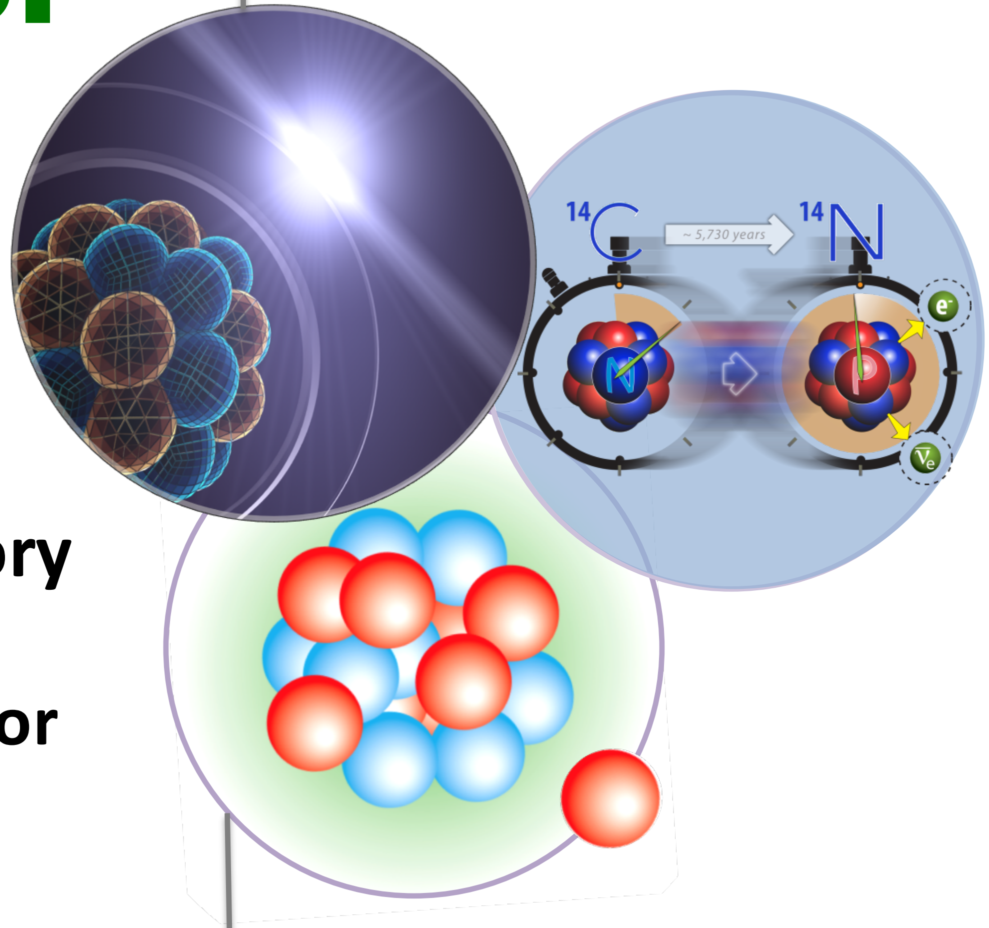
Coupled-cluster calculations of (double-) beta decays



Gaute Hagen
Oak Ridge National Laboratory

Atomic nuclei as laboratories for BSM physics

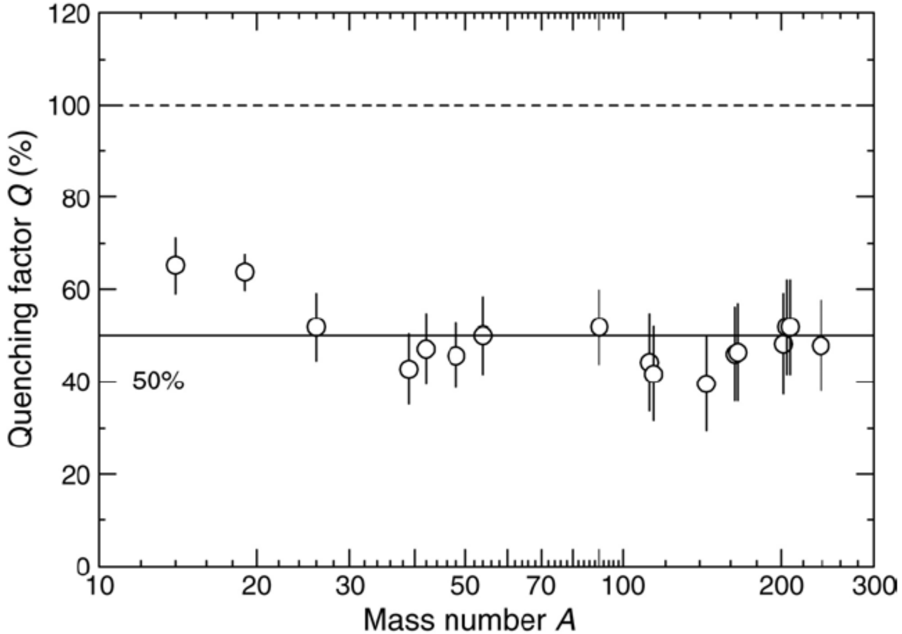
ECT, April 17th, 2019

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

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

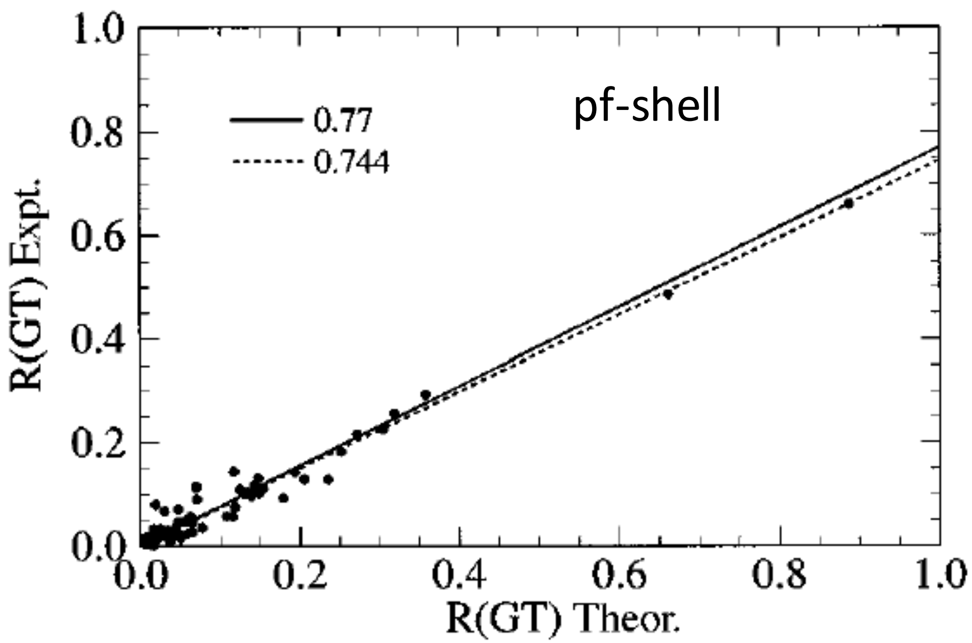
A 50 year old problem:
The puzzle of quenched of beta decays



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)



<u>This work:</u> Focus on strong Gamow-Teller transitions from light to heavy nuclei using state-of-the-art many-body methods with interactions and currents from Chiral EFT

nature physics

LETTERS

https://doi.org/10.1038/s41567-019-0450-7

Discrepancy between experimental and theoretical β-decay rates resolved from first principles

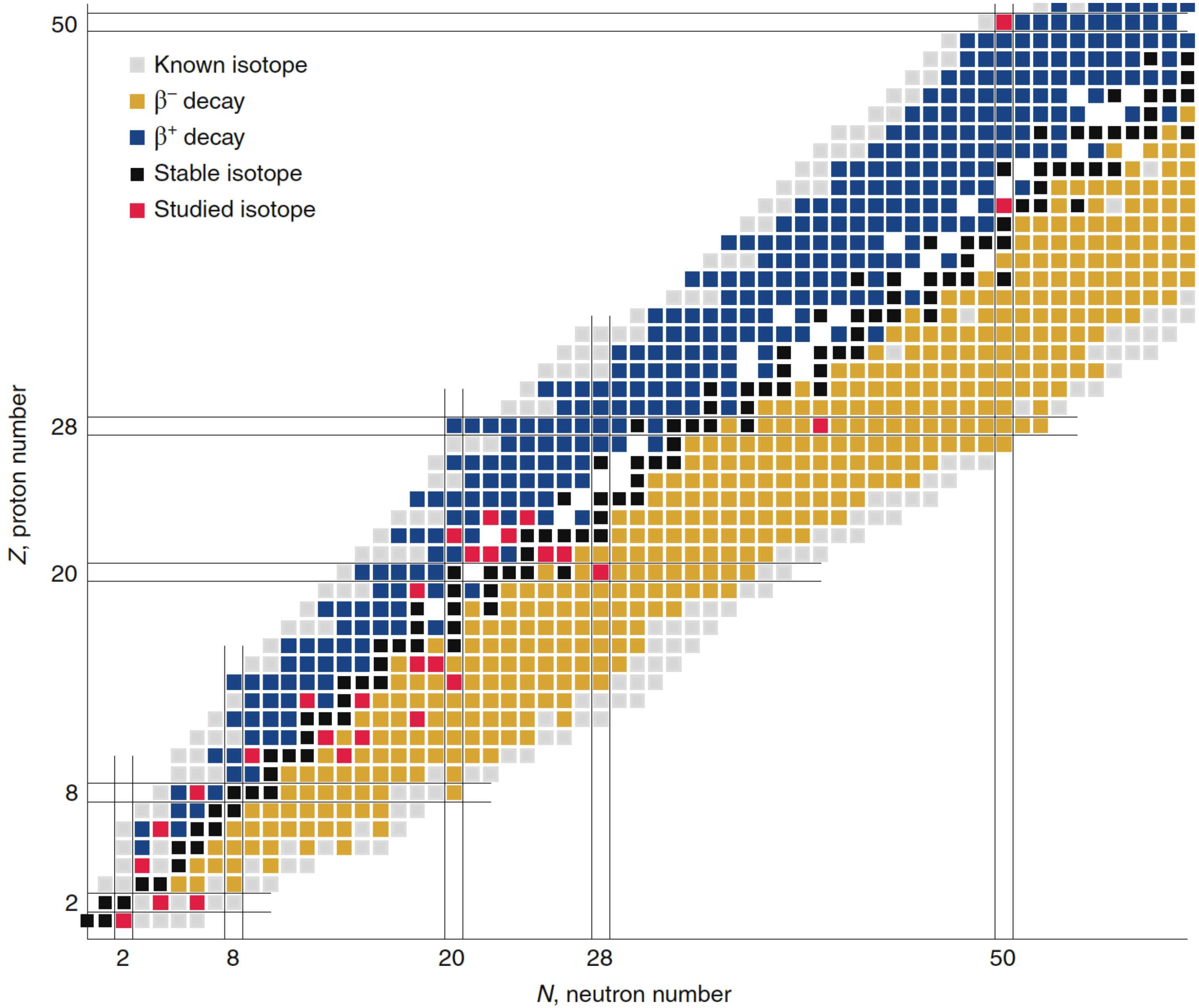
P. Gysbers[1,2], G. Hagen[3,4]*, J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

