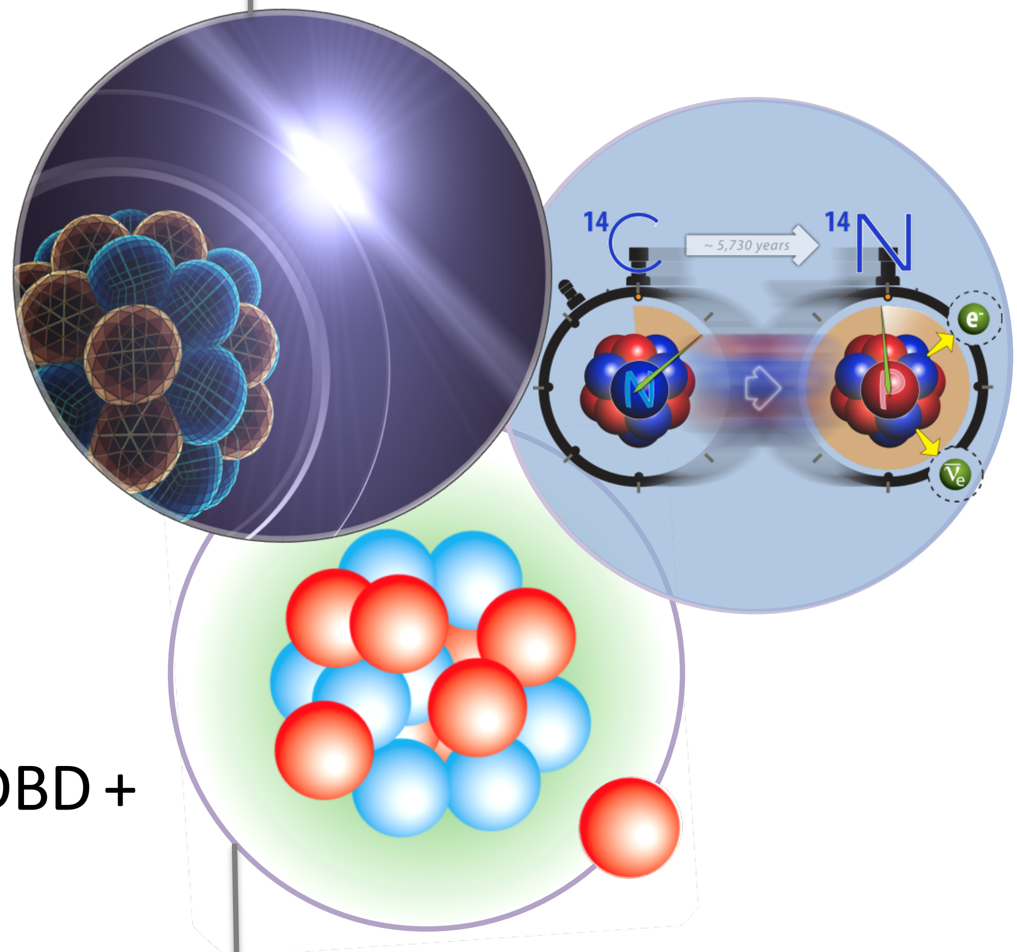
Weak decays from coupled cluster computations

Gaute Hagen

Oak Ridge National Laboratory



Topical Collaboration meeting on DBD + fundamental symmetries

INT, June 20, 2017

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

BSF
United States – Israel
Binational Science Foundation

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Collaborators

@ ORNL / UTK: G. R. Jansen, **T. Morris**, T. Papenbrock, **M. Schuster, Z. H. Sun**

@ Chalmers: **B. Carlsson**, A. Ekström, C. Forssén

@ Hebrew U: N. Barnea, D. Gazit

@ MSU/ U Oslo: M. Hjorth-Jensen

@ Trento: G. Orlandini

@ TRIUMF: S. Bacca, J. Holt, **M. Miorelli**, P. Navratil, **S. R. Stroberg**

@ TU Darmstadt: **C. Drischler**, **C. Stumpf**, K. Hebeler, R. Roth, A. Schwenk, **J. Simonis**

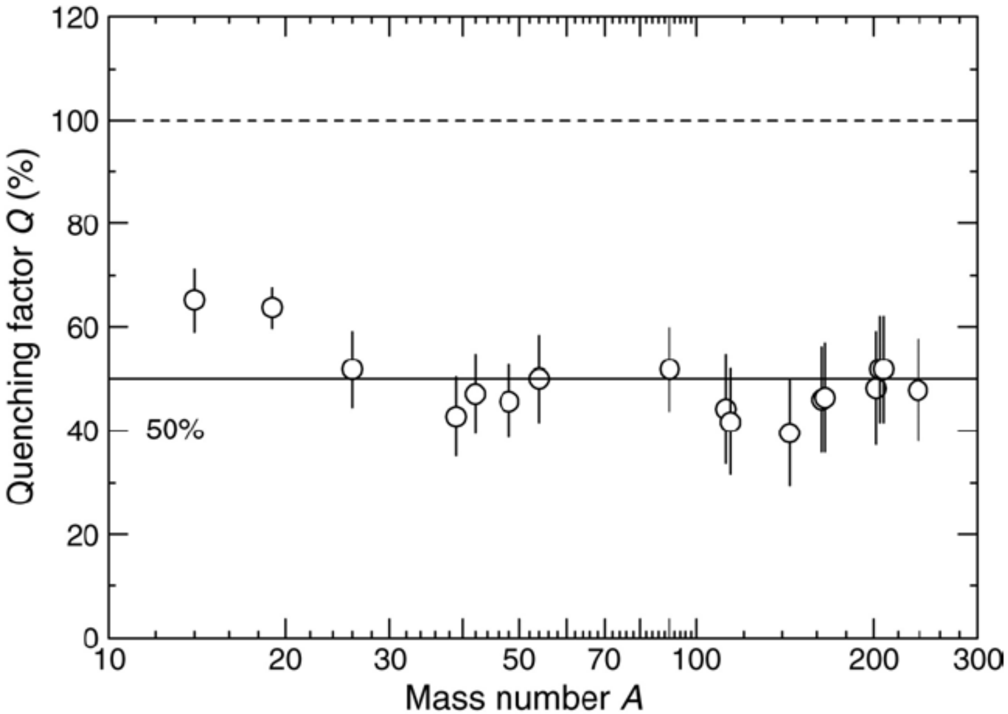
@ LLNL: **K. Wendt**

Outline

- CC computations of beta decays in ^{8}He and ^{14}C. Benchmark GT with other methods (CI-IM-SRG, NCSM).
- The quenching of g_A
- Role of 2BCs and correlations on super allowed Gamow-Teller transition in ^{100}Sn
- Compute $2\nu\beta\beta$ and $0\nu\beta\beta$ decay in ^{48}Ca with full-space coupled-cluster

Quenching of Gamow-Teller strength in nuclei

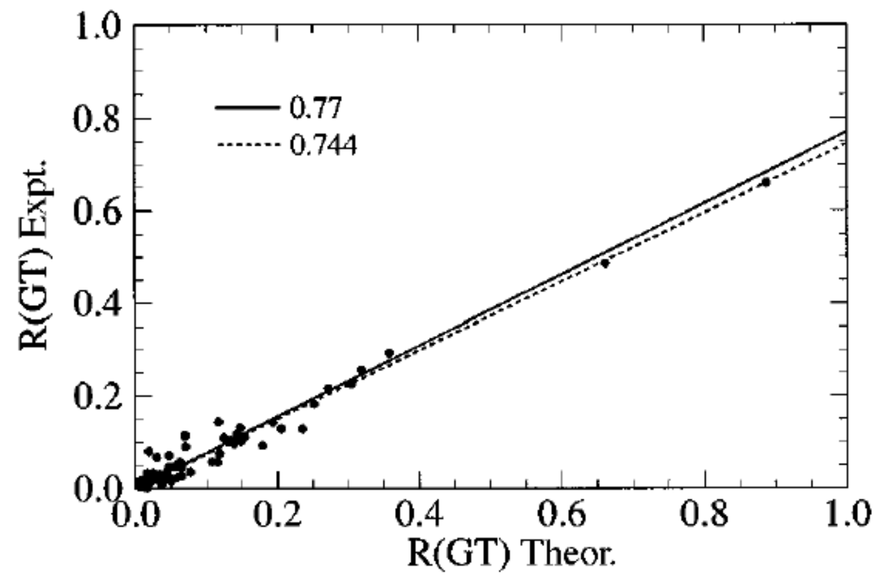
Long-standing problem: Experimental beta-decay strengths quenched compared to theoretical results.



Surprisingly large quenching *Q* (50%) obtained from (*p*,*n*) experiments. The excitation energies were just above the giant Gamow-Teller resonance ~10-15MeV (Gaarde 1983).

- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?
- Meson exchange currents (2BCs)?

G. Martinez-Pinedo et al, PRC **53**, R2602 (1996)

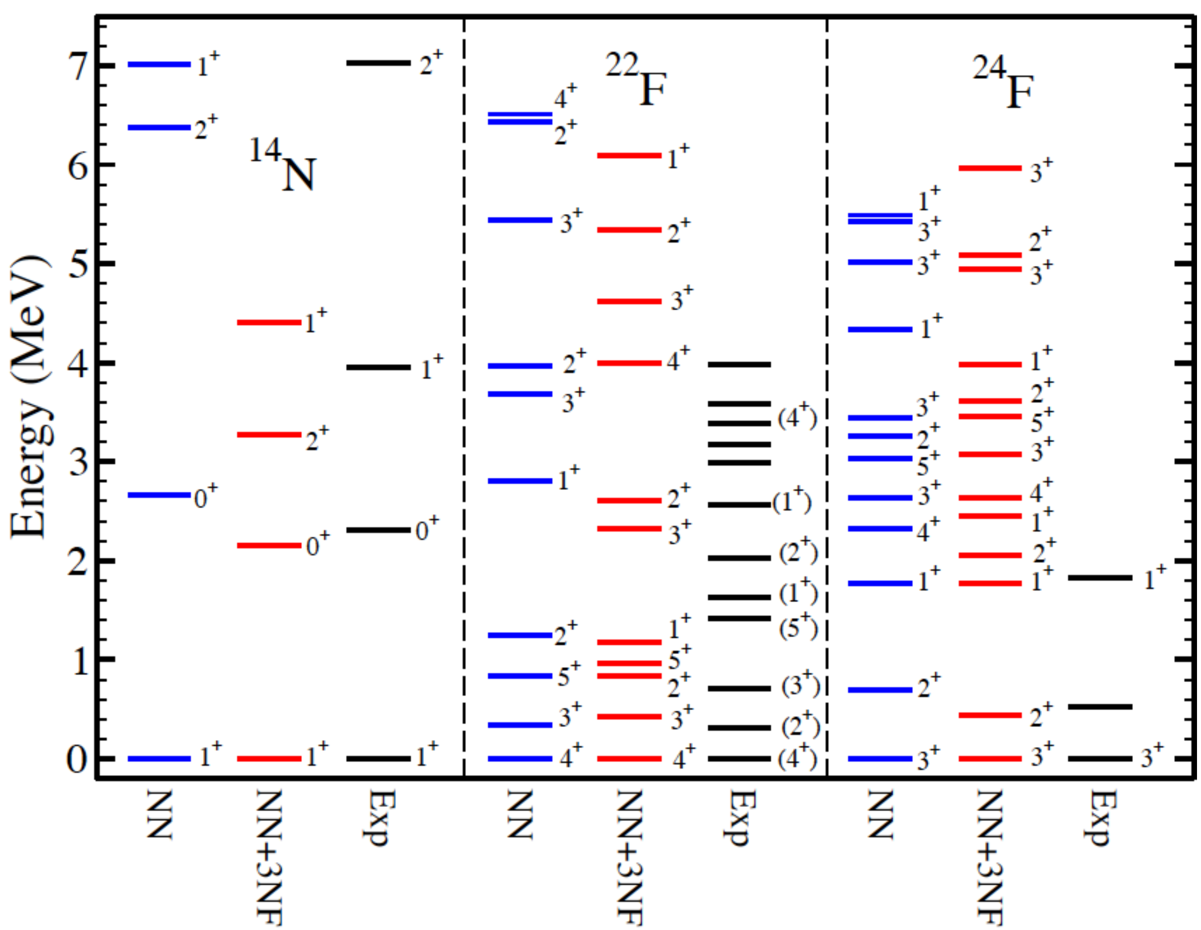


Charge exchange equation-of-motion coupled method

Diagonalize $\overline{H} = e^{-T} H_N e^T$ via a equation-of-motion technique:

$$R_\nu = \sum r_i^a \, p_a^\dagger n_i + \frac{1}{4}\sum r_{ij}^{ab} \, p_a^\dagger N_b^\dagger N_j n_i + \frac{1}{36}\sum r_{ijk}^{abc} \, p_a^\dagger N_b^\dagger N_c^\dagger N_k N_j n_i$$

