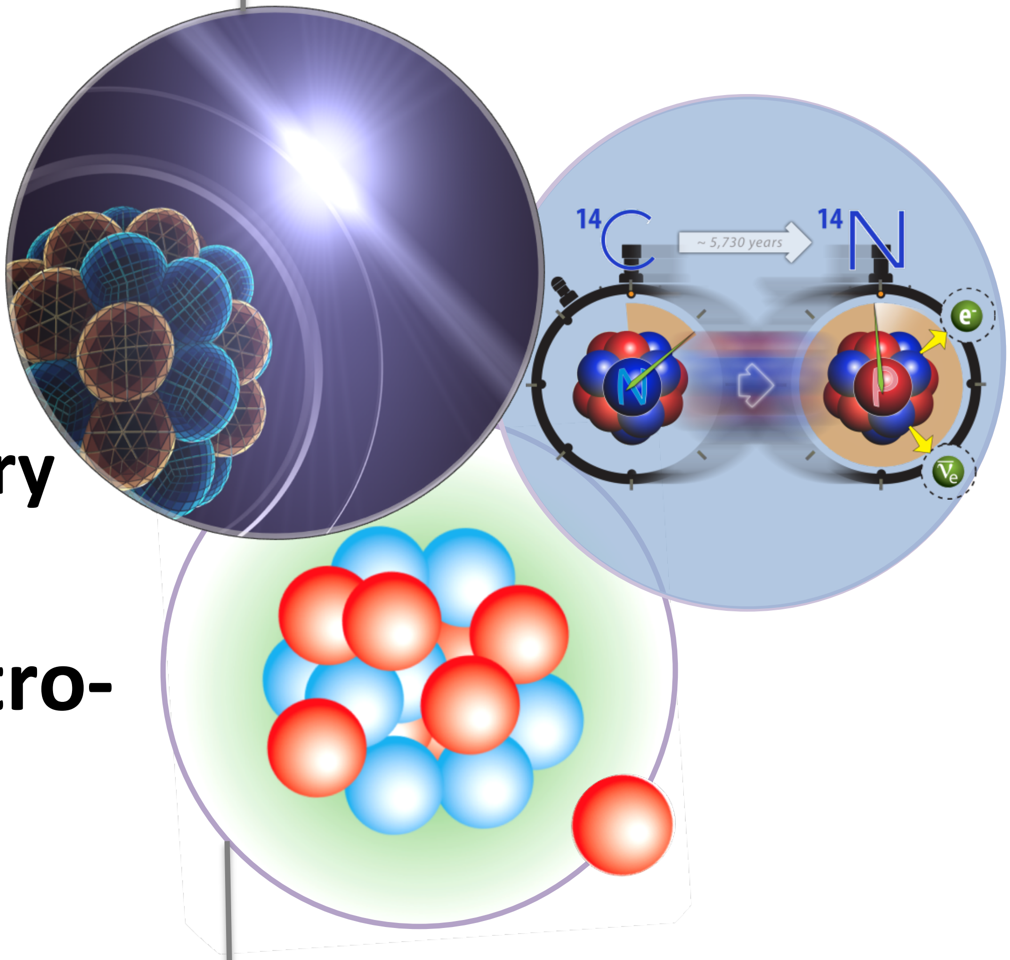
Coupled cluster computations of weak decays

Gaute Hagen
Oak Ridge National Laboratory

Exploring the role of electro-weak currents in Atomic Nuclei

ECT, April 25th, 2018



U.S. DEPARTMENT OF ENERGY

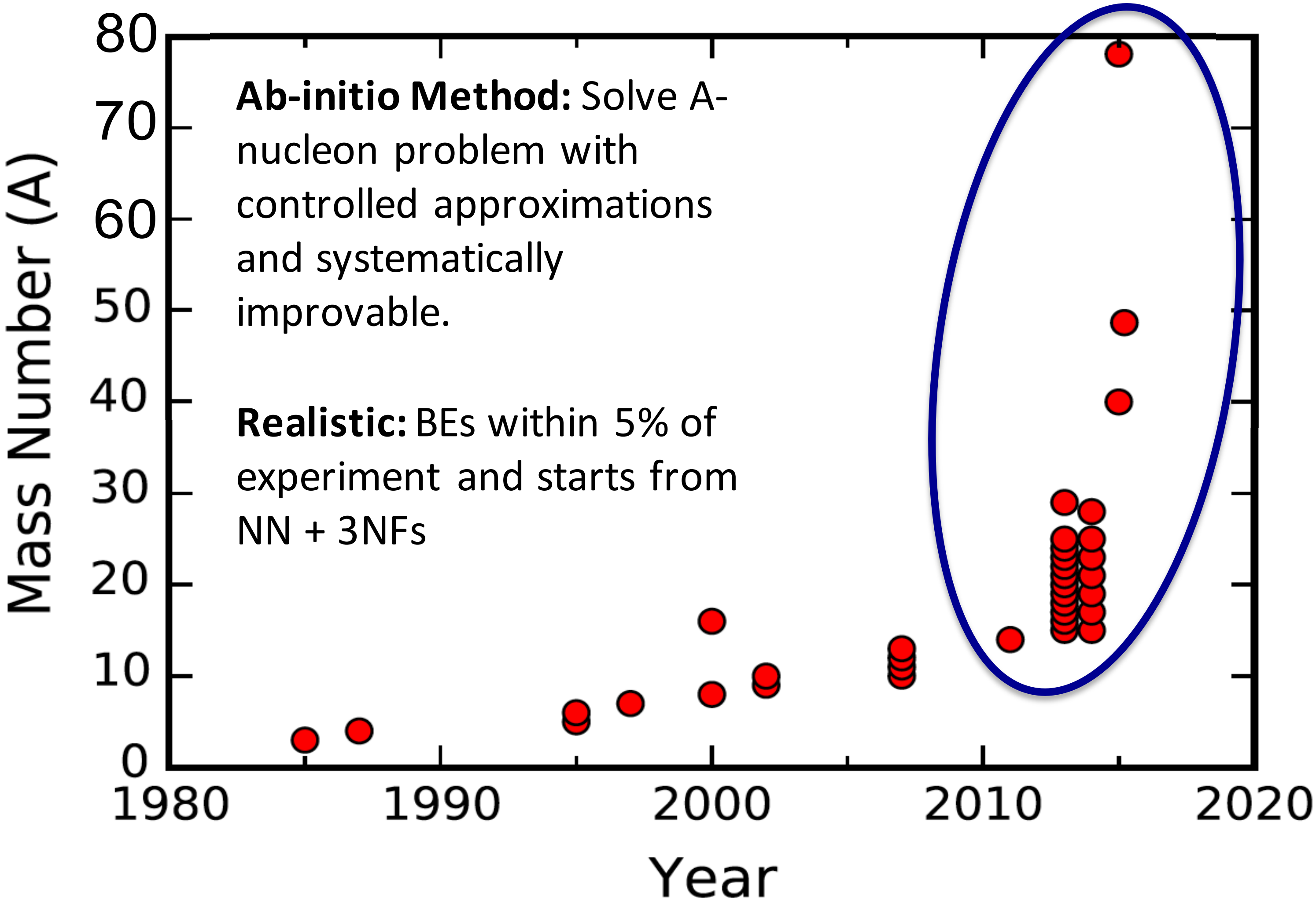
NUCLEI
Nuclear Computational Low-Energy Initiative

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

Trend in realistic ab-initio calculations

Explosion of many-body methods (Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, …)

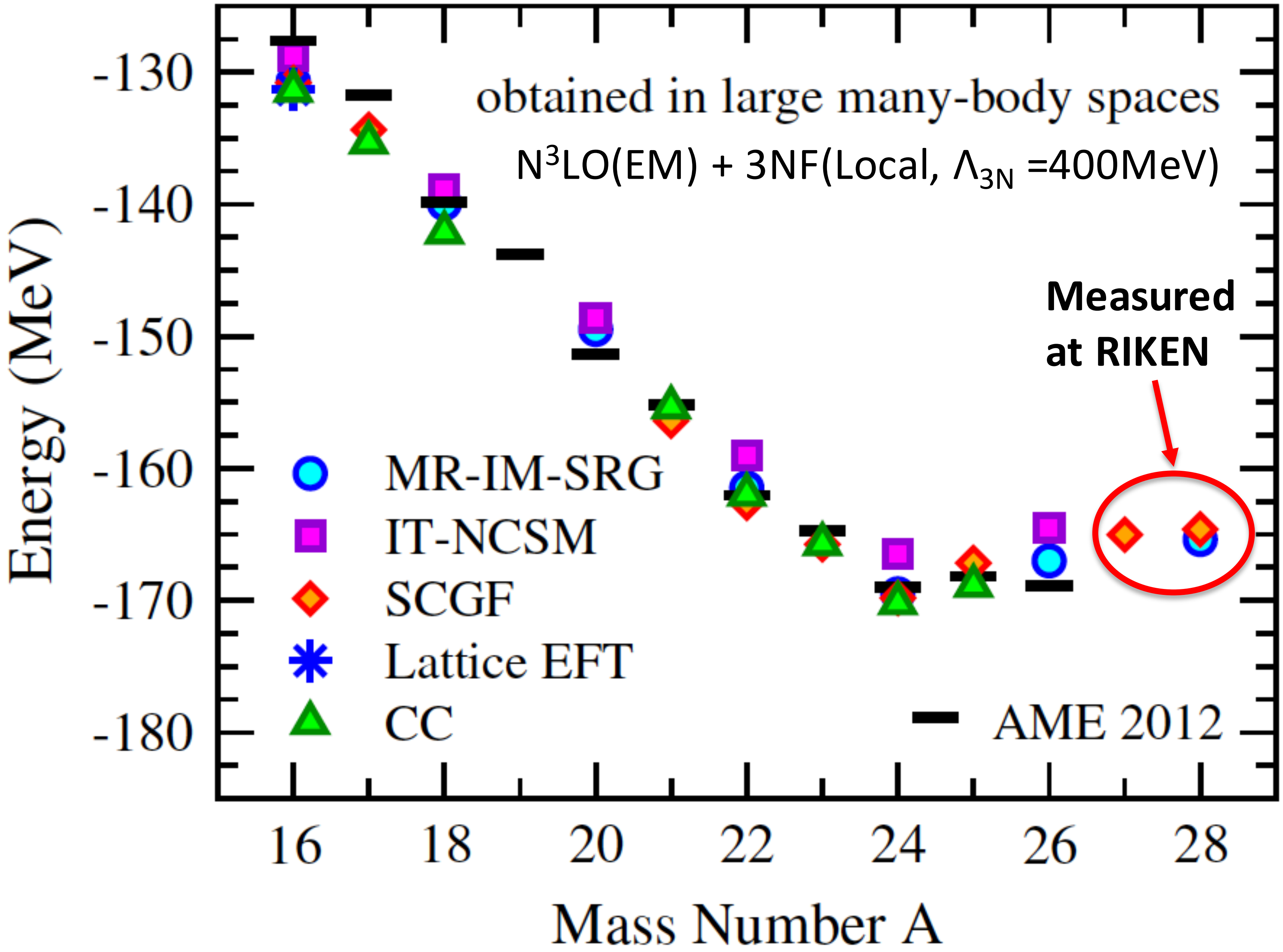
Application of ideas from EFT and renormalization group (V_{low-k}, Similarity Renormalization Group, …)



Ab-initio Method: Solve A-nucleon problem with controlled approximations and systematically improvable.

Realistic: BEs within 5% of experiment and starts from NN + 3NFs

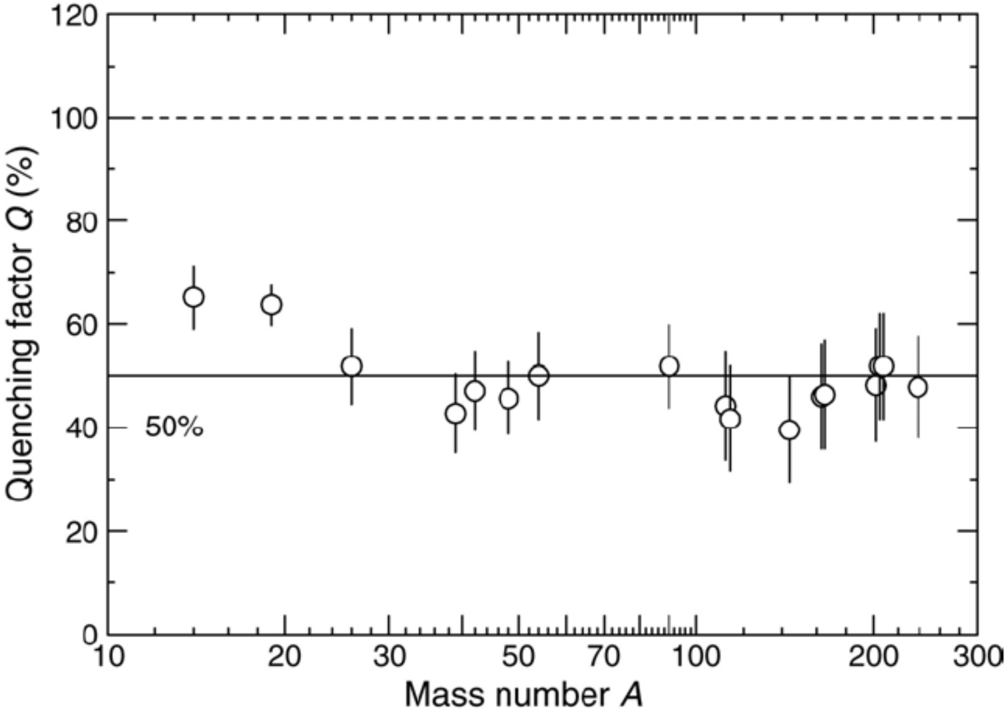
Oxgyen chain with interactions from chiral EFT



Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

The puzzle of quenched of beta decays

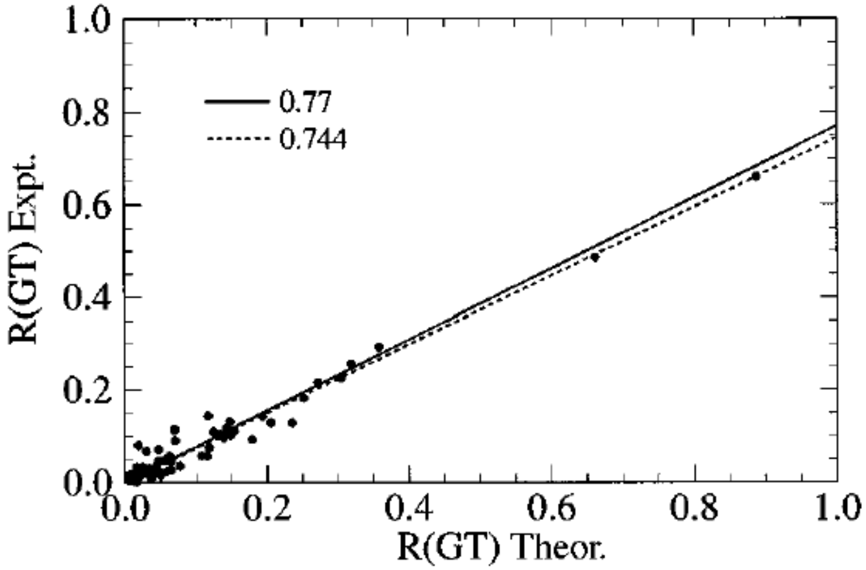
Long-standing problem: Experimental beta-decay strengths quenched compared to theoretical results.



Quenching obtained from charge-exchange (*p*,*n*) experiments. (Gaarde 1983).

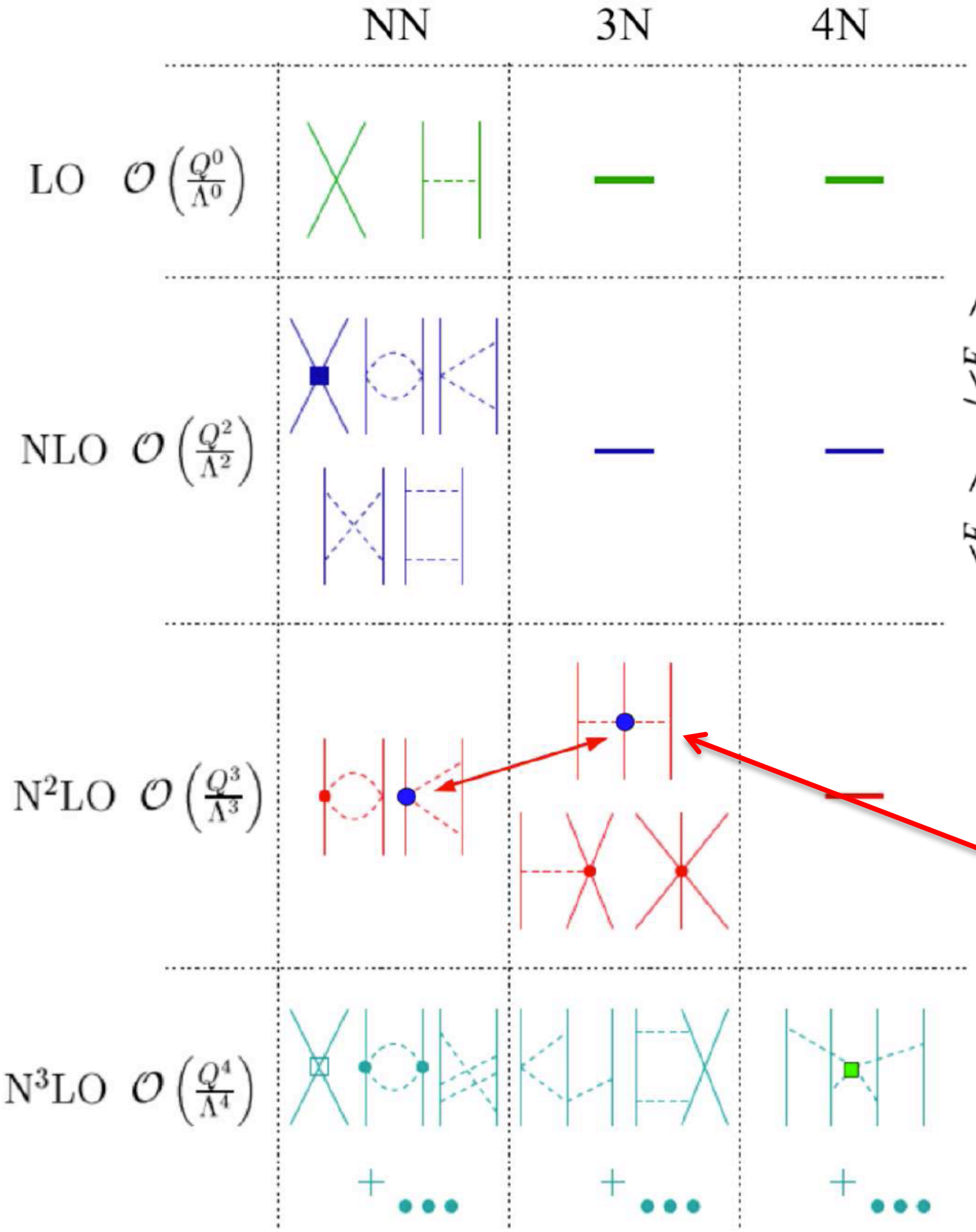
- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?
- Two-body currents (2BCs)?