The dominant decay mode of atomic nuclei is beta decay (β-decay), a process that changes a neutron into a proton (and vice versa). This decay offers a window to physics beyond the standard model, and is at the heart of microphysical processes in stellar explosions and element synthesis in the Universe[1–3]. However, observed β-decay rates in nuclei have been found to be systematically smaller than for free neutrons: this 50-year-old puzzle about the apparent quenching of the fundamental coupling constant by a factor of about 0.75 (ref. [4]) is without a first-principles theoretical explanation. Here, we demonstrate that this quenching arises to a large extent from the coupling of the weak force to two nucleons as well as from strong correlations in the nucleus. We present state-of-the-art computations of β-decays from light- and medium-mass nuclei to ^{100}Sn by combining effective field theories of the strong and weak forces[5] with powerful quantum many-body techniques[6–8]. Our results are consistent with experimental data and have implications for heavy element synthesis in neutron star mergers[9–11] and predictions for the neutrino-less double-β-decay[3], where an analogous quenching puzzle is a source of uncertainty in extracting the neutrino mass scale[12].

data, and precision, from the systematically improvable EFT expansion. Moreover, EFT enables a consistent description of the coupling of weak interactions to two nucleons via two-body currents (2BCs). In the EFT approach, 2BCs enter as subleading corrections to the one-body standard Gamow–Teller operator $\sigma\tau^+$ (with Pauli spin and isospin matrices σ and τ, respectively); they are smaller but significant corrections to weak transitions as three-nucleon forces are smaller but significant corrections to the nuclear interaction[5,17].

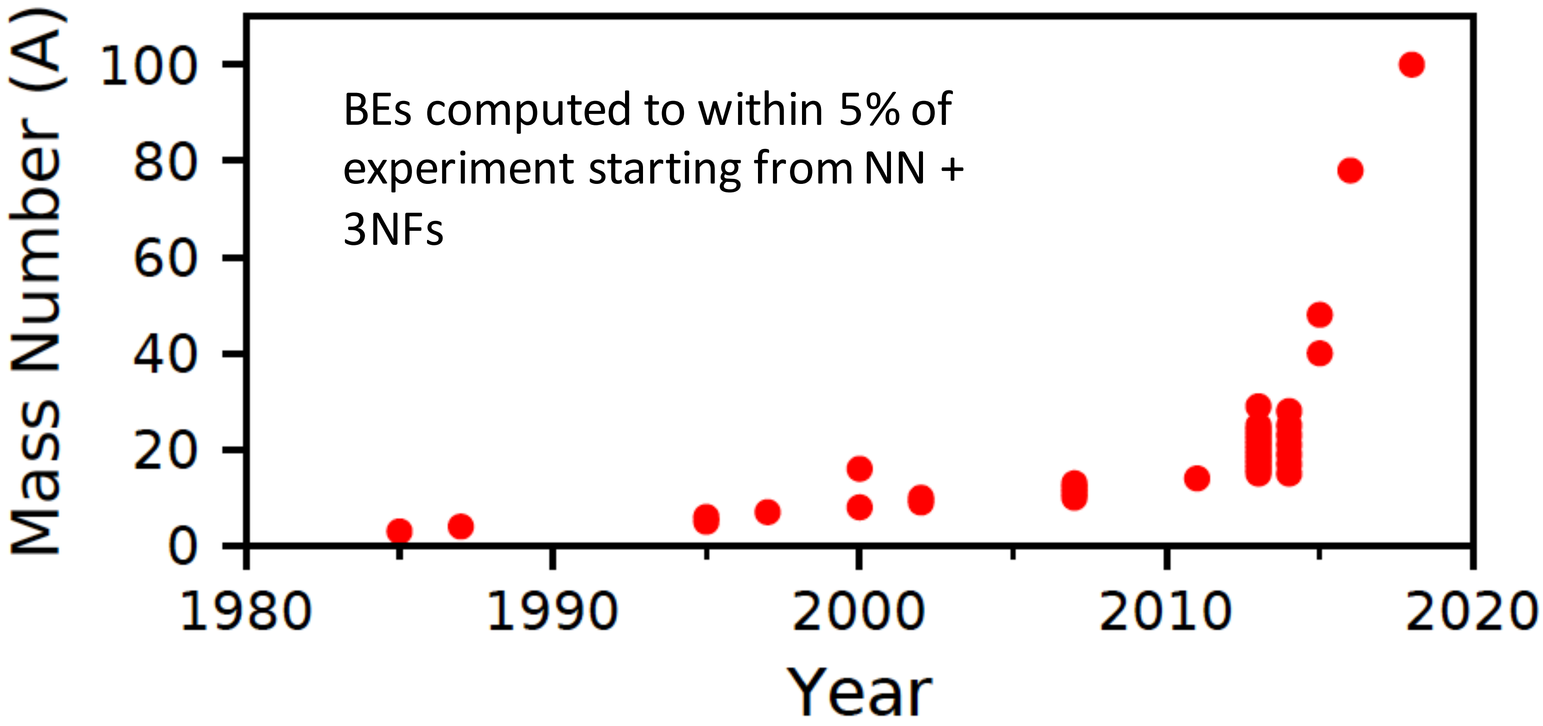
In this work we focus on strong Gamow–Teller transitions, where the effects of quenching should dominate over cancellations due to fine details (as occur in the famous case of the ^{14}C decay used for radiocarbon dating[18,19]). An excellent example is the superallowed β-decay of the doubly magic ^{100}Sn nucleus (Fig. 1), which exhibits the strongest Gamow–Teller strength so far measured in all atomic nuclei[20]. A first-principles description of this exotic decay, in such a heavy nucleus, presents a significant computational challenge. However, its equal 'magic' numbers ($Z=N=50$) of protons and neutrons arranged into complete shells makes ^{100}Sn an ideal candidate for large-scale coupled-cluster calculations[21], while the daughter nucleus ^{100}In can be reached via novel extensions of the high-order charge-exchange coupled-cluster methods developed

Isotopes studied in this work



Arnau Rios, Nature News & Views (2019)
DOI: 10.1038/s41567-019-0483-y

What precision/accuracy can we aim for in ab-initio calculations of nuclei?



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

Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, …

What precision/accuracy can we aim for in ab-initio calculations of nuclei?

Total error budget:

$$\sigma_{Total} =$$
$$\sigma_{model/EFT} + \sigma_{data} + \sigma_{numerical} + \sigma_{method}$$

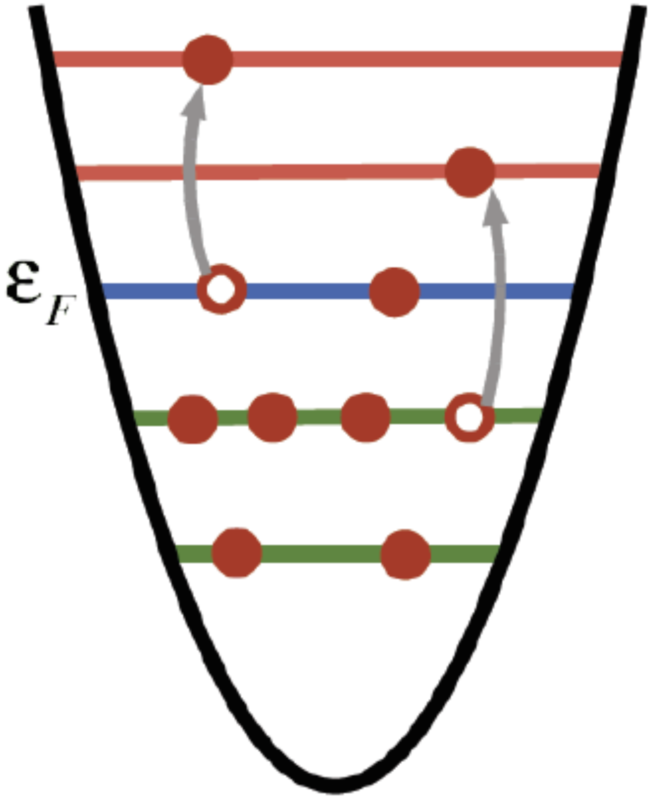
Ab-initio Method: Solve A-nucleon problem with controlled approximations and systematically improvable:

Coupled clusters, Green's function Monte Carlo, In-Medium SRG, Lattice EFT, MCSM, No-Core Shell Model, Self-Consistent Green's Function, UMOA, …

Correlation energy in wavefunction based methods

$$E = E_0 + \Delta E$$

Total energy



Mean-Field Energy

- Easy to calculate
- Provides a starting point for many-body methods

Correlation energy

- Hard to calculate (CC, IM-SRG, NCSM, SCGM)
- Non-observable
- Depends on the employed Hamiltonian and resolution scale