A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)



- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predict several states in neutron rich Fluorine

Charge exchange equation-of-motion coupled method

Diagonalize $\overline{H} = e^{-T} H_N e^{T}$ via a equation-of-motion technique:

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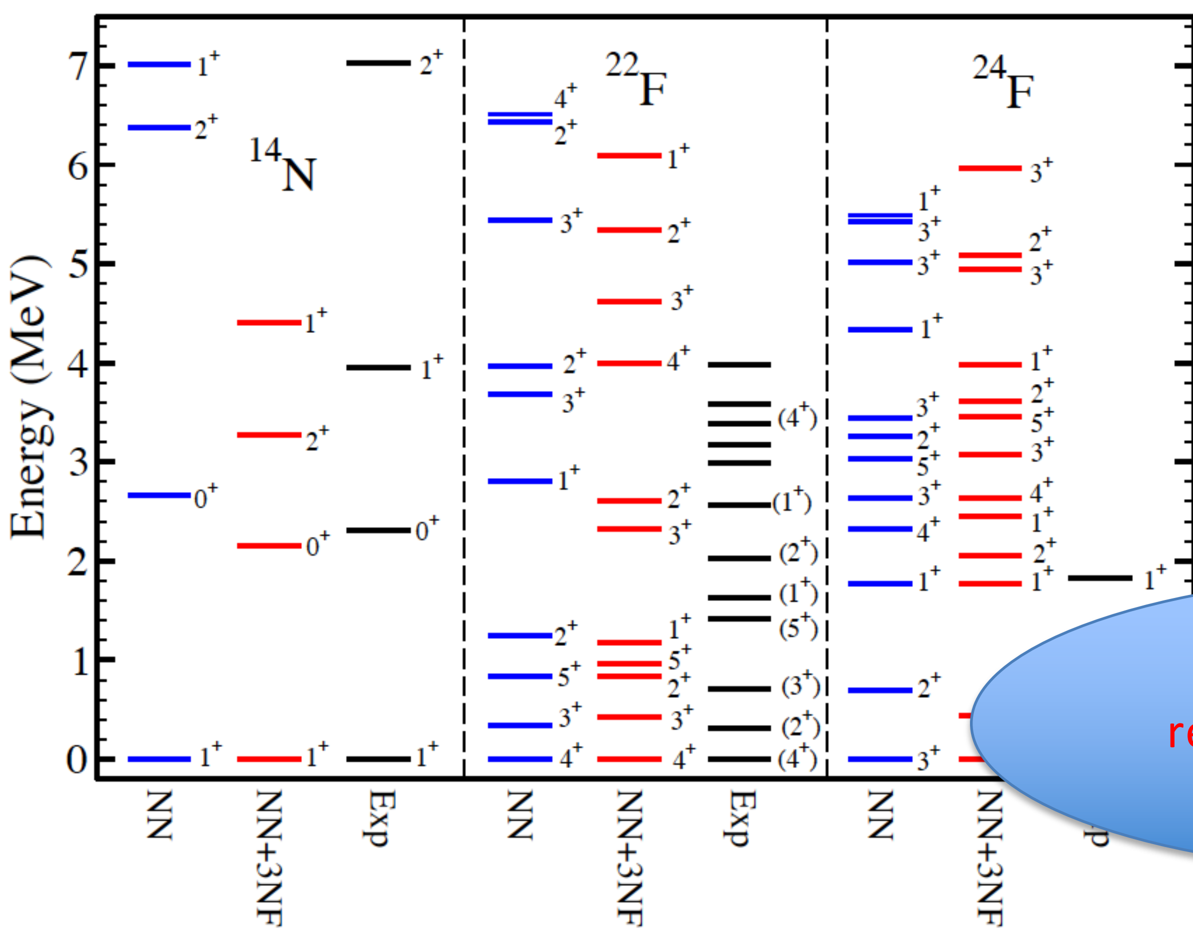

- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with

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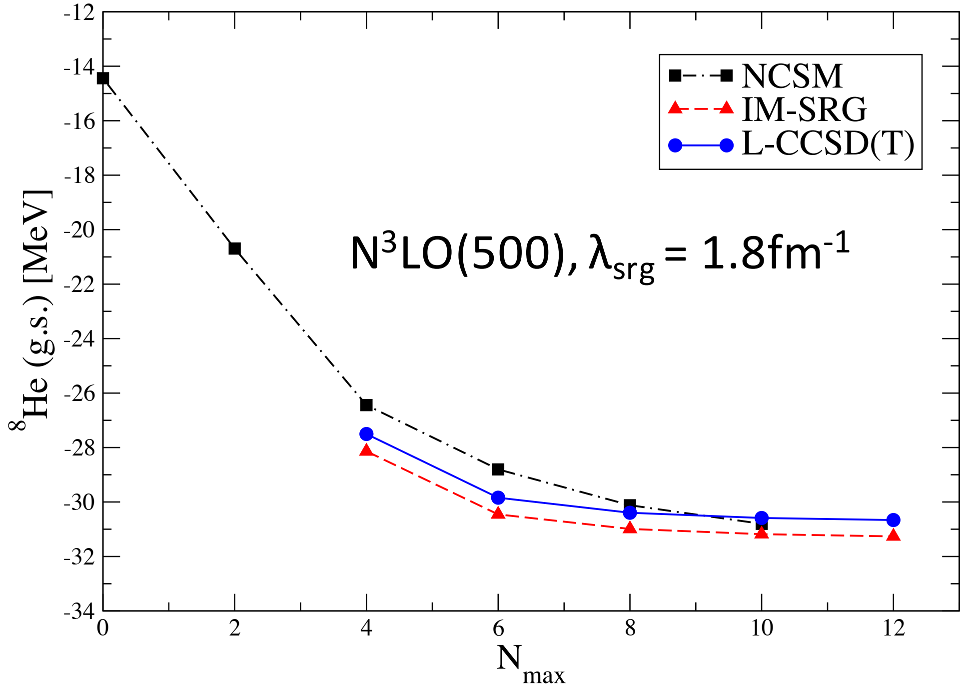
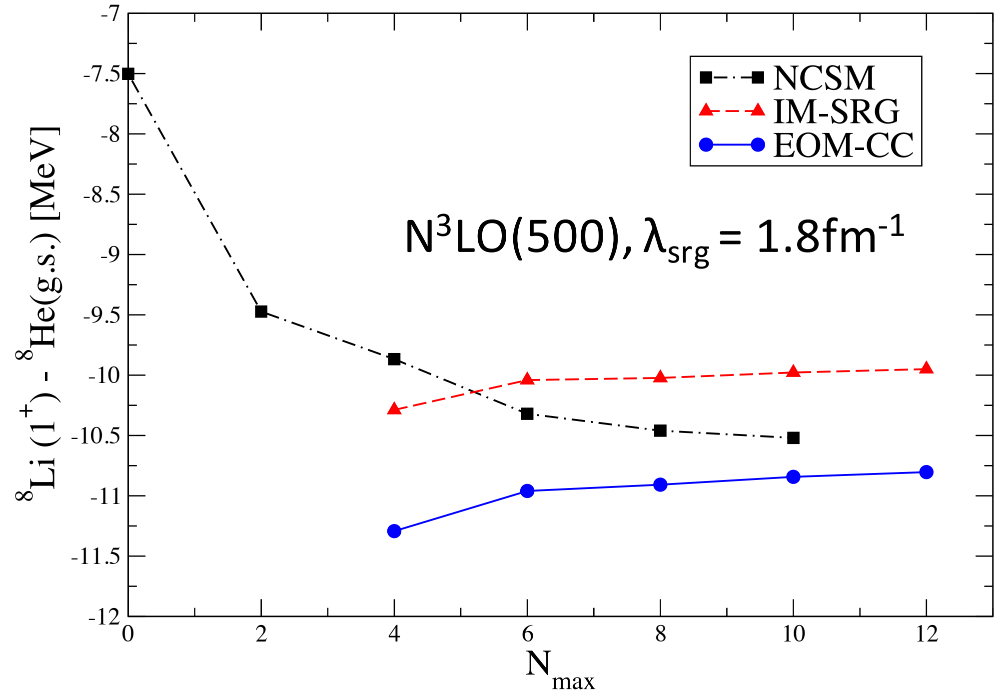
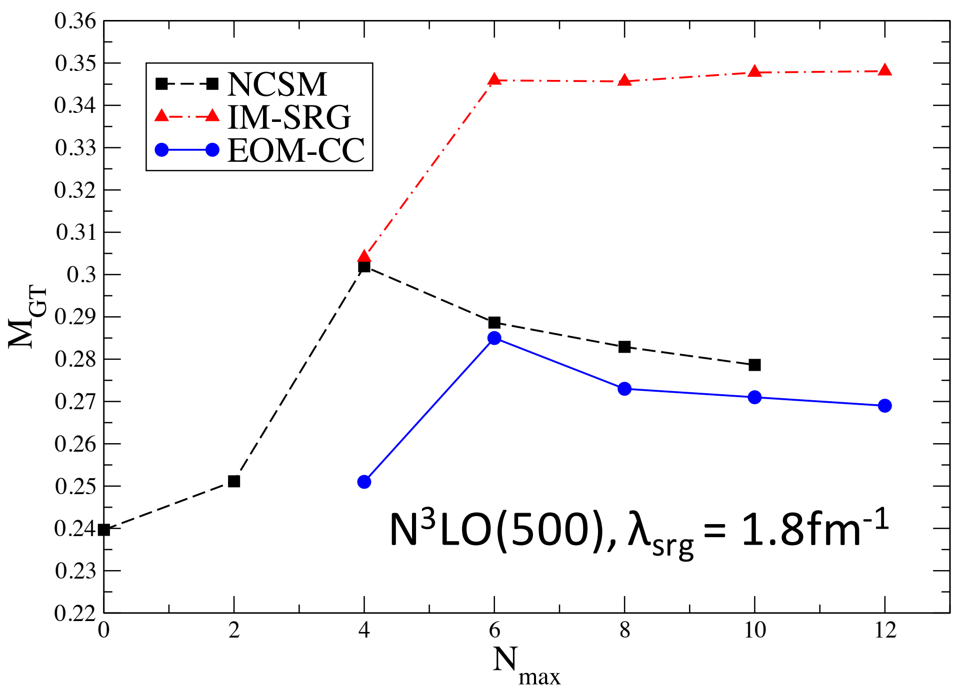
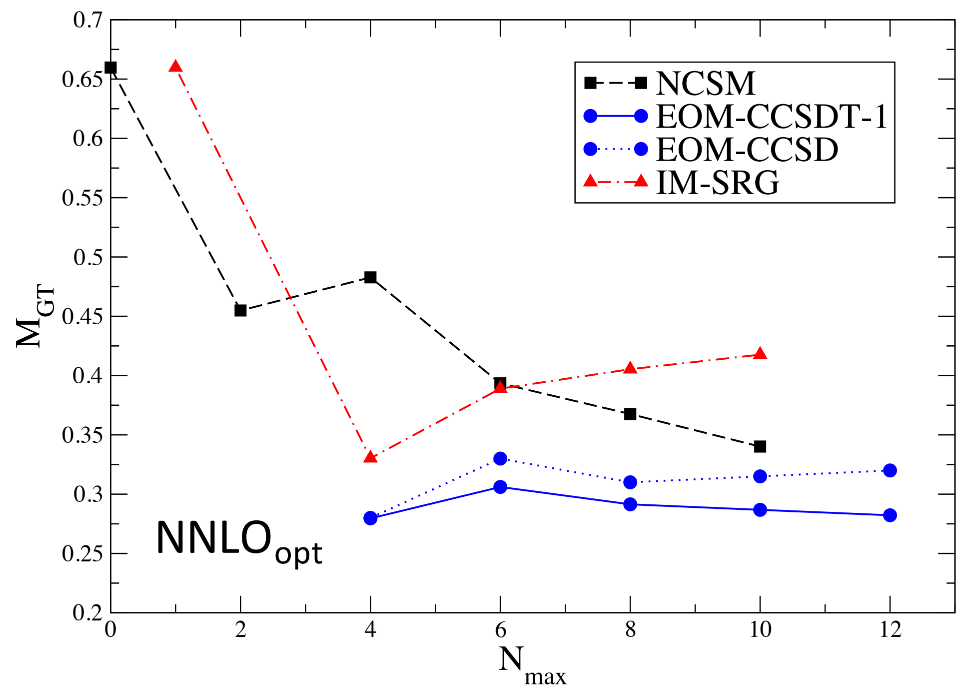
r_{ijk}^{abc} has massive requirements for realistic calcs

