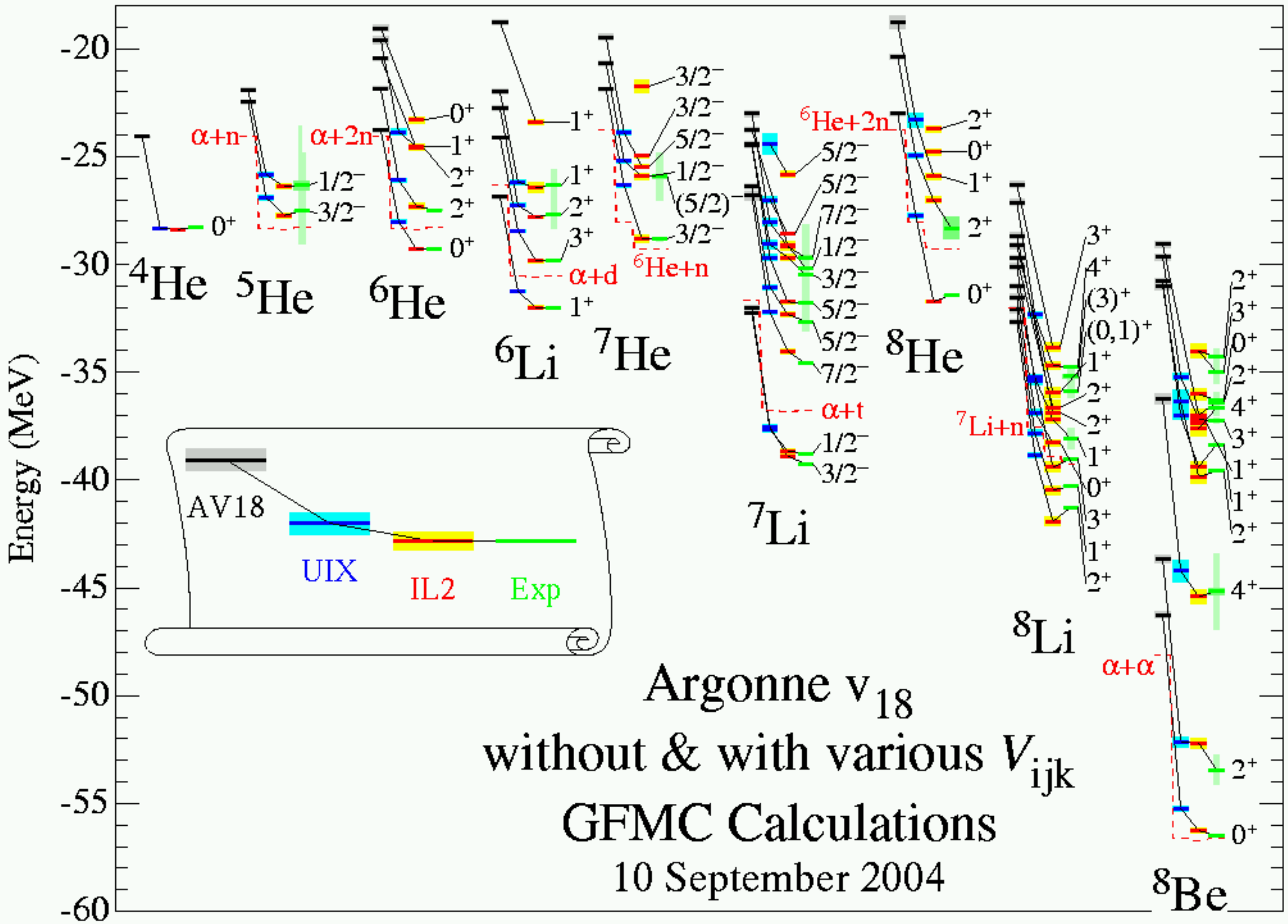
SR-DFT → MR-DFT → NCCI

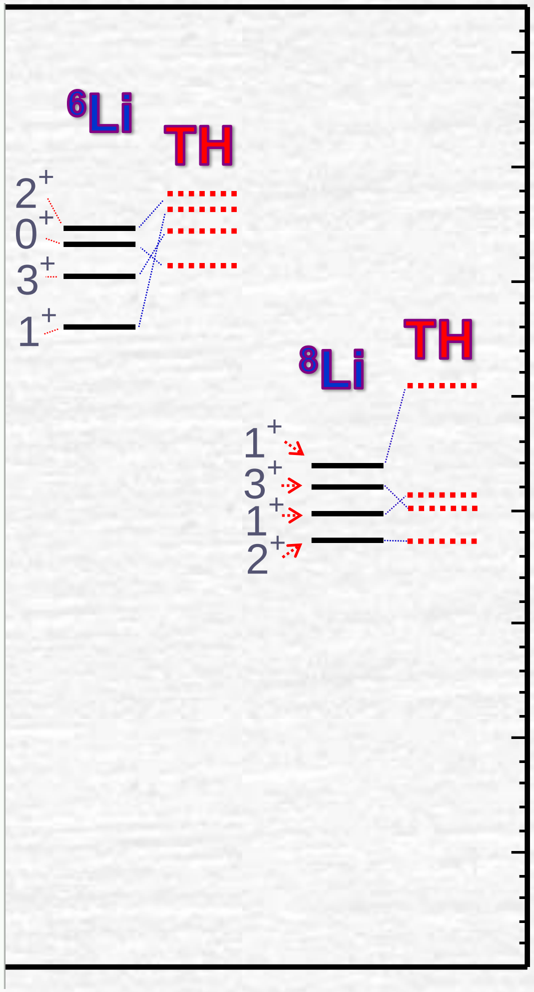


MEAN FIELD
compute a set of n self-consistent Slater determinants corresponding to low-lying p-h excitations
φ_1 φ_2 φ_3 $\cdots$ φ_n
PROJECTION
compute the I-,K- and T-projected states
$\Psi^{(1)}_{TIK}$ $\Psi^{(2)}_{TIK}$ $\Psi^{(3)}_{TIK}$ $\cdots$ $\Psi^{(n)}_{TIK}$
K- AND T-MIXING
compute the K-mixing of Coulomb T-mixed states
$\Psi^{(1)}_{\tilde{T}I\alpha}$ $\Psi^{(2)}_{\tilde{T}I\alpha}$ $\Psi^{(3)}_{\tilde{T}I\alpha}$ $\cdots$ $\Psi^{(n)}_{\tilde{T}I\alpha}$
CONFIGURATION INTERACTION
solve the Hill-Wheeler equation
E_k , $|I_k\rangle$

PRELIMINARY

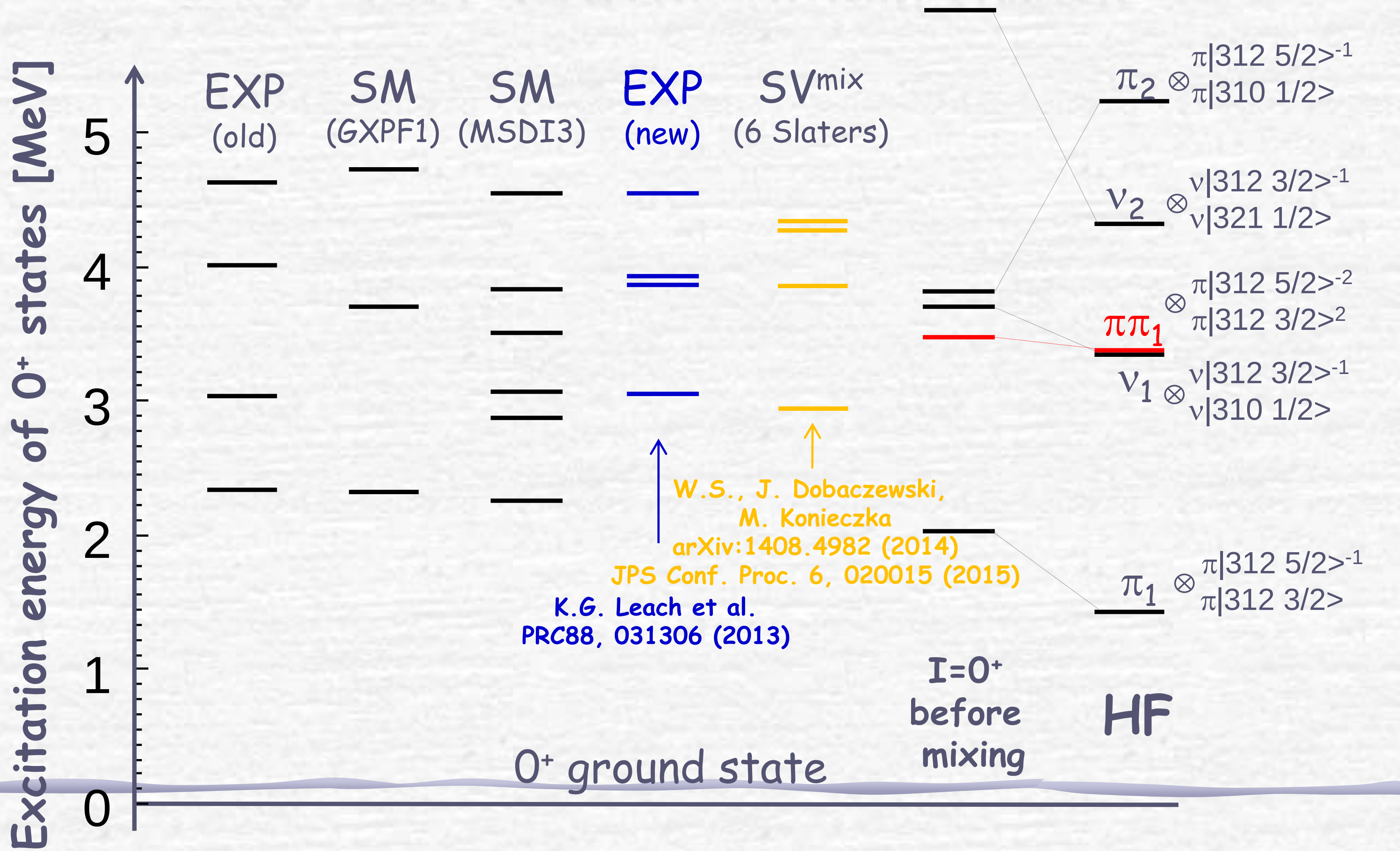
(mixing of states projected from three-four p-h configurations)