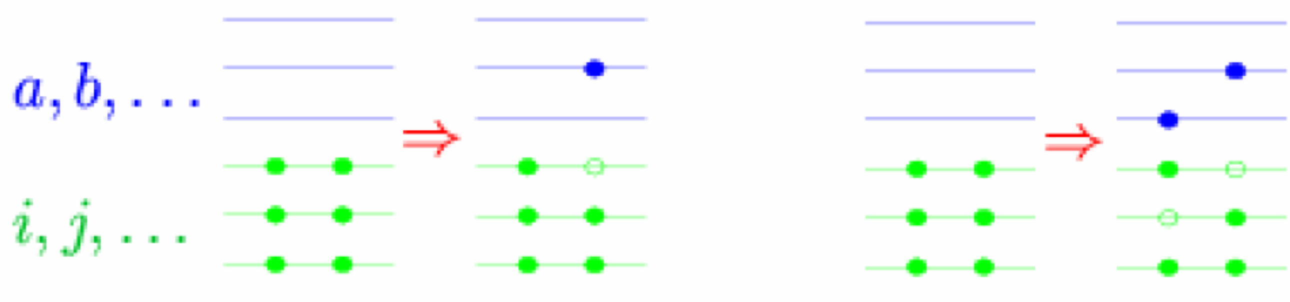
Coupled-cluster method (CCSD approximation)

Ansatz:

$$
\begin{aligned}
|\Psi\rangle &= e^{T}|\Phi\rangle \\
T &= T_1 + T_2 + \ldots \\
T_1 &= \sum_{ia} t_i^a a_a^\dagger a_i \\
T_2 &= \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i
\end{aligned}
$$

- ☺ Scales gently (polynomial) with increasing problem size o^2u^4 .
- ☺ Truncation is the only approximation.
- ☺ Size extensive (error scales with A)
- ☹ Most efficient for closed (sub-)shell nuclei

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



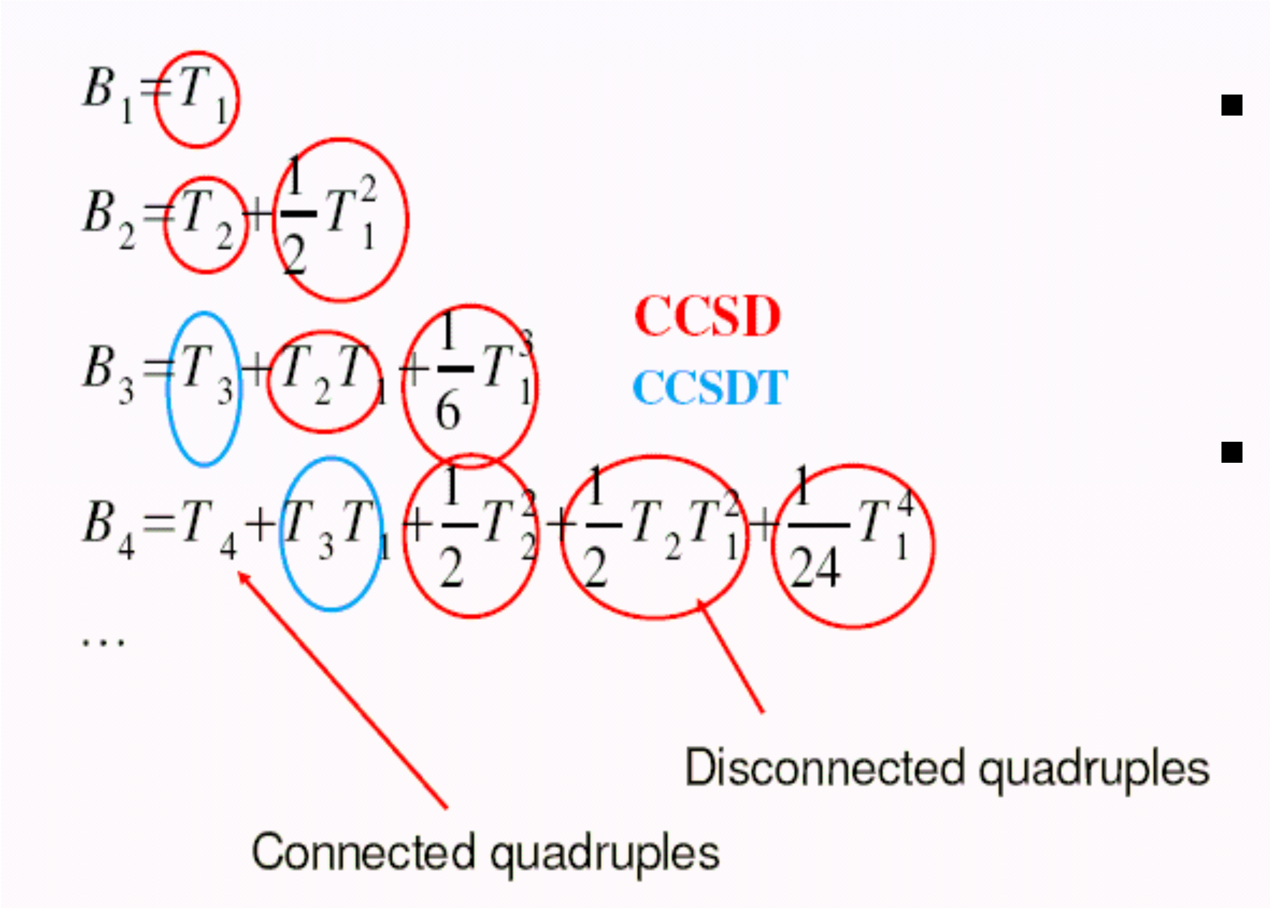
Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle
\end{aligned}
$$

Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

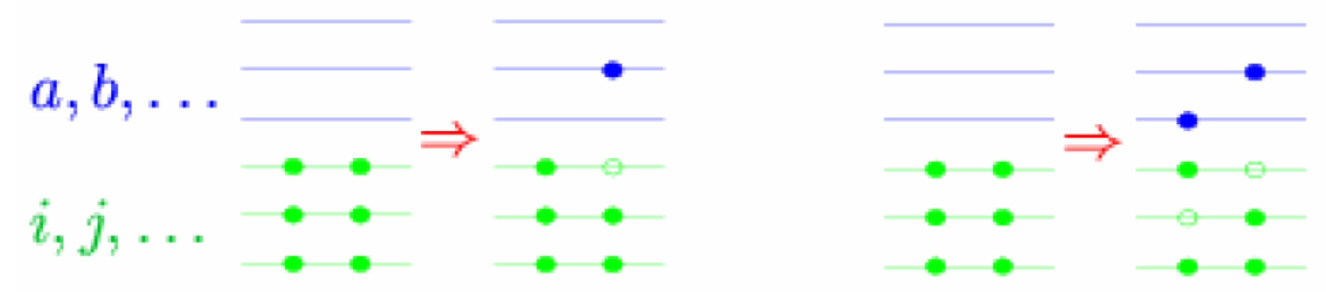
$$
\overline{H} \equiv e^{-T} H e^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
$$

Coupled-cluster method

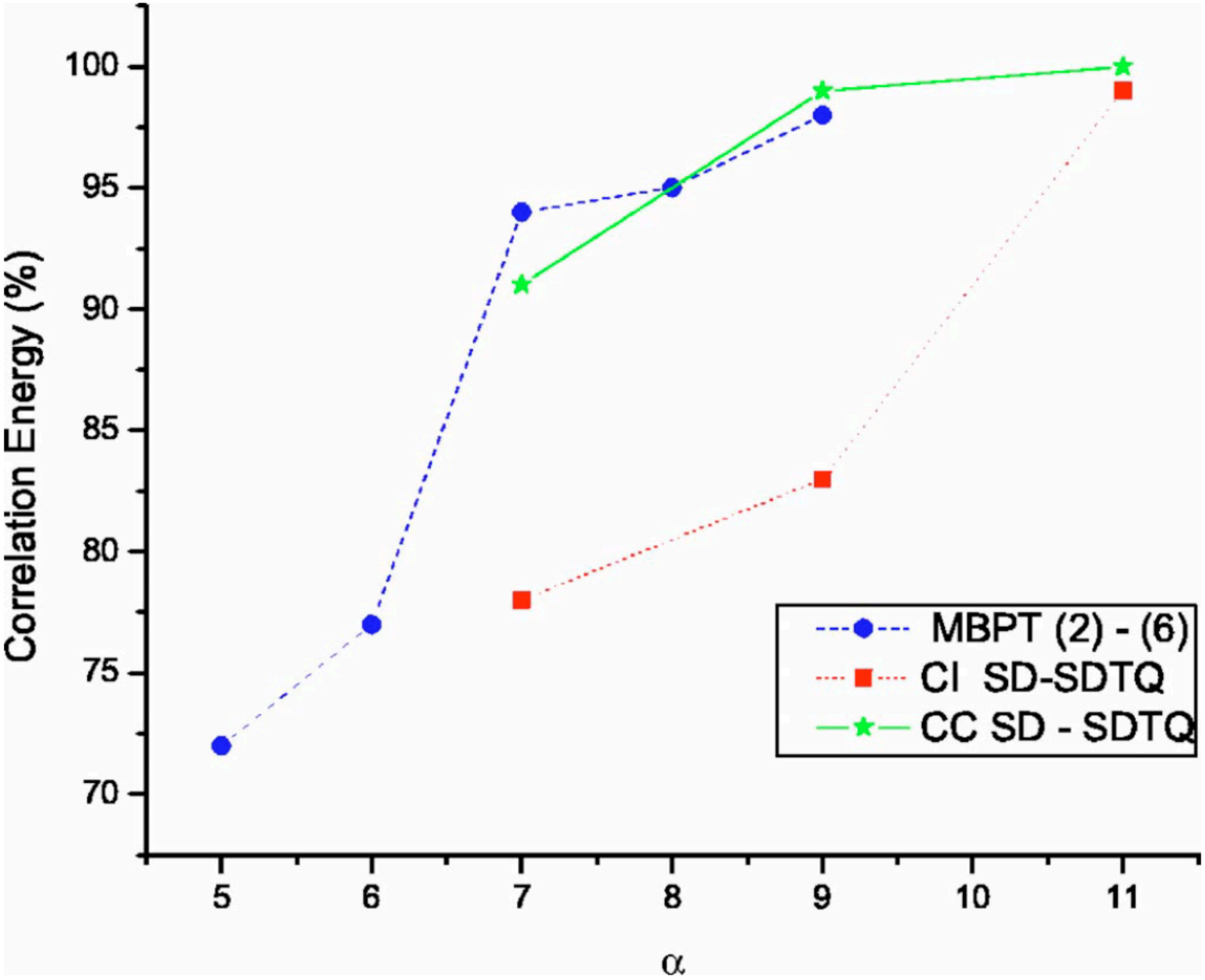


- CCSD captures most of the 3p3h and 4p4h excitations (scales as $n_o^2 n_u^4$)
- In order to describe α −cluster states need to include full quadruples (CCSDTQ) (scales $n_o^4 n_u^6$)

Correlations are *exponentiated* 1p-1h and 2p-2h excitations. Part of np-nh excitations included!