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

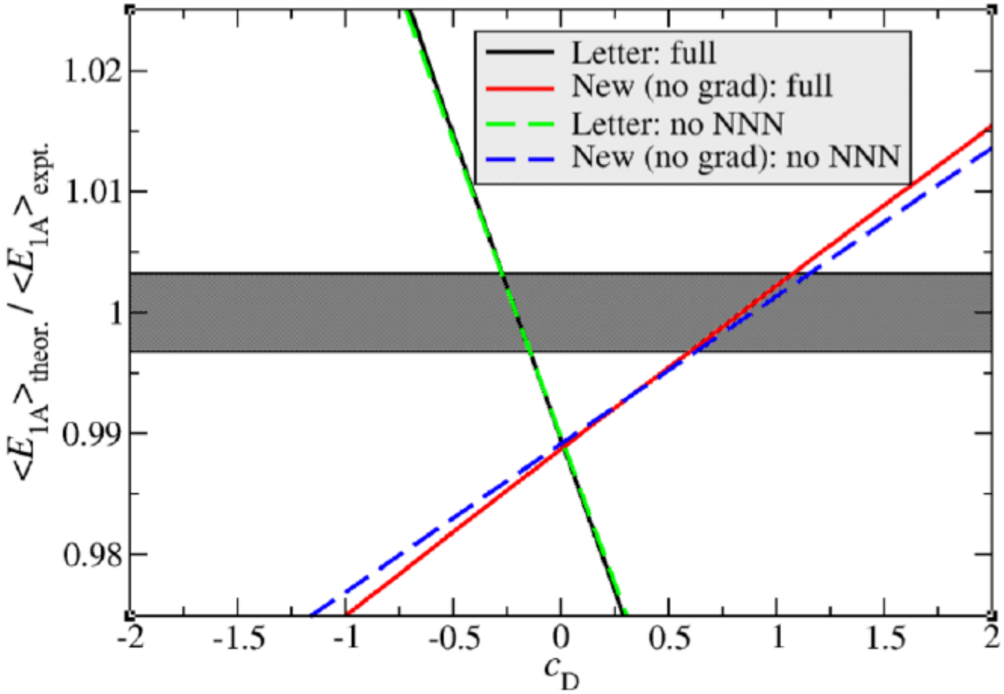


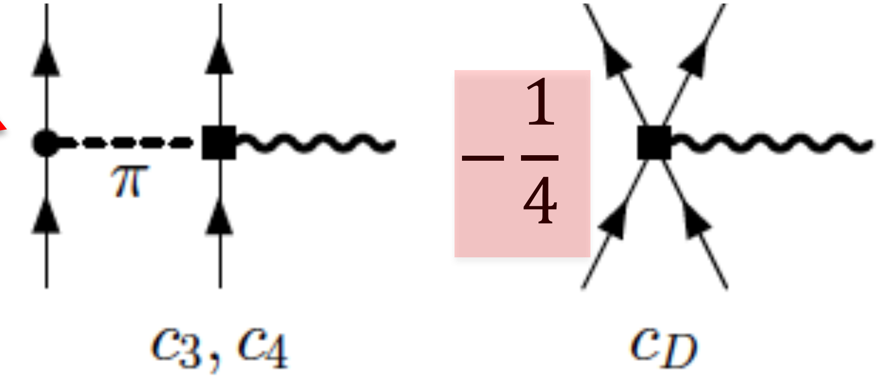
Nuclear forces from chiral effective field theory

[Weinberg; van Kolck; Epelbaum *et al.*; Entem & Machleidt; …]

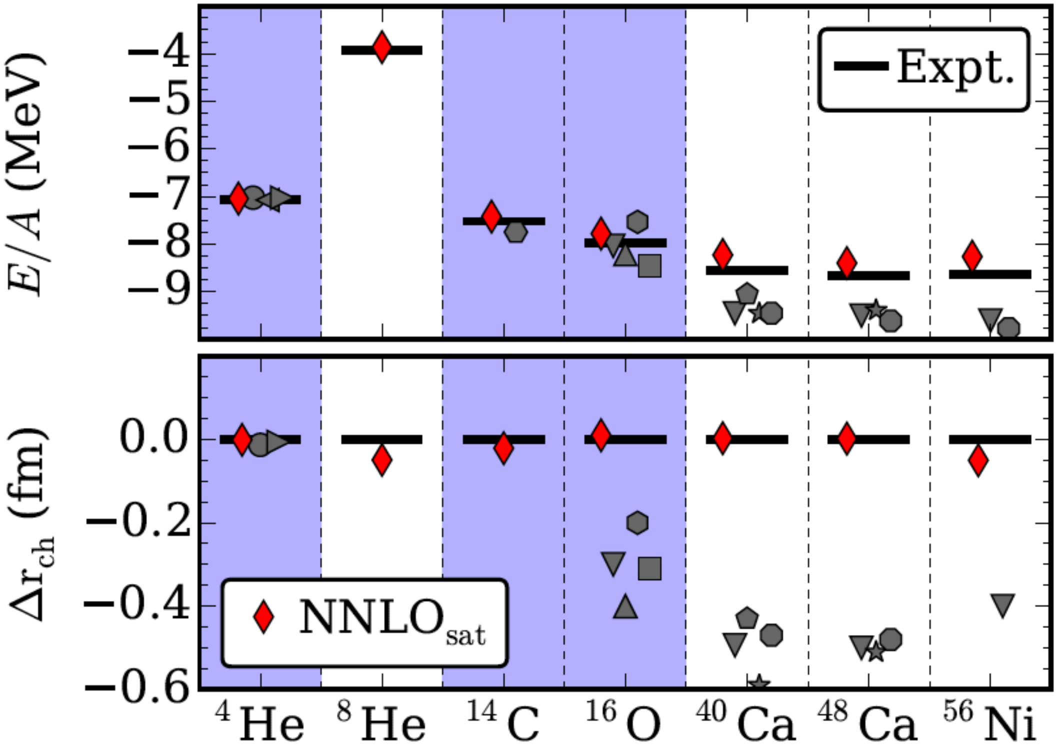


From Sofia Quaglioni and Kyle Wendt





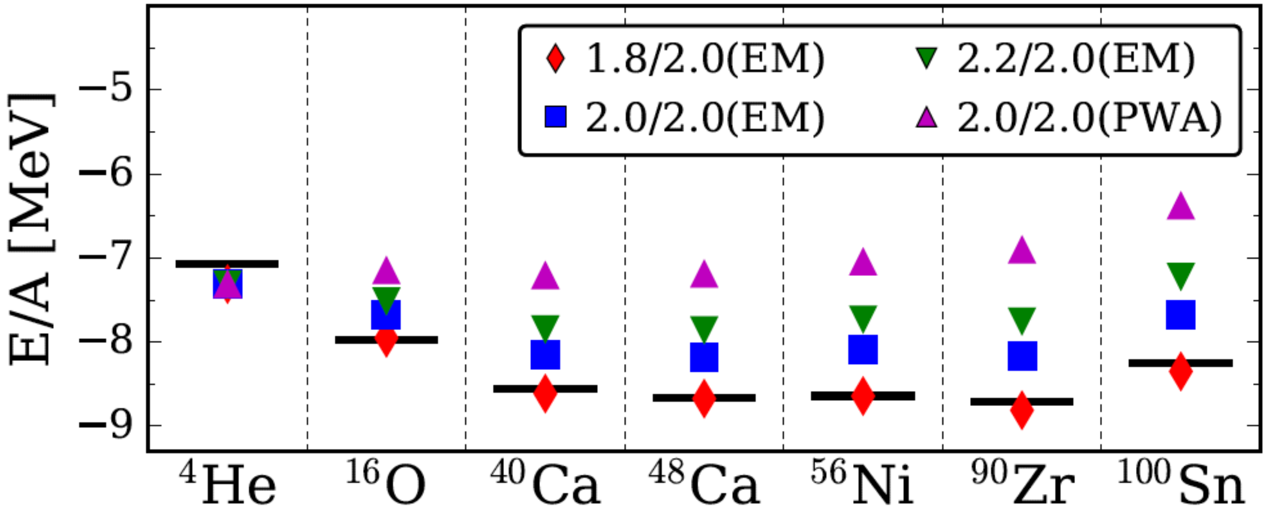
A family of interactions from chiral EFT



NNLO$_{sat}$: Accurate radii and BEs

- Simultaneous optimization of NN and 3NFs
- Include charge radii and binding energies of ^{3}H, ^{3,4}He, ^{14}C, ^{16}O in the optimization
- Harder interaction: difficult to converge beyond ^{56}Ni

A. Ekström *et al*, Phys. Rev. C **91**, 051301(R) (2015).



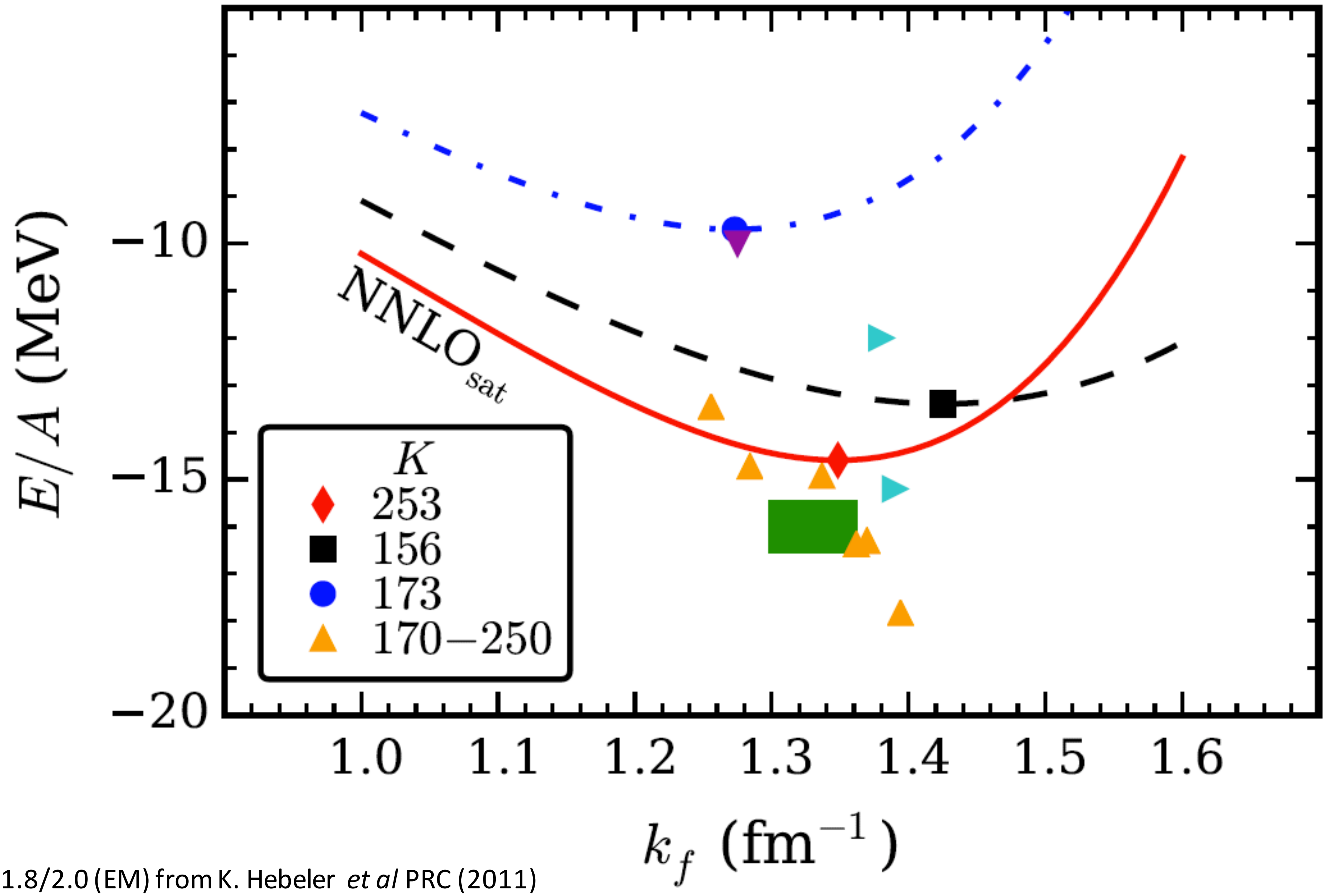
1.8/2.0(EM): Accurate BEs

Soft interaction: SRG NN from Entem & Machleidt with 3NF from chiral EFT

K. Hebeler *et al* PRC (2011).

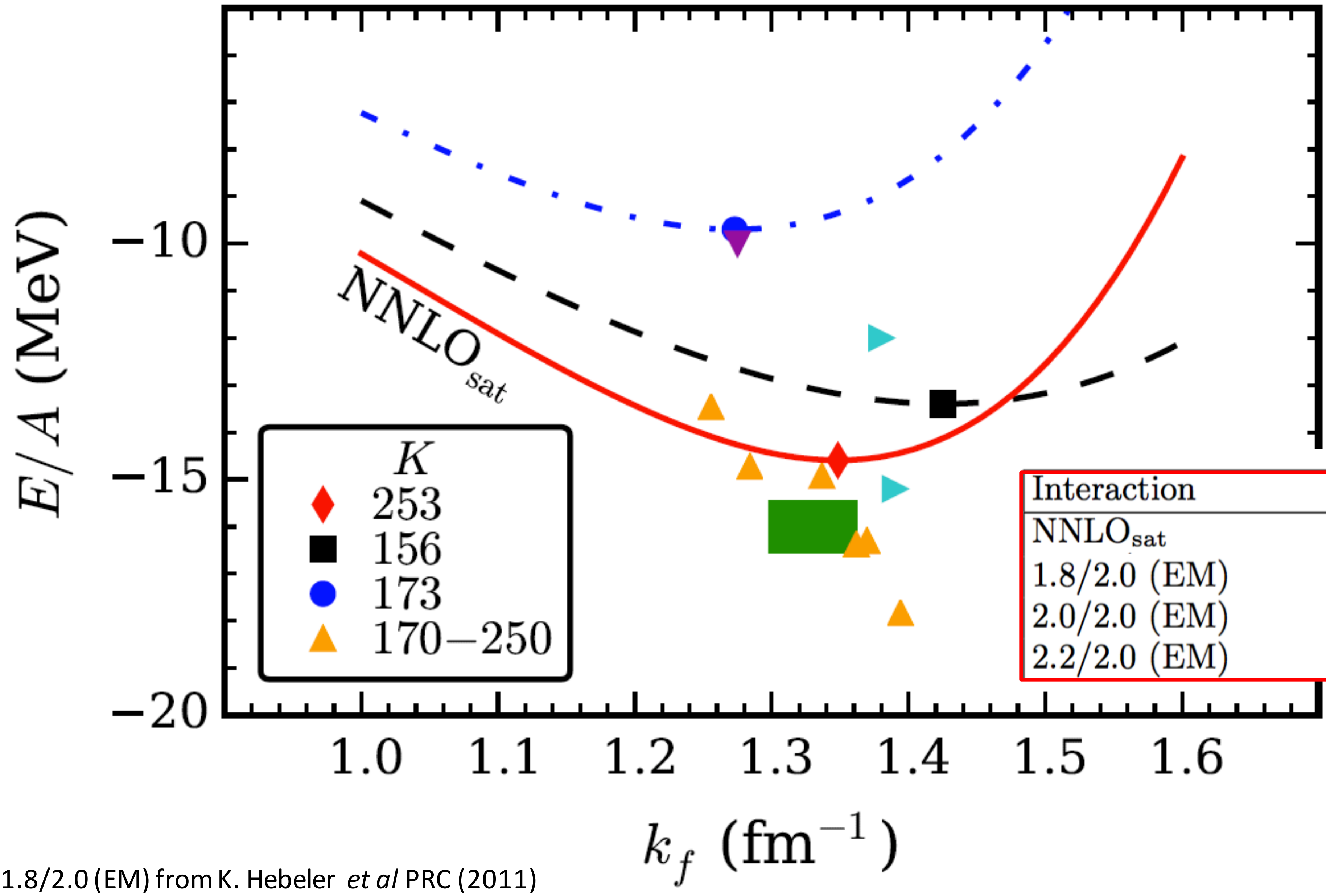
T. Morris *et al*, arXiv:1709.02786 (2017).