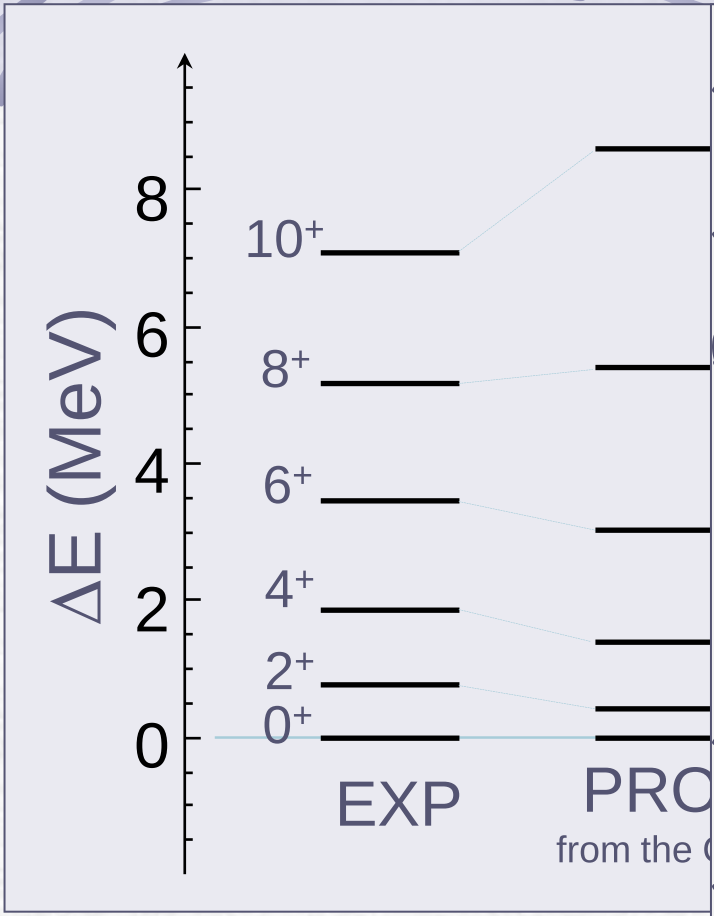


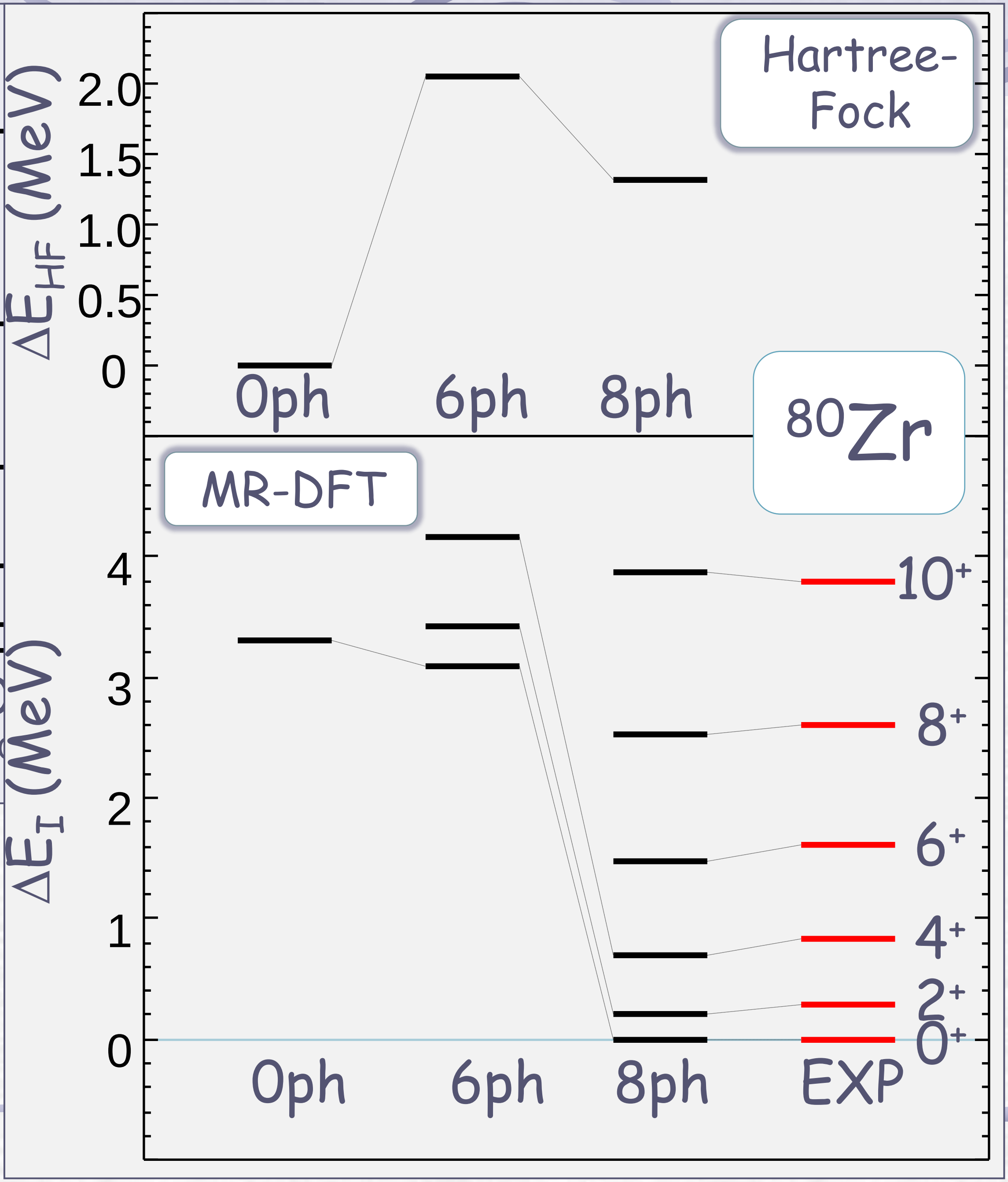
No-core configuration-interaction formalism based on the isospin and angular momentum projected DFT

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



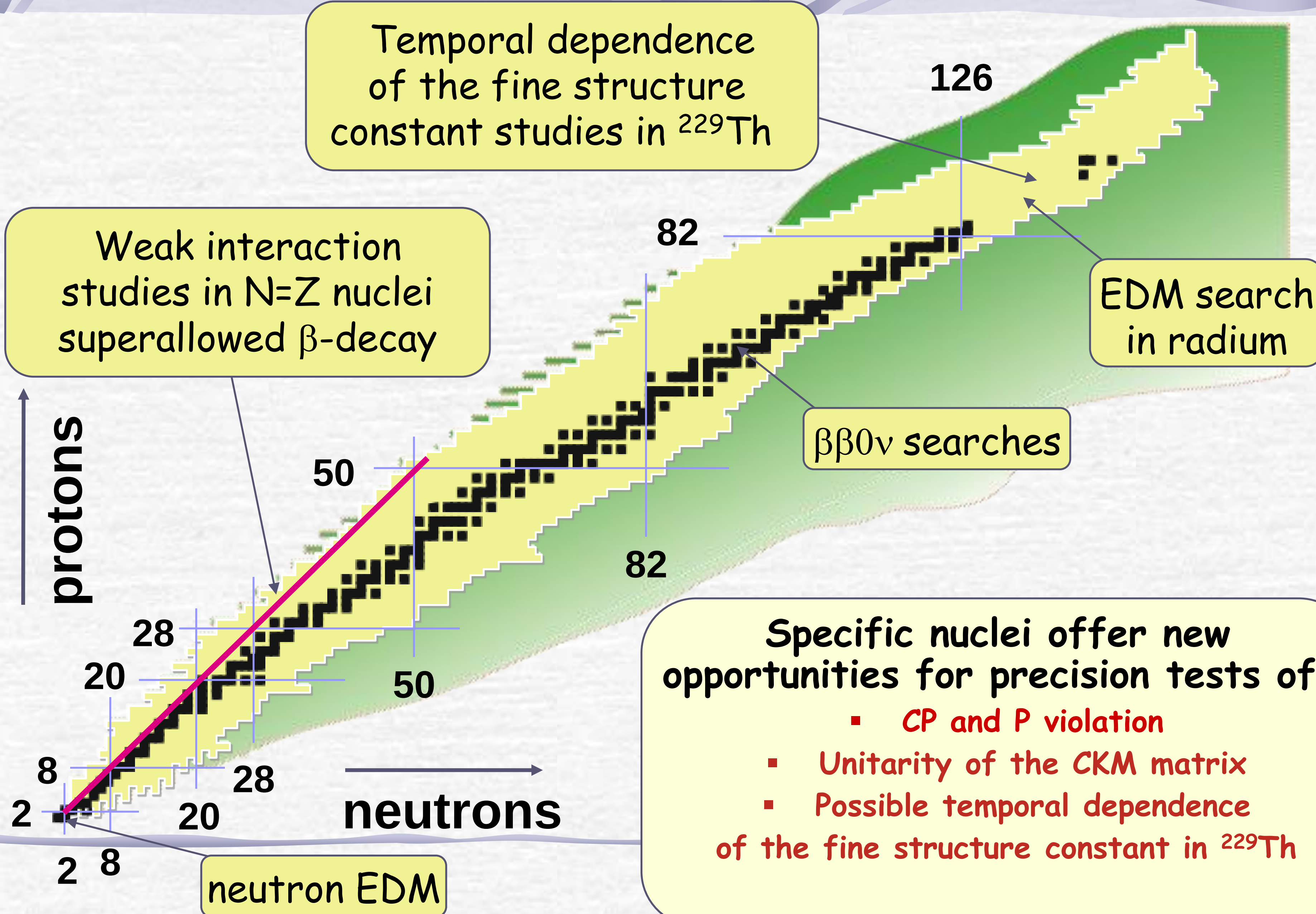
W.Satuła, J.Dobaczewski & M.Konieczka, arXiv:1408.4982; JPS Conf. Proc. 6, 020015 (2015)





COLLECTIVE BANDS

Testing the fundamental symmetries of nature

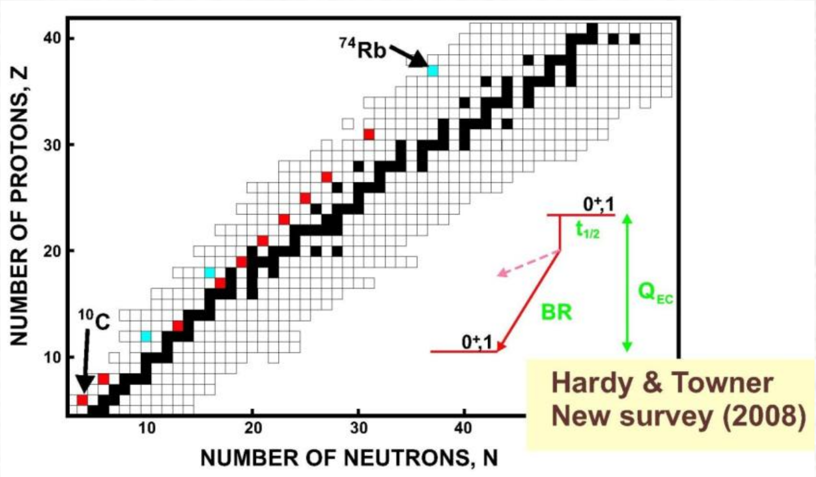


Specific nuclei offer new opportunities for precision tests of:

- *CP and P violation*
- Unitarity of the CKM matrix
- Possible temporal dependence of the fine structure constant in ^{229}Th