Coupled-cluster method



Bartlett & Musial Rev. Mod. Phys. (2007)

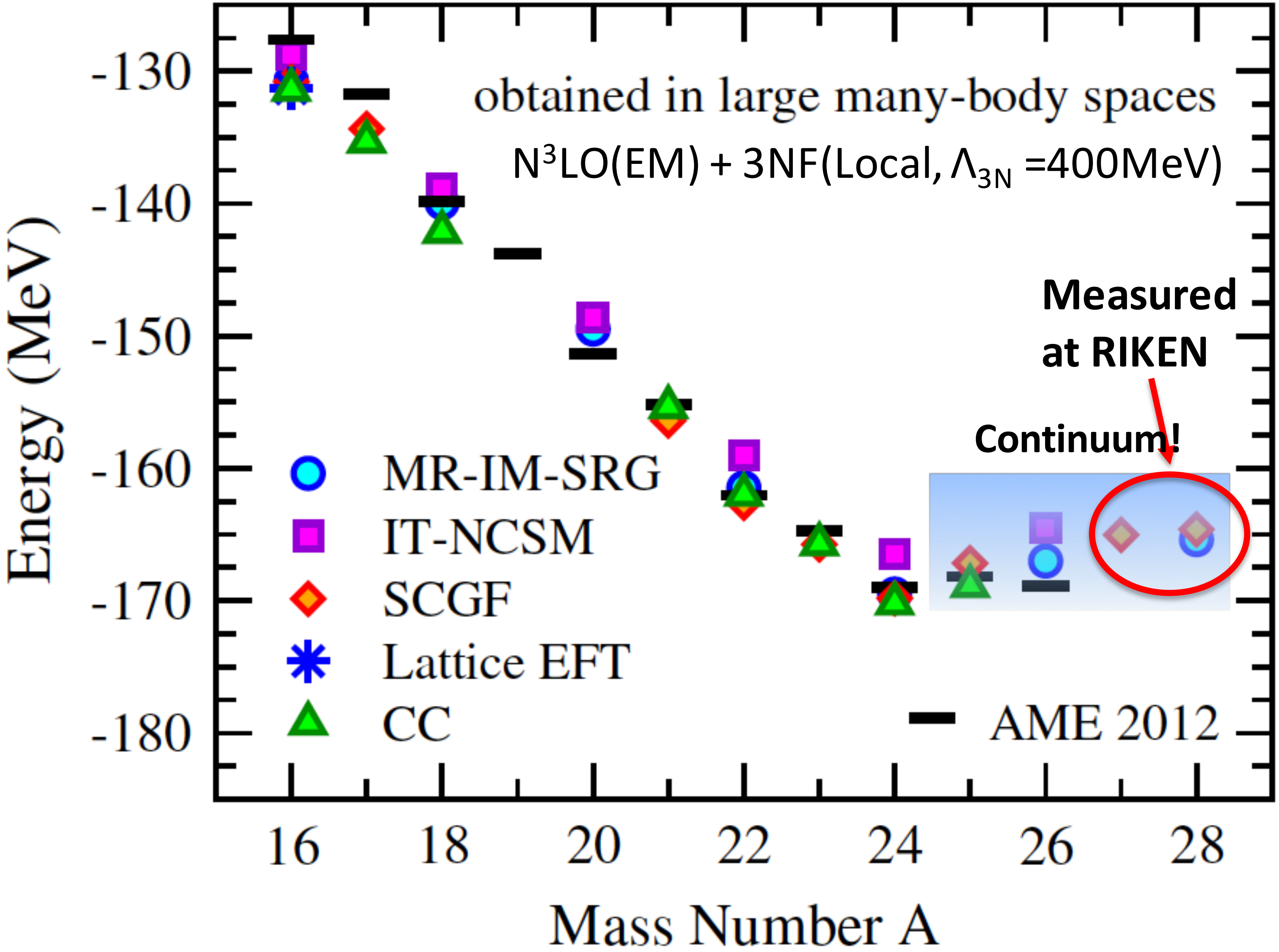
Coupled-cluster method

Energies	^{16}O	^{22}O	^{24}O	^{28}O
($\Lambda_\chi = 500$ MeV)				
E_0	25.946	46.52	50.74	63.85
ΔE_{CCSD}	−133.53	−171.31	−185.17	−200.63
ΔE_3	−13.31	−19.61	−19.91	−20.23
E	−120.89	−144.40	−154.34	−157.01
($\Lambda_\chi = 600$ MeV)				
E_0	22.08	46.33	52.94	68.57
ΔE_{CCSD}	−119.04	−156.51	−168.49	−182.42
ΔE_3	−14.95	−20.71	−22.49	−22.86
E	−111.91	−130.89	−138.04	−136.71
Experiment	−127.62	−162.03	−168.38	

G. Hagen, et al, Phys. Rev. C 80, 021306 (2009).

$\Delta E_3 \sim 10 - 13\%$

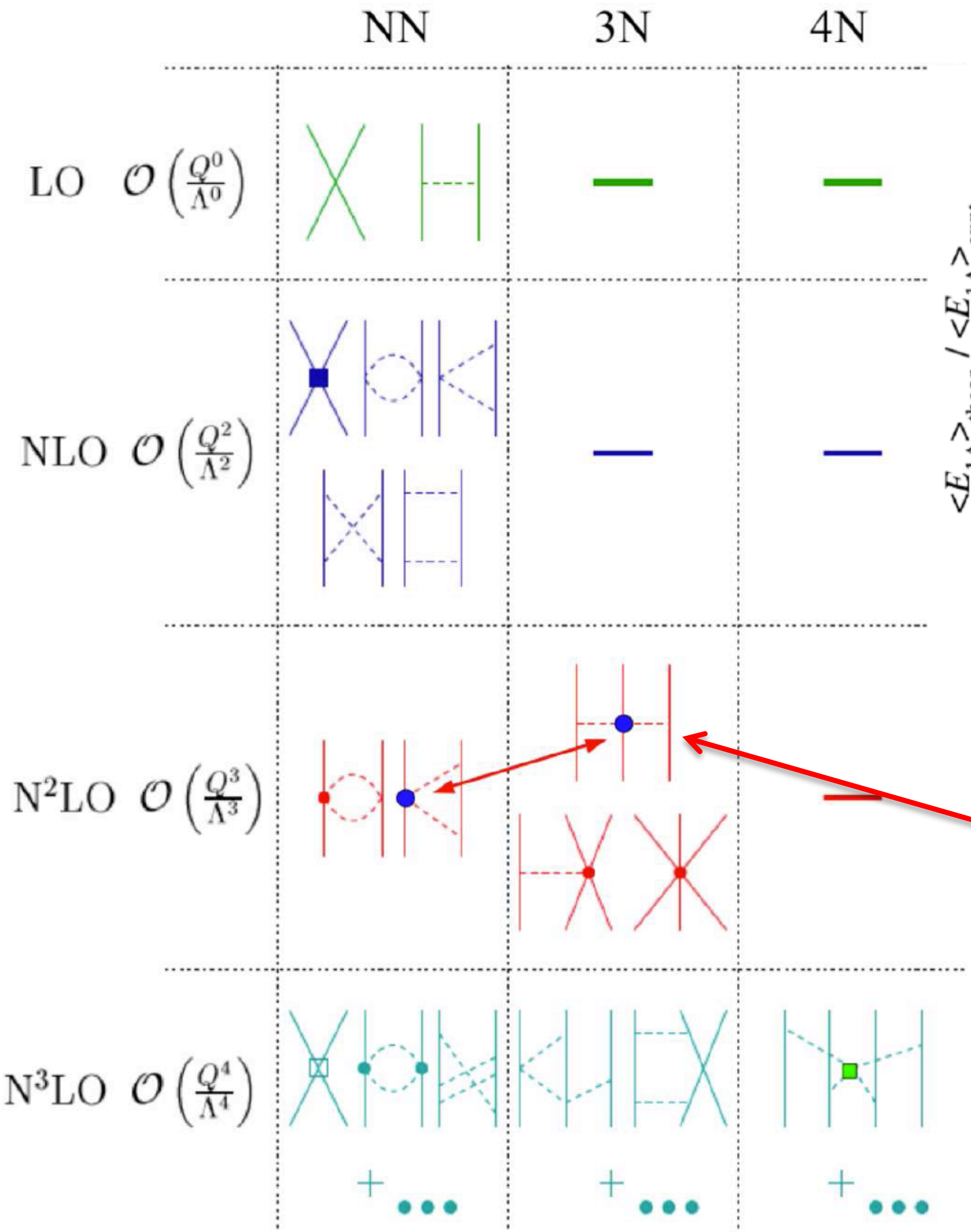
Oxgyen chain with interactions from chiral EFT