Benchmarks for Gamow-Teller transitions in ^{8}He





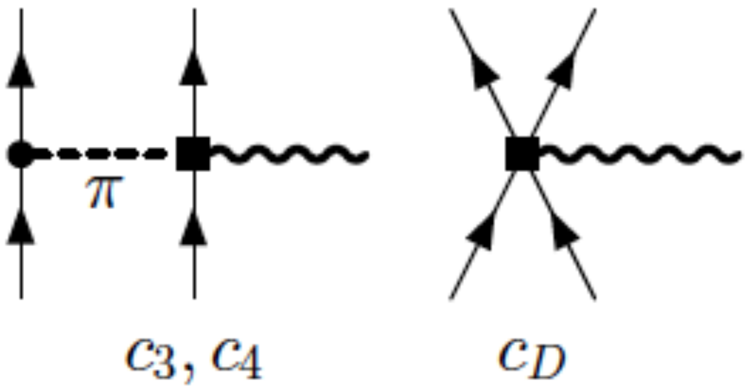




Normal ordered one- and two-body current

Gamow-Teller matrix element:

$$\hat{O}_{\mathrm{GT}} \equiv \hat{O}_{\mathrm{GT}}^{(1)} + \hat{O}_{\mathrm{GT}}^{(2)} \equiv g_A^{-1}\sqrt{3\pi}E_1^A$$



Normal ordered operator:

$$\hat{O}_{\mathrm{GT}} = O_N^0 + O_N^1 + O_N^2$$

$$O_N^0 = \sum_{i \le E_f} \langle i|O^{(1)}|i\rangle + \frac{1}{2}\sum_{i,j \le E_f} \langle ij|O^{(2)}|ij\rangle$$

$$O_N^1 = \sum_{pq} \langle p|O^{(1)}|q\rangle\{p^\dagger q\} + \sum_{pq}\sum_{i \le E_f} \langle pi|O^{(2)}|qi\rangle\{p^\dagger q\}$$

$$O_N^2 = \frac{1}{4}\sum_{pqrs} \langle pq|O^{(2)}|rs\rangle\{p^\dagger q^\dagger s r\}$$

One- and two-body currents and normal ordering in Coupled-Cluster

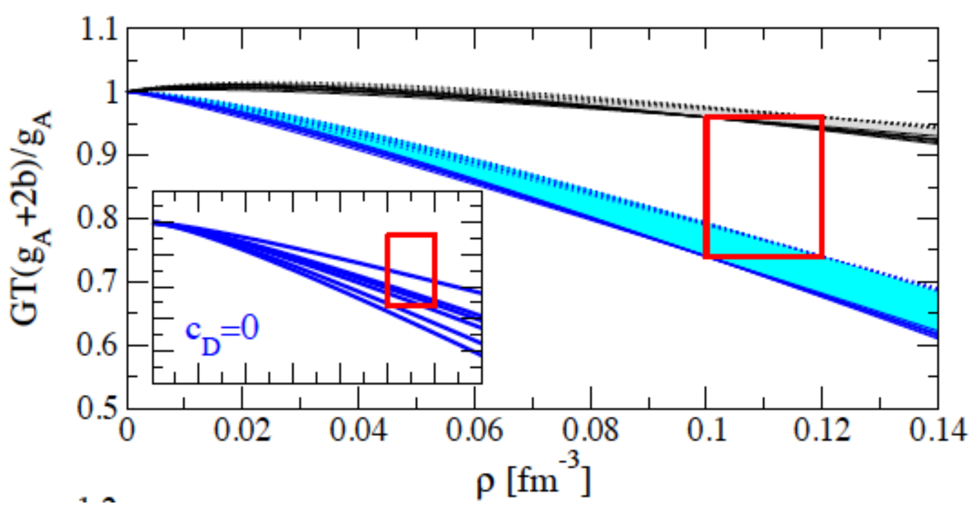
CCSD similarity transformed normal-ordered current operator: $T = T_1 + T_2$

3-body terms

6-body terms

$$\overline{O_{\mathrm{GT}}} = e^{-T} O_N e^T = e^{-T} O_N^1 e^T + e^{-T} O_N^2 e^T$$

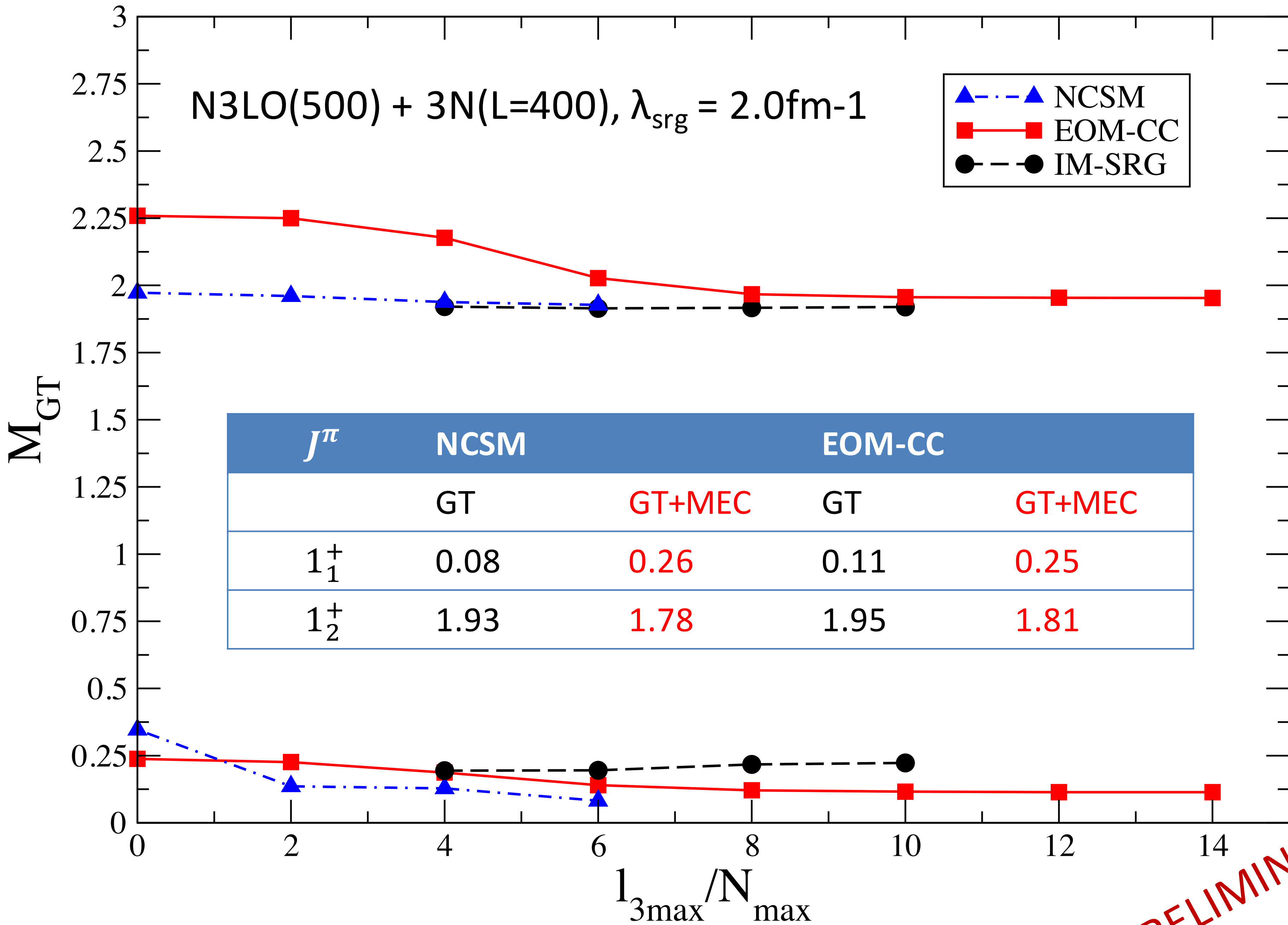
Normal-ordered 1-body approximation



J. Menéndez, D. Gazit, A. Schwenk
PRL 107, 062501 (2011)

Normal order with respect to free Fermi gas. One-body normal ordered approximation gives quenching of g_A by a factor q = 0.74…0.96 for different set of couplings constants