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

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



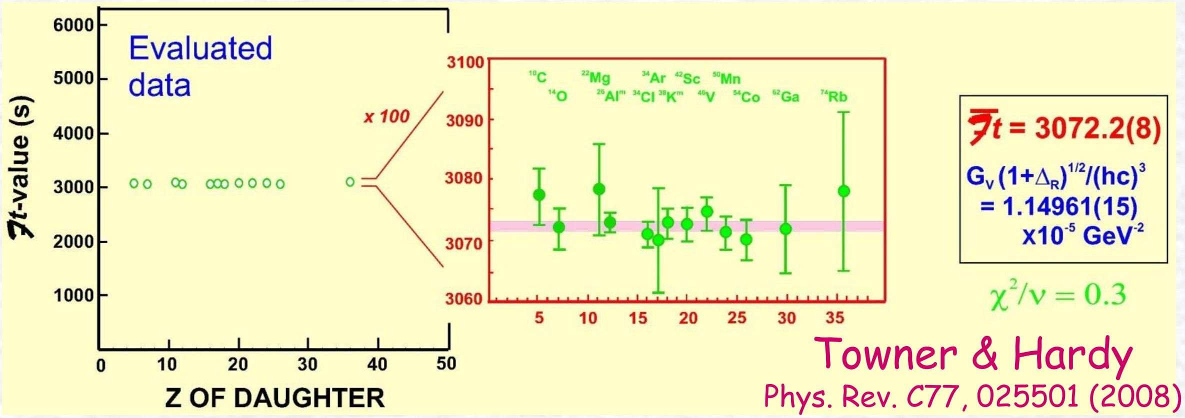
10 cases measured with accuracy ***ft*** ~0.1%
3 cases measured with accuracy ***ft*** ~0.3%

→ 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%



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

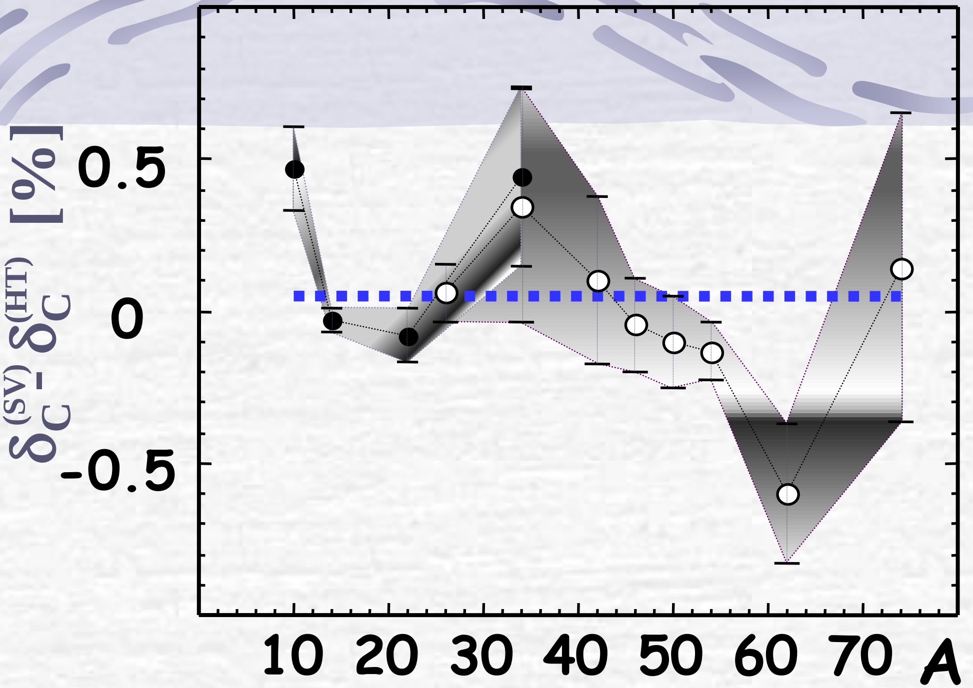
→ test of unitarity of the CKM matrix

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

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

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

0.9490(4) 0.0507(4) <0.0001



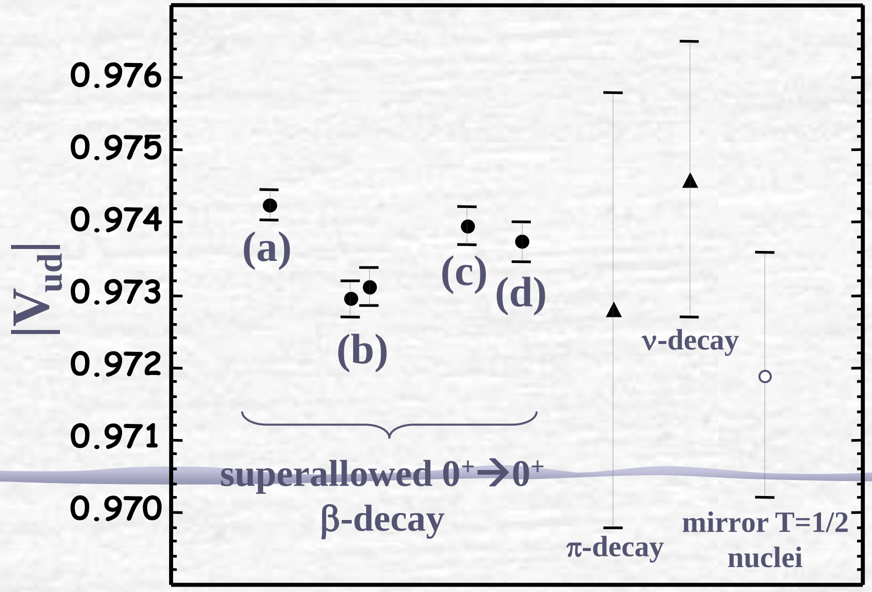
(a) I.S. Towner and J. C. Hardy, Phys. Rev. C **77**, 025501(2008).

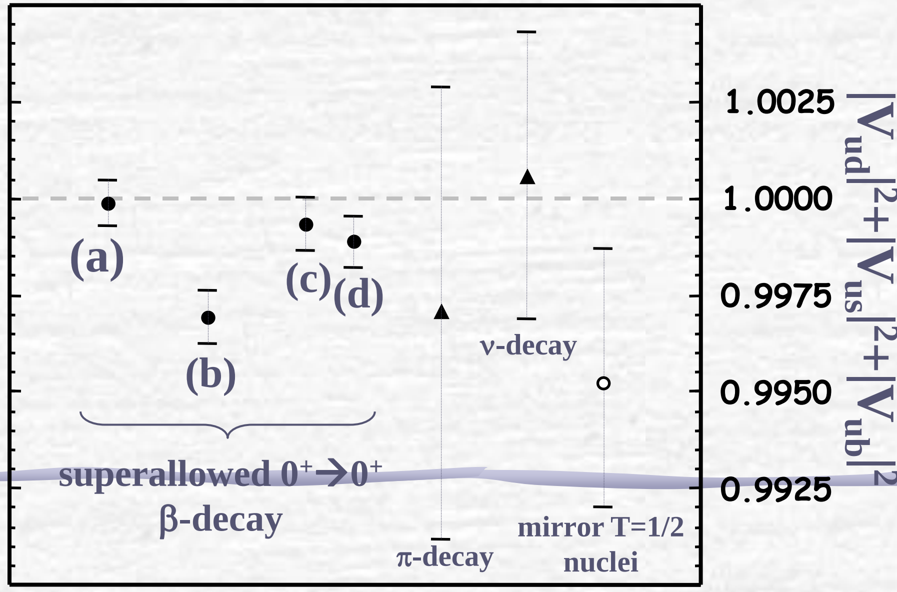
(b) H. Liang, N. V. Giai, and J. Meng, Phys. Rev. C **79**,064316 (2009).

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

O. Naviliat-Cuncic and N. Severijns, Eur. Phys. J. A **42**, 327 (2009); Phys. Rev. Lett. **102**, 142302 (2009).

$|V_{ud}|$ & unitarity – world survey

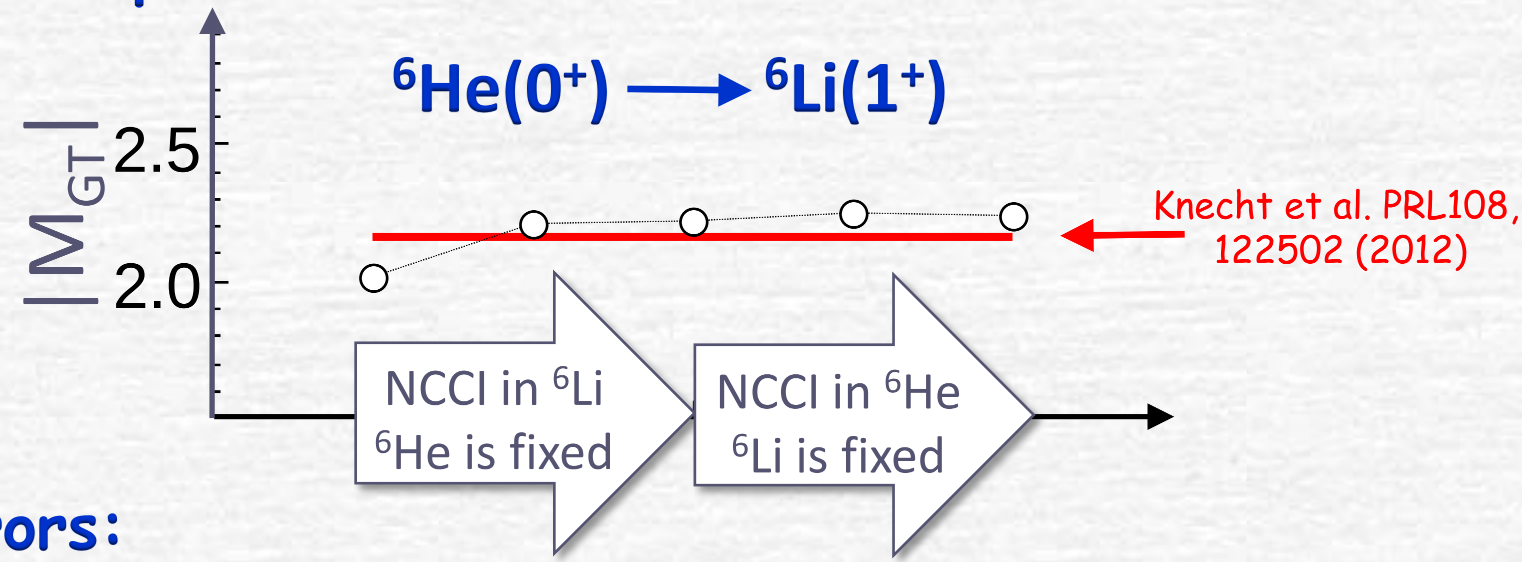




Gamow-Teller and Fermi matrix elements in T=1/2 sd- and ft- mirrors. The NCCI study