Saturation in nuclear matter from chiral interactions



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

Saturation in nuclear matter from chiral interactions

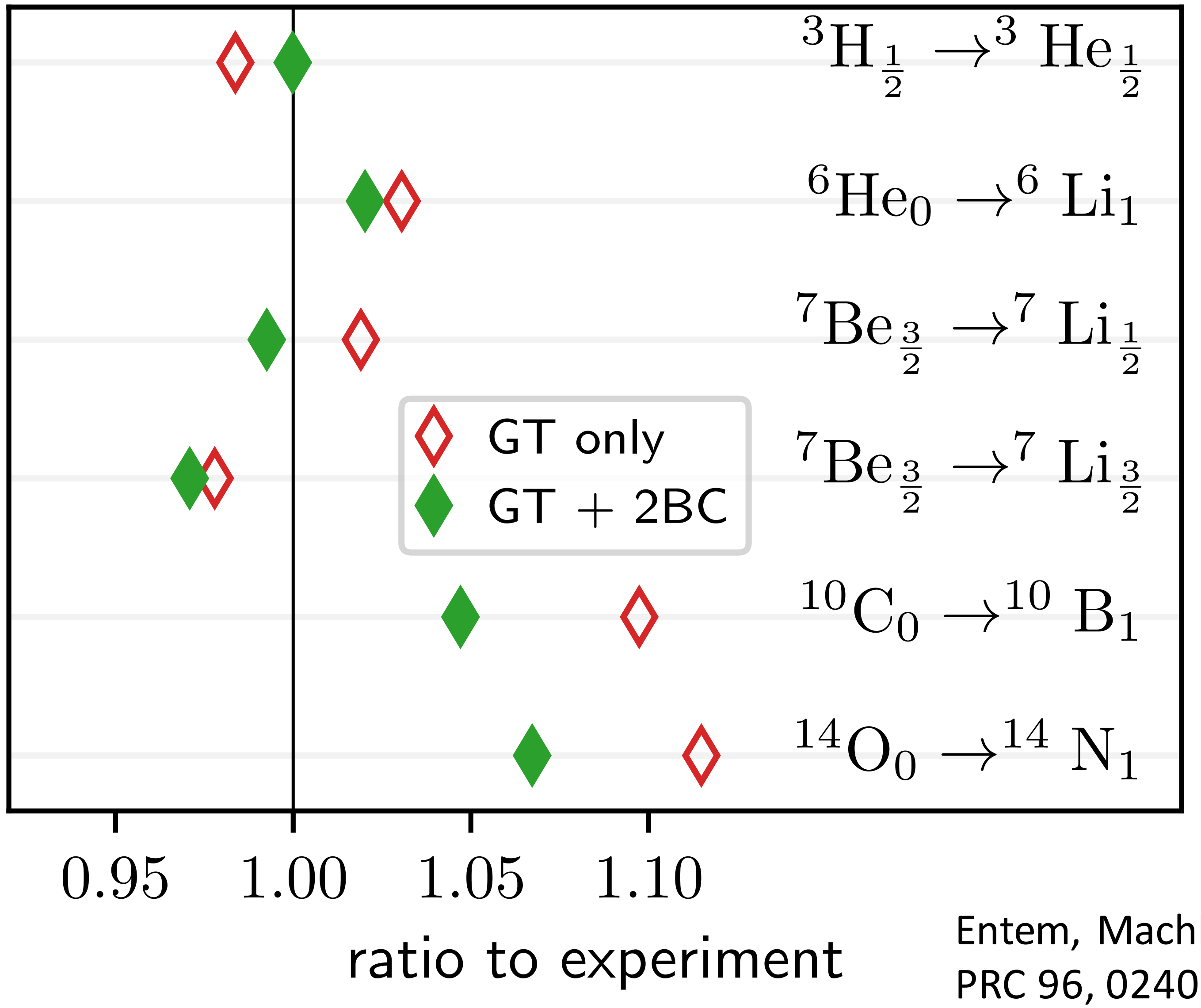


Interaction	c_D
NNLO$_{\text{sat}}$	0.817
1.8/2.0 (EM)	1.264
2.0/2.0 (EM)	1.271
2.2/2.0 (EM)	1.214

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

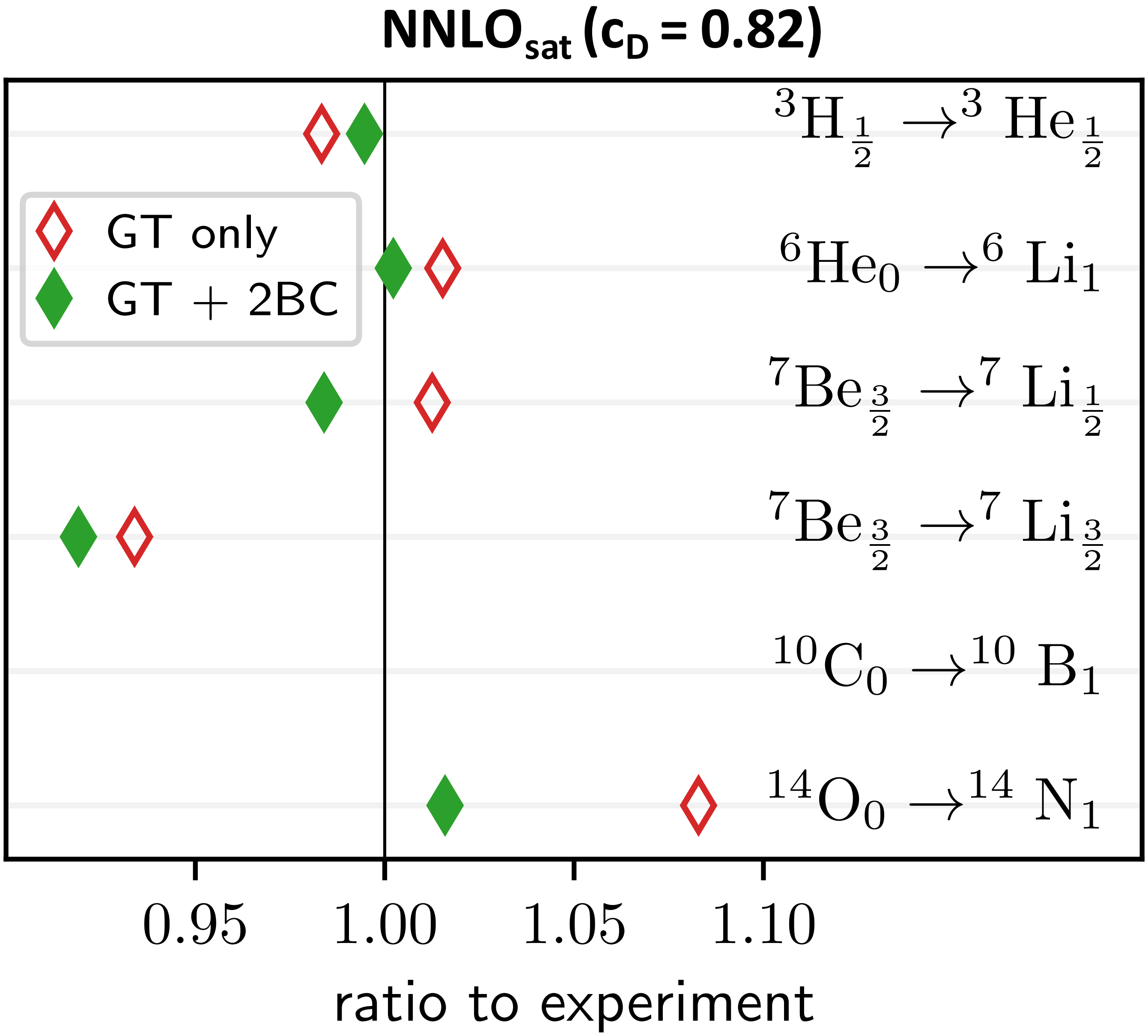
Theory to experiment ratios for beta decays in light nuclei from NCSM

N4LO(EM) + $3N_{lnl}$ SRG-evolved to $2.0 fm^{-1}$ ($c_D = -1.8$)



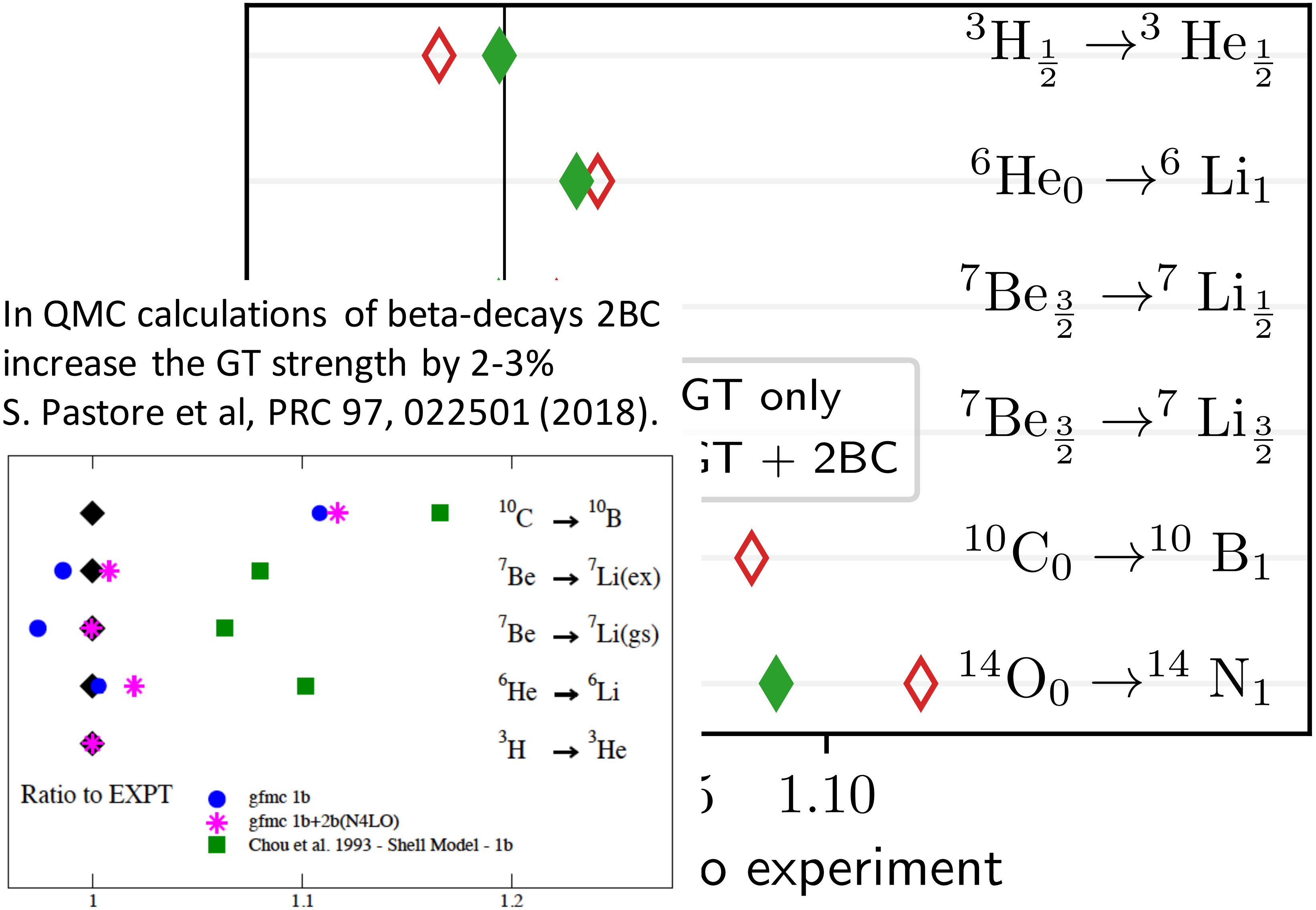
Entem, Machleidt & Nosyk,
PRC 96, 024004 (2017)

Theory to experiment ratios for beta decays in light nuclei from NCSM



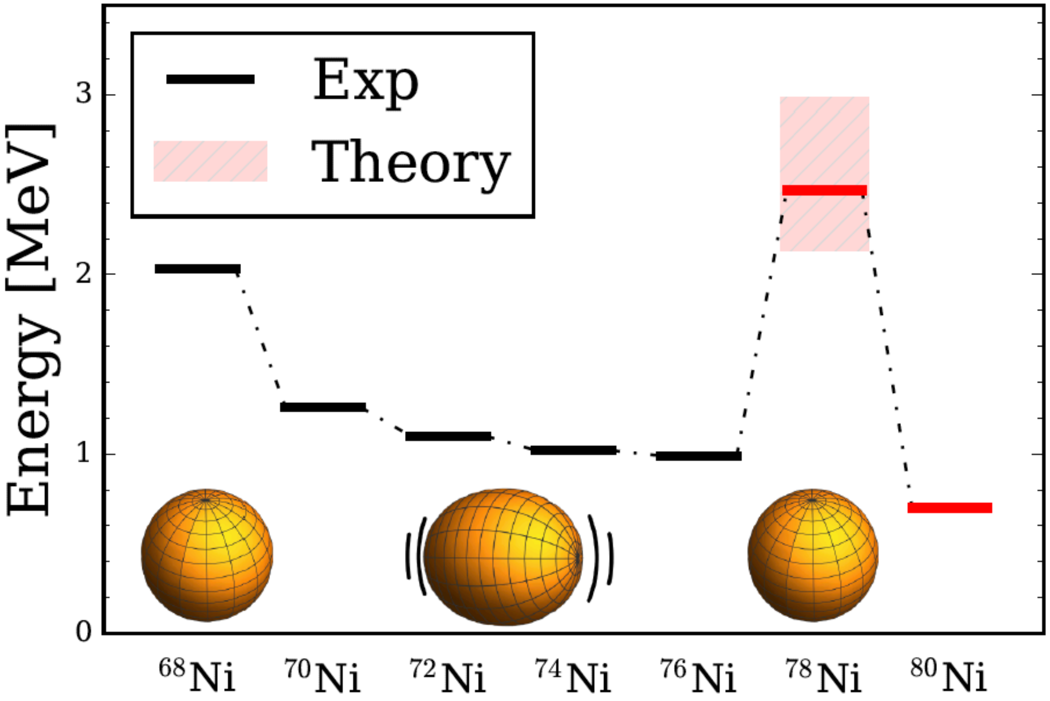
Theory to experiment ratios for beta decays in light nuclei from NCSM

N3LO(EM) + $3N_{lnl}$ SRG-evolved to $2.0\mathrm{fm}^{-1}$ ($c_D = 0.7$)



In QMC calculations of beta-decays 2BC increase the GT strength by 2-3%
S. Pastore et al, PRC 97, 022501 (2018).

Structure of ^{78}Ni from first principles

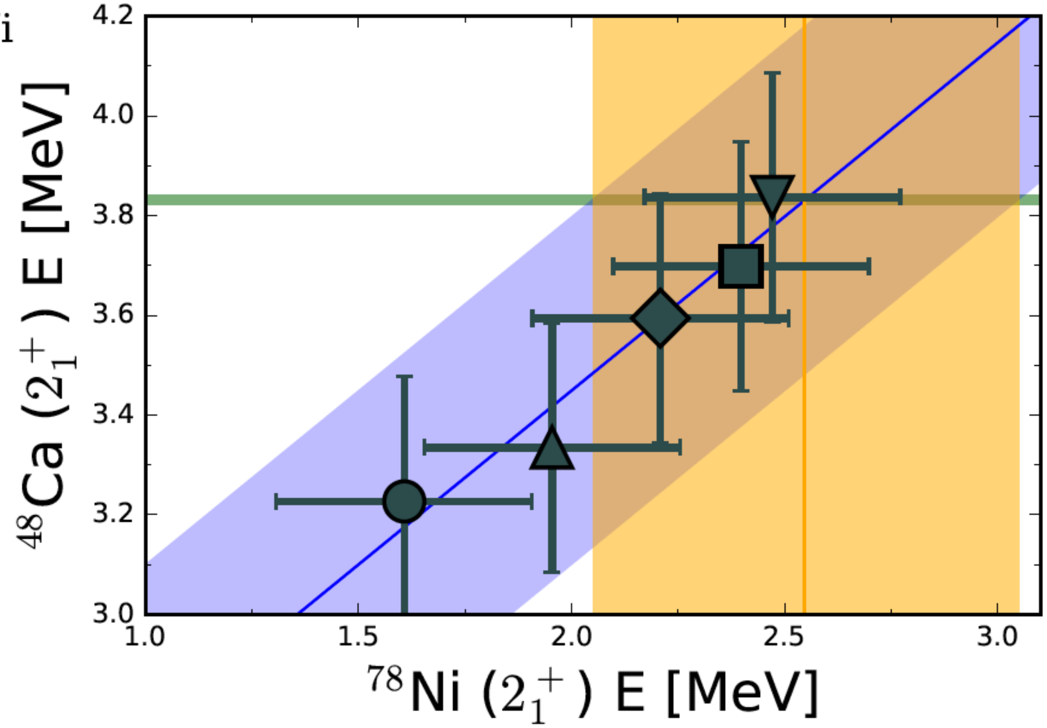


A high 2^+ energy in ^{78}Ni indicates that this nucleus is doubly magic

A measurement of this state has been made at RIBF, RIKEN
R. Taniuchi *et al.*, in preparation

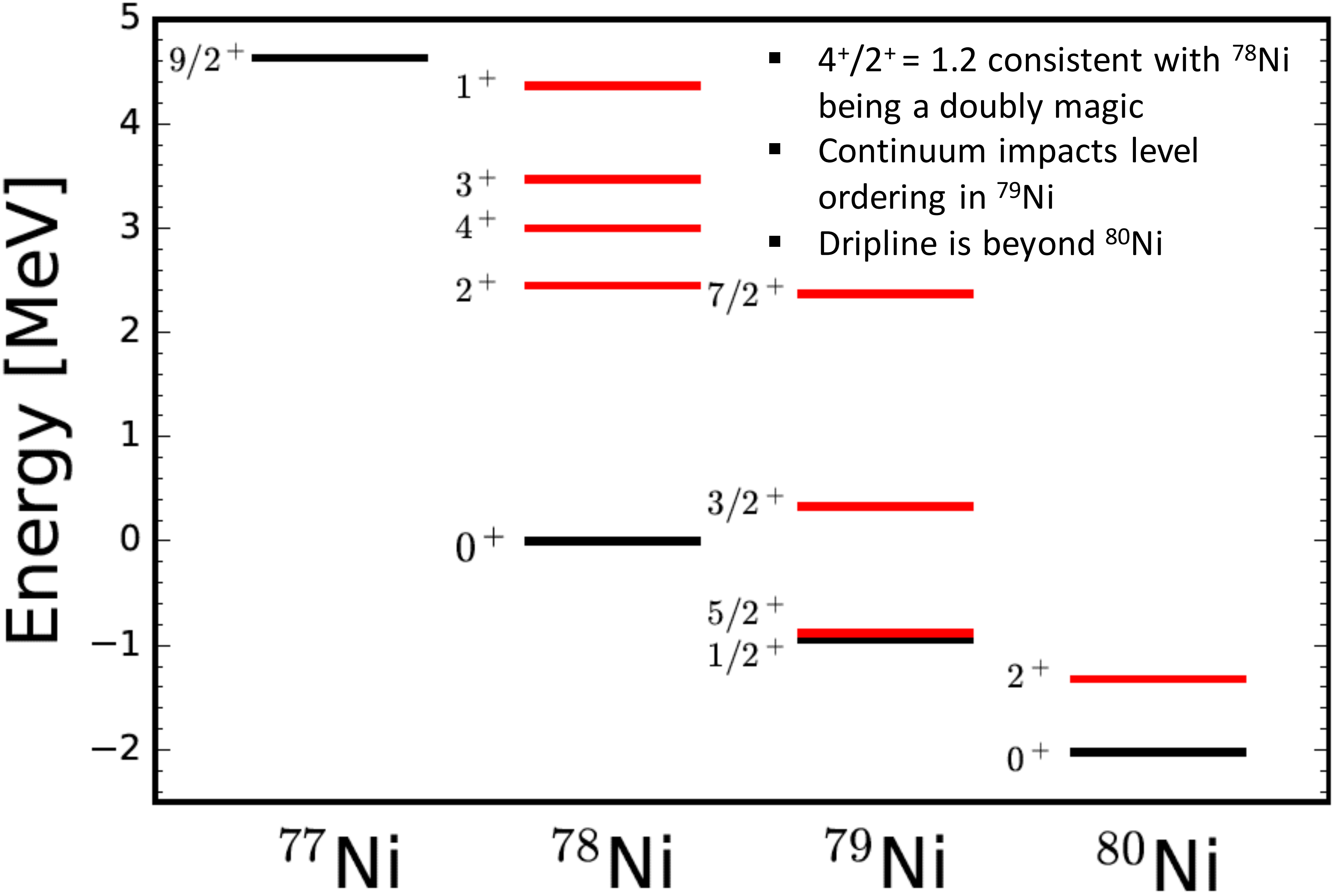
Consistent with recent shell-model studies
F. Nowacki *et al.*, PRL 117, 272501 (2016)

- From an observed correlation we predict the 2^+ excited state in ^{78}Ni using the experimental data for the 2^+ state in ^{48}Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



G. Hagen, G. R. Jansen, and T. Papenbrock
Phys. Rev. Lett. **117**, 172501 (2016)

Excited states in ^{78}Ni and its neighbors



- $4^+/2^+$ = 1.2 consistent with ^{78}Ni being a doubly magic
- Continuum impacts level ordering in ^{79}Ni
- Dripline is beyond ^{80}Ni