Benchmarks for Gamow-Teller transitions in ^{14}C

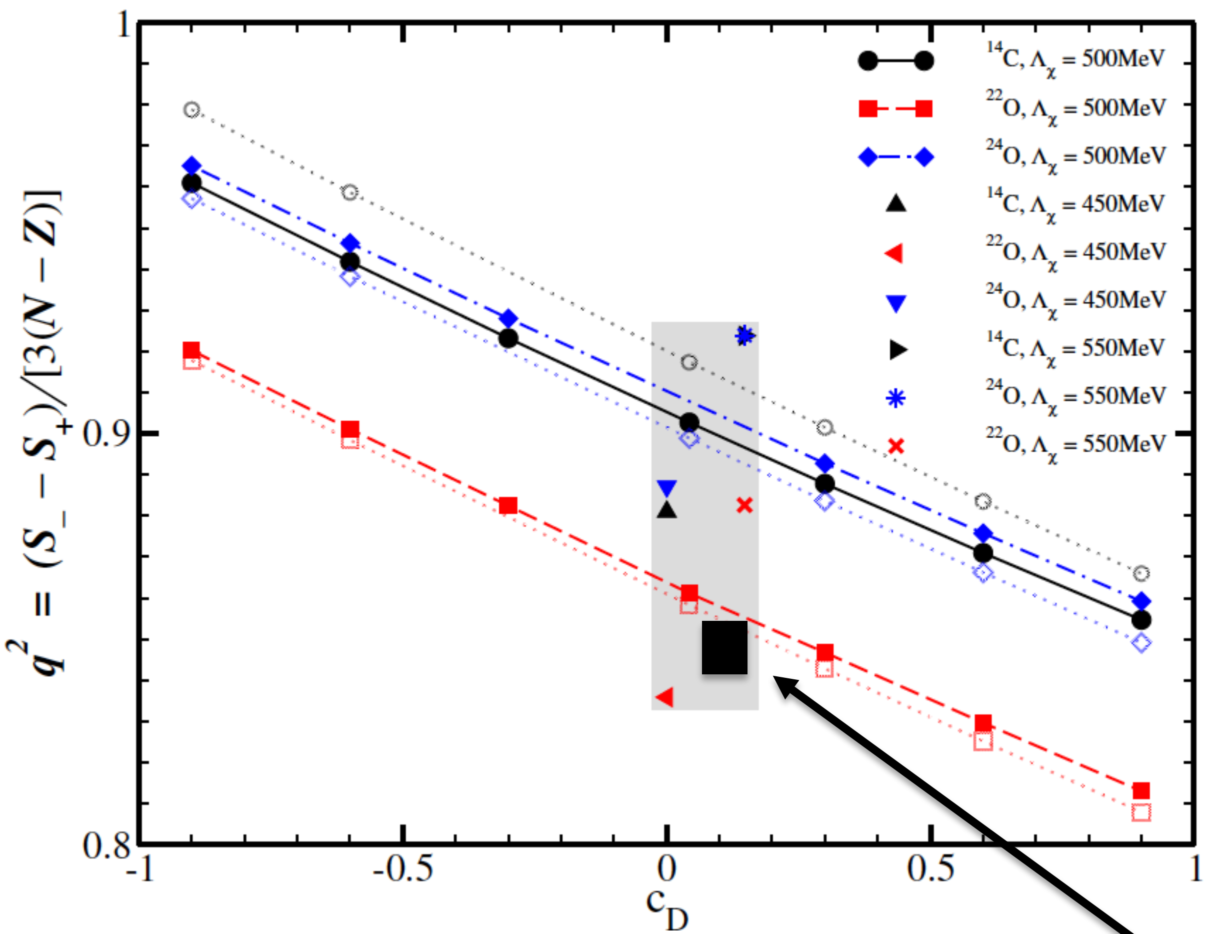


J^{π}	NCSM		EOM-CC	
	GT	GT+MEC	GT	GT+MEC
1^+_1	0.08	0.26	0.11	0.25
1^+_2	1.93	1.78	1.95	1.81

PRELIMINARY

Quenching of Ikeda sum rule in ^{14}C

$$S^{\mathrm{N}}(\mathrm{GT}) = S^{\mathrm{N}}(\mathrm{GT}^-) - S^{\mathrm{N}}(\mathrm{GT}^+) = 3(N - Z)$$



Quenching factor:

$$Q = \frac{S^-_{\mathrm{GT}}(\omega^-_{\mathrm{top}}) - S^+_{\mathrm{GT}}(\omega^+_{\mathrm{top}})}{3(N-Z)}$$

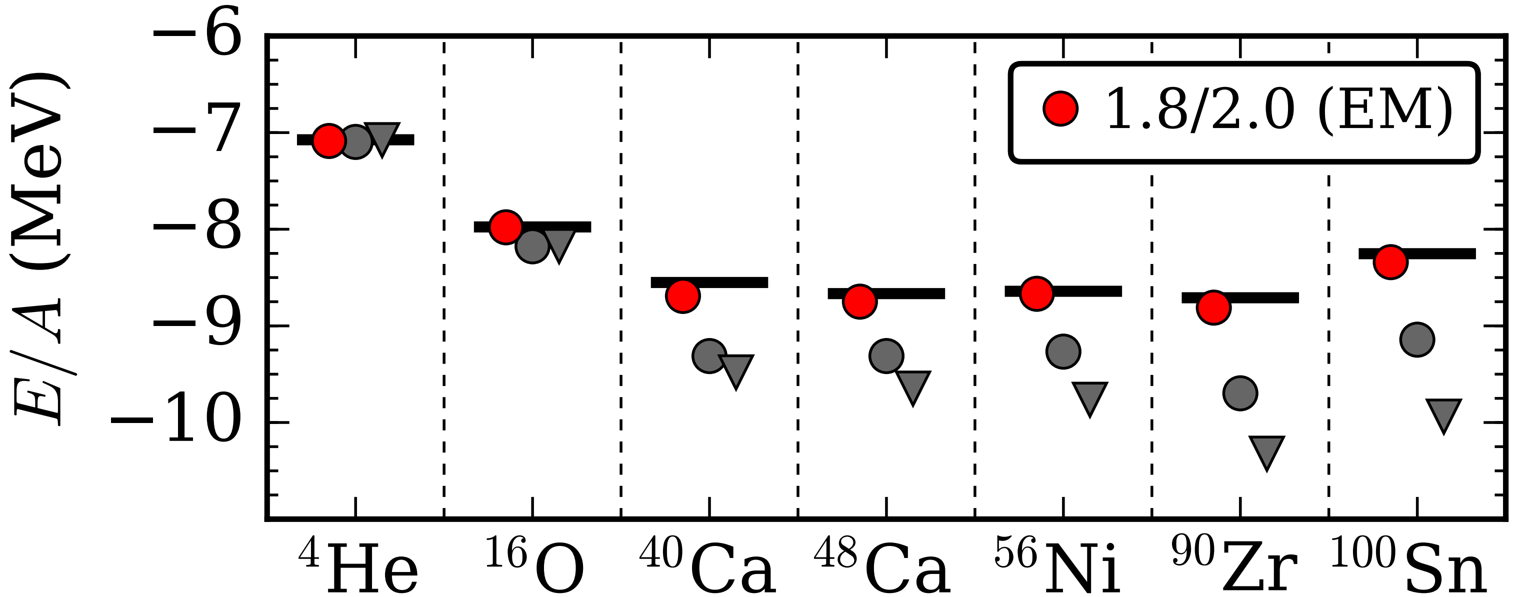
Sum rule calculated in CC:

$$S_- = \langle\Lambda|\overline{\hat{O}^\dagger_{\mathrm{GT}}} \cdot \overline{\hat{O}_{\mathrm{GT}}}|\mathrm{HF}\rangle$$
$$S_+ = \langle\Lambda|\overline{\hat{O}_{\mathrm{GT}}} \cdot \overline{\hat{O}^\dagger_{\mathrm{GT}}}|\mathrm{HF}\rangle$$

N3LO(500) + 3N(L=400), λ_{srg} = 2.0fm-1

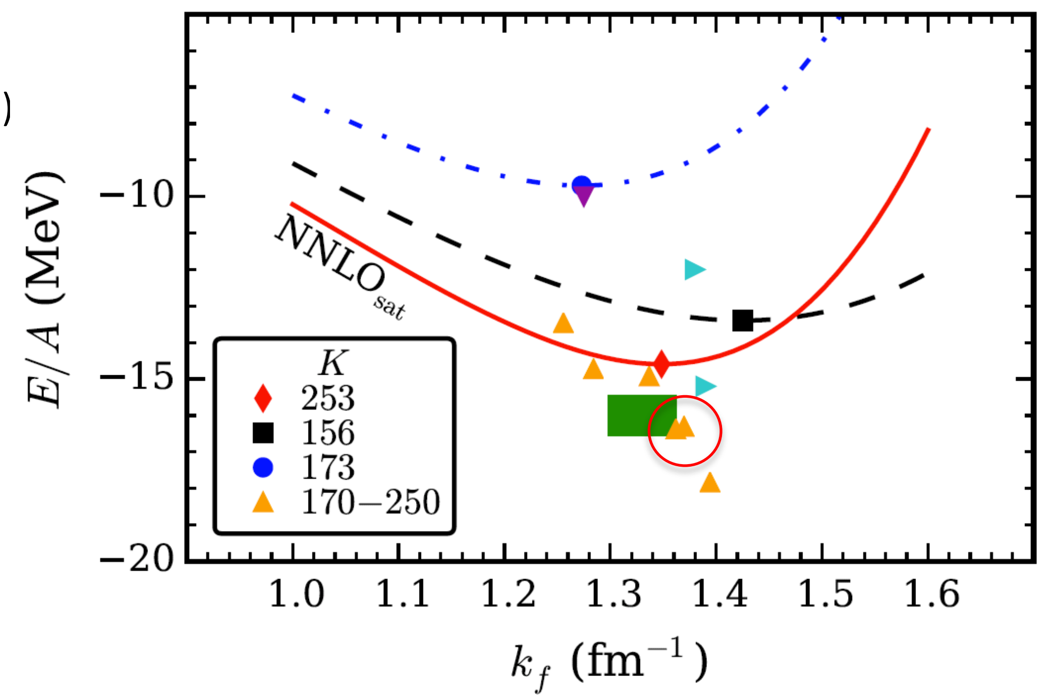
A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