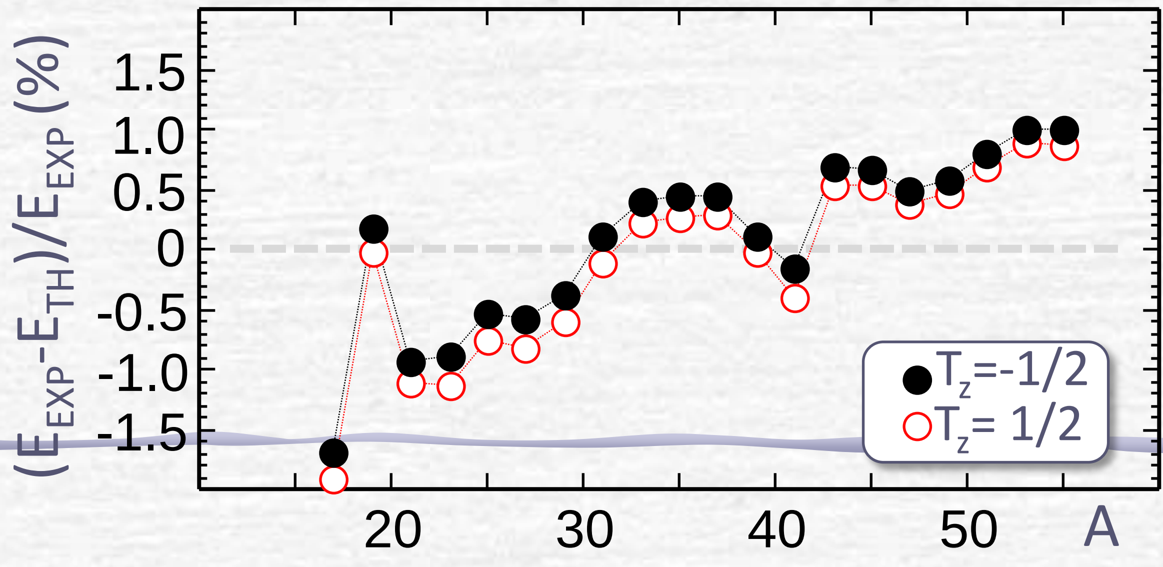
M.Konieczka, P.Bączyk, W.Satuła arXiv:1509.04480

Proof-of-principle calculation:



T=1/2 mirrors:

- masses:



$|g_A M_{GT}|$

Shell-model:

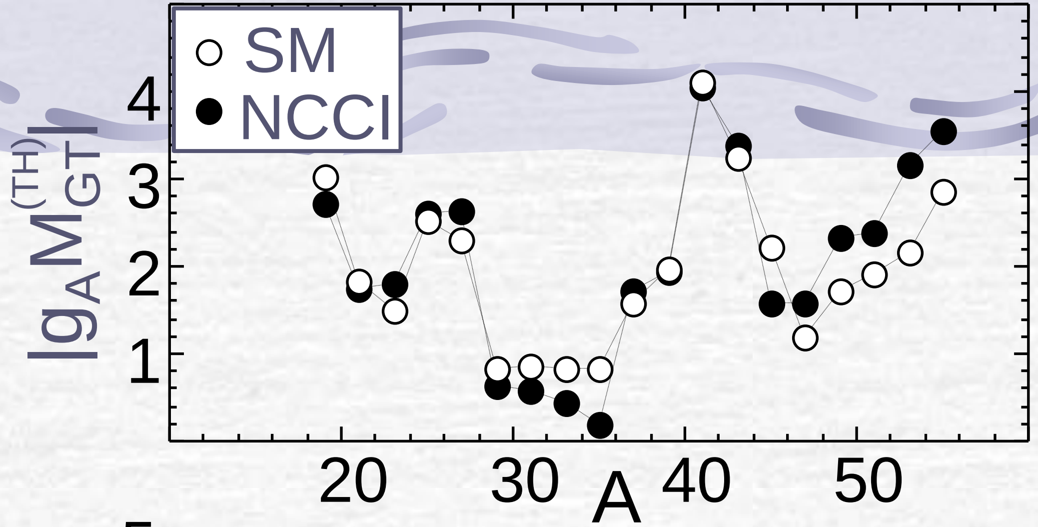
B. A. Brown and B. H. Wildenthal, Atomic Data and Nuclear Data Tables **33**, 347 (1985).

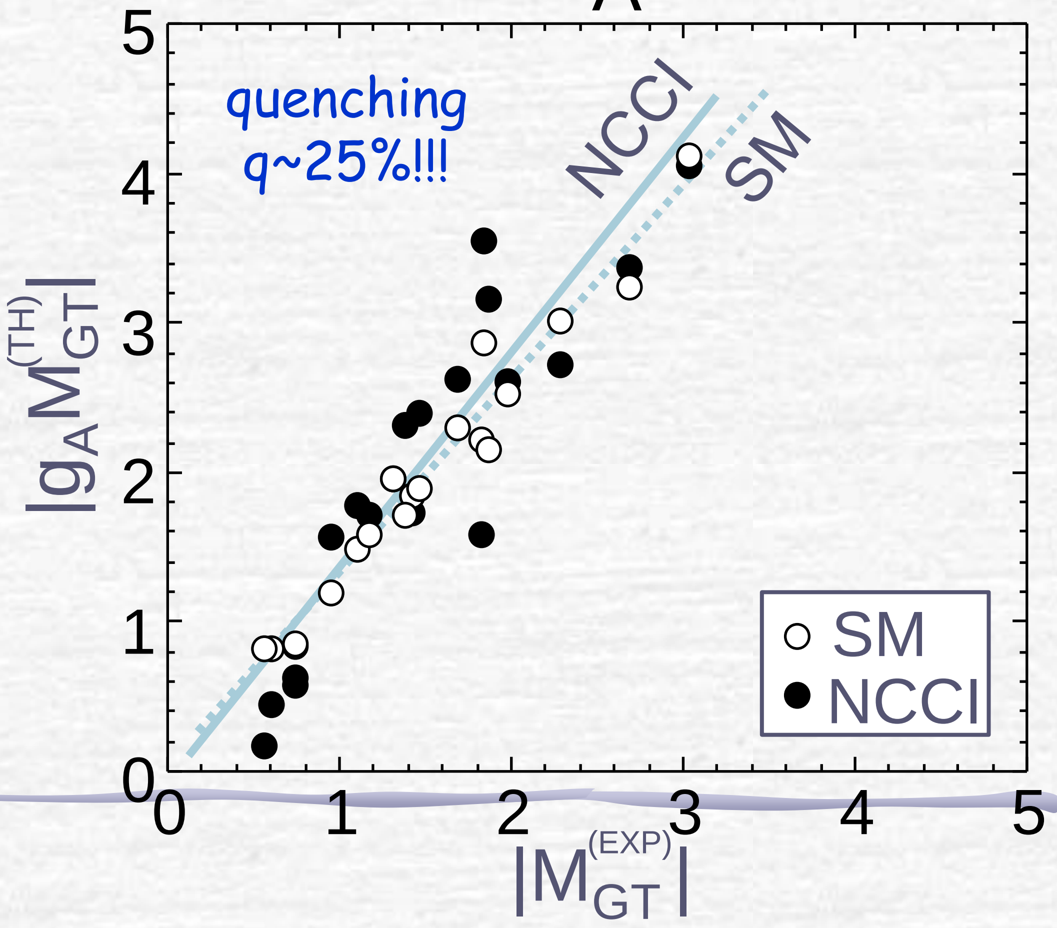
G. Martinez-Pinedo *et al.*, Phys. Rev. **C 53**, R2602 (1996).

T. Sekine *et al.*, Nucl. Phys. **A 467**, (1987).

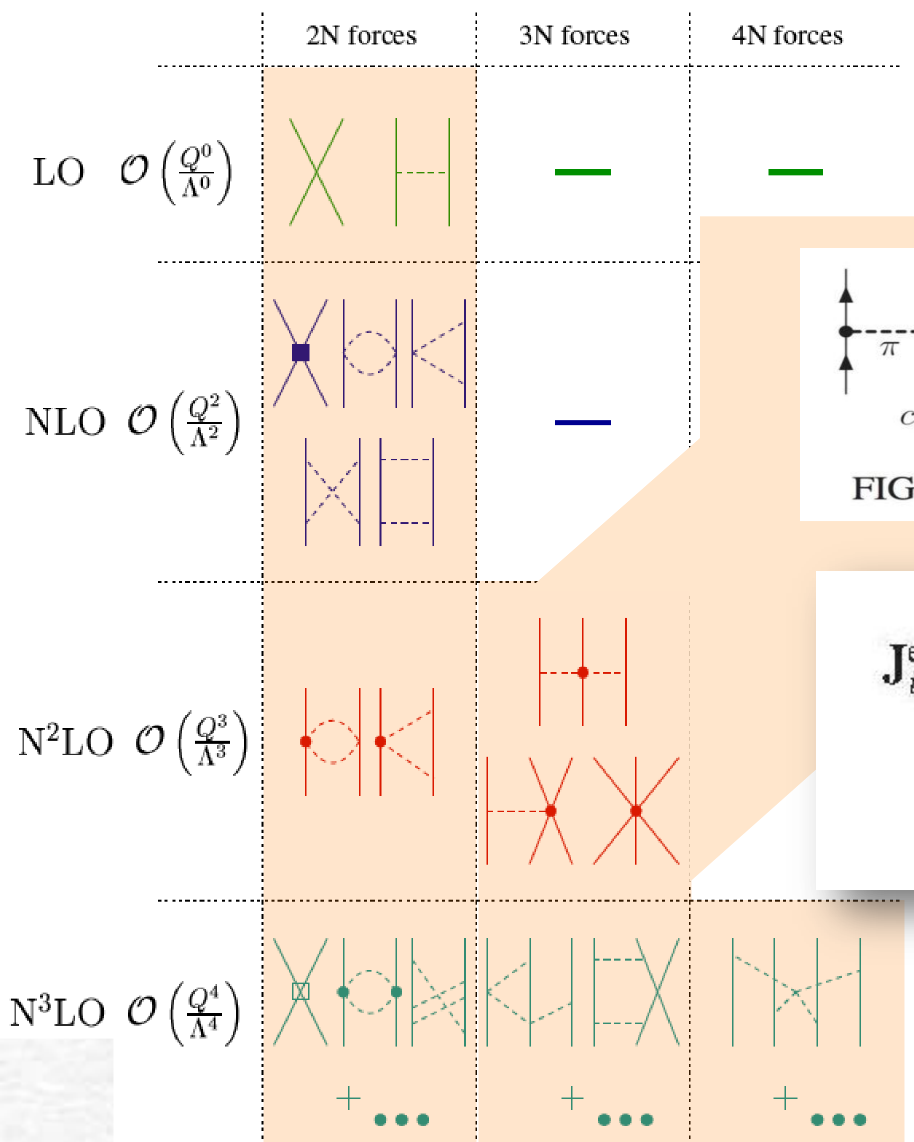
NCCI vs shell-model:

- The NCCI takes into account a core and core-polarization
- Completely different model spaces
- Different treatment of correlations
- Different interactions





Renormalization of axial-vector coupling constant by 2B-currents



c_i from πN and NN:

$$c_1 = -0.9^{+0.2}_{-0.5}\ ,\ c_3 = -4.7^{+1.2}_{-1.0}\ ,\ c_4 = 3.5^{+0.5}_{-0.2}$$

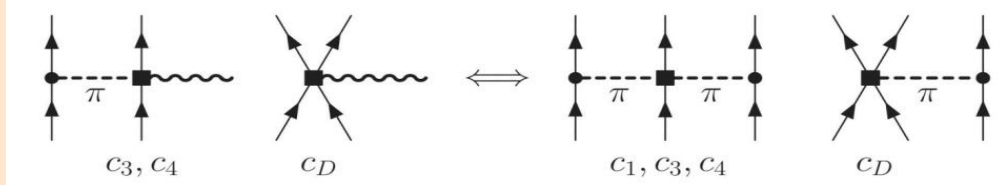


FIG. 1. Chiral $2b$ currents and $3N$ force contributions.