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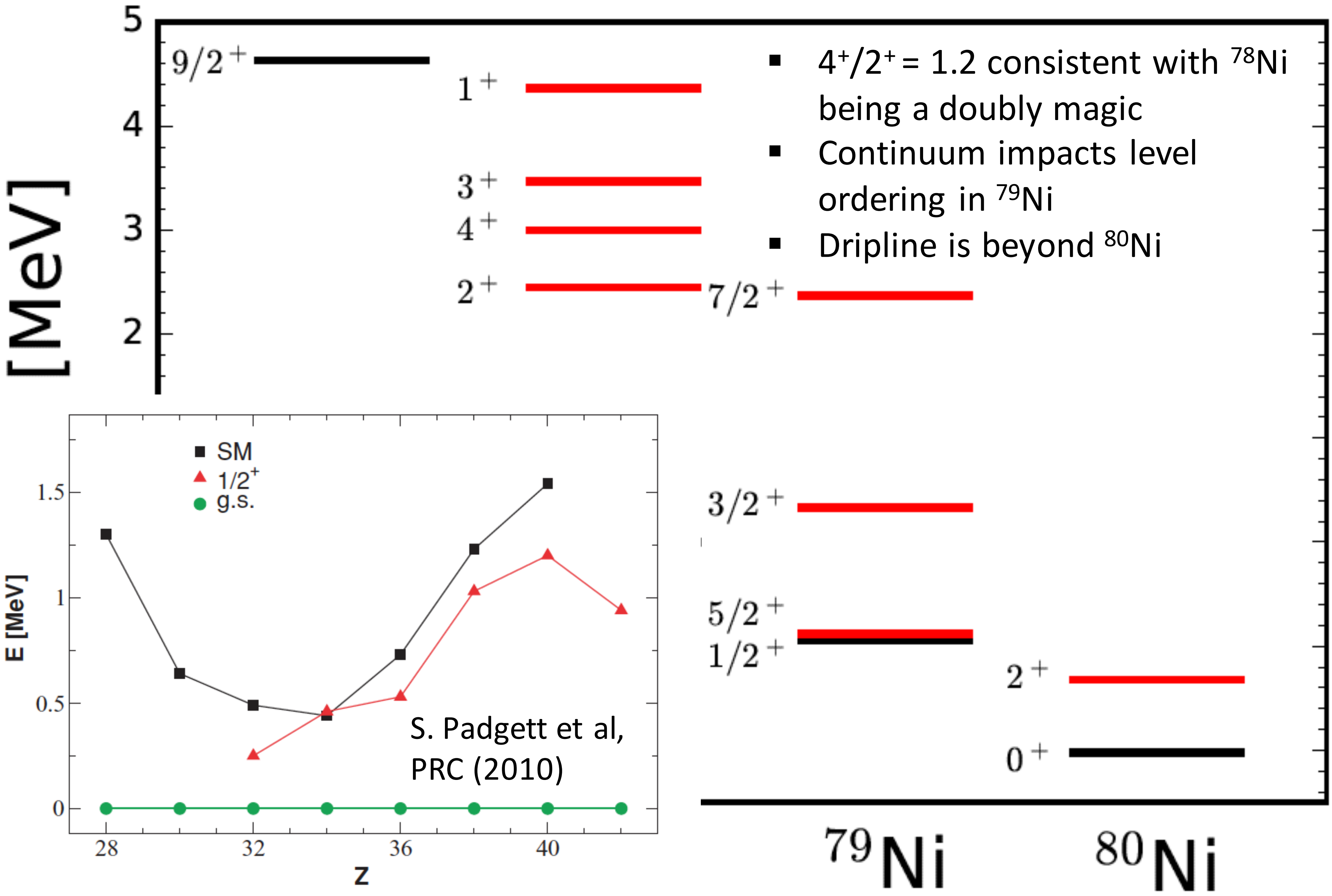

S. Padgett et al, PRC (2010)

Excited states in ^{78}Ni and its neighbors

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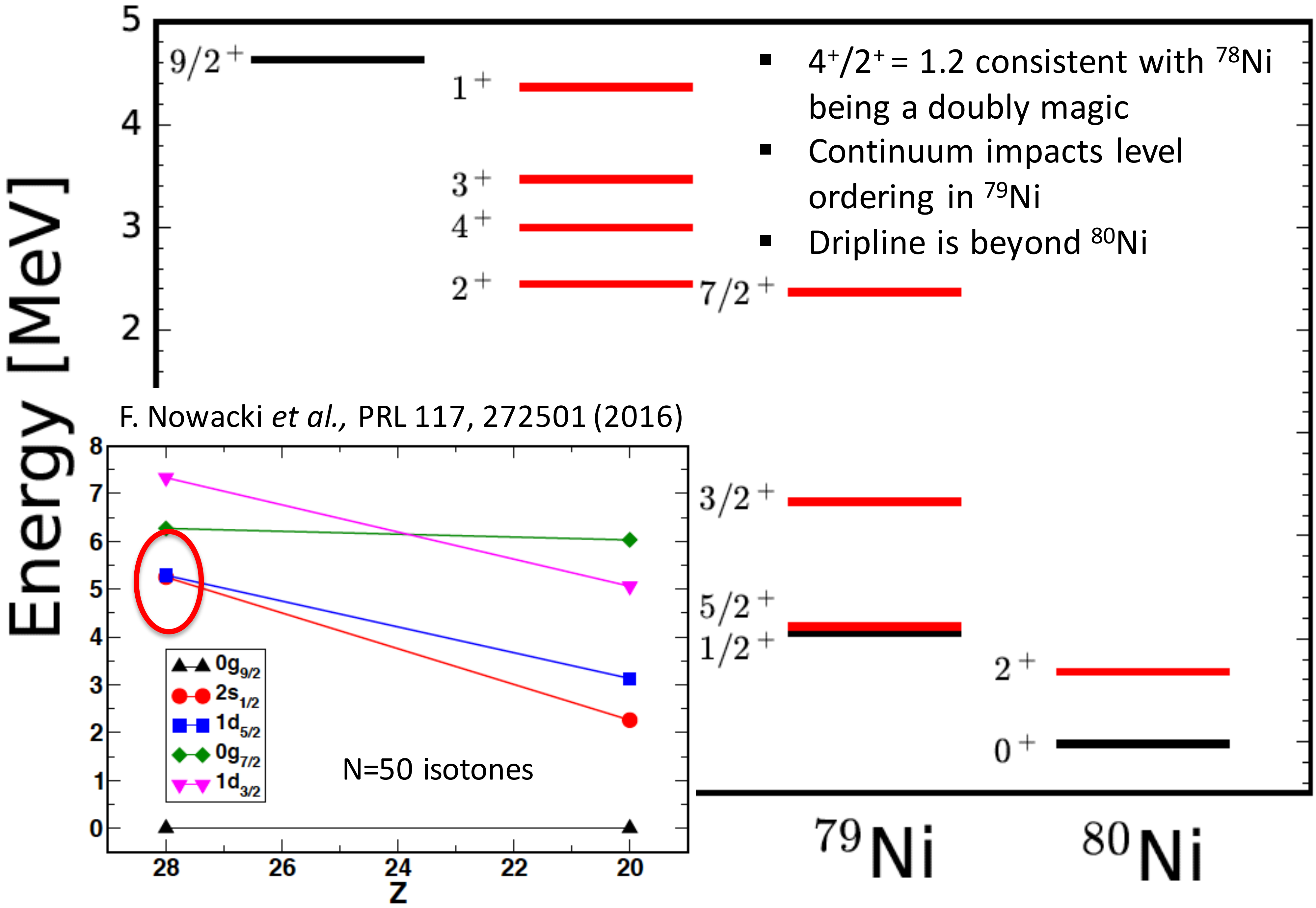
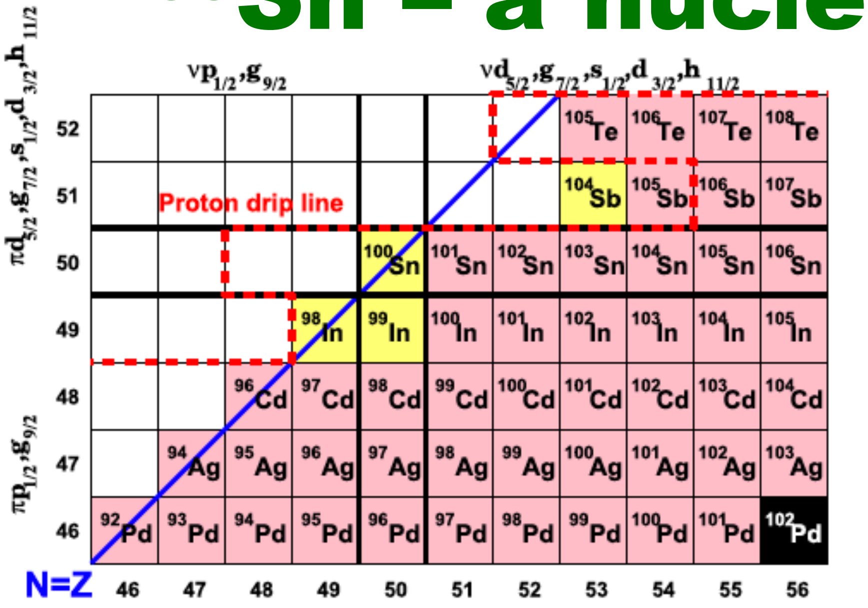


F. Nowacki *et al.*, PRL 117, 272501 (2016)

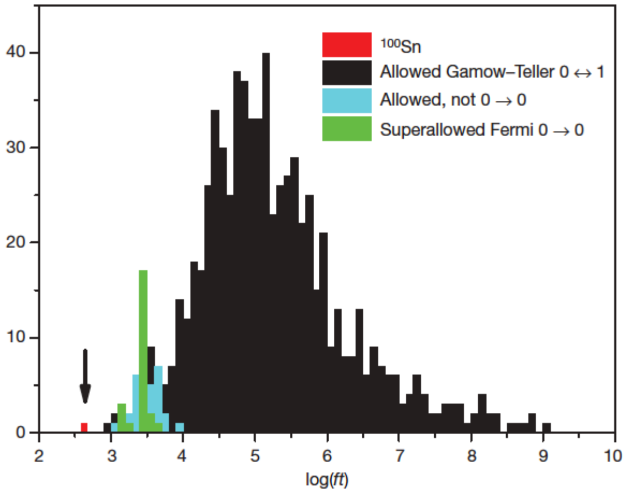
^{100}Sn – a nucleus of superlatives



	46	47	48	49	50	51	52	53	54	55	56
52								^{105}Te	^{106}Te	^{107}Te	^{108}Te
51								^{104}Sb	^{105}Sb	^{106}Sb	^{107}Sb
50					^{100}Sn	^{101}Sn	^{102}Sn	^{103}Sn	^{104}Sn	^{105}Sn	^{106}Sn
49				^{98}In	^{99}In	^{100}In	^{101}In	^{102}In	^{103}In	^{104}In	^{105}In
48			^{96}Cd	^{97}Cd	^{98}Cd	^{99}Cd	^{100}Cd	^{101}Cd	^{102}Cd	^{103}Cd	^{104}Cd
47		^{94}Ag	^{95}Ag	^{96}Ag	^{97}Ag	^{98}Ag	^{99}Ag	^{100}Ag	^{101}Ag	^{102}Ag	^{103}Ag
46	^{92}Pd	^{93}Pd	^{94}Pd	^{95}Pd	^{96}Pd	^{97}Pd	^{98}Pd	^{99}Pd	^{100}Pd	^{101}Pd	^{102}Pd

🟨	**Nucleus produced with known half-life**
🟥	**Nucleus with known excited states**
⬛	**Stable nucleus**

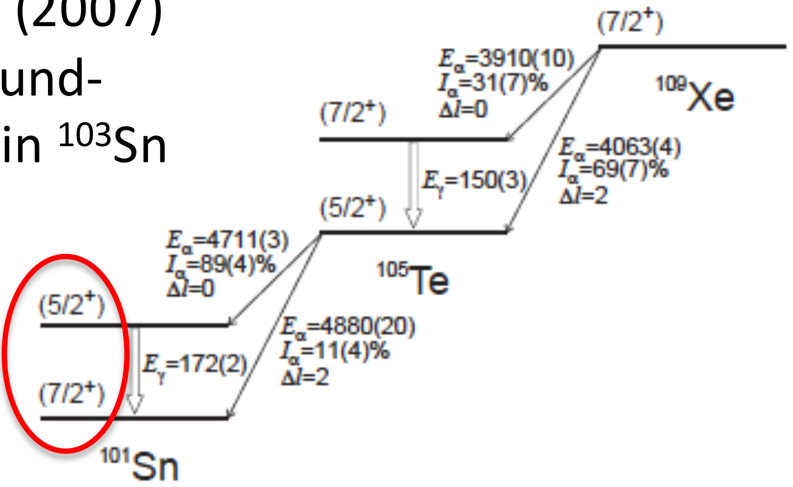
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



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)

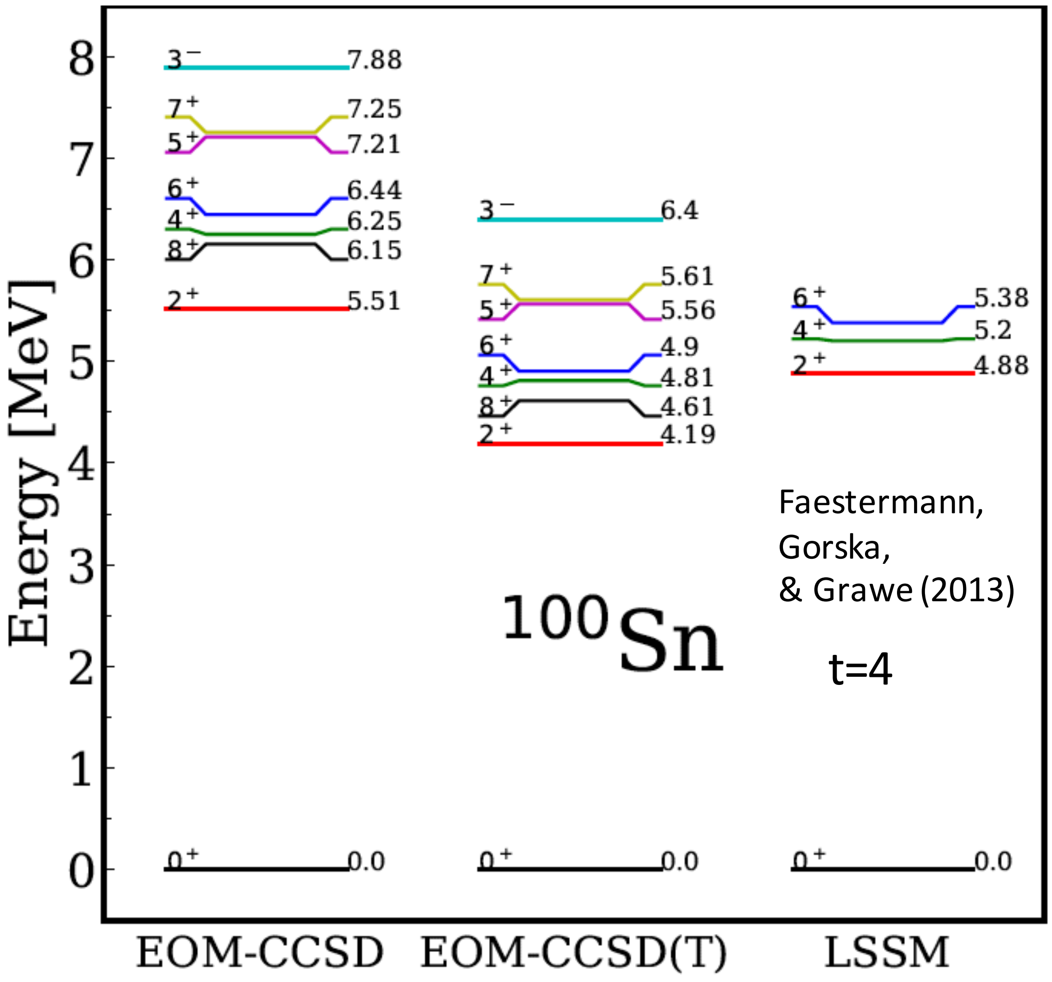


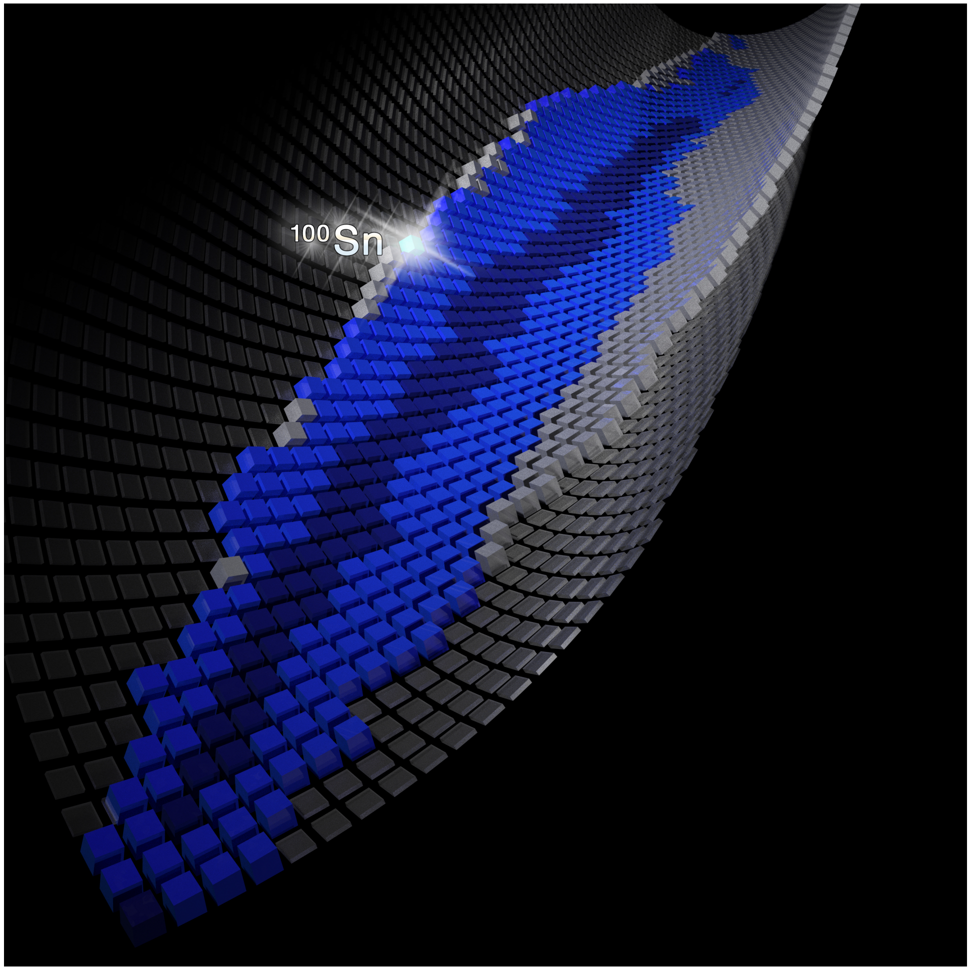
PHYSICAL REVIEW LETTERS **120,** 152503 (2018)