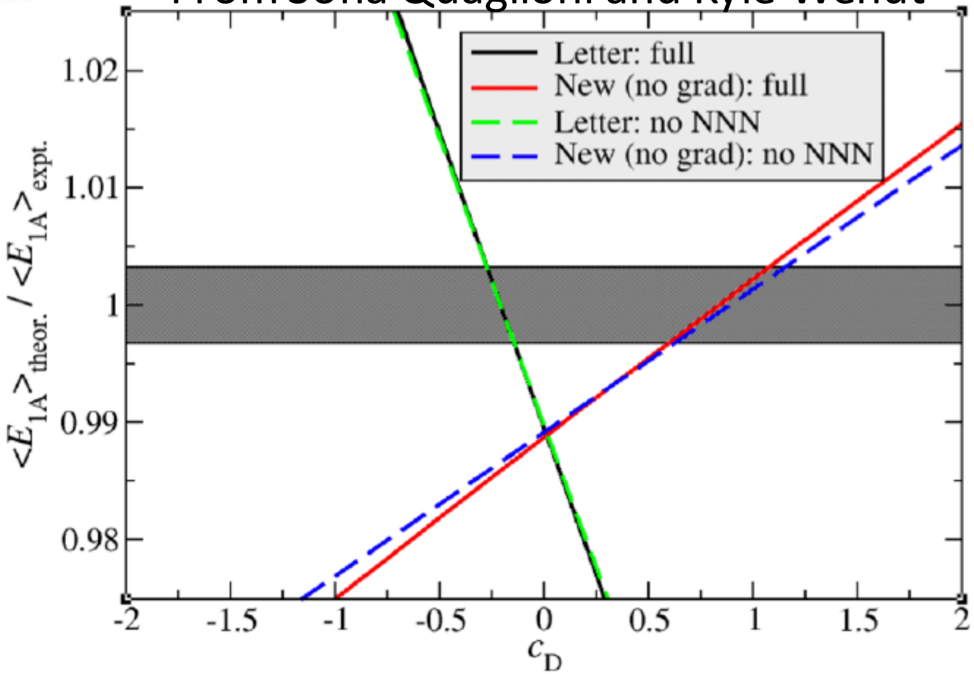
Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

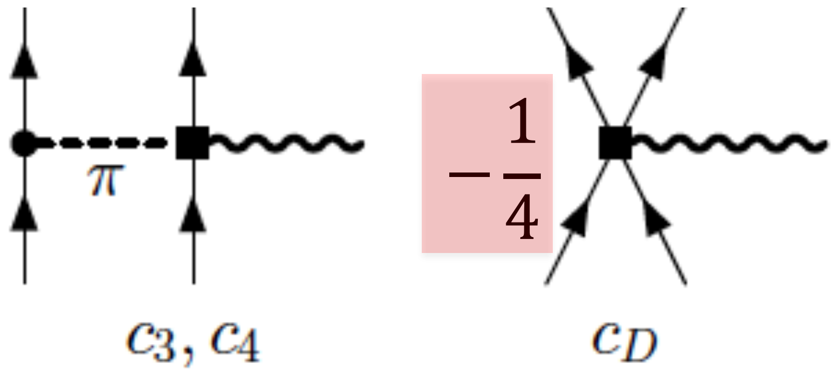
Nuclear forces from chiral effective field theory

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



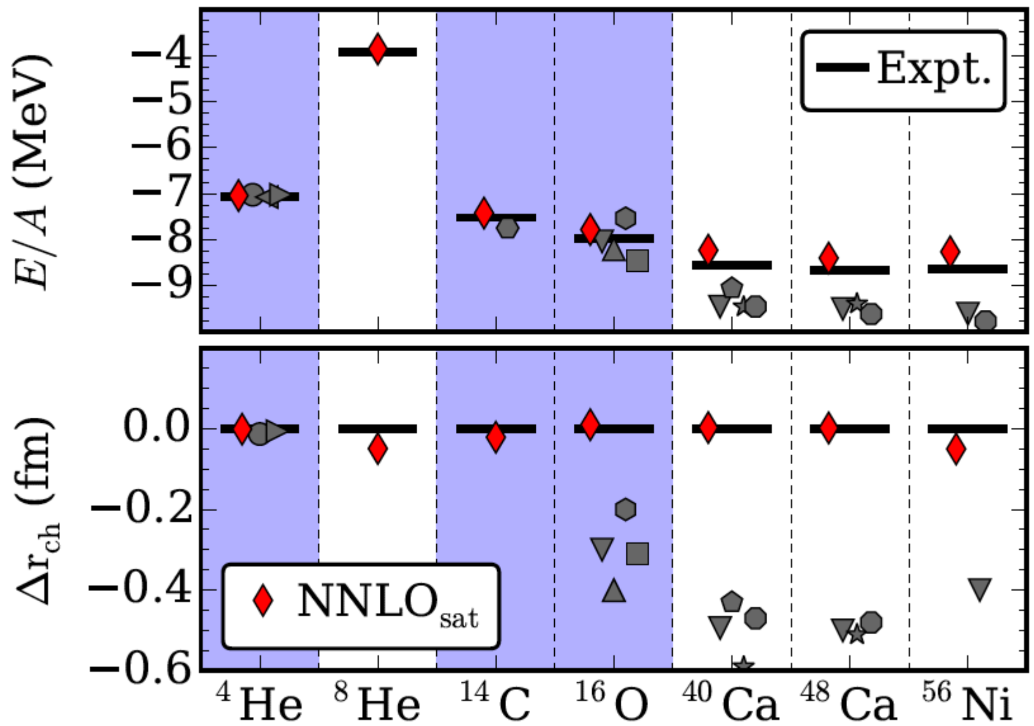
From Sofia Quaglioni and Kyle Wendt





Chiral EFT offers consistency between forces and currents

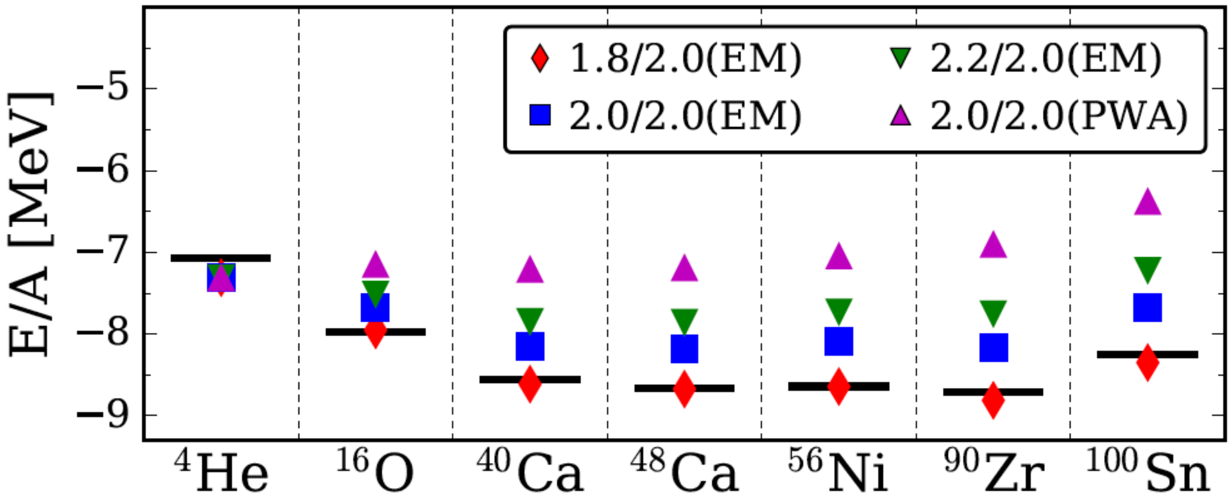
A family of interactions from chiral EFT



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

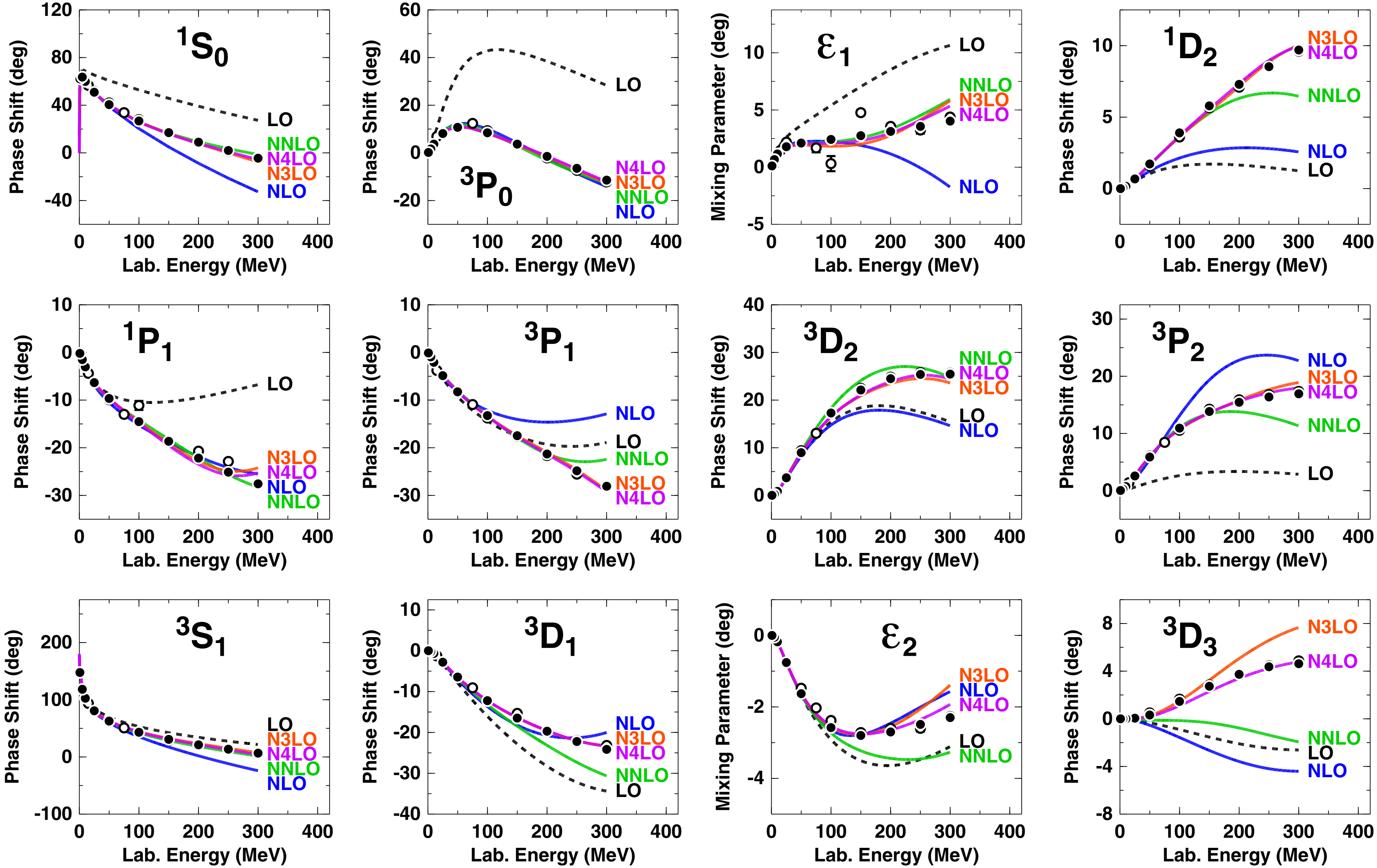
K. Hebeler *et al* PRC (2011).