Menendez et al. PRL107, 062501 (2011)

$$\mathbf{J}^{\text{eff}}_{i,2b} = -g_A \boldsymbol{\sigma}_i \boldsymbol{\tau}_i^- \frac{\rho}{F_\pi^2}\left[\frac{c_D}{g_A \Lambda_\chi} + \frac{2}{3} c_3 \frac{\mathbf{p}^2}{4m_\pi^2 + \mathbf{p}^2} + I(\rho, P)\left(\frac{1}{3}(2c_4 - c_3) + \frac{1}{6m}\right)\right],$$

β$^-$ decays of ^{14}C and $^{22;24}$O

Ekstrom et al. PRL 113, 262504 (2014)

q^2~0.84-0.92 (from Ikeda sum rule)

q~0.9

See also:

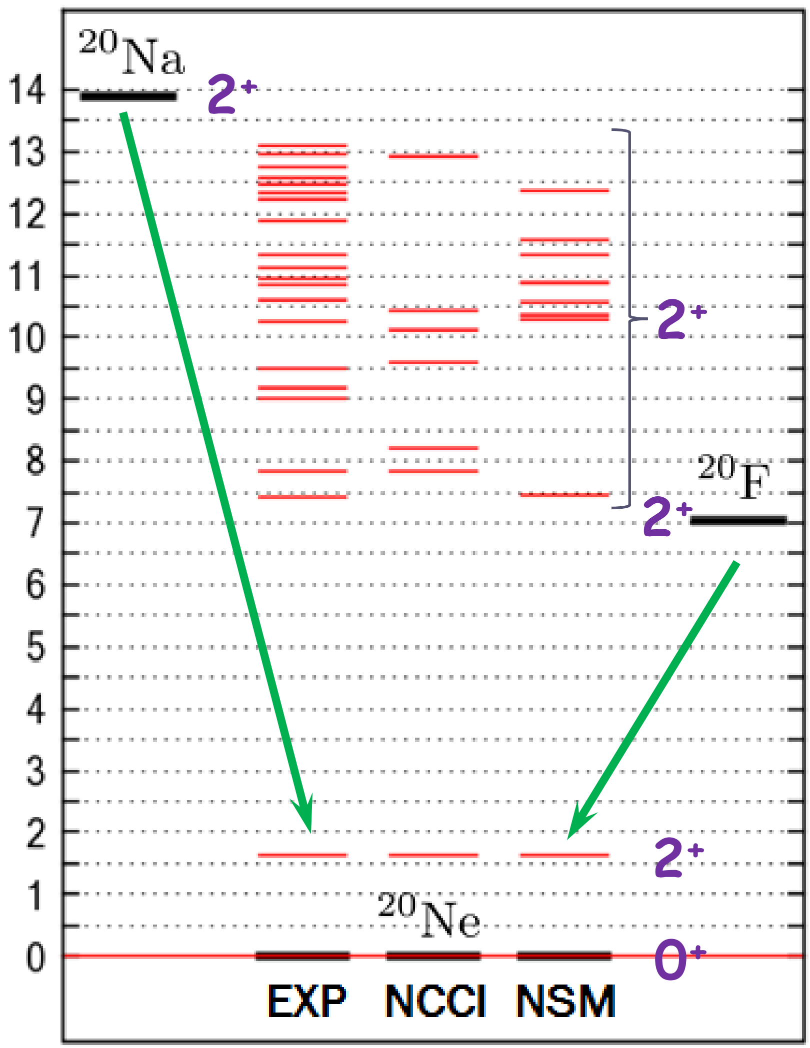
Klos et al. PRC89, 029901 (2013)

Engel et al. PRC89, 064308 (2013)

GT beta decay to excited states

(from Maciek Konieczka)

Beta decay to ^{20}Ne; 6 SD in NCCI



Gamow-Teller matrix elements for ^{20}Na→^{20}Ne

ITn	NCCI	NSM	EXP
2 0 1	0.326	0.551	0.450
2 1 1	0.752	0.774	0.532
2 0 2	2.343	2.171	–
2 1 2	0.198	0.181	–
2 0 3	0.980	1.322	1.133
2 1 3	0.531	0.384	–

Isospin symmetry breaking effects in GT decays of T=1 nuclei

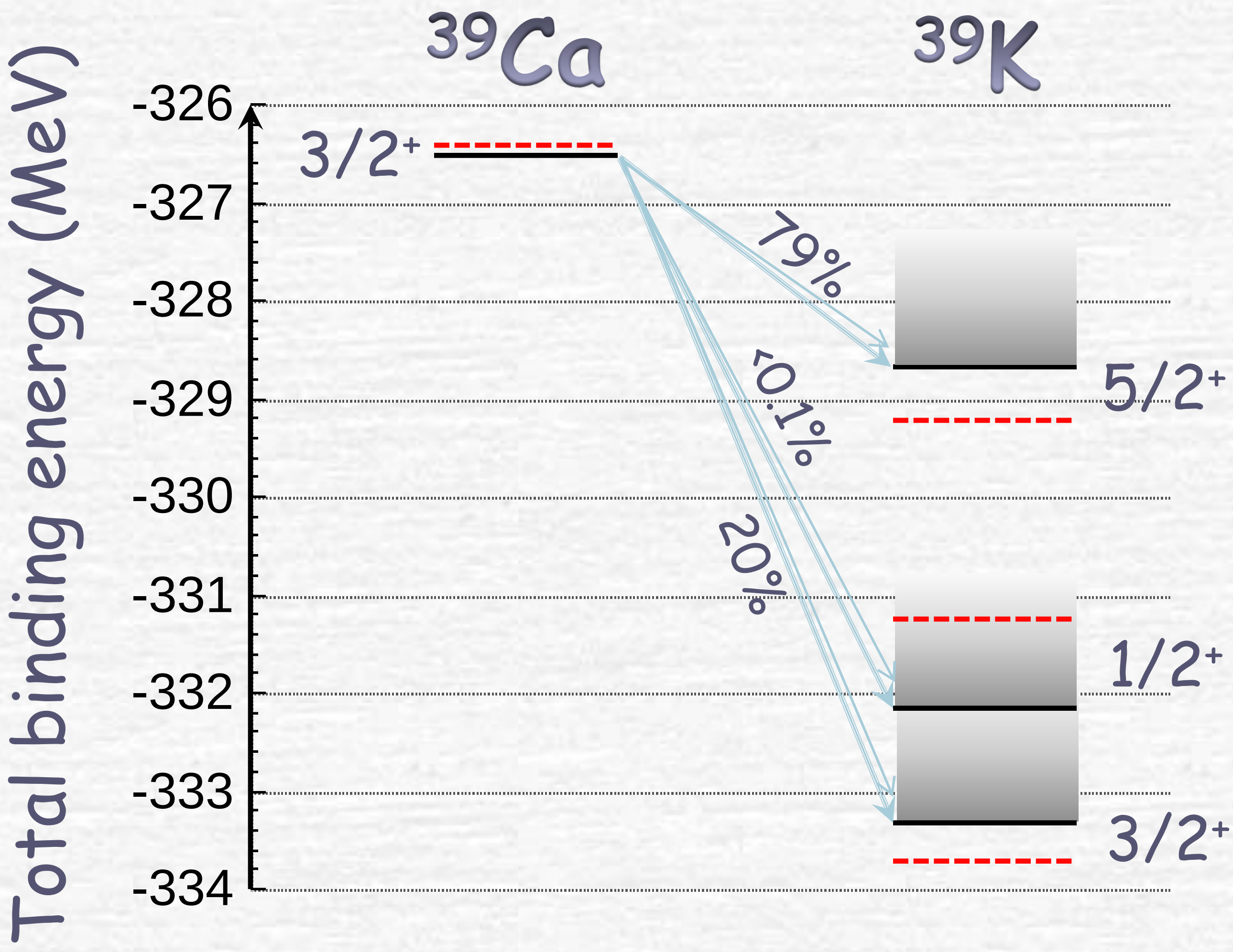
$$|M_{GT-}| - |M_{GT\pm}|$$

β^-	$\beta^\pm$	MR-DFT	EXP
$^{18}Ne \to ^{18}F$	$^{18}F \to ^{18}O$	0.012	0.008
$^{20}Na \to ^{20}Ne$	$^{20}F \to ^{20}Ne$	0.003	-0.023
$^{24}Al \to ^{24}Mg$	$^{24}Na \to ^{24}Mg$	0.002	0.006
$^{28}P \to ^{28}Si$	$^{28}Al \to ^{28}Si$	0.035	0.015
$^{30}S \to ^{30}P$	$^{30}P \to ^{30}Si$	-0.009	-0.017
$^{32}P \to ^{32}S$	$^{32}Cl \to ^{32}S$	0.000	0.034

VERY PRELIMINARY RESULTS !!!