Editors' Suggestion

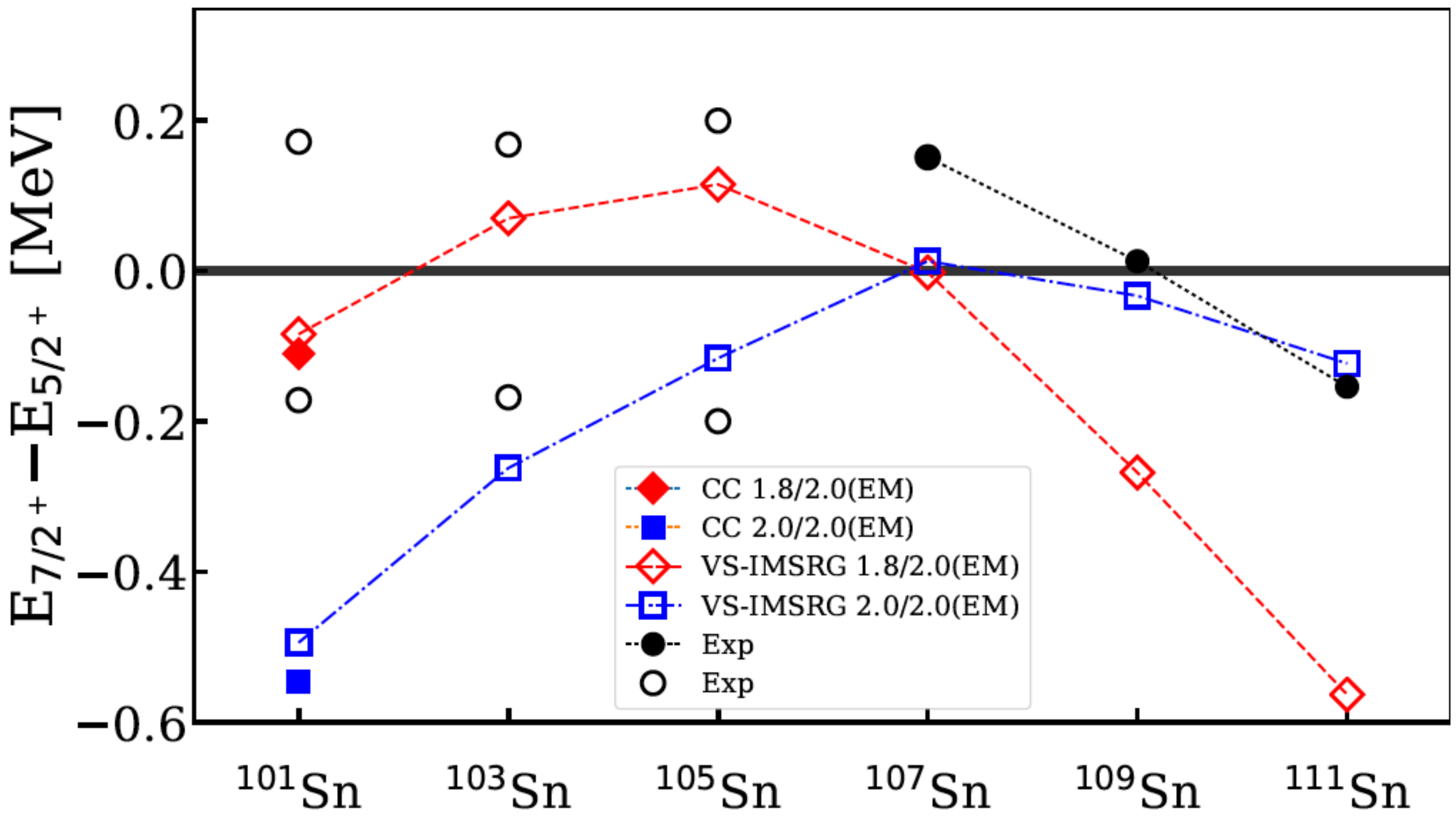
Structure of the Lightest Tin Isotopes

T. D. Morris,[1,2] J. Simonis,[3,4] S. R. Stroberg,[5,6] C. Stumpf,[3] G. Hagen,[2,1] J. D. Holt,[5] G. R. Jansen,[7,2]
T. Papenbrock,[1,2] R. Roth,[3] and A. Schwenk[3,4,8]





Structure of the ligthest tin isotopes

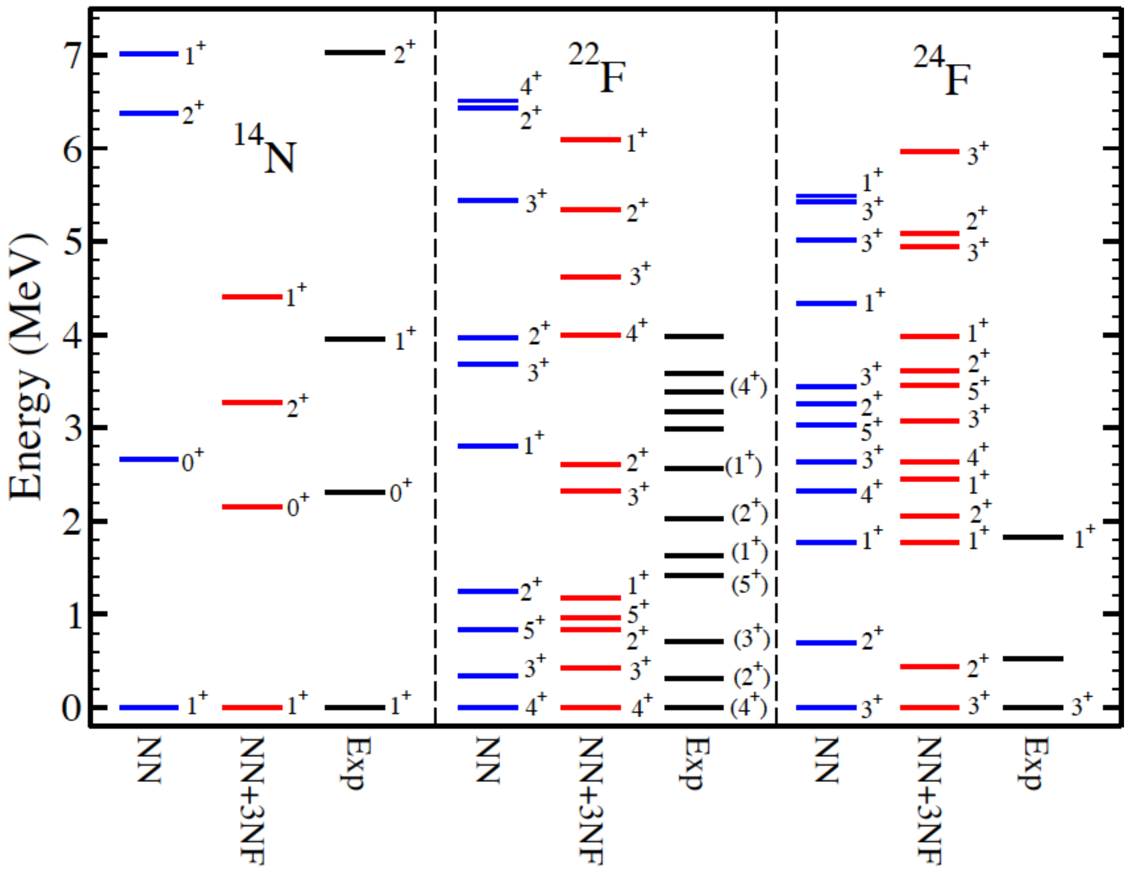


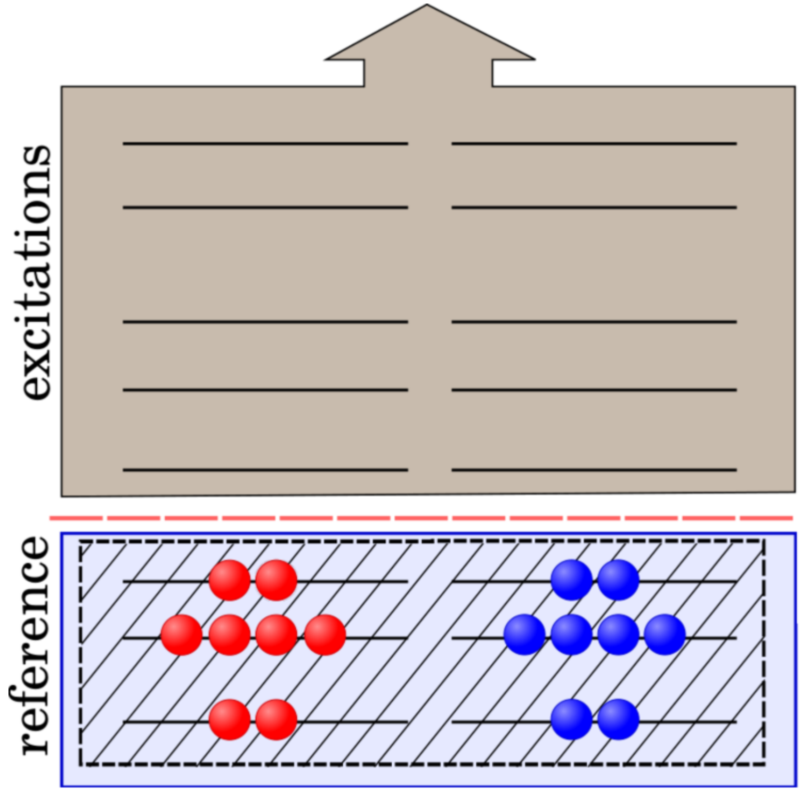
- Splitting between 7/2$^+$ and 5/2$^+$ reproduced
- Ground-state spins of $^{101\text{-}121}$Sn will be measured at CERN (CRIS collaboration)

Coupled cluster calculations of beta-decay partners

Diagonalize $\overline{H} = e^{-T} H_N e^{T}$ via a novel 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)

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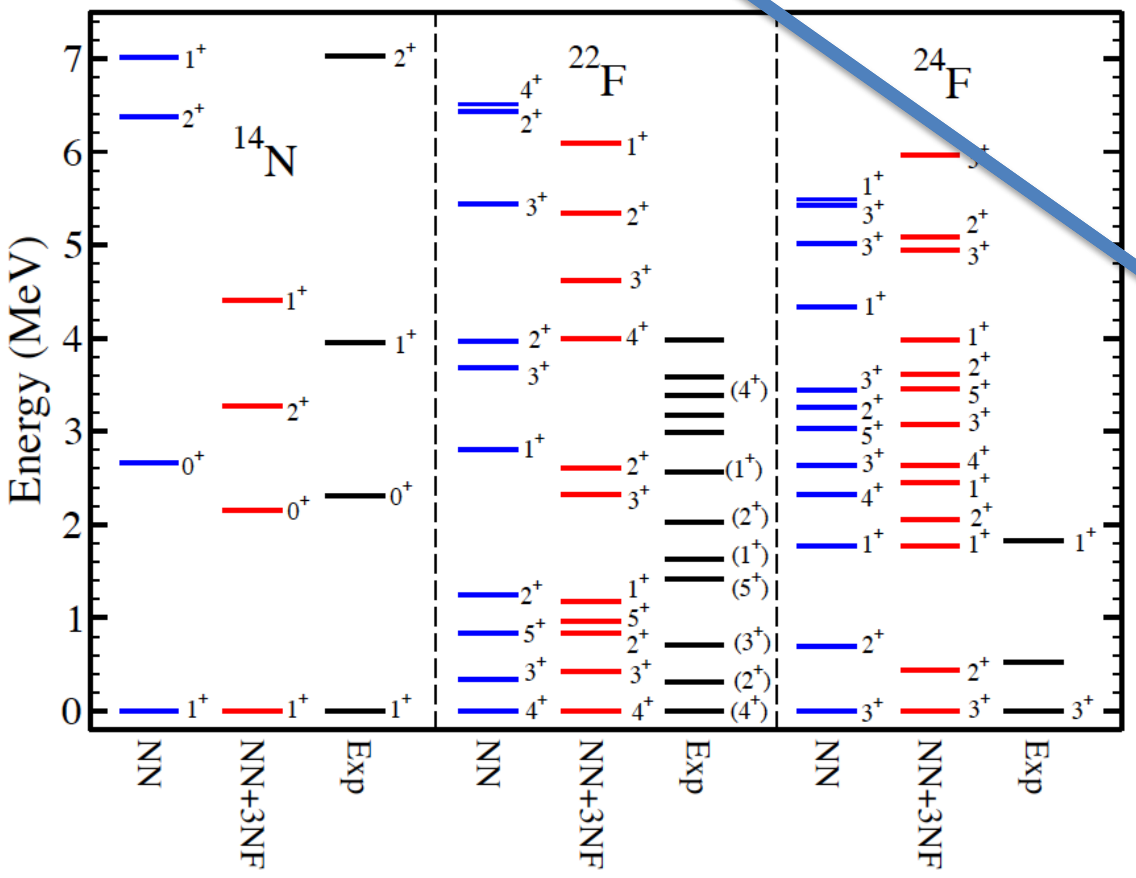

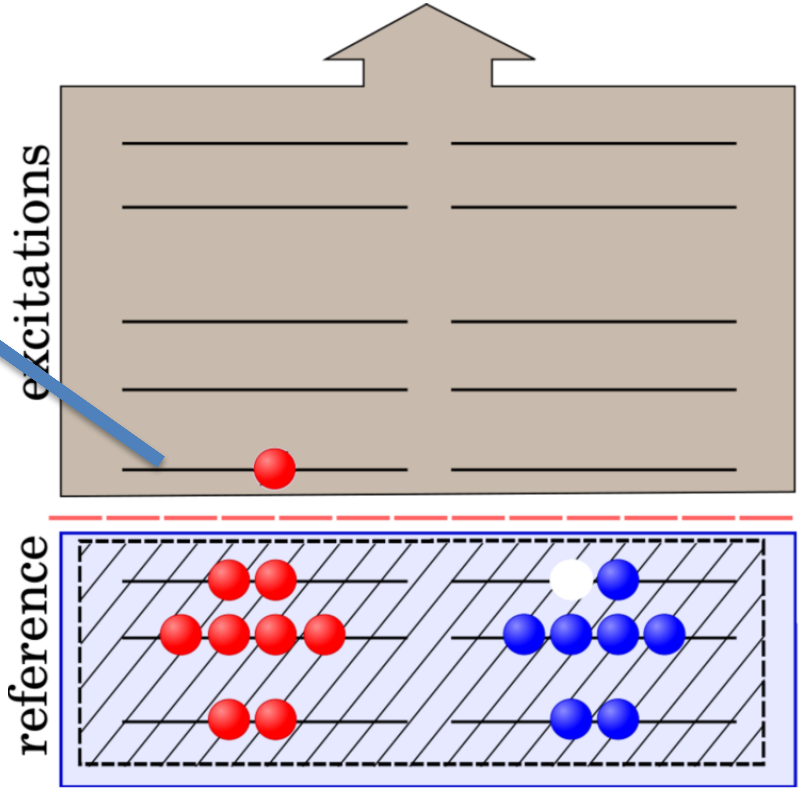

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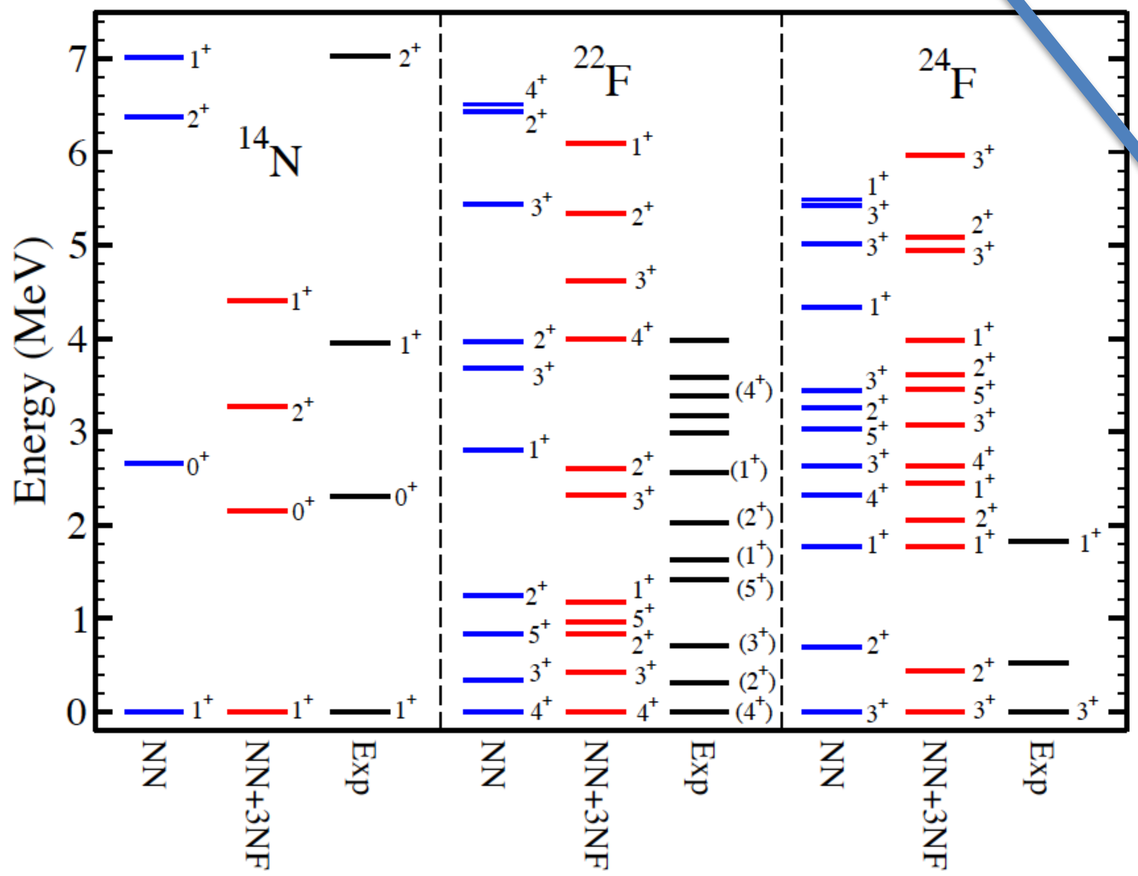