Accurate BEs from light → heavy → infinite matter from a chiral interaction

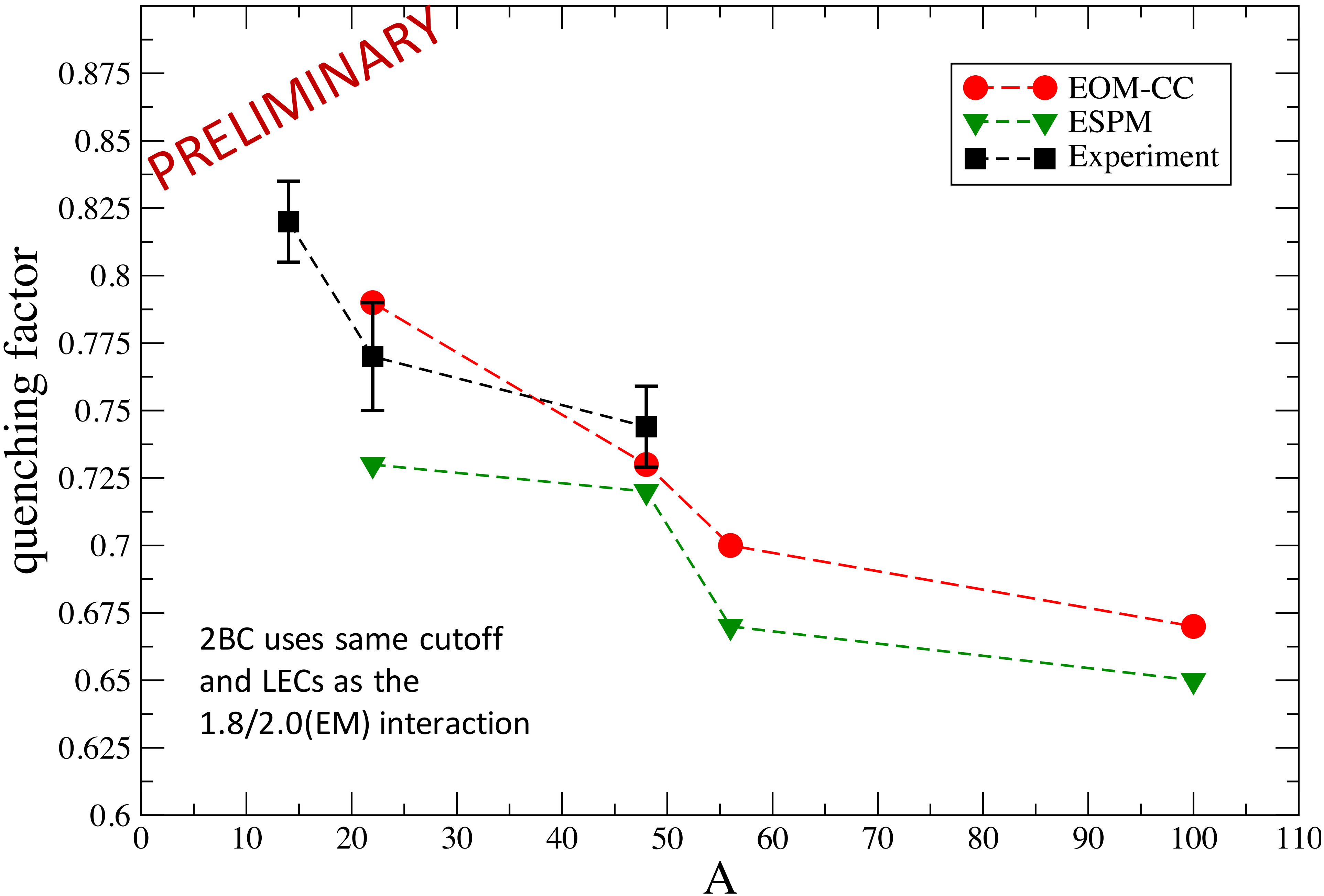


1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

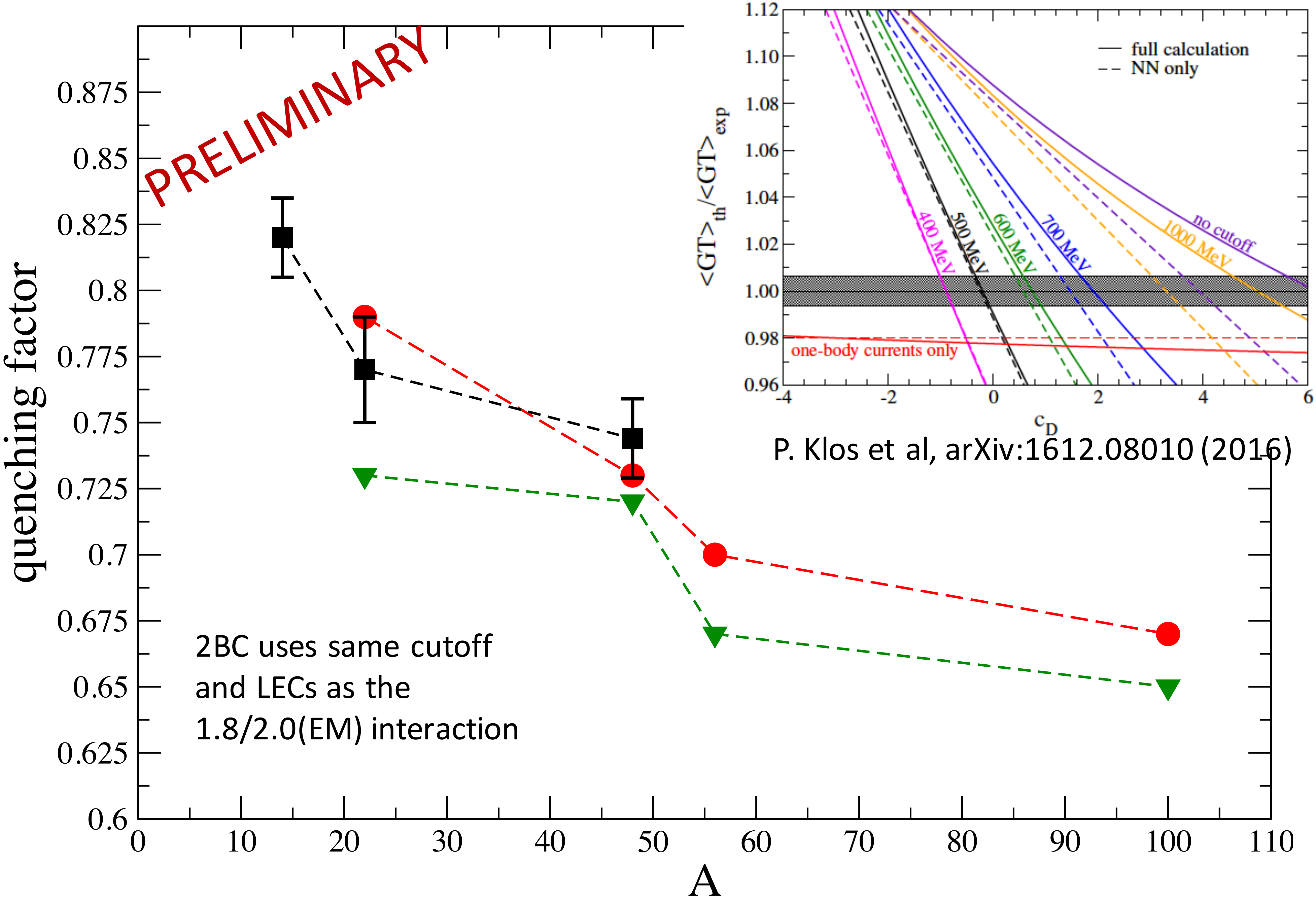
- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate



Quenching of g_A from two-body currents

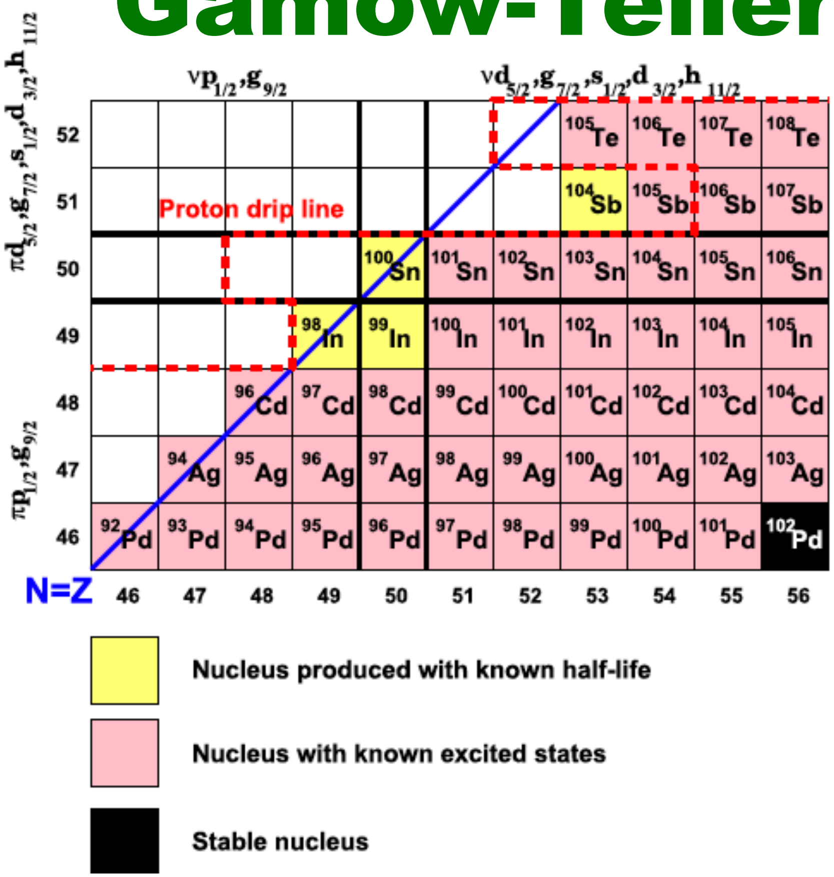


Quenching of g_A from two-body currents

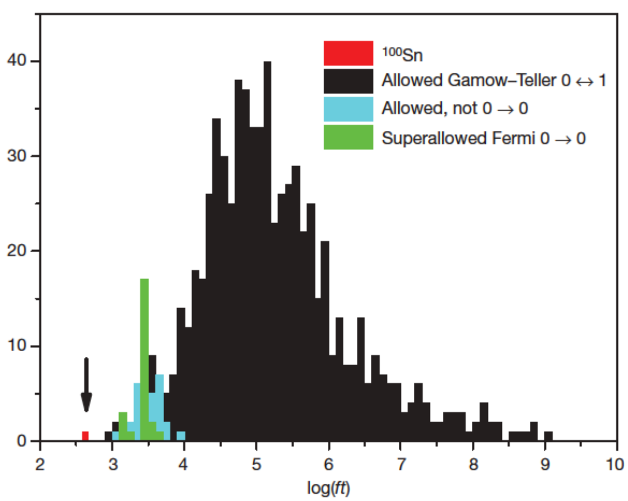


P. Klos et al, arXiv:1612.08010 (2016)

Gamow-Teller transition in ^{100}Sn



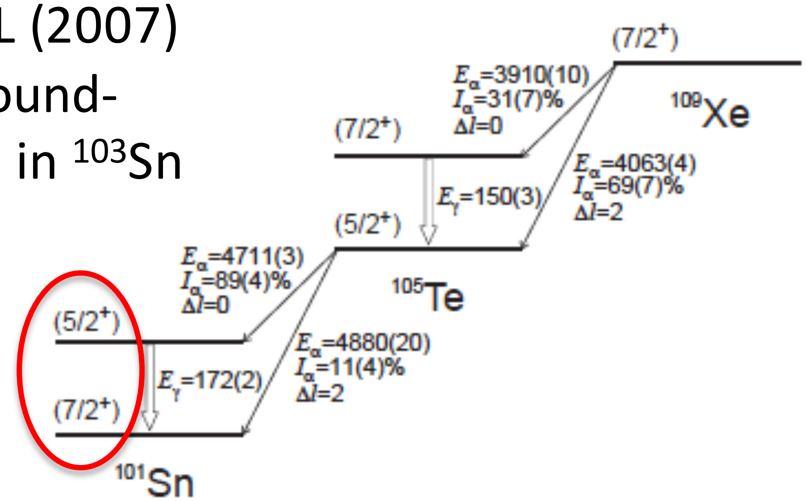
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



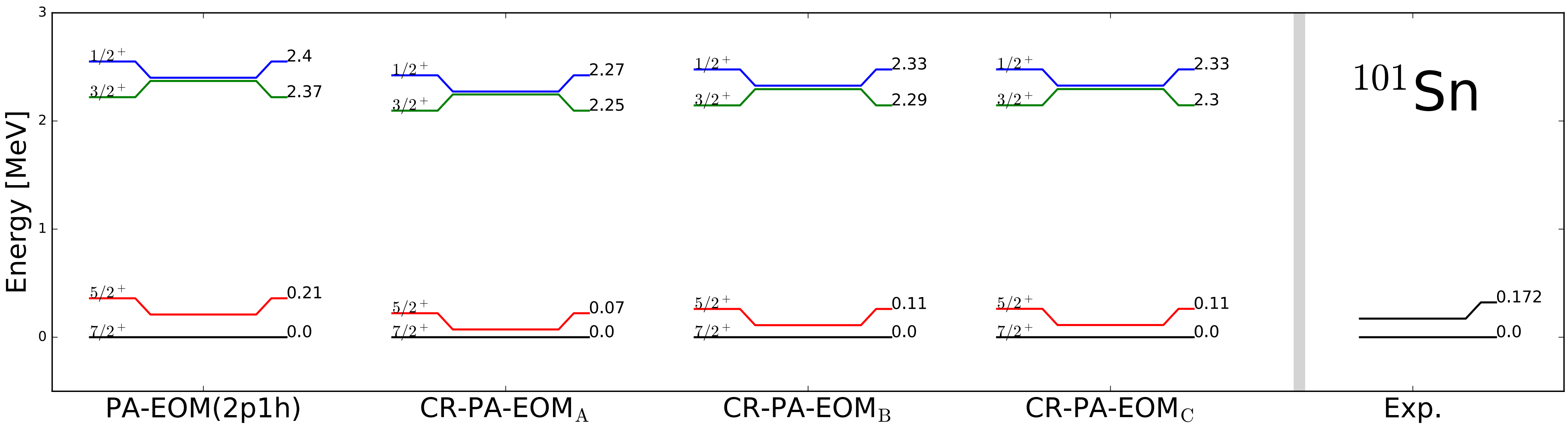
Hinke et al, Nature (2012)