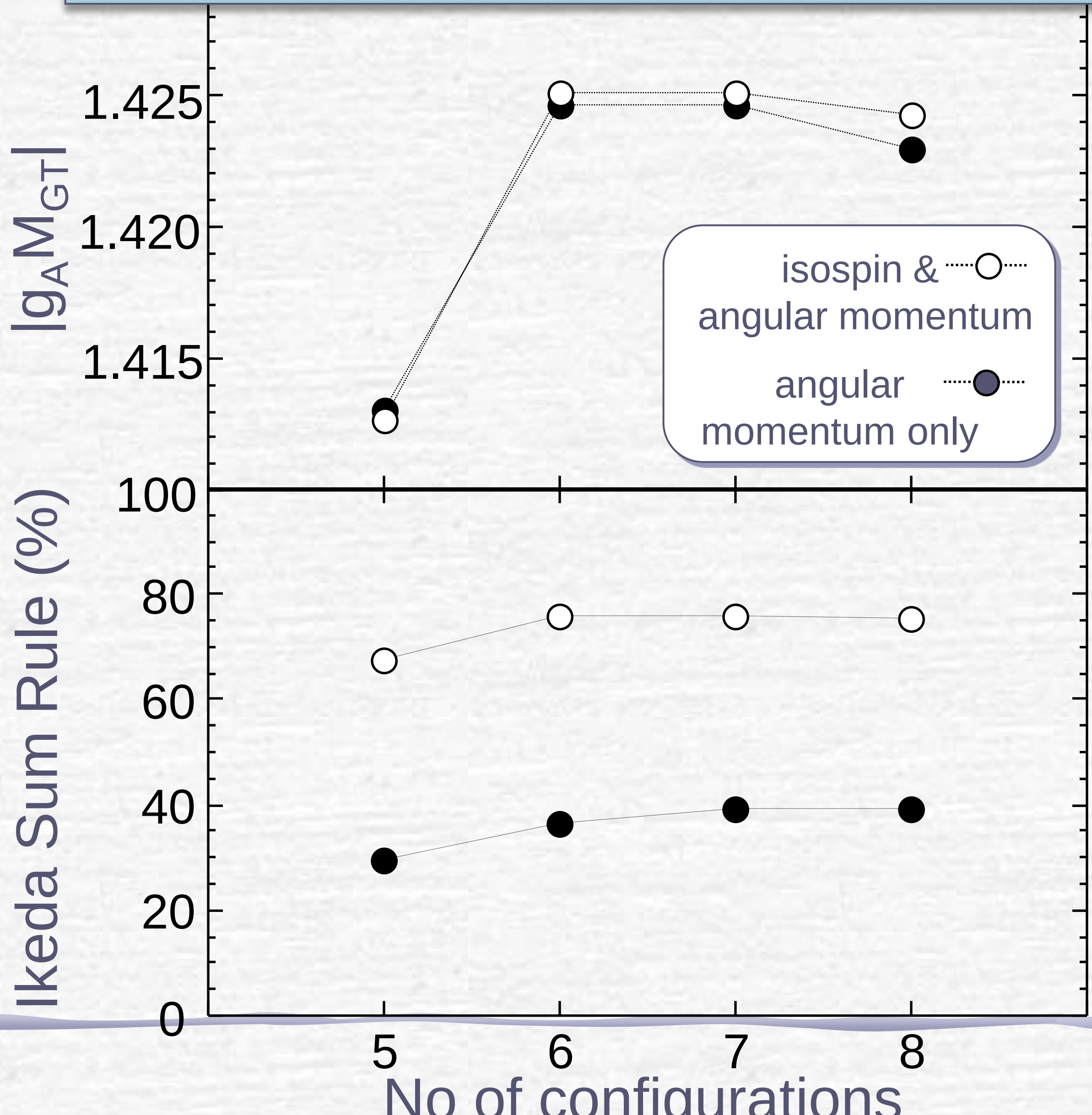
NSM fom Brown, Wildenthal, Atomic and Nuclear Data Tables 33 (1985)

Ikeda sum rule for GT operator



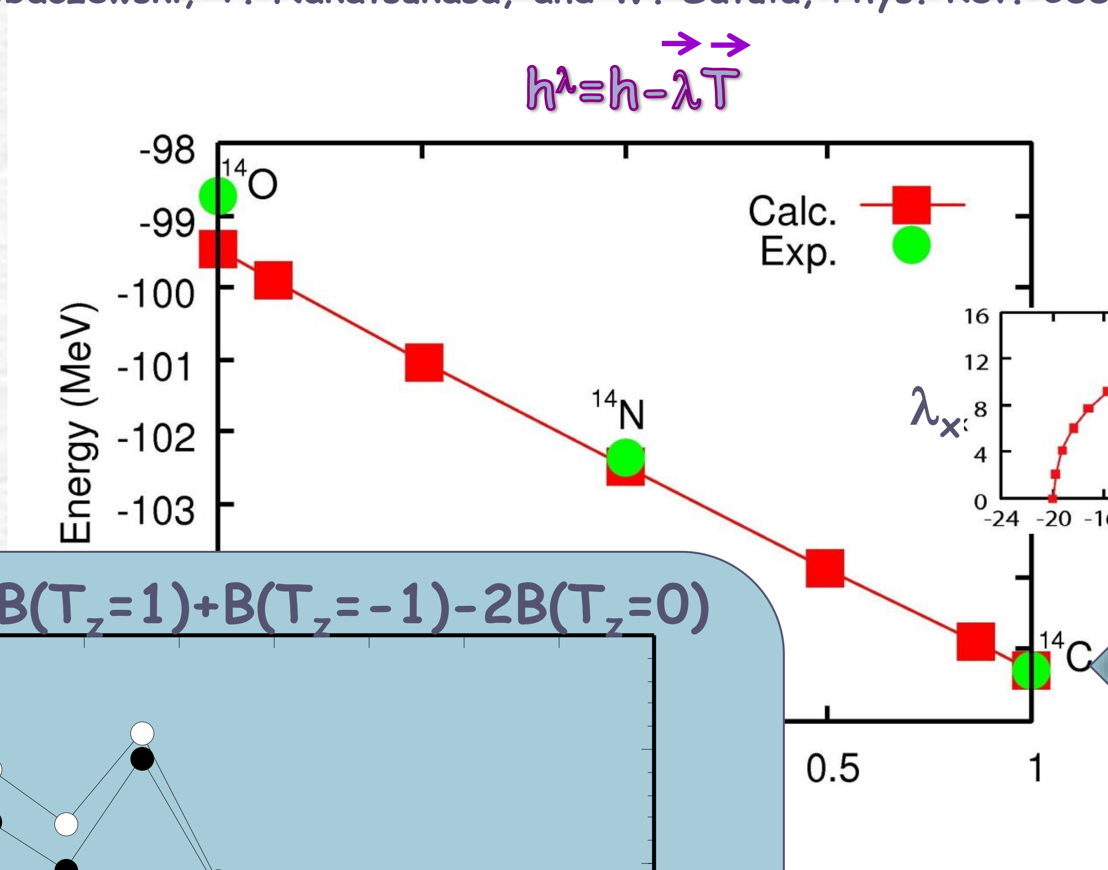
8 p-h configs

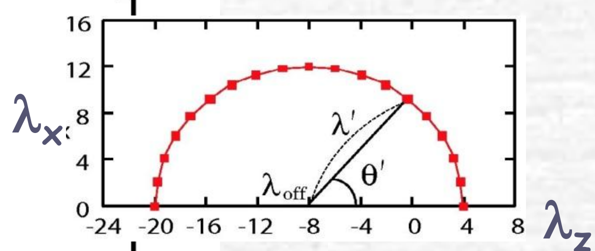
$^{23}Mg \longrightarrow ^{23}Na \longrightarrow$ ~80%



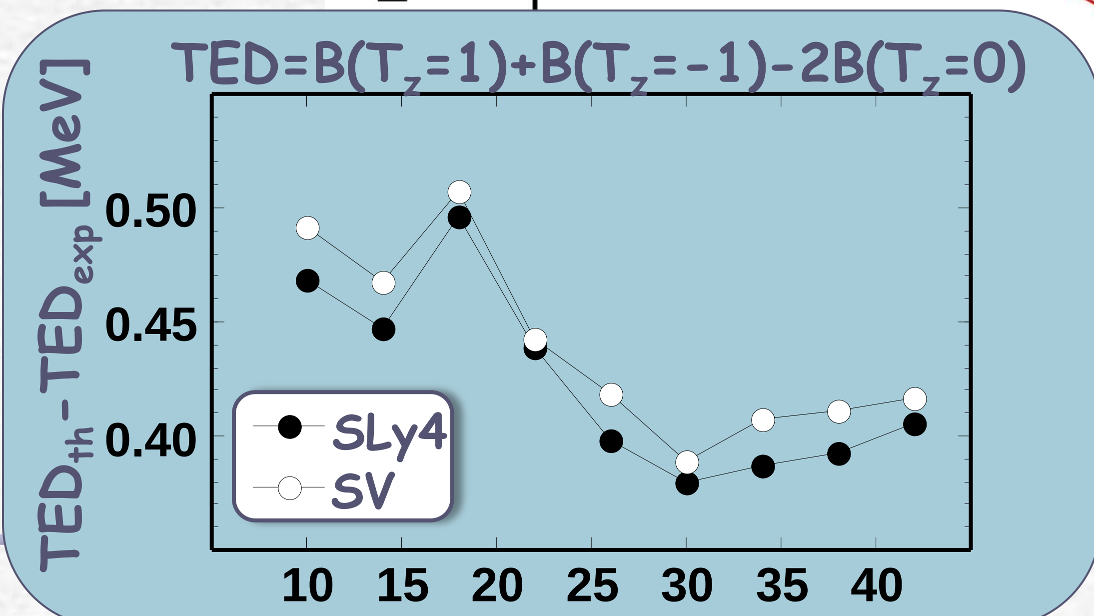
T=1, I=0$^+$ isobaric analogue states from self-consistent 3D-isocranked HF: $h^\lambda = h - \vec{\lambda}\vec{T}$

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





normalized:
theory (red curve)
shifted
by 3.2MeV



separable solution

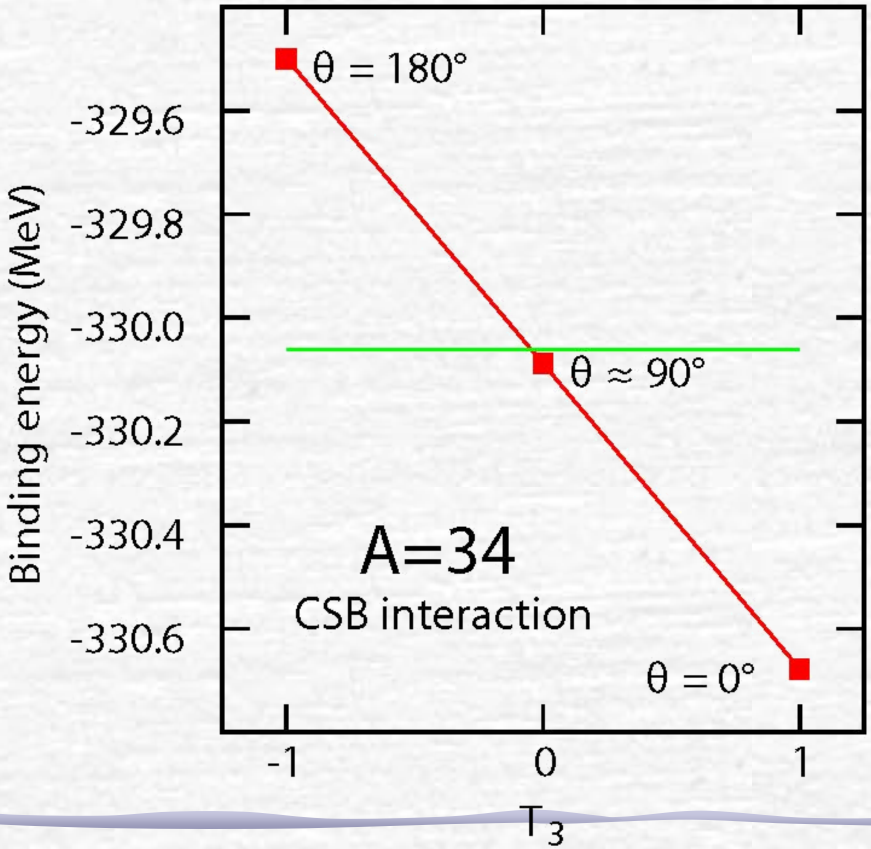
CSB and CIB local corrections to the Skyrme force
(class II (CIB) and III (CSB) Henley-Miller forces)

$$\hat{V}^{\rm II}(i,j) = \frac{1}{2} t_0^{\rm II}\,\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\left(1 - x_0^{\rm II}\hat{P}^\sigma_{ij}\right)\left[3\hat{\tau}_3(i)\hat{\tau}_3(j) - \hat{\vec{\tau}}(i)\circ\hat{\vec{\tau}}(j)\right],$$