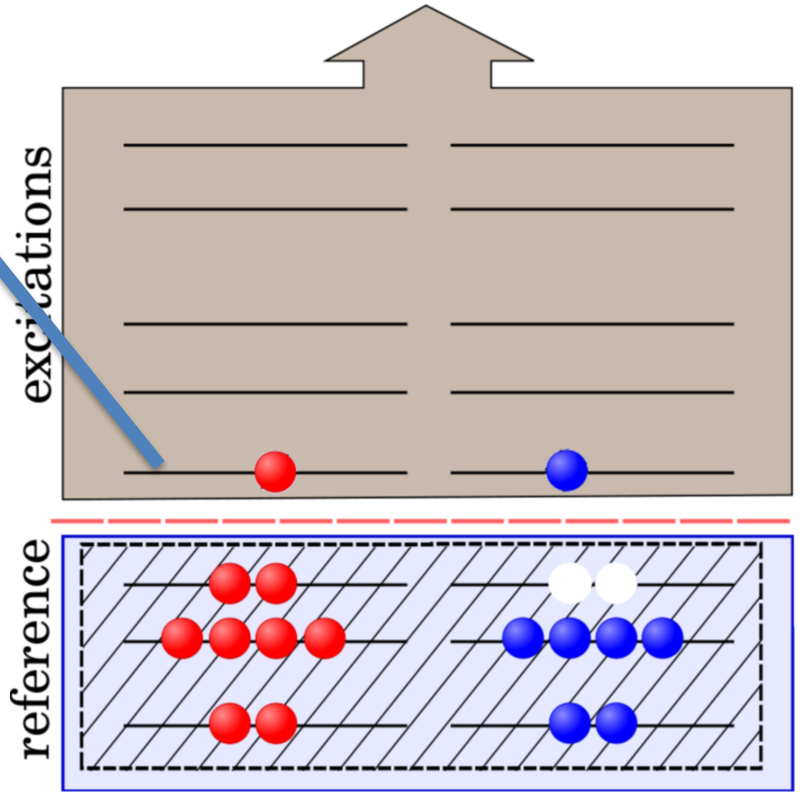

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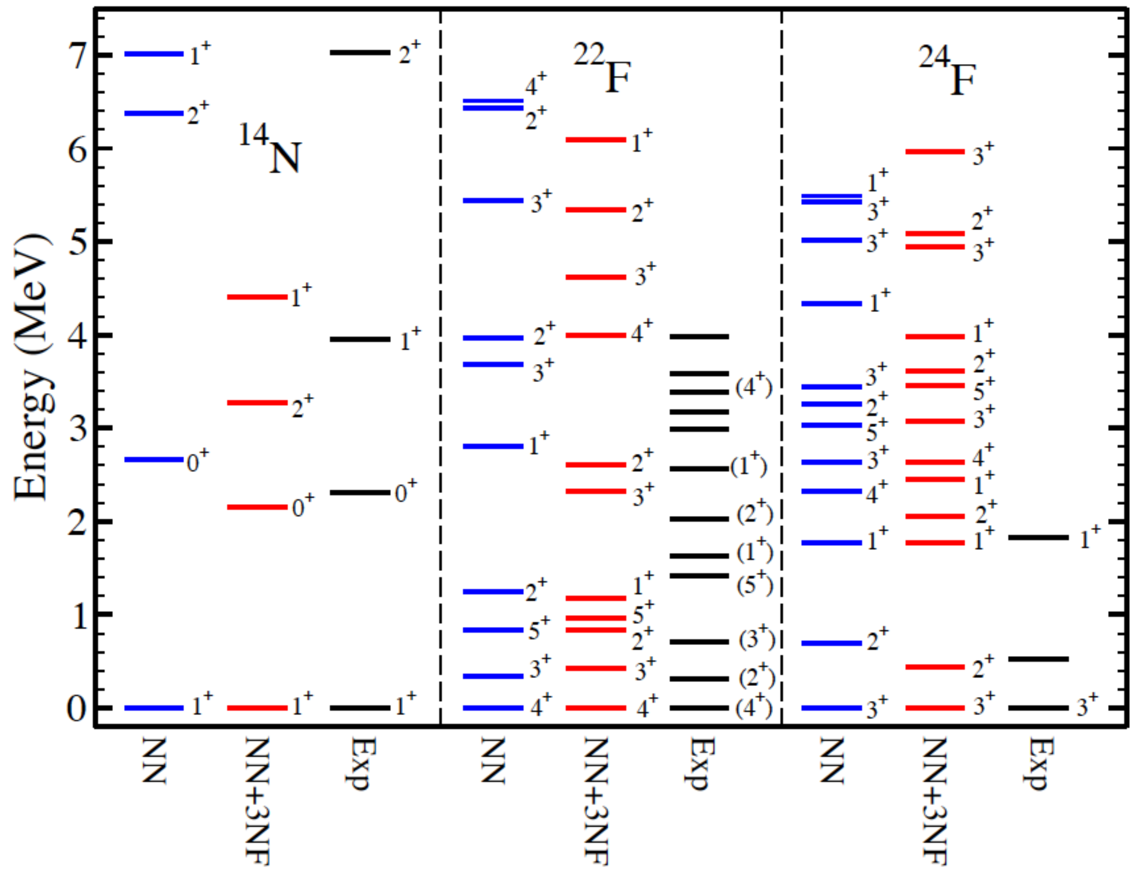

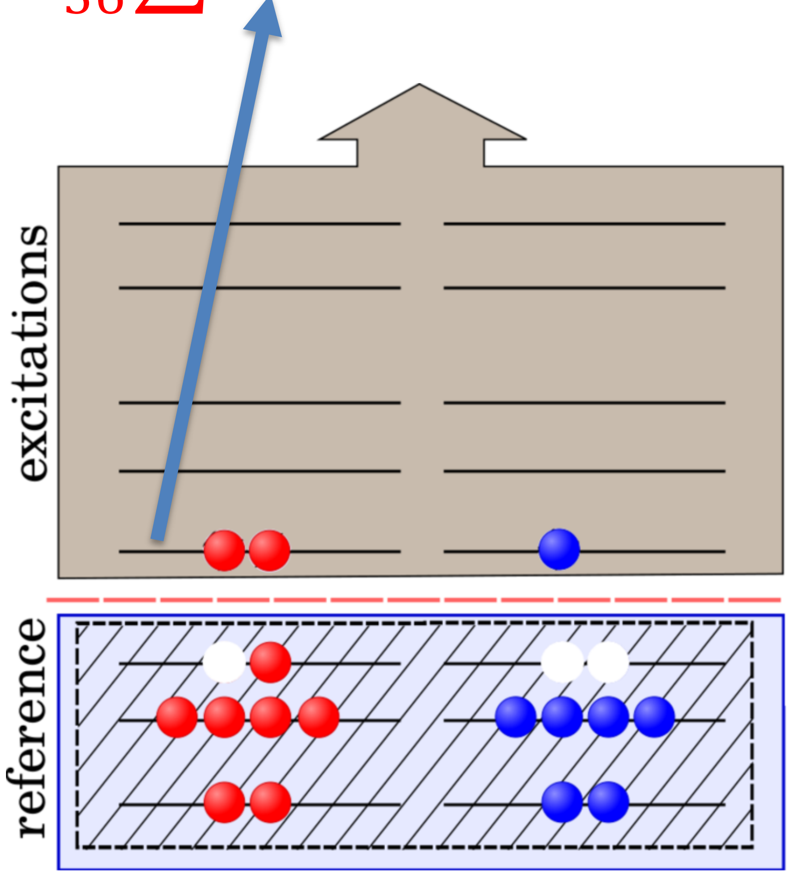

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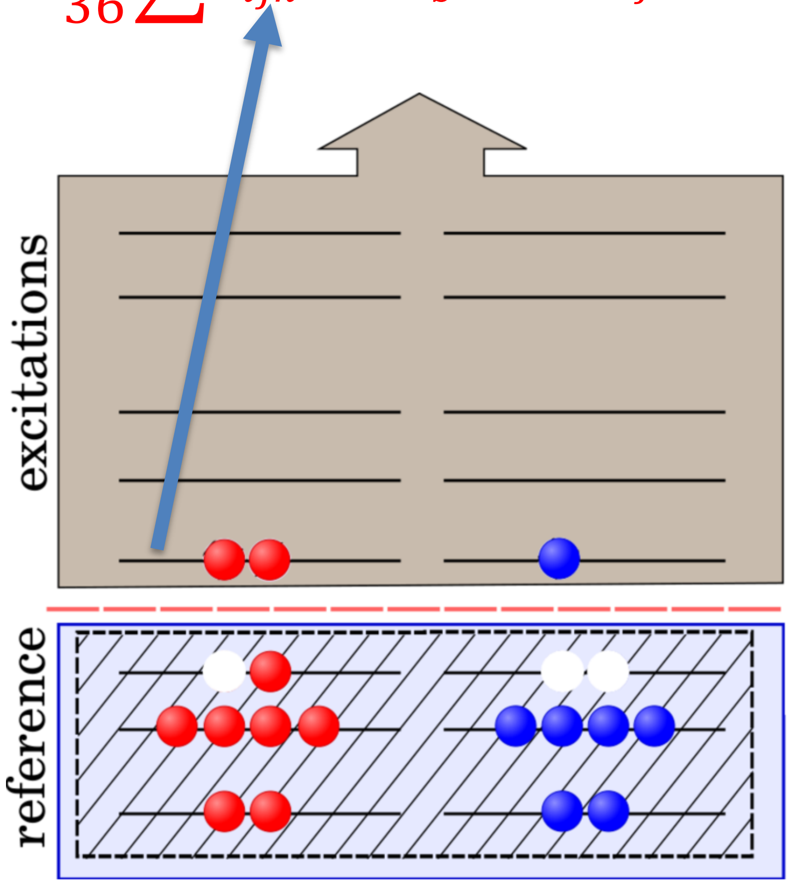
Introduce an energy cut on allowed three-particle three-hole excitations:

$$\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\max}$$

$$\tilde{e}_p = |N_p - N_F|$$

measures the difference of number of harmonic oscillator shells wrt the Fermi surface.



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

Charge exchange EOM-CCSDT-1

$$\bar{H}_{CCSDT-1} = \begin{bmatrix} \langle S|\bar{H}|S\rangle & \langle D|\bar{H}|S\rangle & \langle T|V|S\rangle \\ \langle S|\bar{H}|D\rangle & \langle D|\bar{H}|D\rangle & \langle T|V|D\rangle \\ \langle S|V|T\rangle & \langle D|V|T\rangle & \langle T|F|T\rangle \end{bmatrix}$$

Charge exchange EOM-CCSDT-1

P-space

$$\bar{H}_{CCSDT-1} = \begin{bmatrix} \langle S|\bar{H}|S\rangle & \langle D|\bar{H}|S\rangle & \langle T|V|S\rangle \\ \langle S|\bar{H}|D\rangle & \langle D|\bar{H}|D\rangle & \langle T|V|D\rangle \\ \langle S|V|T\rangle & \langle D|V|T\rangle & \langle T|F|T\rangle \end{bmatrix}$$

Q-space

Charge exchange EOM-CCSDT-1

P-space

$$\overline{H}_{CCSDT-1} = \begin{bmatrix} \langle S|\overline{H}|S\rangle & \langle D|\overline{H}|S\rangle & \langle T|V|S\rangle \\ \langle S|\overline{H}|D\rangle & \langle D|\overline{H}|D\rangle & \langle T|V|D\rangle \\ \langle S|V|T\rangle & \langle D|V|T\rangle & \langle T|F|T\rangle \end{bmatrix}$$

Q-space

- Bloch-Horowitz is exact; iterative solution poss.

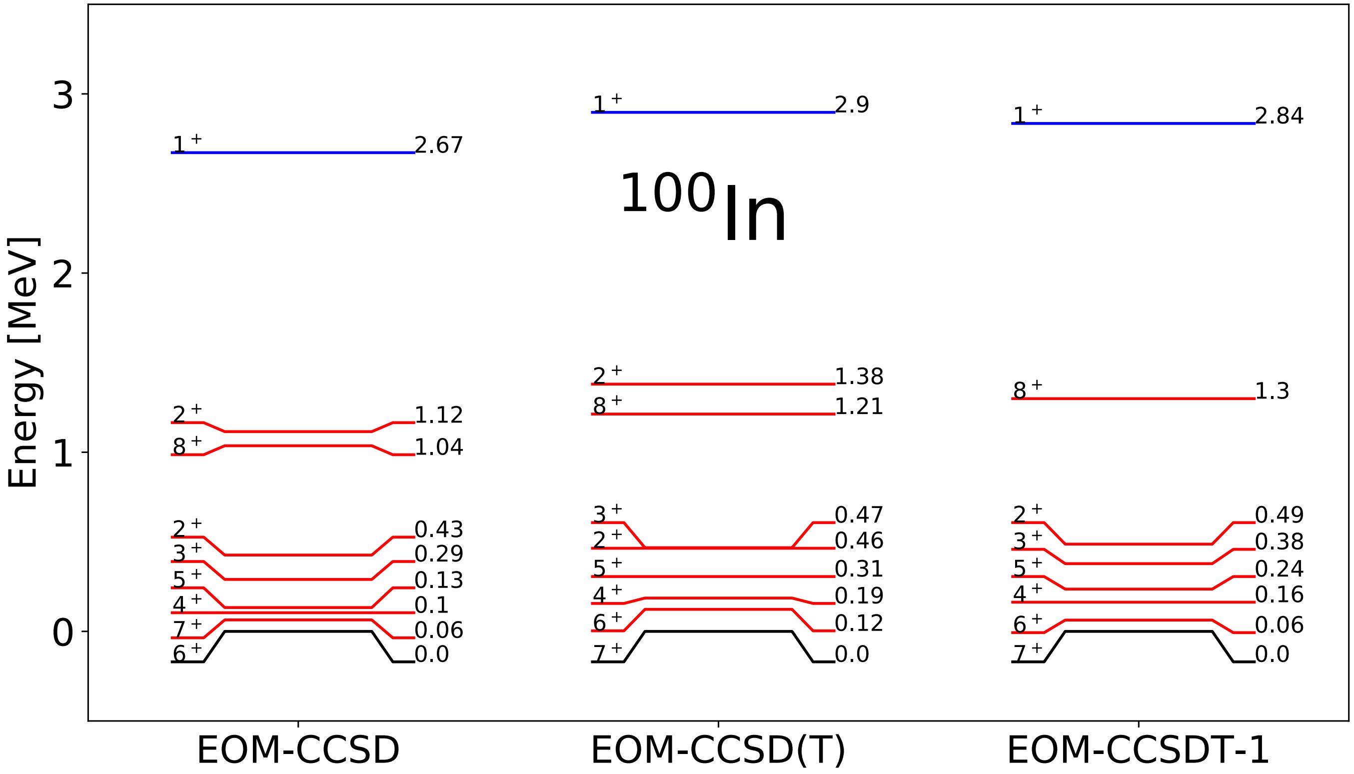
$$\overline{H}_{PP}R_P + \overline{H}_{PQ}(\omega - \overline{H}_{QQ})^{-1}\overline{H}_{QP}R_P = \omega R_P$$

- No large memory required for lanczos vectors
- Can only solve for one state at a time
- Reduces matrix dimension from ~10^9 to ~10^6
- Method scales as N^7

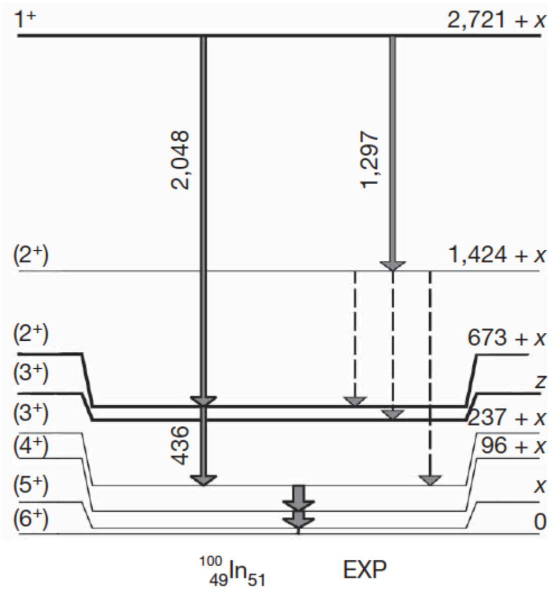
W. C. Haxton and C.-L. Song Phys. Rev. Lett. **84** (2000); W. C. Haxton Phys. Rev. C **77**, 034005 (2008)
C. E. Smith, J. Chem. Phys. **122**, 054110 (2005)

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

1.8/2.0 (EM)



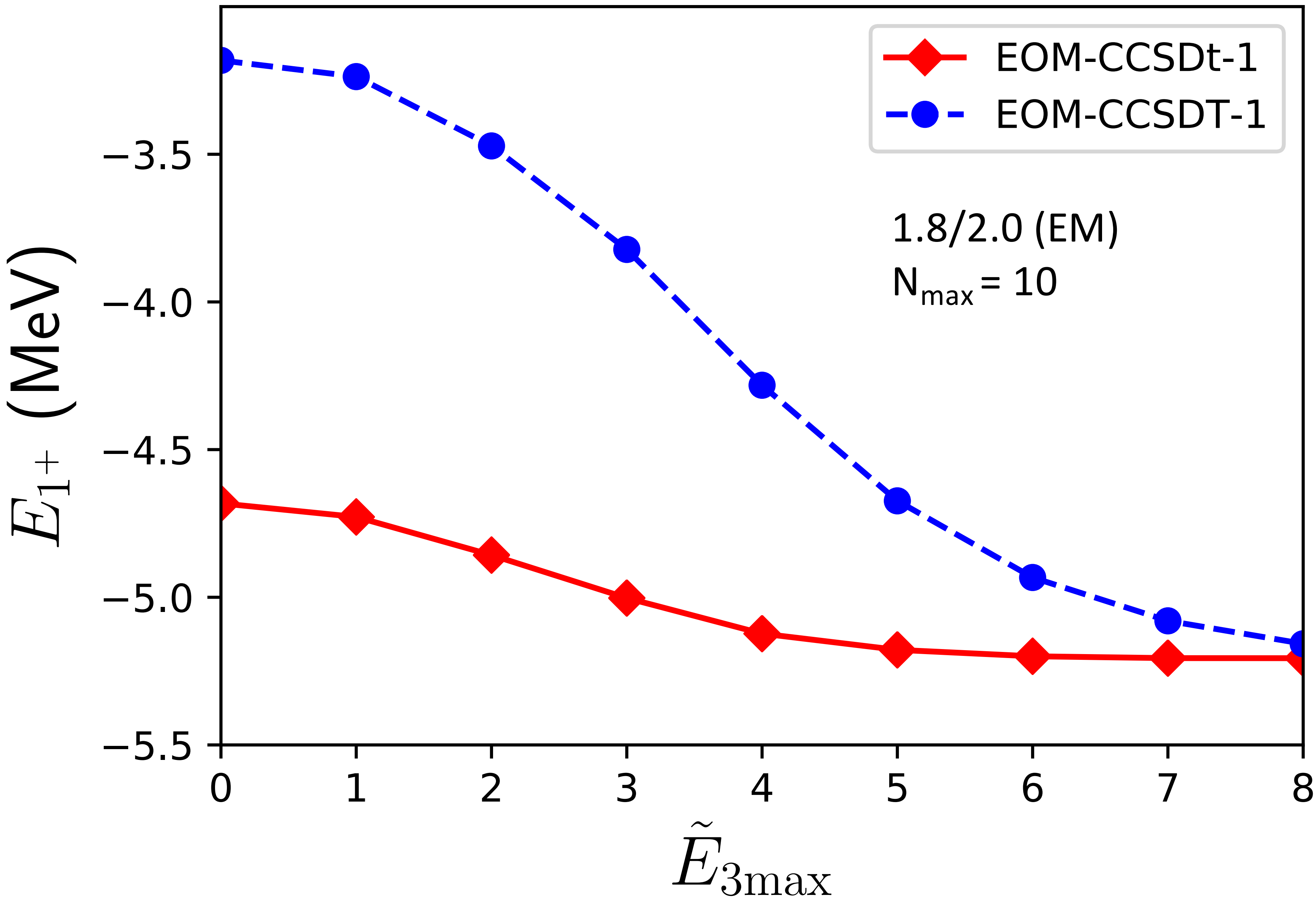
Hinke et al, Nature (2012)