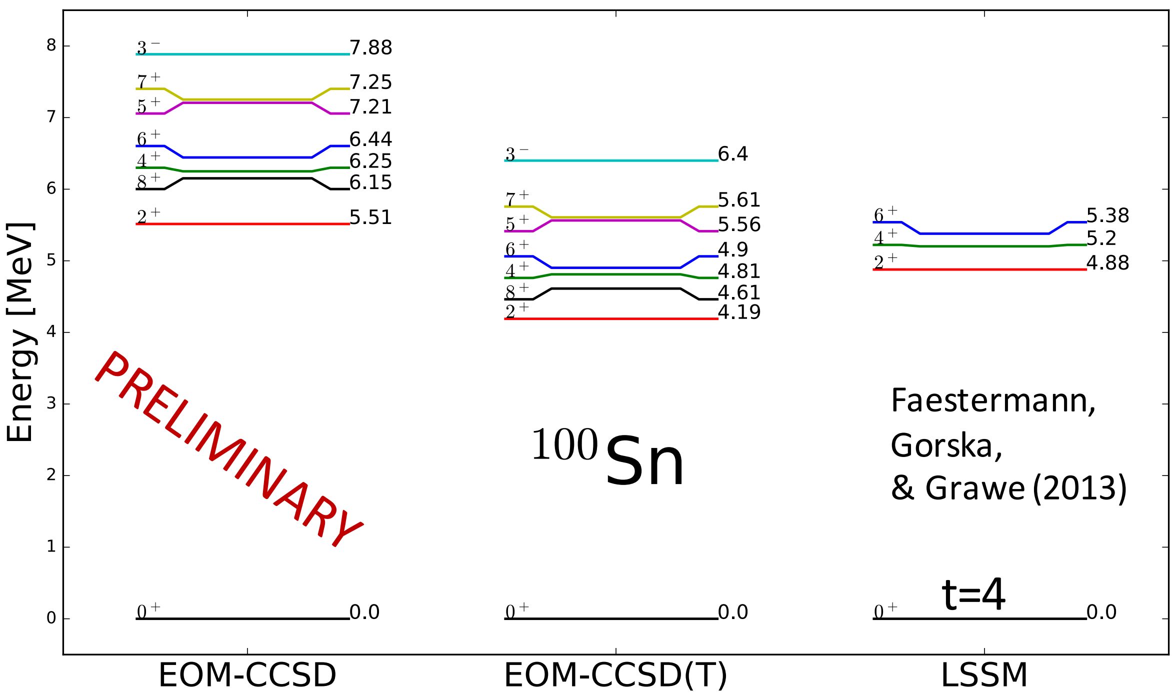
Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in ^{103}Sn

Darby et al, PRL (2010)



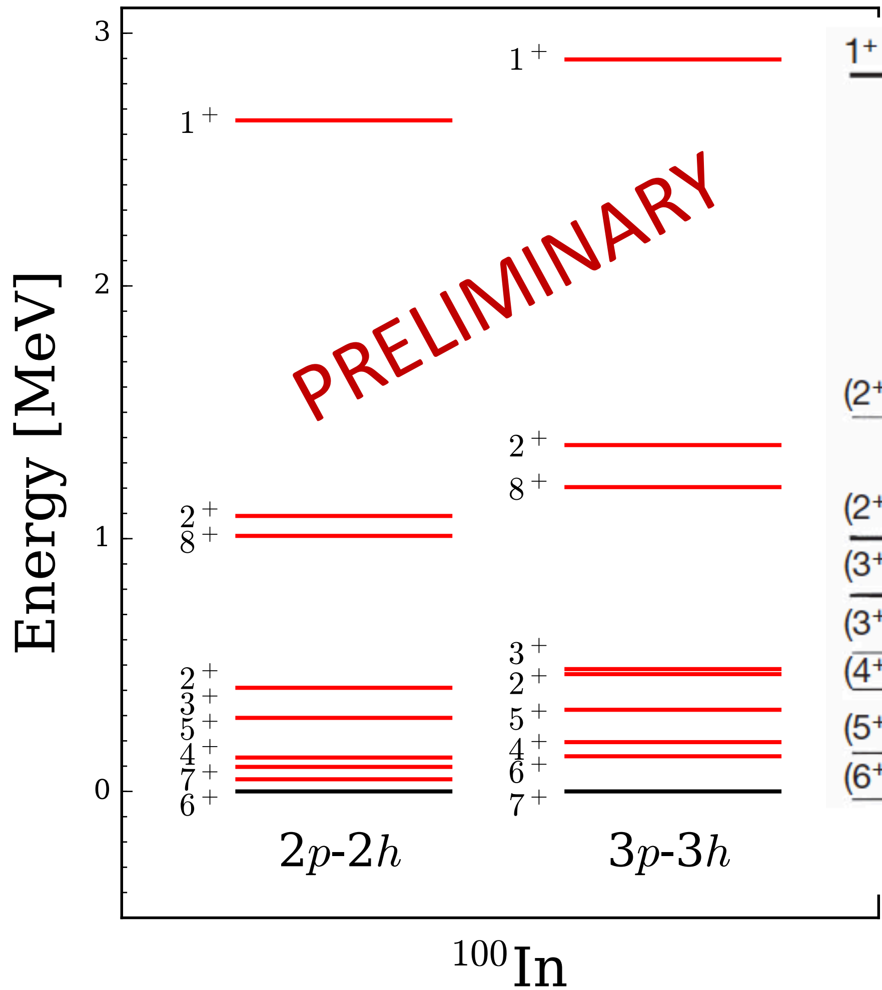
Structure of the ligthest tin isotopes

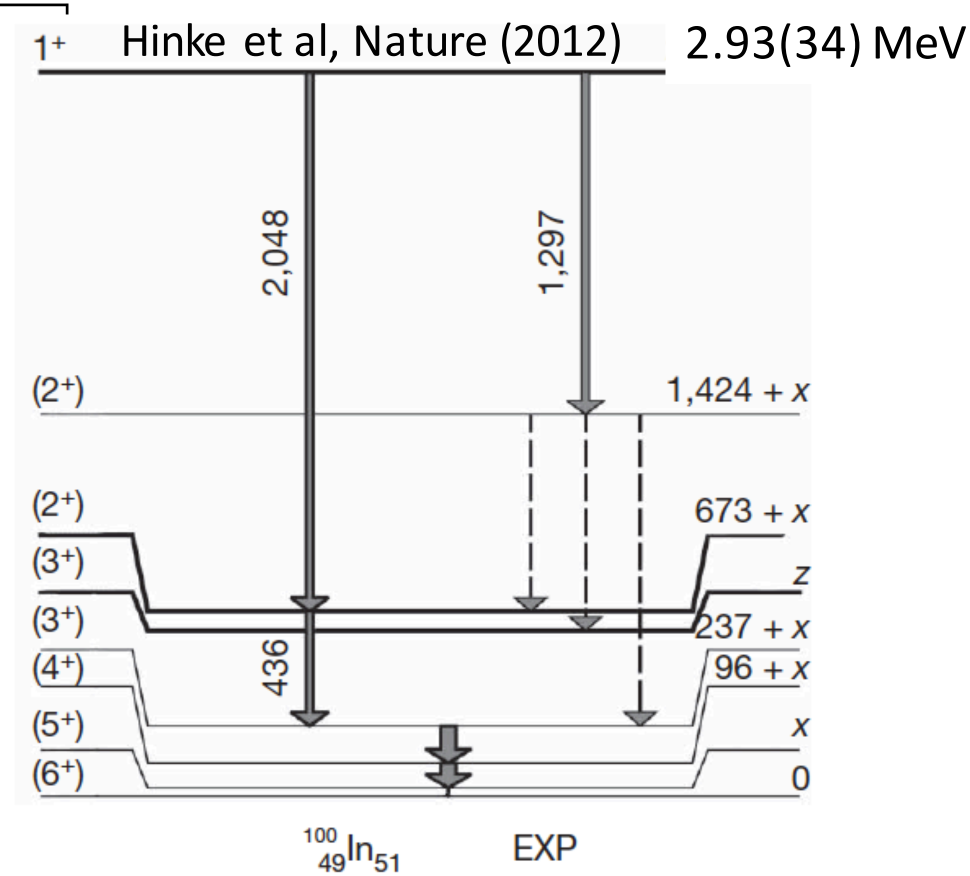




- High 2^+ energy in ^{100}Sn
- Predict $7/2^+$ ground-state in ^{101}Sn
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced
- Ground-state spins of $^{101-121}$Sn will be measured at CERN (CRIS collaboration)

^{100}In from charge exchange coupled-cluster equation-of-motion method



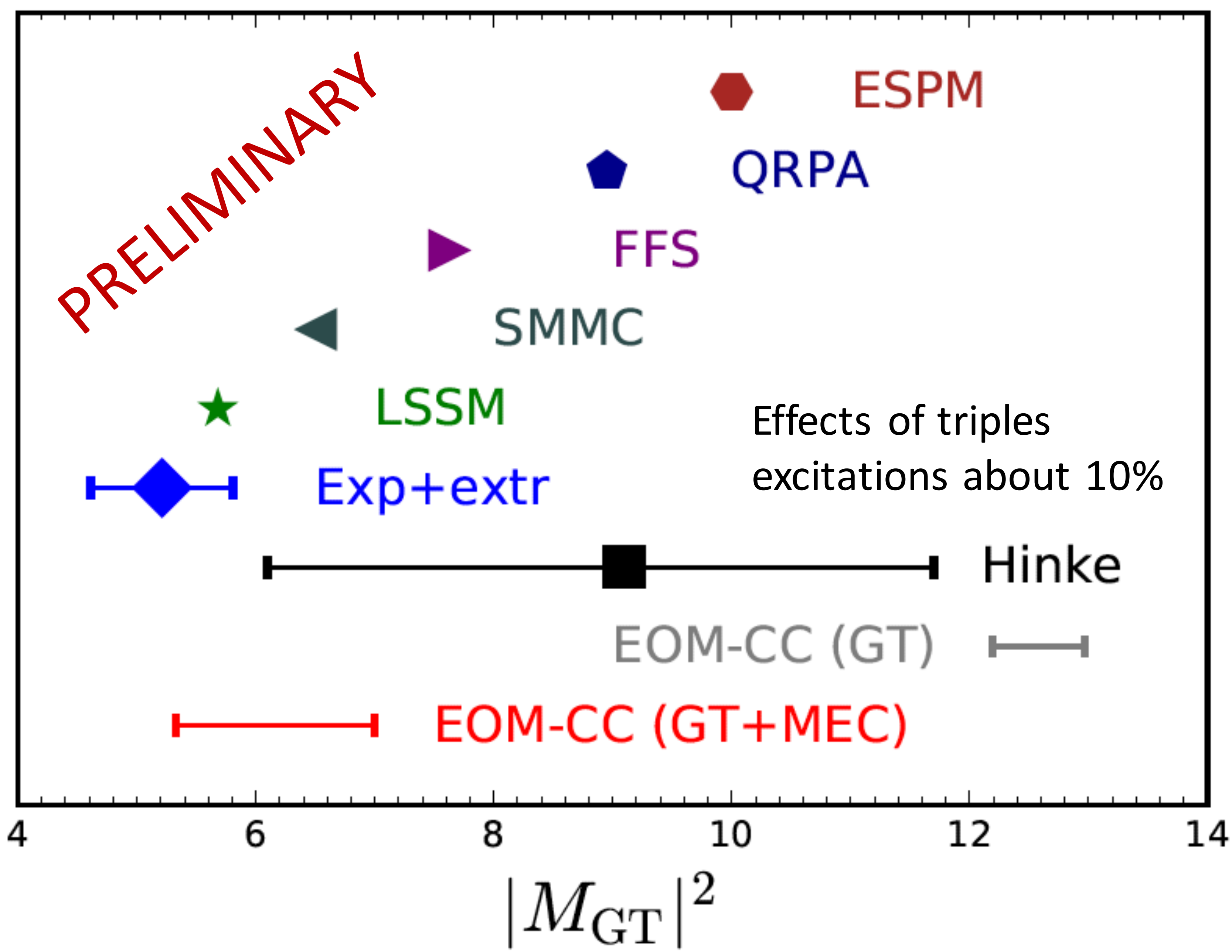


3p-3h charge-exchange EOM:

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

- Reproduce known 1^+ state at 2.93(34) MeV
- Predict a 7^+ ground-state for ^{100}In
- Ground-state spin of ^{100}In can be measured by CRIS collab. at CERN