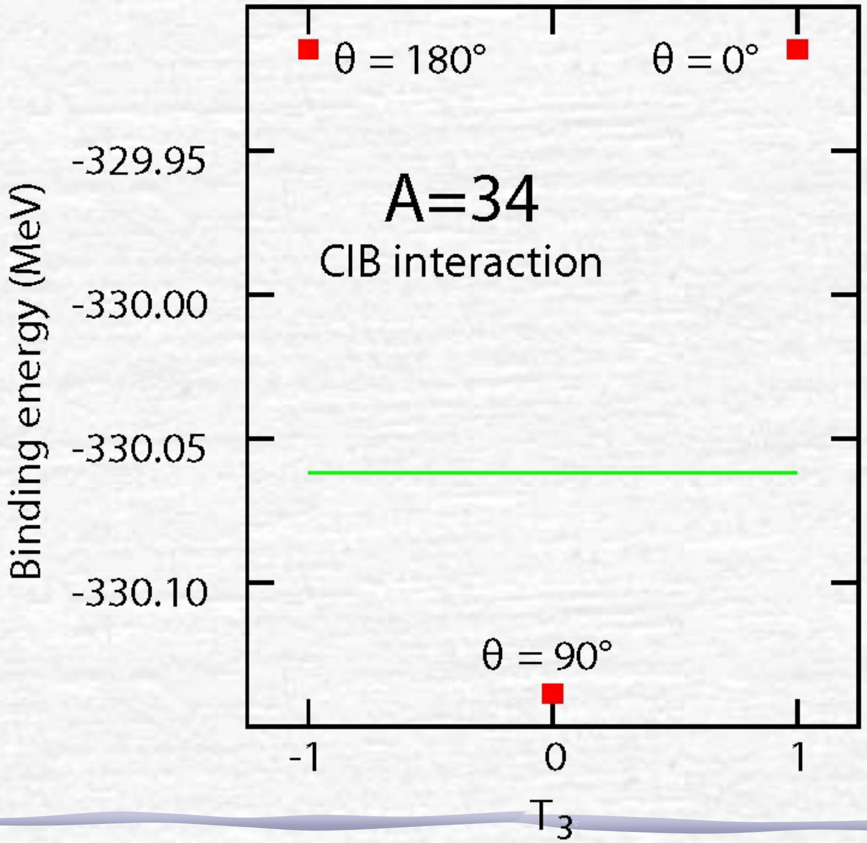
$$\hat{V}^{\rm III}(i,j) = \frac{1}{2} t_0^{\rm III}\,\delta(\boldsymbol{r}_i - \boldsymbol{r}_j)\left(1 - x_0^{\rm III}\hat{P}^\sigma_{ij}\right)\left[\hat{\tau}_3(i) + \hat{\tau}_3(j)\right],$$

$$\mathcal{H}_{\rm II} = \tfrac{1}{2} t_0^{\rm II}\left(1 - x_0^{\rm II}\right)\left(\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pm} - \boldsymbol{s}_n^2 - \boldsymbol{s}_p^2 + 2\boldsymbol{s}_n\cdot\boldsymbol{s}_p + 2\boldsymbol{s}_{np}\cdot\boldsymbol{s}_{pn}\right),$$

$$\mathcal{H}_{\rm III} = \tfrac{1}{2} t_0^{\rm III}\left(1 - x_0^{\rm III}\right)\left(\rho_n^2 - \rho_p^2 - \boldsymbol{s}_n^2 + \boldsymbol{s}_p^2\right),$$



CSB corrects for MDE



CIB corrects for TDE

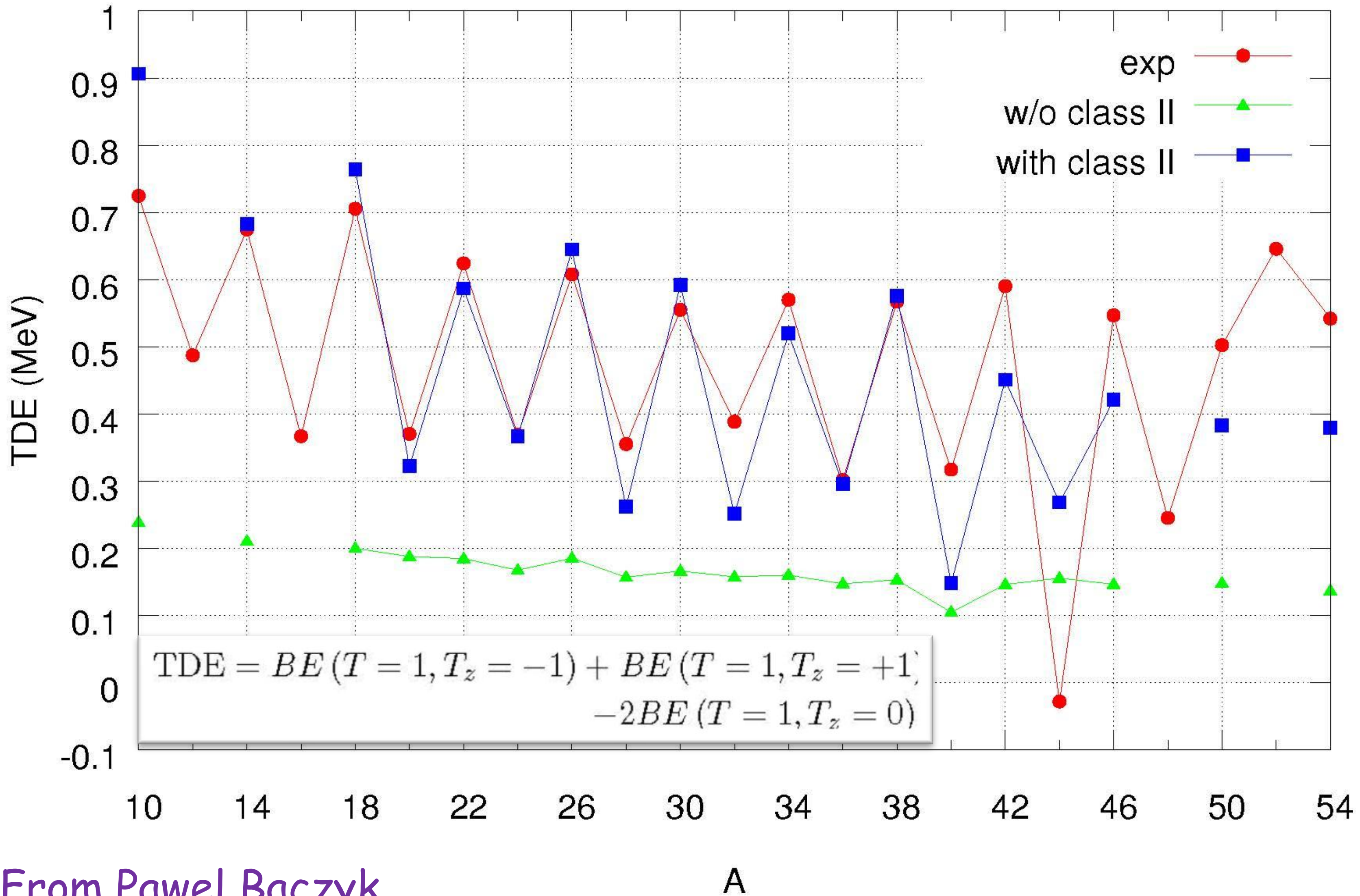
CSB and CIB local corrections to the Skyrme force

$$\hat{V}^{\rm II}(i,j) = \frac{1}{2} t_0^{\rm II}\,\delta\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)\left(1 - x_0^{\rm II}\,\hat{P}^\sigma_{ij}\right)\left[3\hat{\tau}_3(i)\hat{\tau}_3(j) - \hat{\vec{\tau}}(i)\circ\hat{\vec{\tau}}(j)\right],$$

$$\hat{V}^{\rm III}(i,j) = \frac{1}{2} t_0^{\rm III}\,\delta\left(\boldsymbol{r}_i - \boldsymbol{r}_j\right)\left(1 - x_0^{\rm III}\,\hat{P}^\sigma_{ij}\right)\left[\hat{\tau}_3(i) + \hat{\tau}_3(j)\right],$$

$$\mathcal{H}_{\rm II} = \tfrac{1}{2} t_0^{\rm II}\left(1 - x_0^{\rm II}\right)\left(\rho_n^2 + \rho_p^2 - 2\rho_n\rho_p - 2\rho_{np}\rho_{pn} - \boldsymbol{s}_n^2 - \boldsymbol{s}_p^2 + 2\boldsymbol{s}_n\cdot\boldsymbol{s}_p + 2\boldsymbol{s}_{np}\cdot\boldsymbol{s}_{pn}\right),$$

$$\mathcal{H}_{\rm III} = \tfrac{1}{2} t_0^{\rm III}\left(1 - x_0^{\rm III}\right)\left(\rho_n^2 - \rho_p^2 - \boldsymbol{s}_n^2 + \boldsymbol{s}_p^2\right),$$



From Pawel Baczyk

Challenges for Low-Energy Nuclear Theory

- Perform proof-of-principle lattice QCD calculation for the lightest nuclei
- Develop first-principles framework for light, medium-mass nuclei, and nuclear matter from 0.1 to twice the saturation density
- Derive predictive nuclear energy density functional rooted in first-principles theory
- Carry out predictive and quantified calculations of nuclear matrix elements for fundamental symmetry tests.
- Unify the fields of nuclear structure and reactions.
- Develop predictive microscopic model of fusion and fission that will provide the missing data for astrophysics and nuclear energy research.
- Develop and utilize tools for quantification of theoretical uncertainties.
- Provide the microscopic explanation for observed, and new, (partial-) dynamical symmetries and simple patterns

Perspectives are not bad!