T. Morris *et al*, PRL (2018).

PHYSICAL REVIEW C **96**, 024004 (2017)

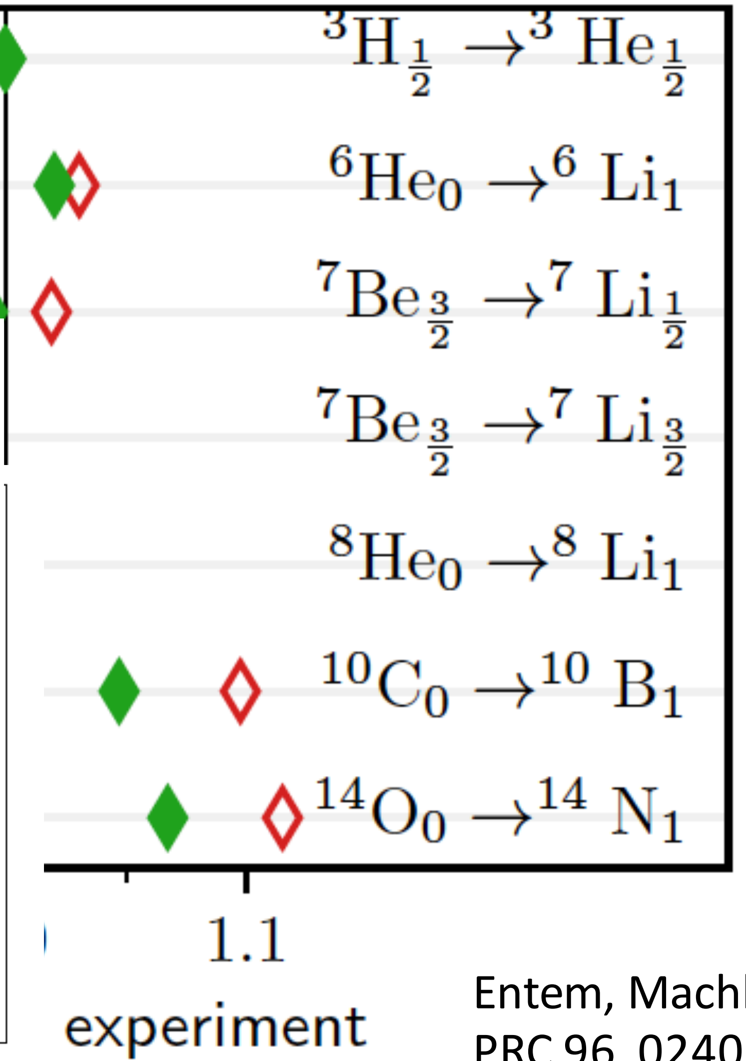
High-quality two-nucleon potentials up to fifth order of the chiral expansion

D. R. Entem,[1,*] R. Machleidt,[2,†] and Y. Nosyk[2]

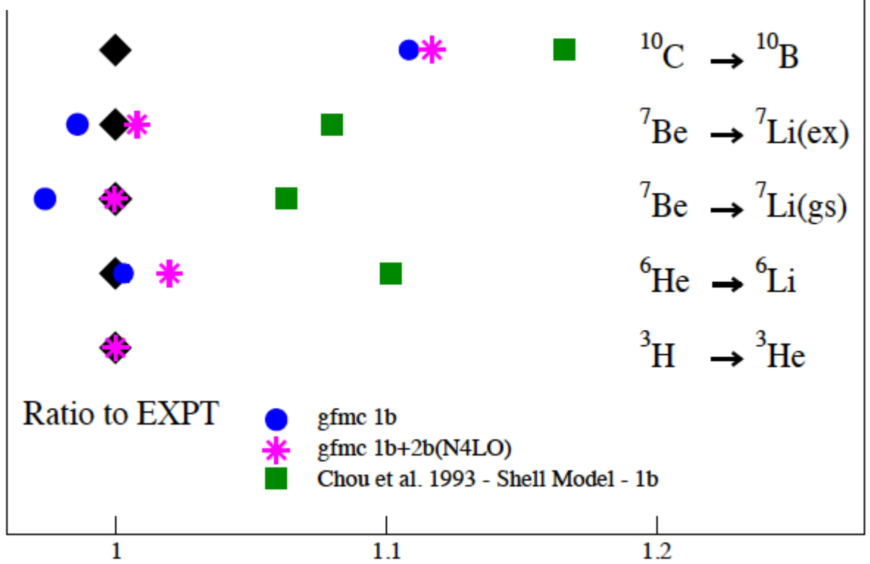


Theory to experiment ratios for beta decays in light nuclei from NCSM

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

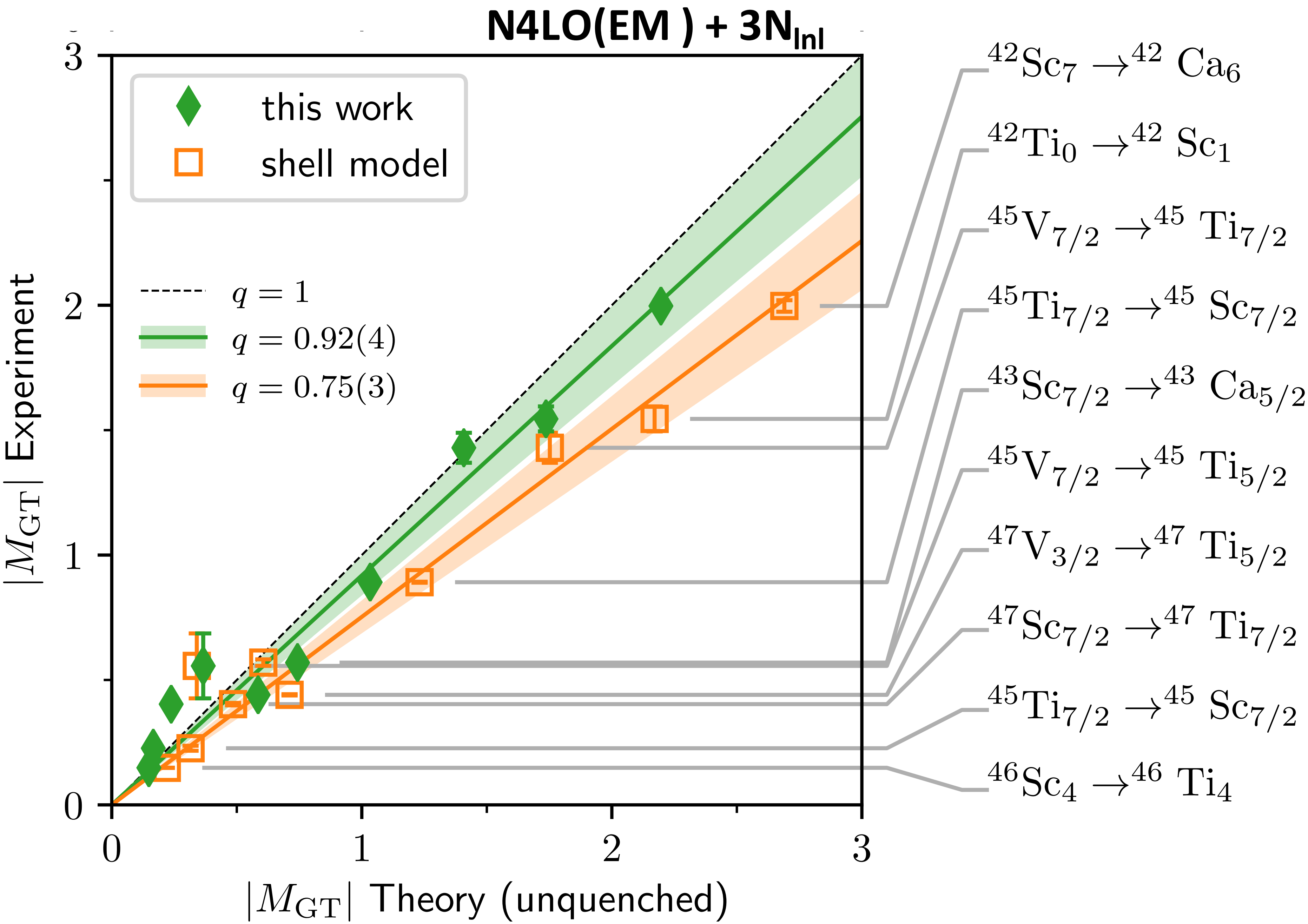


In QMC calculations of beta-decays 2BC increase the GT strength by 2-3%
S. Pastore et al, PRC 97, 022501 (2018).