Charge-exchange EOM-CC with perturbative corrections accounting for excluded 3p3h states:

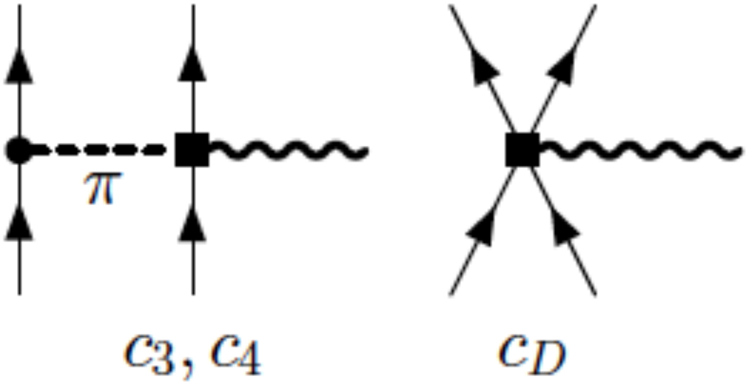
$$\Delta\omega_\mu = \langle\Phi_0|L_\mu \overline{H}_{PQ'}(\omega_\mu - \overline{H}_{Q'Q'})^{-1}\overline{H}_{Q'P}R_\mu|\Phi_0\rangle$$

Convergence of excited states in ^{100}In



Normal ordered one- and two-body current

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



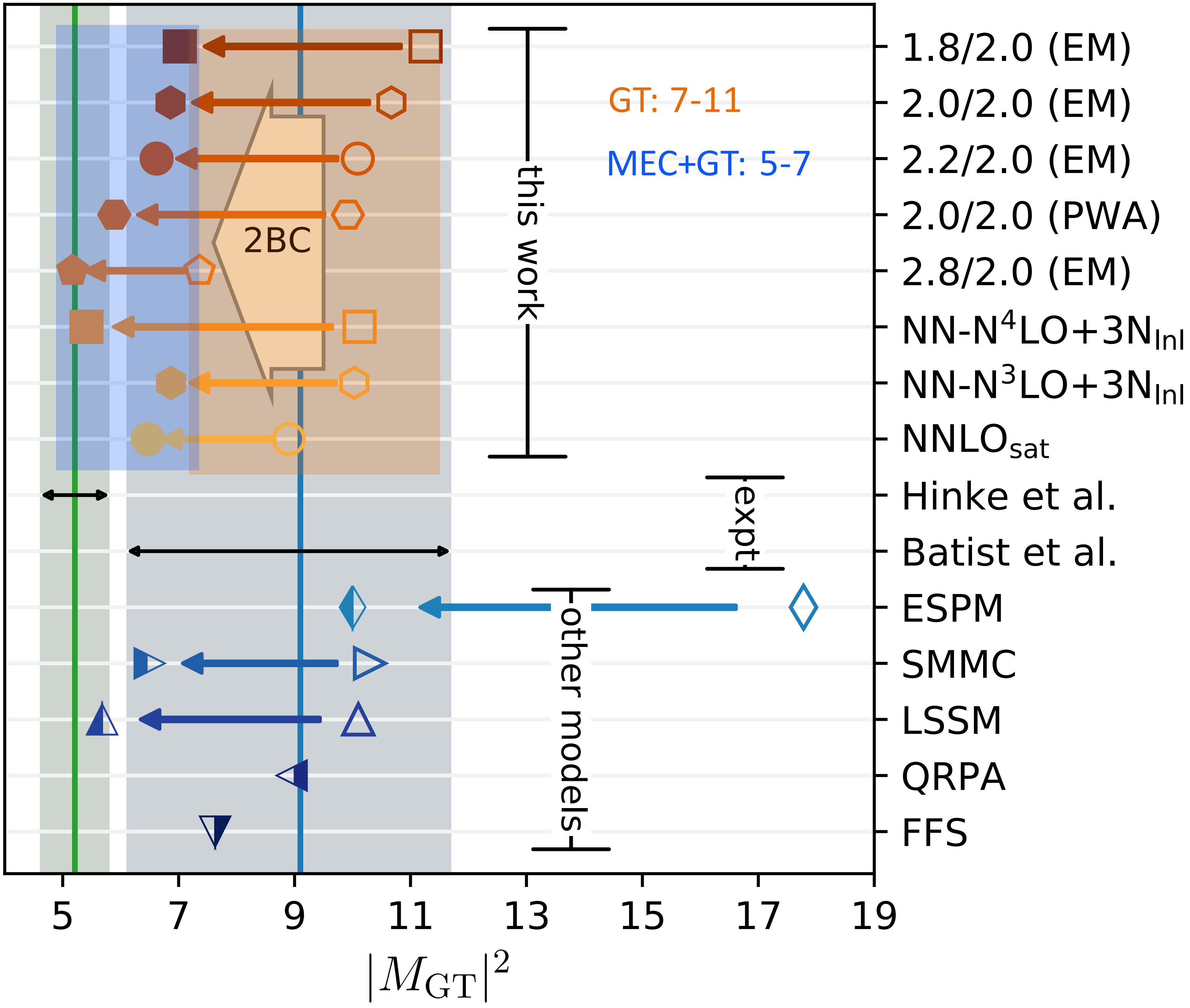
Normal ordered operator:

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

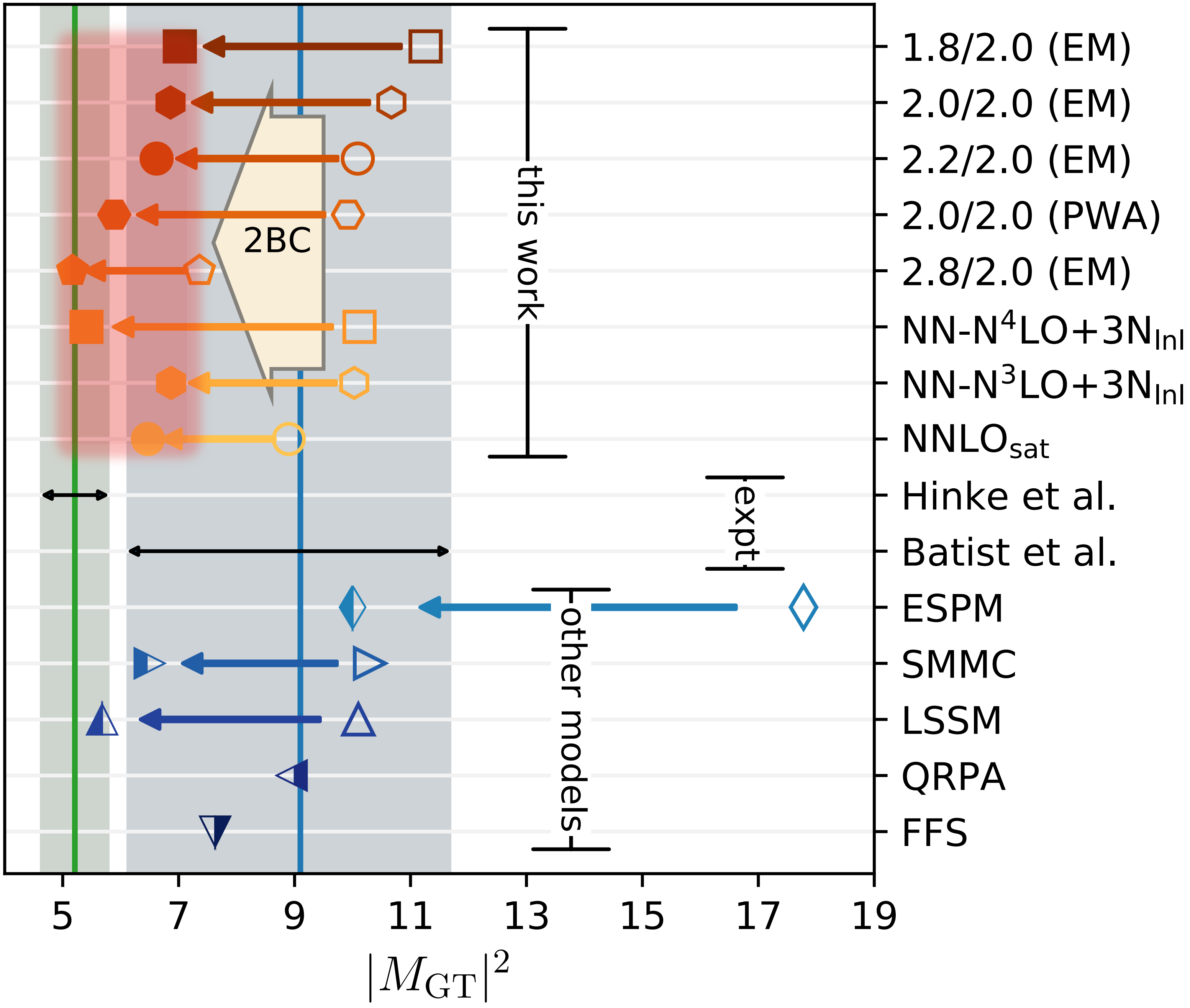
Benchmark between NCSM and CC for the large transition in ^{14}O using NNLO$_{\mathrm{sat}}$

Method	$\lvert M_{\mathrm{GT}}(\sigma\tau)\rvert$	$\lvert M_{\mathrm{GT}}\rvert$
EOM-CCSD	2.15	2.08
EOM-CCSDT-1	1.77	1.69
NCSM	1.80(3)	1.69(3)

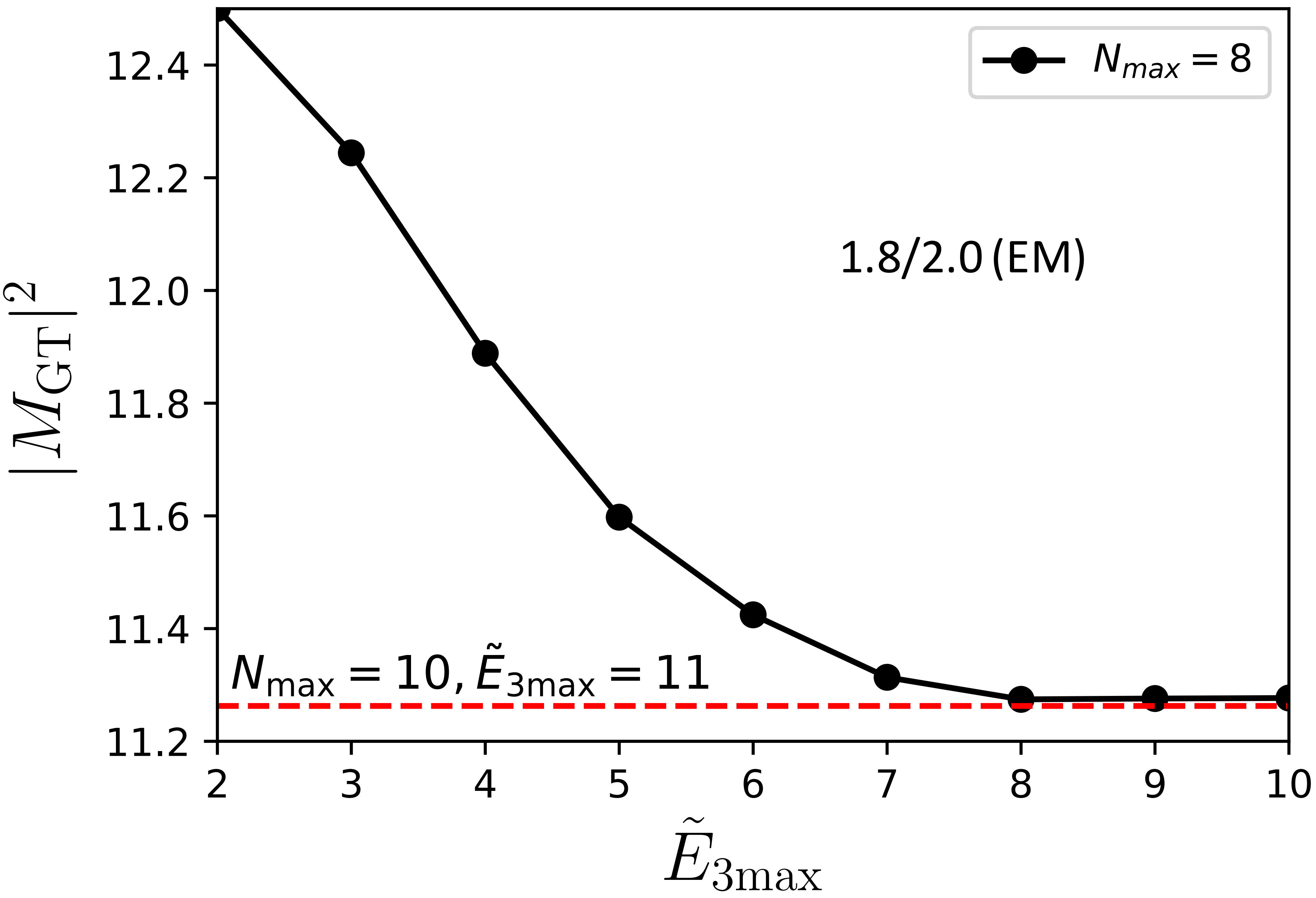
Super allowed Gamow-Teller decay of ^{100}Sn



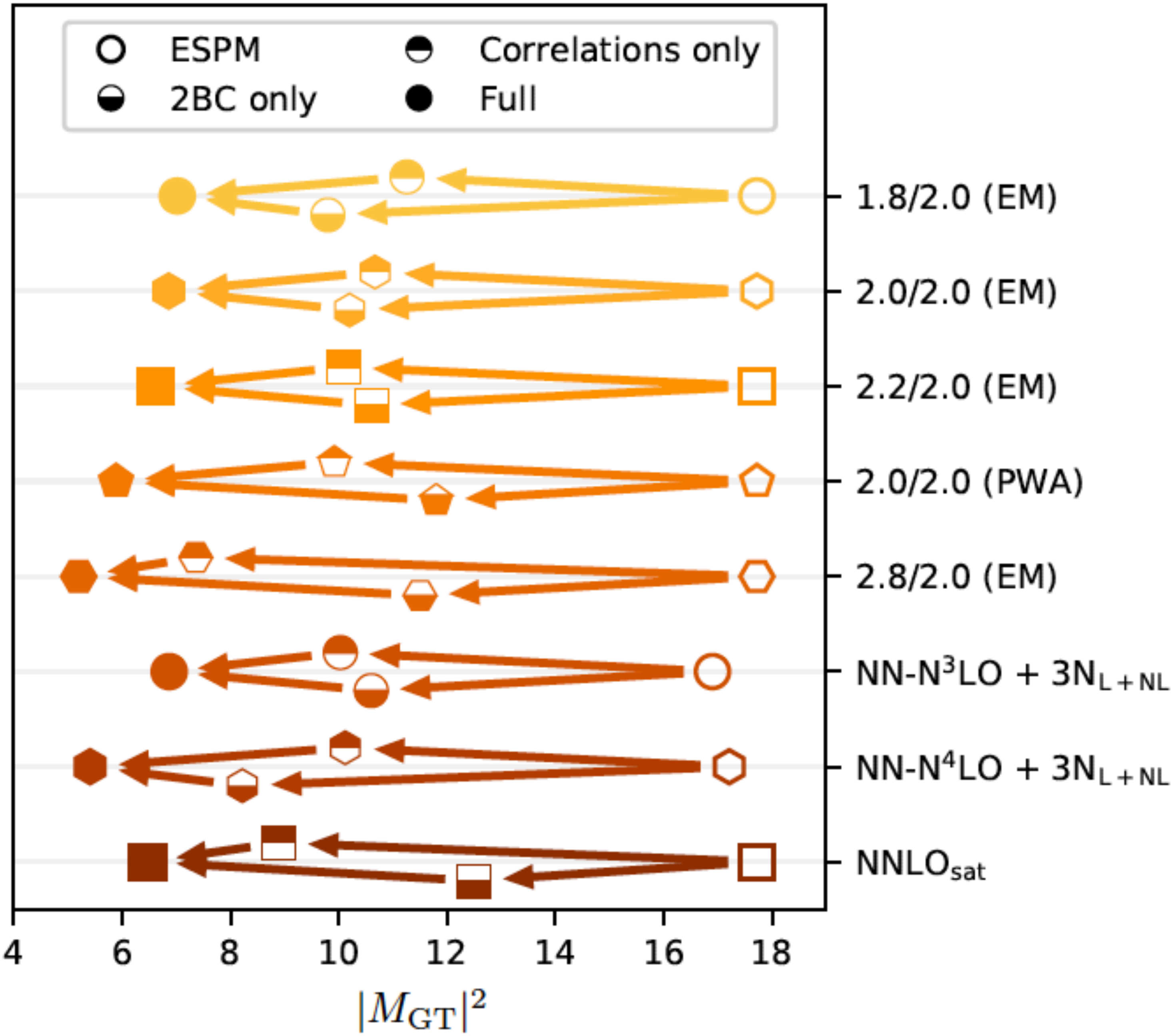
Super allowed Gamow-Teller decay of ^{100}Sn



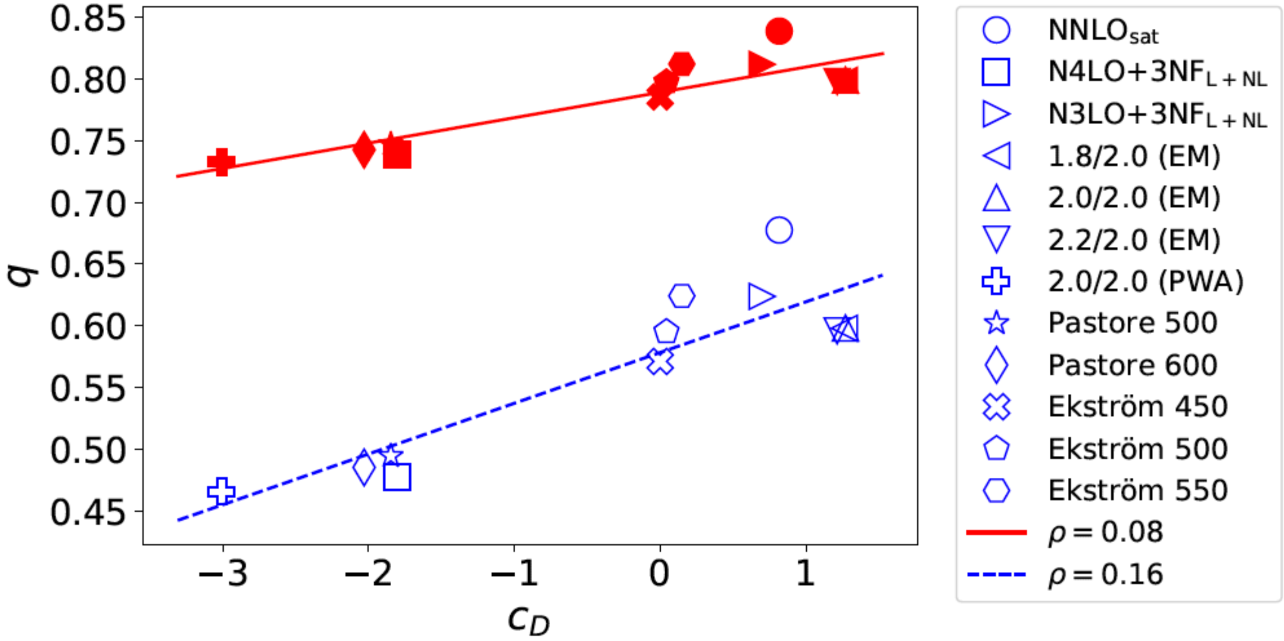
Convergence of GT transition in ^{100}Sn



Role of 2BC and correlations in ^{100}Sn



A simple interpretation of the quenching of beta decays



Contributions pion exchange to the 2BC gives roughly half of the necessary quenching

Contributions from the short range part accounts for a smaller part.