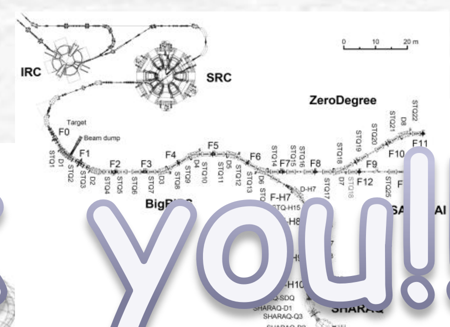
"The purpose of computing is insight, not numbers"

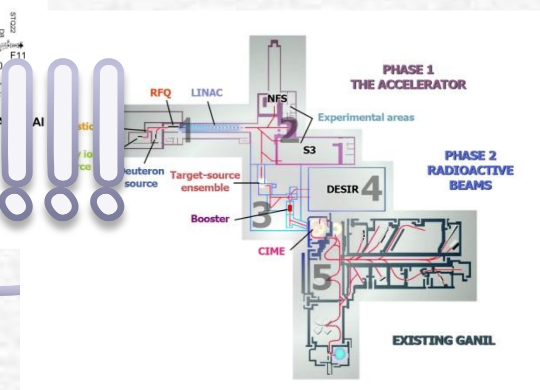
(Richard Hamming, 1962)

"According to Einstein's theory, if we move the computer real fast, we can go back in time and recover the files you accidentally deleted."

- because of high-performance computing
- and new high-precision data, in particular, on short lived nuclei

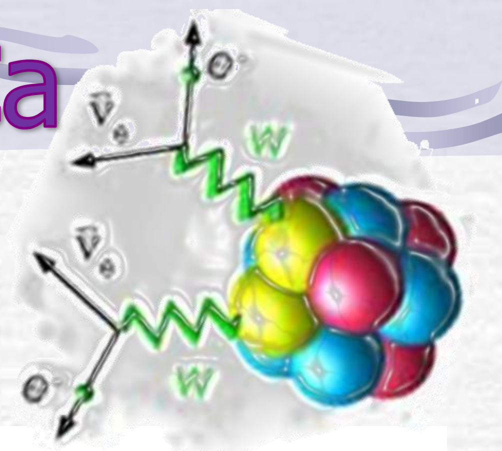
Radioactive Ion Beam Facilities Worldwide





Thank you!!!

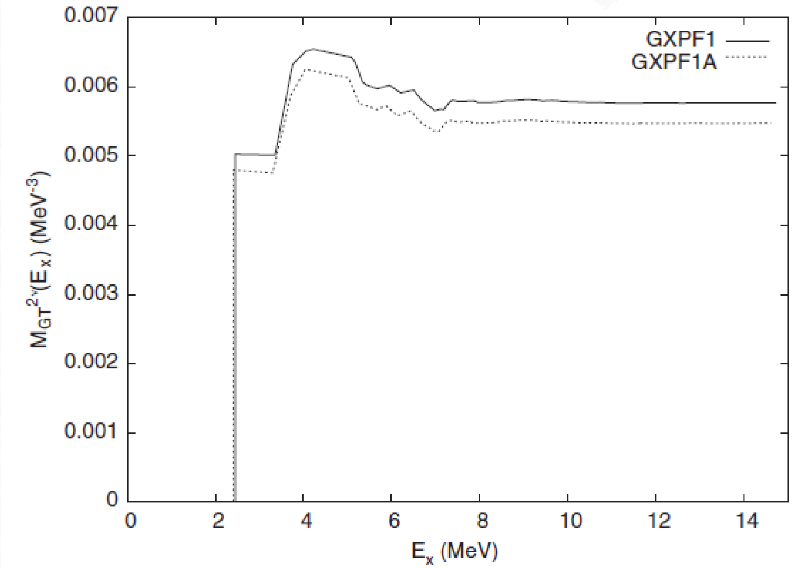
Double beta decay of ^{48}Ca



$$|M_{GT}^{2\nu\beta\beta}| = \sum_n \frac{\langle \Psi_f, I=0 | \hat{O}_{GT} | \Psi_n^{int}, I=1\rangle \langle \Psi_n^{int}, I=1 | \hat{O}_{GT} | \Psi_i, I=0\rangle}{(\frac{1}{2}Q_{\beta\beta}(\Psi_f, I=0) + E(\Psi_n^{int}) - M_i)/m_e + 1}$$

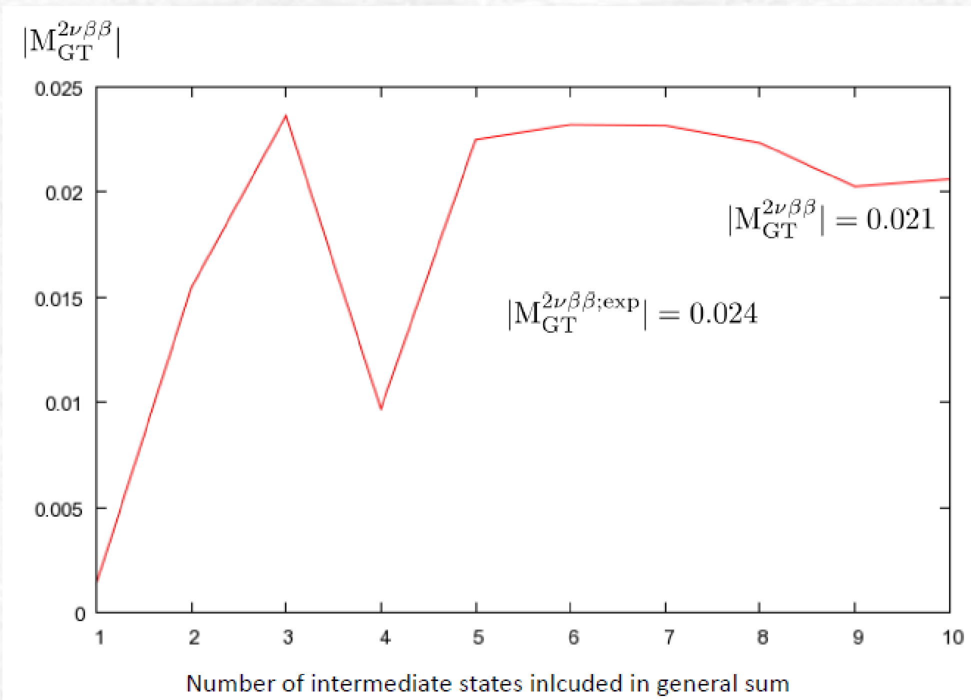
J. Suhonen, O. Civitarese, Physics Reports 300 (1998)

NSM uses **more** than
250 intermediate states!!!



Horoi, Stoica, Brown; Phys Rev. C **75**, 034303 (2007)

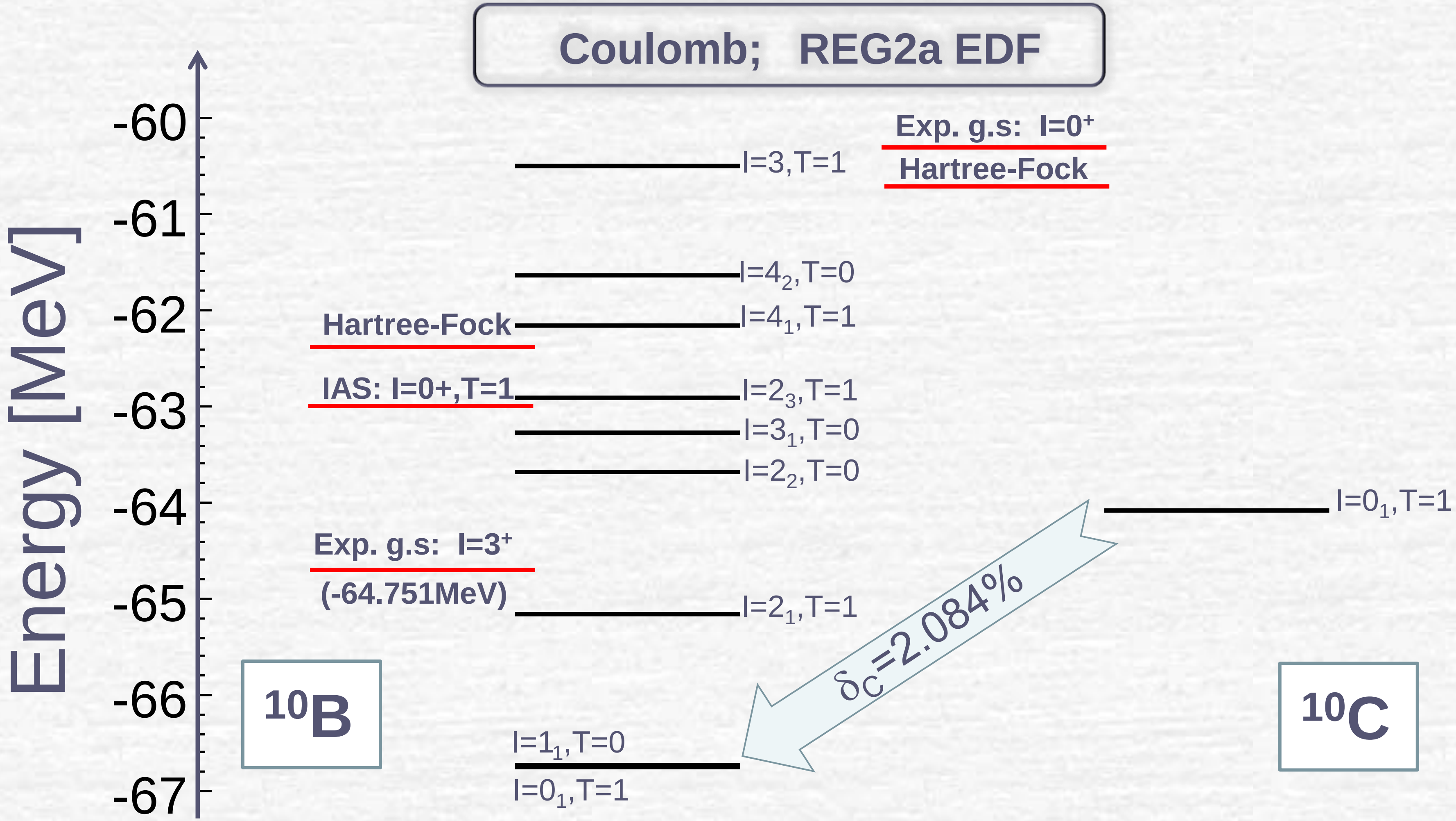
VERY PRELIMINARY RESULTS !!!



10 intermediate states only:

$E(1_1^+)$	2.901	$E(1_6^+)$	8.598
$E(1_2^+)$	4.028	$E(1_7^+)$	10.250
$E(1_3^+)$	4.669	$E(1_8^+)$	14.042
$E(1_4^+)$	5.356	$E(1_9^+)$	15.495
$E(1_5^+)$	6.931	$E(1_{10}^+)$	40.419

Projection from anti-aligned HF state
BDR regularized functional REG2



ΔE_{th}=2.597 MeV; ΔE_{exp}=2.690 MeV