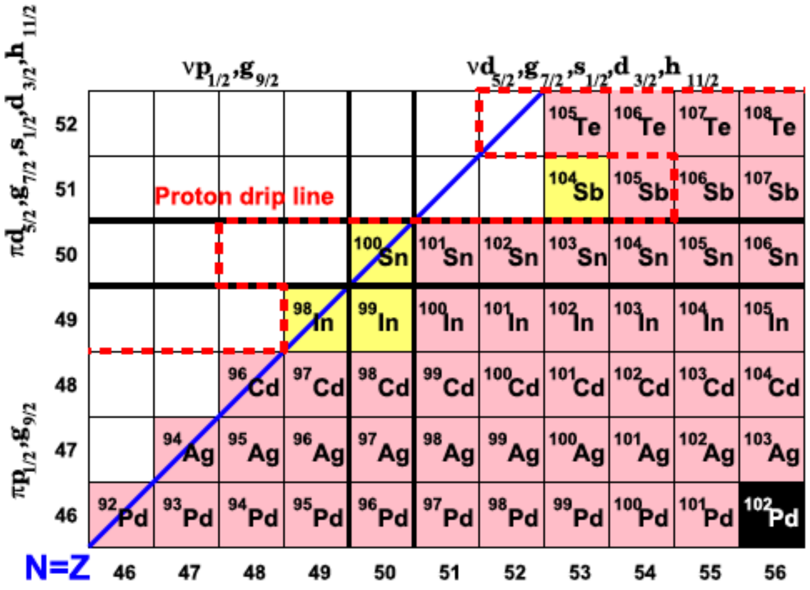


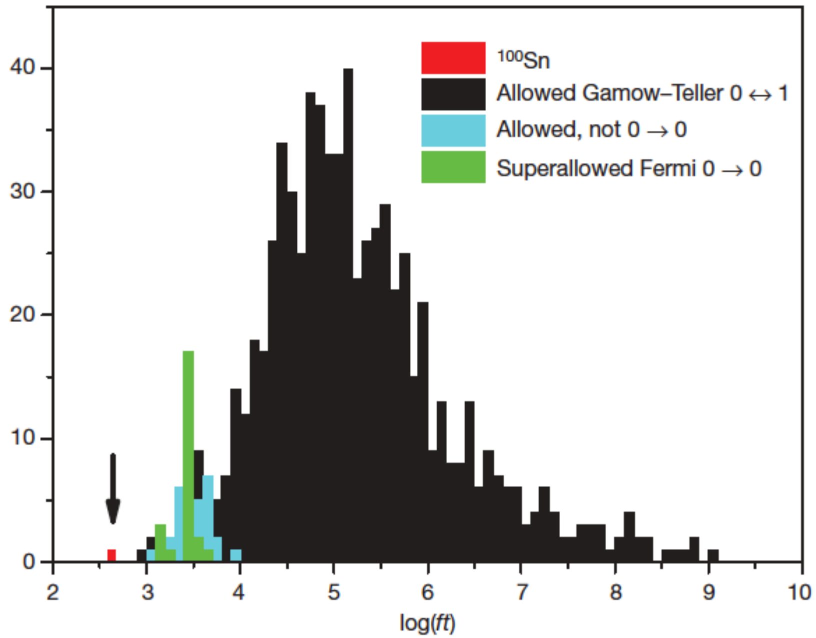
Entem, Machleidt & Nosyk, PRC 96, 024004 (2017)

The role of 2BC in the pf-shell



^{100}Sn – a nucleus of superlatives





Hinke et al, Nature (2012)

- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- Ideal nucleus for high-order CC approaches

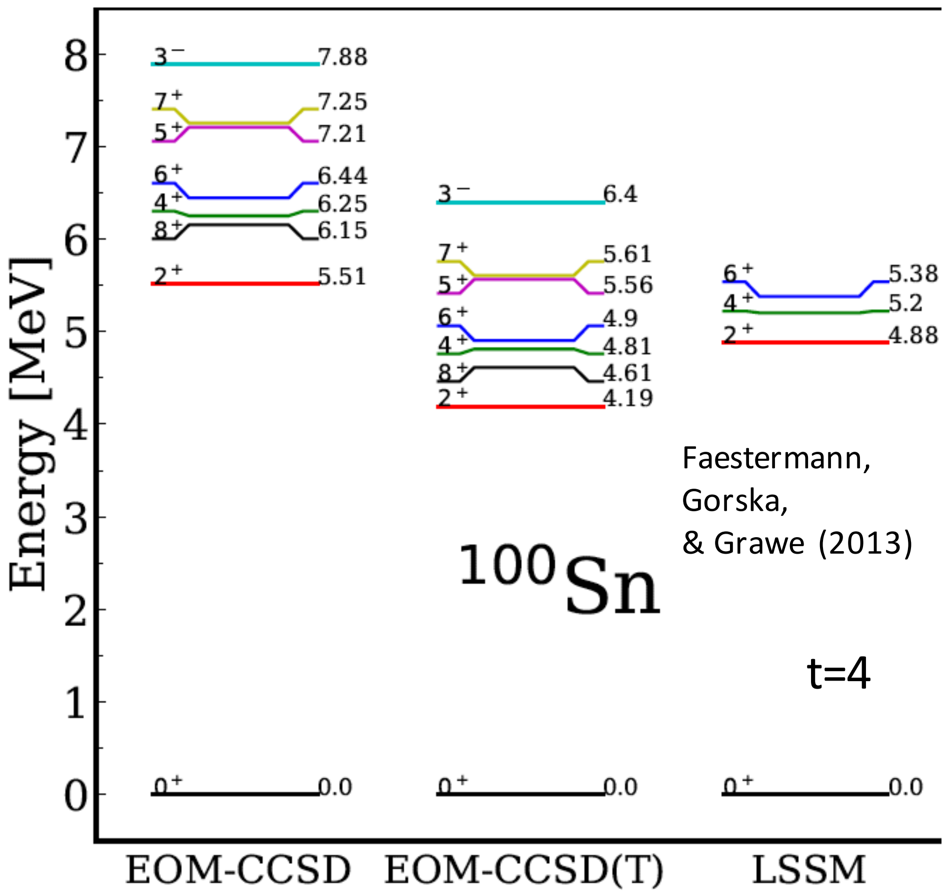
Quantify the effect of quenching from correlations and 2BCs

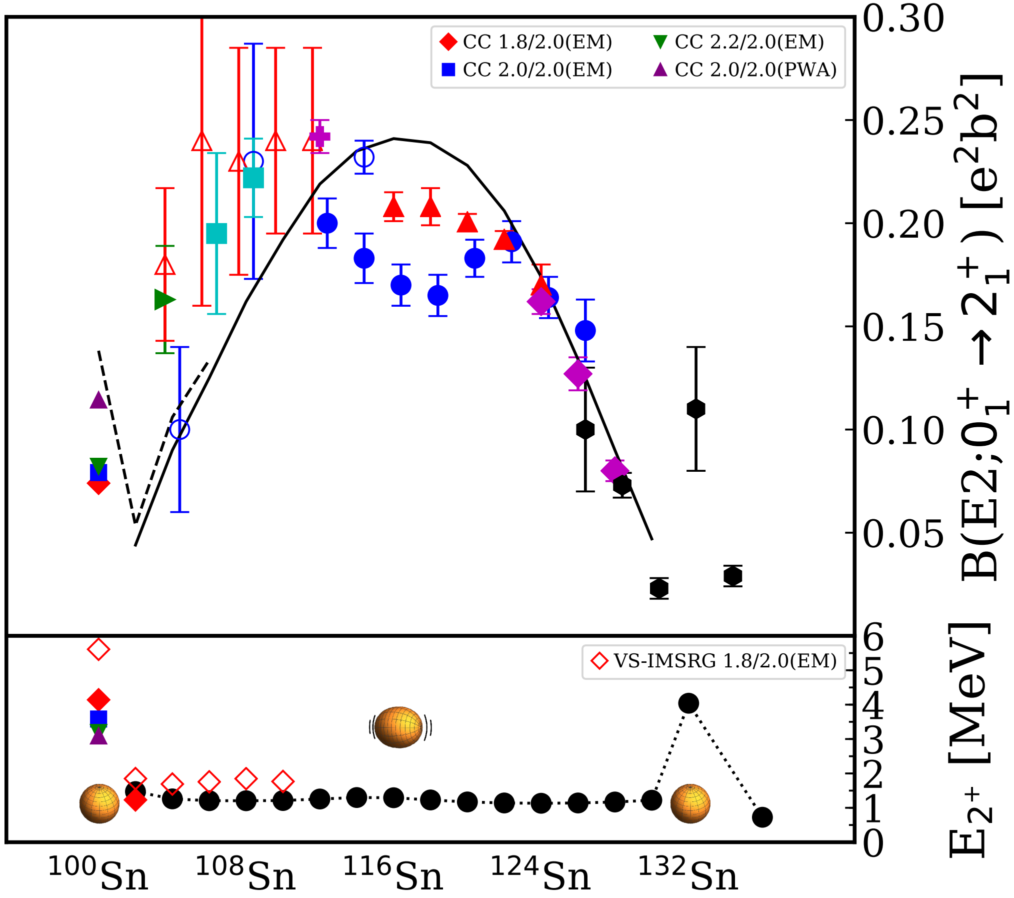
PHYSICAL REVIEW LETTERS 120, 152503 (2018)

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]



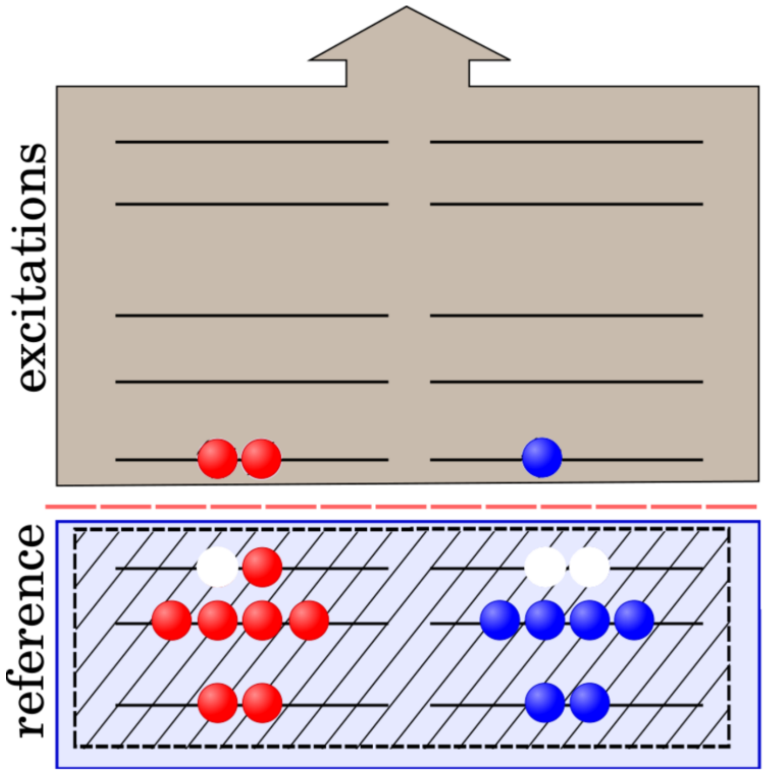


Coupled cluster calculations of beta-decay partners

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

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

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.