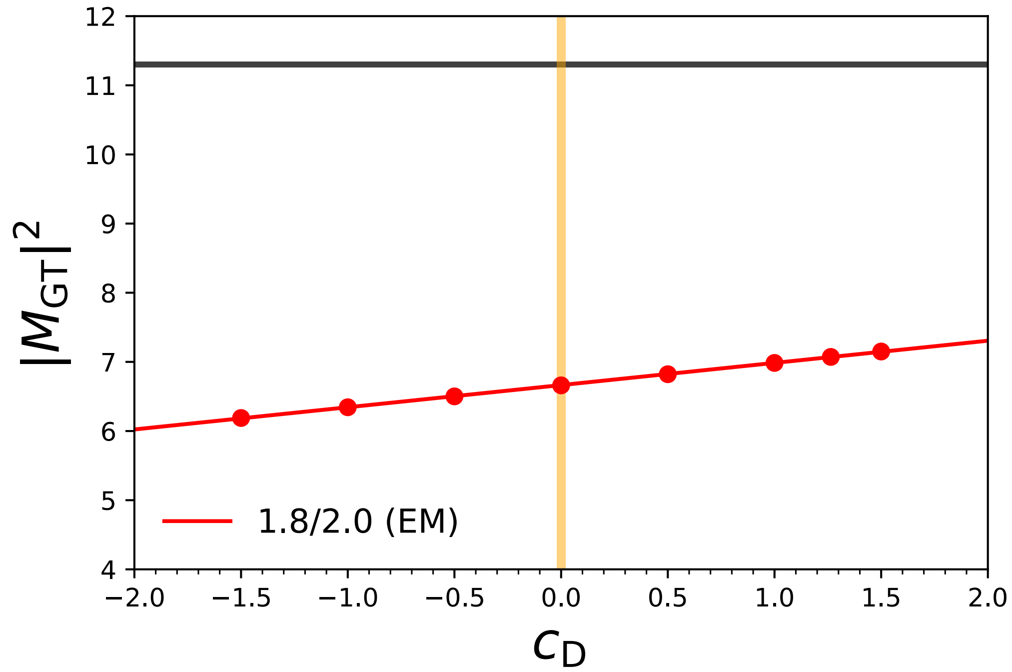
J. Menéndez, D. Gazit, A. Schwenk
PRL 107, 062501 (2011)

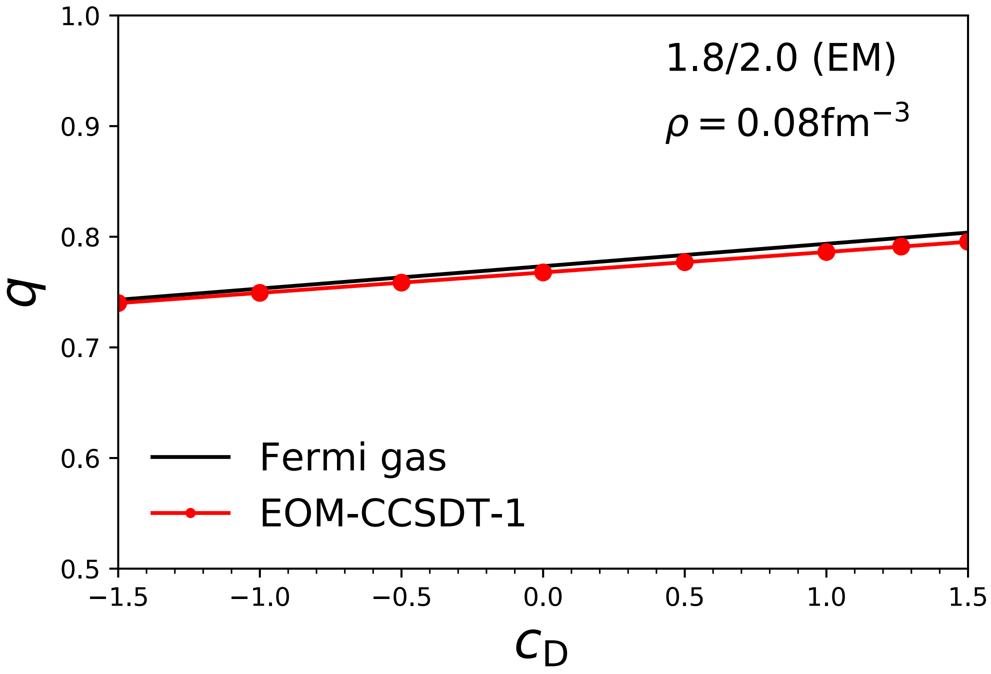
One-body normal ordering of 2BC in free Fermi gas

$$q \approx 1 - \frac{\rho \hbar^3 c^3}{F_\pi^2}\left(-\frac{c_D}{4 g_A \Lambda} + \frac{I}{3}(2c_4 - c_3) + \frac{I}{6m}\right)$$

Interaction	c_D	$2c_4 - c_3$	Λ_χ [GeV]	Ref.
NNLO$_{\rm sat}$	0.817	11.46	0.7	[24]
NN-N^{4}LO +3N$_{\rm lnl}$	−1.8	13.88	0.7	
NN-N^{3}LO +3N$_{\rm lnl}$	0.7	14.0	0.7	[25]
1.8/2.0 (EM)	1.264	14.0	0.7	[23]
2.0/2.0 (EM)	1.271	14.0	0.7	[23]
2.2/2.0 (EM)	1.214	14.0	0.7	[23]
2.0/2.0 (PWA)	−3.007	12.7	0.7	[23]
Pastore 500	−1.847	14.0	1.0	[26]
Pastore 600	−2.03	14.13	1.0	[26]
Ekström 450	0.0004	13.22	0.7	[48]
Ekström 500	0.0431	12.50	0.7	[48]
Ekström 550	0.1488	11.71	0.7	[48]

The small role of short-ranged 2BC on GT decay





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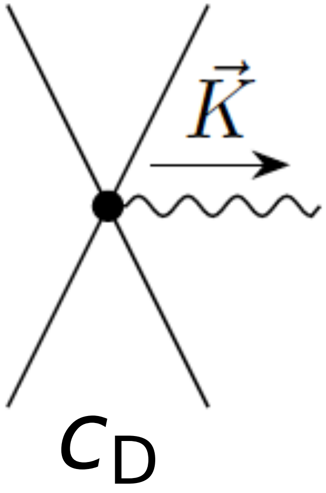
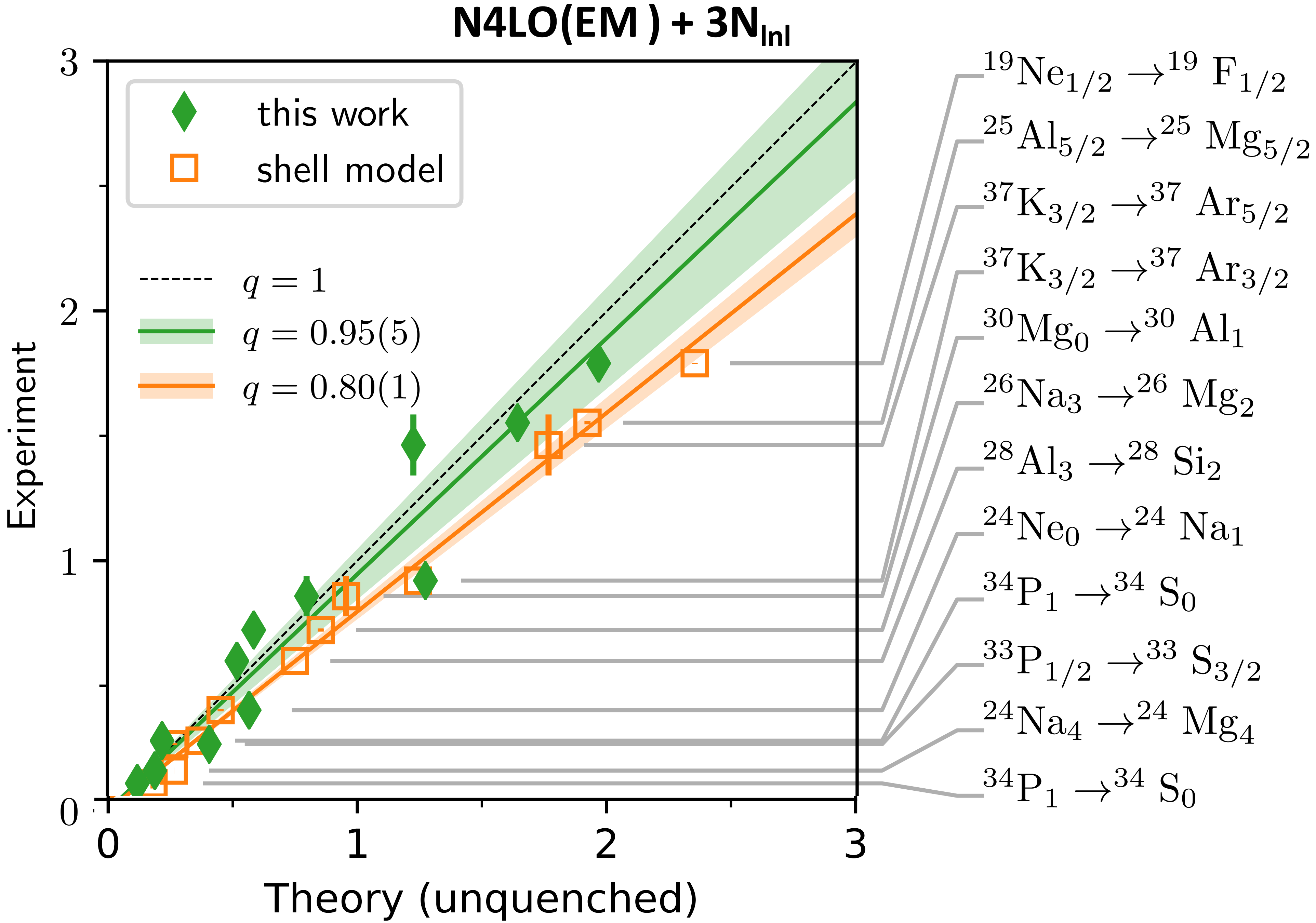
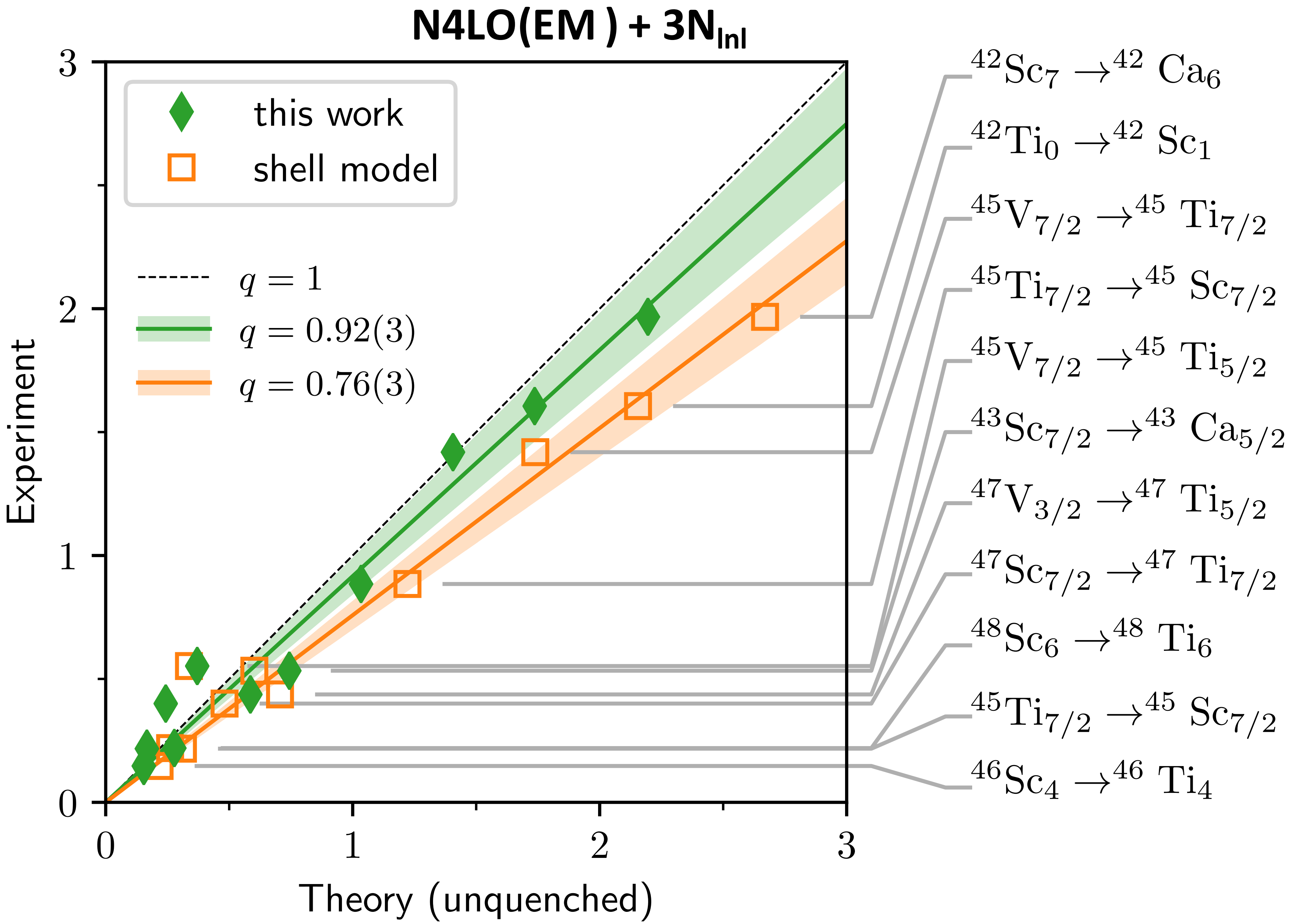


Short-ranged contact term of 2BC (heavy meson exchange)

The role of 2BC in the sd-shell

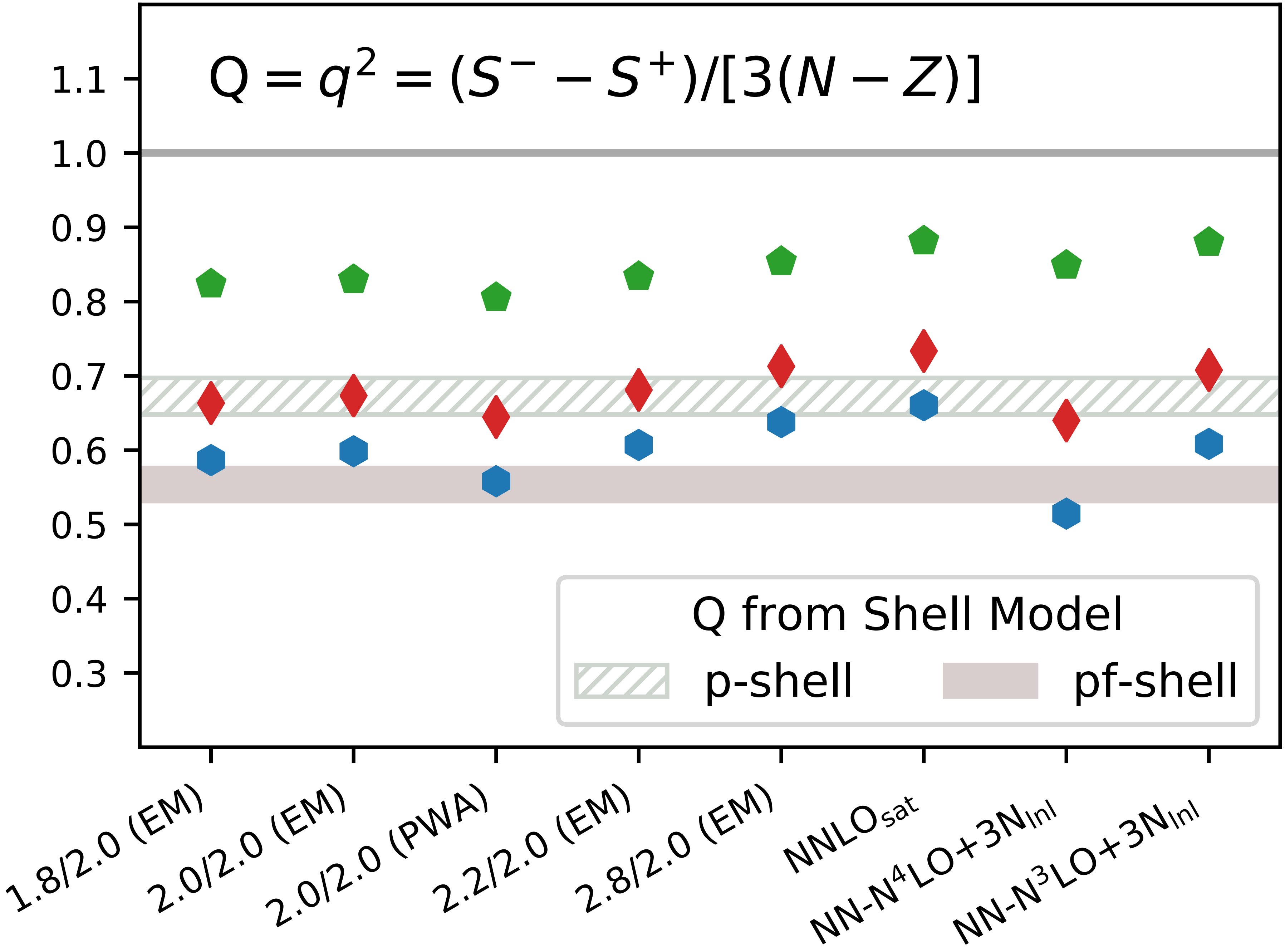


The role of 2BC in the pf-shell



N4LO(EM) + $3N_{lnl}$

Quenching of Ikeda sum-rule from 2BC



Summary

- Forces and 2BCs from chiral EFT explain (to large extent) the quenching of GT strength in atomic nuclei
- Make predictions for the super allowed GT transition in ^{100}Sn