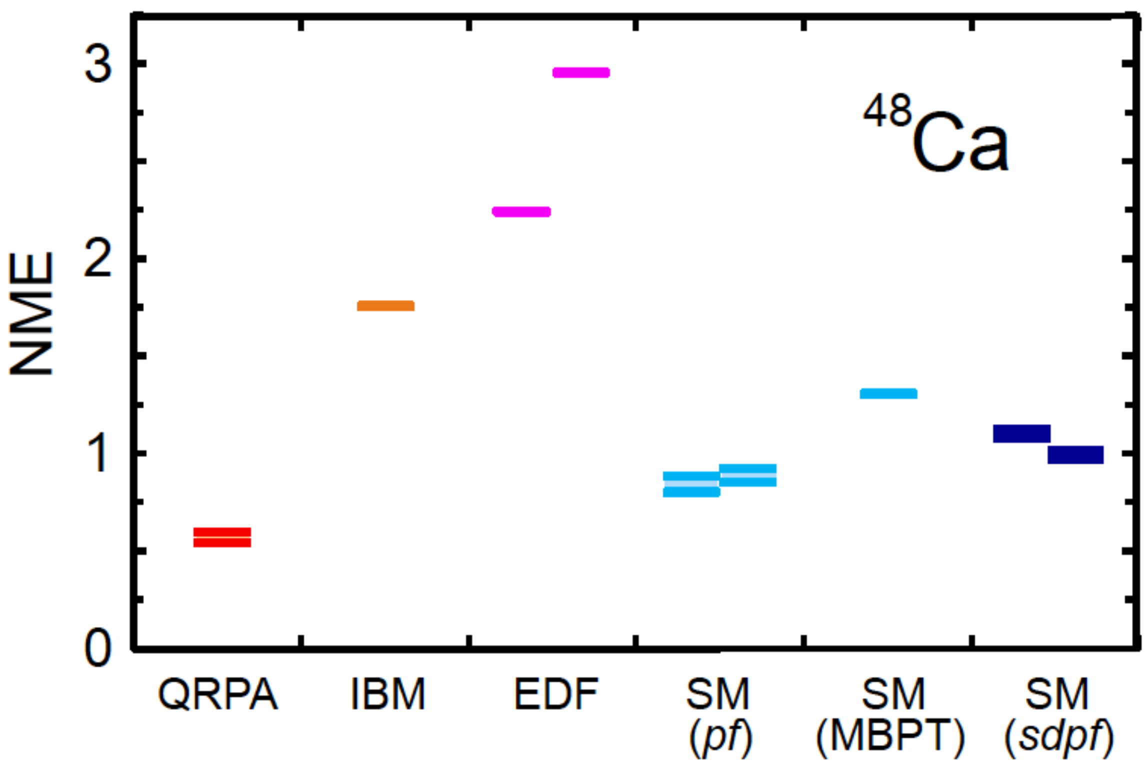
Super allowed Gamow-Teller decay of ^{100}Sn



Neutrinoless ββ-decay of ^{48}Ca

$$\left[T_{1/2}^{0\nu}\left(0_i^+ \to 0_f^+\right)\right]^{-1} = G^{0\nu}|M^{0\nu}|^2\left(\frac{\langle m_{\beta\beta}\rangle}{m_e}\right)^2$$

0νββ



Nuclear matrix element for neutrinoless double beta decay in ^{48}Ca using different methods. From Y. Iwata et al, PRL (2016).

- The NME for 0νββ differ by a factor two or three depending on the method
- Need to determine the NME more precisely with quantified uncertainties
- What does ab-initio calculations add to this picture?

Neutrinoless ββ-decay of ^{48}Ca

$$|\langle ^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle|^2 = \langle ^{48}\mathrm{Ti}|O|^{48}\mathrm{Ca}\rangle\langle ^{48}\mathrm{Ca}|O^\dagger|^{48}\mathrm{Ti}\rangle$$

Closure approximation with Gamow-Teller, Fermi and Tensor contributions:

$$M^{0\nu}_{GT} + \left(\frac{g_V}{g_A}\right)^2 M^{0\nu}_F + M^{0\nu}_T$$

The ground-state of ^{48}Ca is computed in the CCSD approximation:

$$\overline{H}_N|\Phi_0\rangle = E_0|\Phi_0\rangle,\ \ \overline{H}_N = e^{-T}H_N e^{T},\ \ T = T_1 + T_2$$

The CC energy functional is expressed in term of left/right ground-states

$$\langle\Phi_0|(1+\Lambda)\overline{H}_N|\Phi_0\rangle = E_0,\ \ \langle\Phi_0|(1+\Lambda)|\Phi_0\rangle = 1.$$

$$\Lambda = \sum_{ia}\lambda_a^i a_a a_i^\dagger + \frac{1}{2}\sum_{ijab}\lambda_{ab}^{ij} a_b a_a a_i^\dagger a_j^\dagger$$

Neutrinoless ββ-decay of ^{48}Ca

^{48}Ti is computed using a double charge exchange equation of motion method with 2p2h and 3p3h excitations

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

$$\langle\Phi_0| L_\mu \overline{H}_N = \langle\Phi_0| L_\mu E_\mu$$

$$R_\mu = \frac{1}{4}\sum_{ijab} r_{ij}^{ab} p_a^\dagger p_b^\dagger n_i n_j + \frac{1}{36}\sum_{ijkabc} r_{ijk}^{abc} p_a^\dagger p_b^\dagger N_c^\dagger N_k n_i n_j$$

$$L_\mu = \frac{1}{4}\sum_{ijab} l_{ab}^{ij} p_b p_a n_i^\dagger n_j^\dagger + \frac{1}{36}\sum_{ijkabc} l_{abc}^{ijj} p_a p_b N_c N_k^\dagger n_i^\dagger n_j^\dagger$$

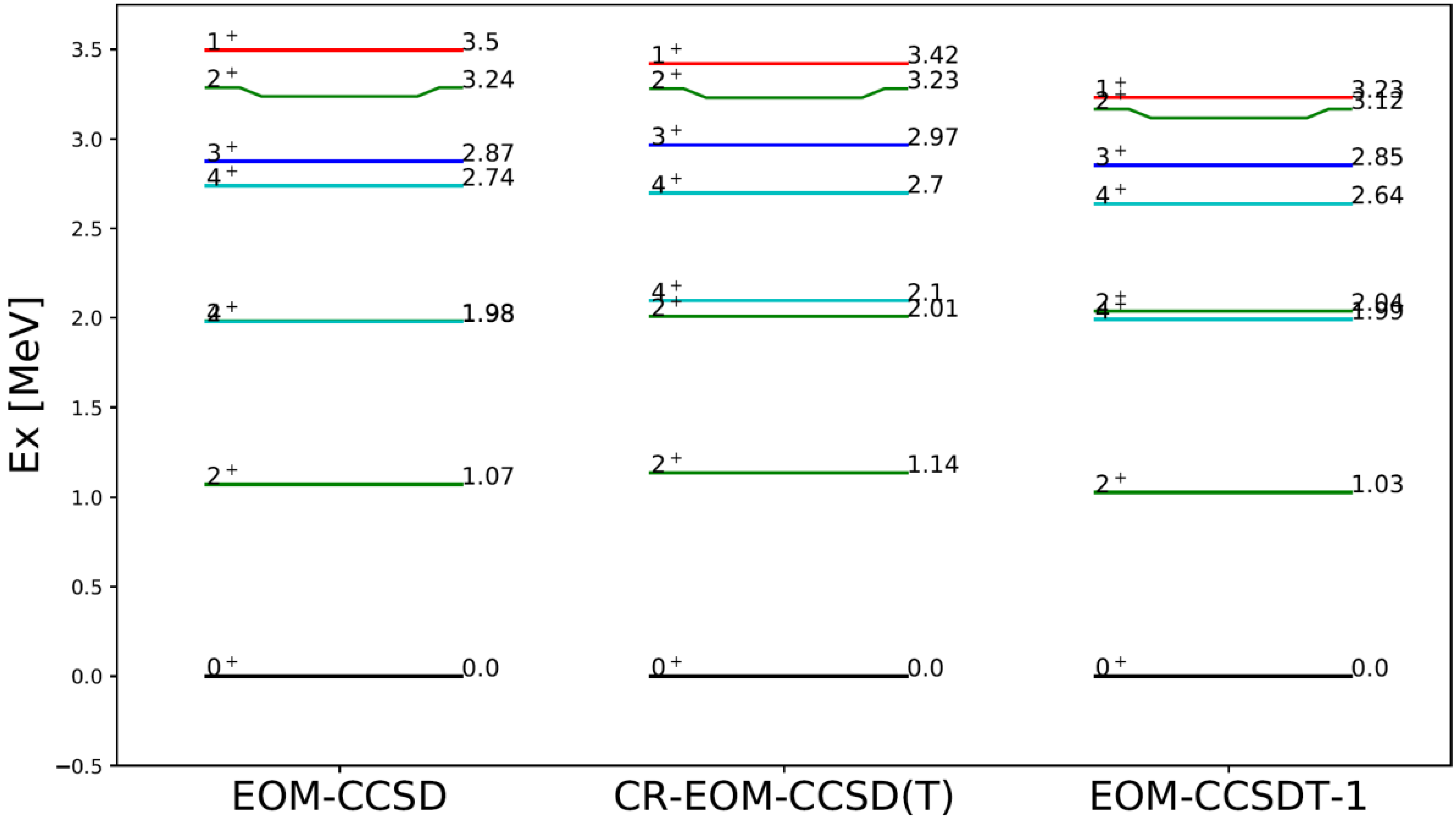
The Nuclear matrix element for 0νββ in ^{48}Ca is given by:

$$|\langle {}^{48}\mathrm{Ti}|O|{}^{48}\mathrm{Ca}\rangle|^2 = \langle {}^{48}\mathrm{Ti}|O|{}^{48}\mathrm{Ca}\rangle\langle {}^{48}\mathrm{Ca}|O^\dagger|{}^{48}\mathrm{Ti}\rangle$$

$$= \langle\Phi_0|L_0\overline{O}_N|\Phi_0\rangle\langle\Phi_0|(1+\Lambda)\overline{O^\dagger}_N R_0|\Phi_0\rangle$$

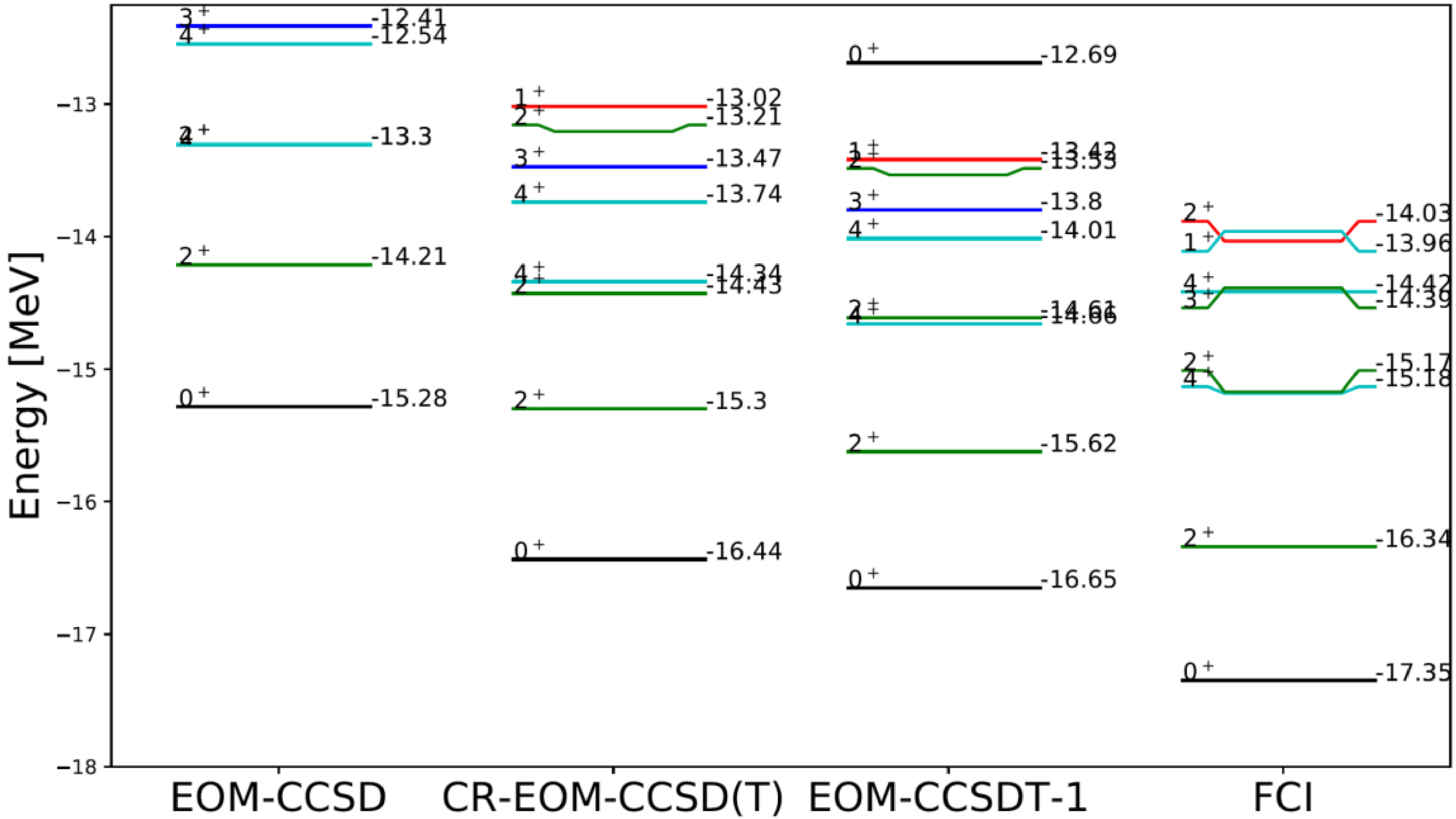
^{48}Ti from CR-EOM-CCSD(T)

$$R_\nu = \frac{1}{4}\sum r_{ij}^{ab}\, p_a^\dagger p_b^\dagger n_j n_i + \frac{1}{3!^2}\sum r_{ijk}^{abc}\, p_a^\dagger p_b^\dagger N_c^\dagger N_k n_j n_i$$

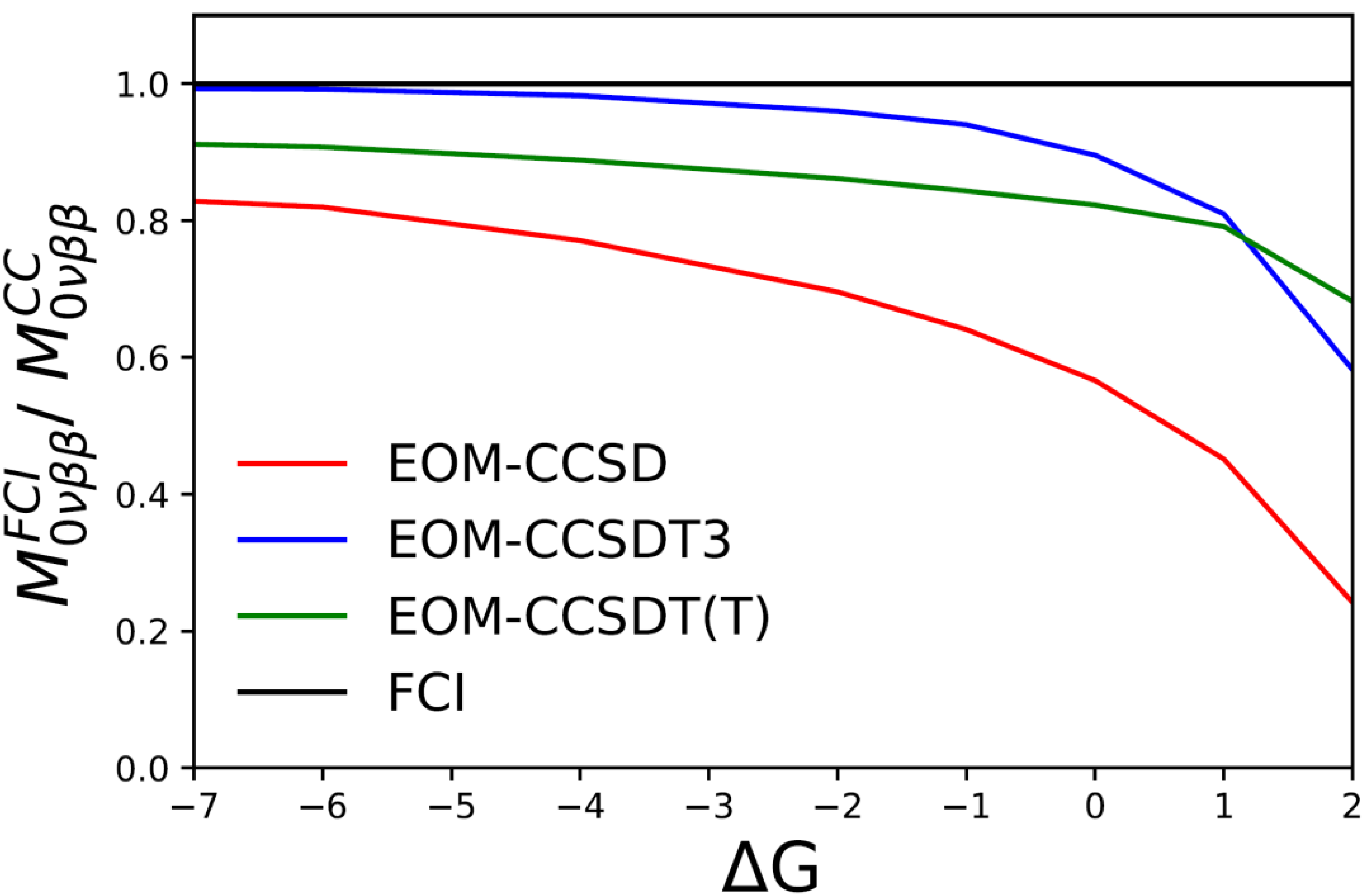


^{48}Ti from CR-EOM-CCSD(T)

$$R_\nu = \frac{1}{4}\sum r_{ij}^{ab}\, p_a^\dagger p_b^\dagger n_j n_i \qquad + \frac{1}{3!^2}\sum r_{ijk}^{abc}\, p_a^\dagger p_b^\dagger N_c^\dagger N_k n_j n_i$$



EOM-CR-CCSD(T)

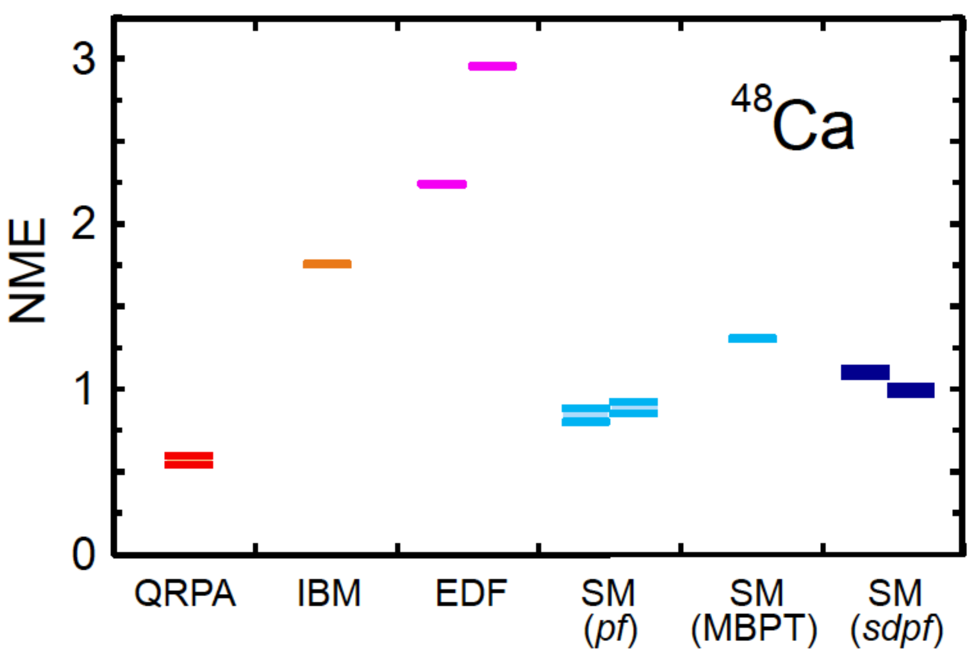


$M^{FCI}_{0\nu\beta\beta} / M^{CC}_{0\nu\beta\beta}$
0.0
0.2
0.4
0.6
0.8
1.0
−7
−6
−5
−4
−3
−2
−1
0
1
2
ΔG
EOM-CCSD
EOM-CCSDT3
EOM-CCSDT(T)
FCI

Neutrinoless ββ-decay of ^{48}Ca

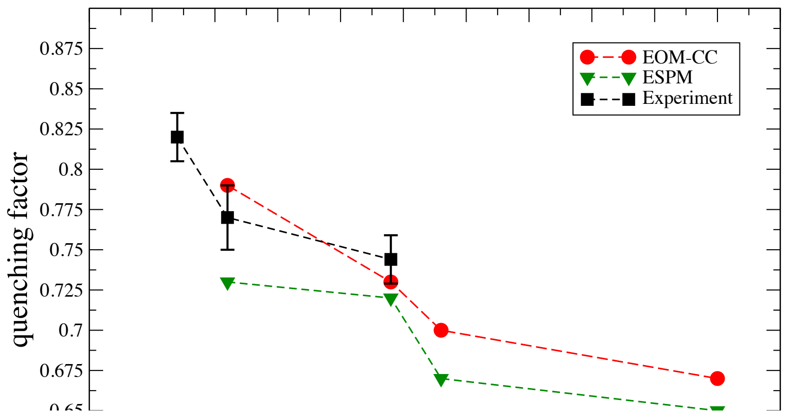
PRELIMINARY

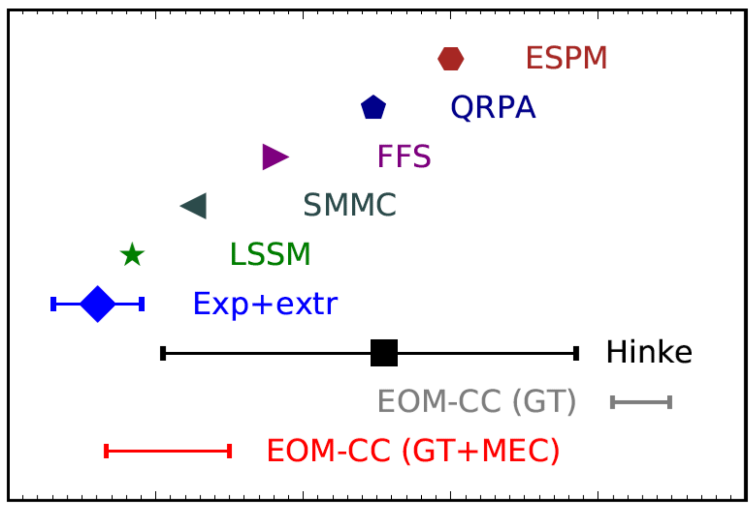
NME for $0\nu\beta\beta$			
Method	GT	Fermi	Tensor
CCSD	0.97	0.31	-0.12
CCSDT-1(10)	0.44	0.09	-0.11
CCSDT-1(12)	0.50	0.11	-0.11
CCSDT-1(14)	0.45	0.10	-0.11



- NME computed with the chiral NN + 3N interaction 1.8/2.0 (EM) [K. Hebeler *et al* PRC (2011)]
- Model-space N_{max} =10, hw = 22MeV.
- Not converged with respect to model-space or truncation in 3p3h amplitudes
- Preliminary CC results agree with QRPA

Summary





NME for $0\nu\beta\beta$			
Method	GT	Fermi	Tensor
CCSD	0.97	0.31	-0.12
CCSDT-1(10)	0.44	0.09	-0.11
CCSDT-1(12)	0.50	0.11	-0.11
CCSDT-1(14)	0.45	0.10	-0.11

- Quenching of GT strength in nuclei from two-body currents
- Super allowed GT transition in ^{100}Sn
- The NME for $0\nu\beta\beta$ in ^{48}Ca from coupled-cluster calcualtions