Charge exchange EOM-CCSDT-1

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

P-space (upper-left 2×2 block); Q-space

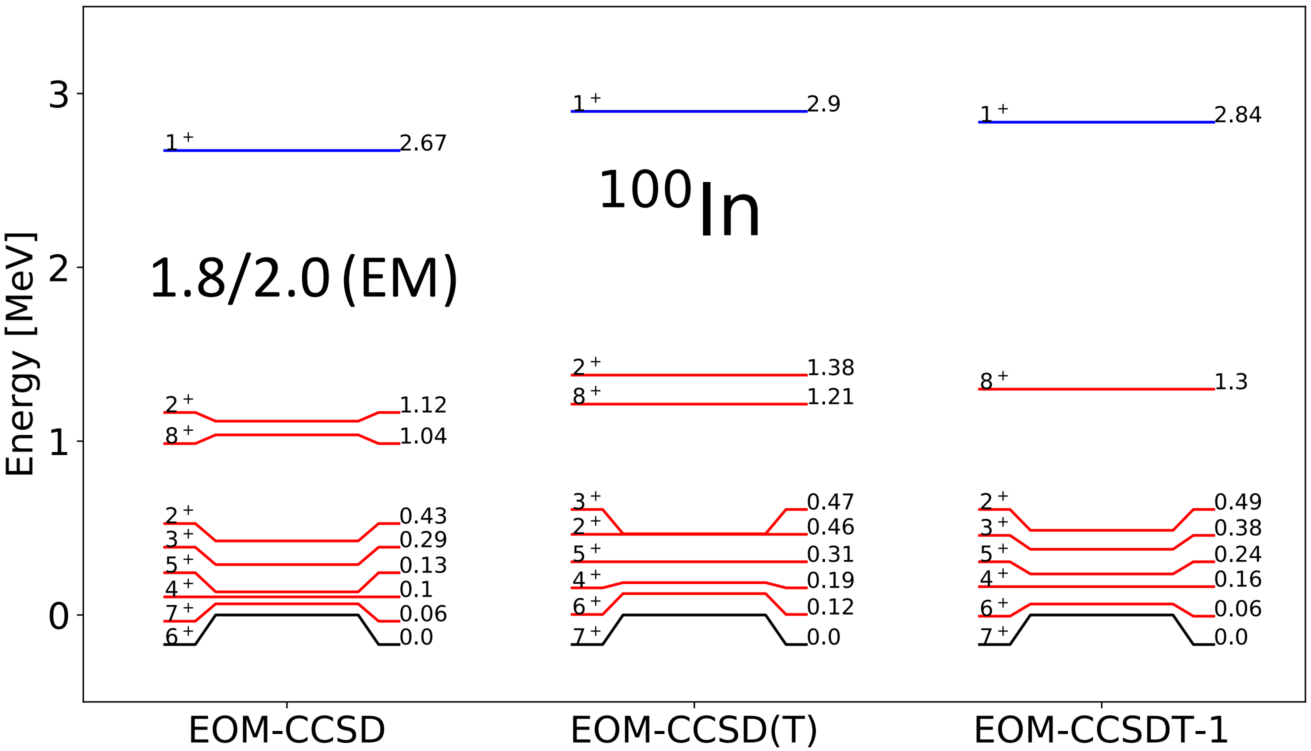
- Bloch-Horowitz is exact; iterative solution poss.

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

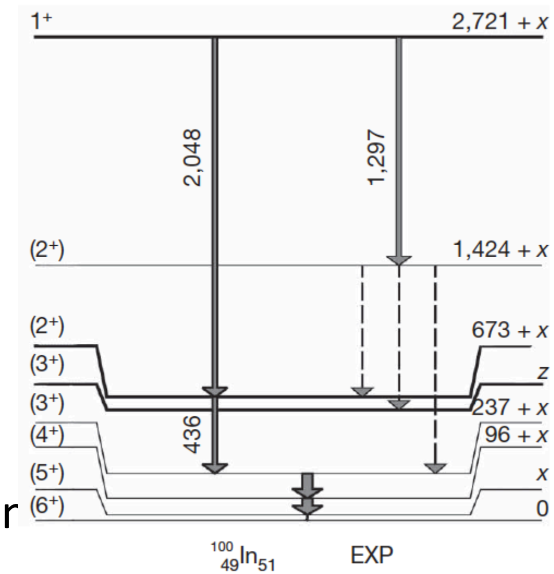
- Q-space is restricted to: $\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\max}$
- No large memory required for lanczos vectors
- Can only solve for one state at a time
- Reduces matrix dimension from ~10^9 to ~10^6

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)

Spectrum of daughter nucleus ^{100}In



Hinke et al, Nature (2012)



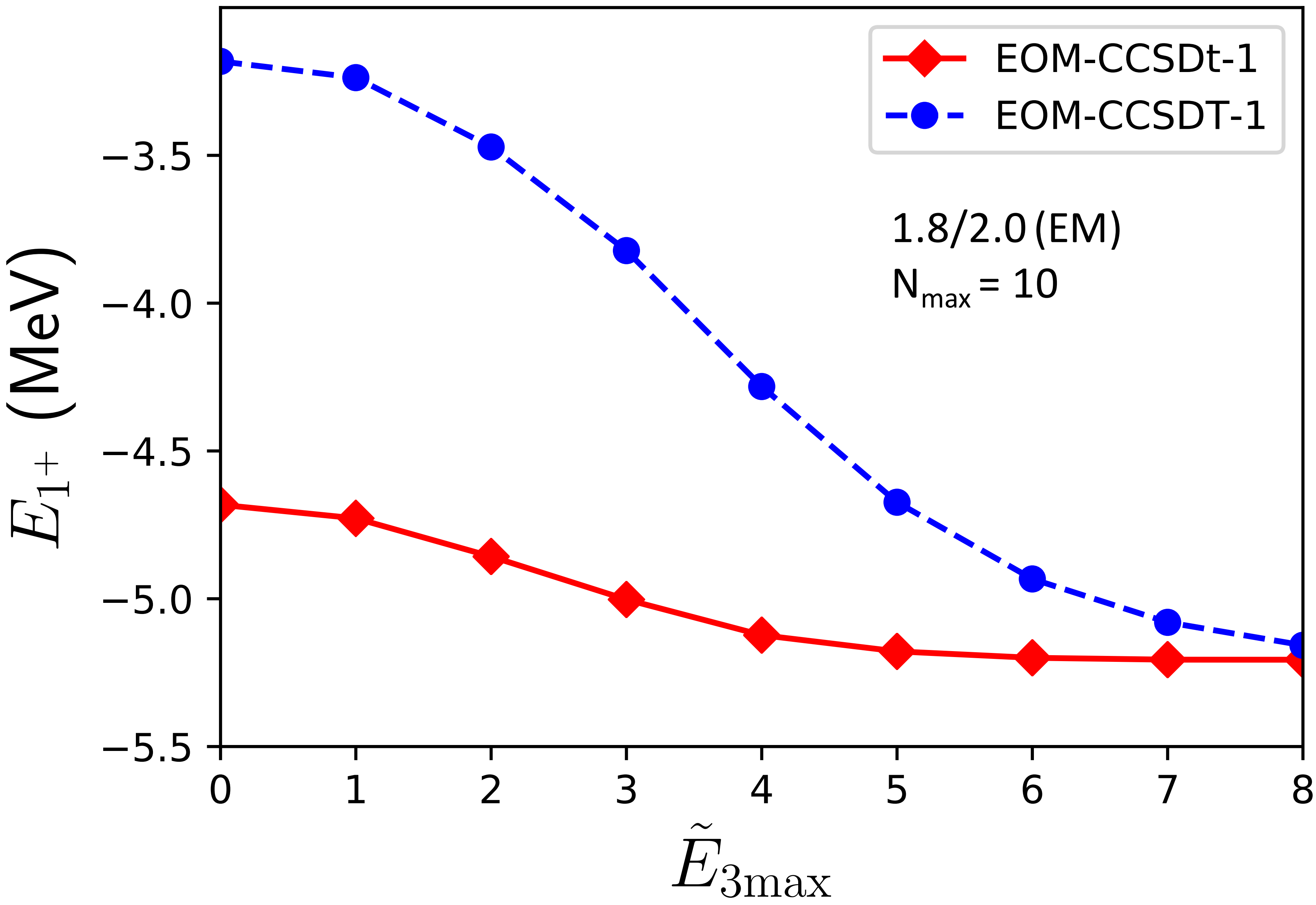
Q-space: $\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\mathrm{max}}$

Everything outside Q we label Q’

Use perturbative approach to calculate contribution from Q’:

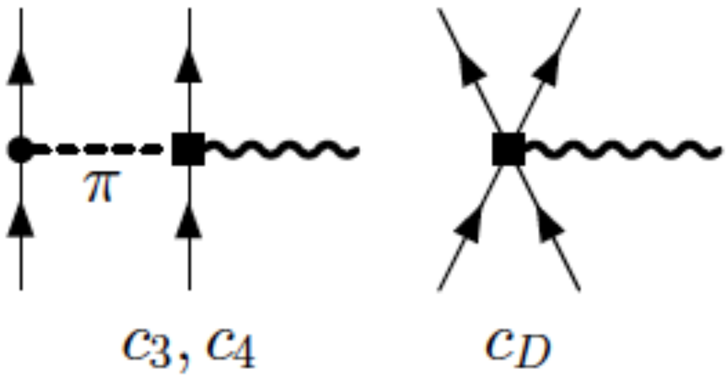
$$\Delta\omega_\mu = \langle \Phi_0 | L_\mu \overline{H}_{PQ'} (\omega_\mu - \overline{H}_{Q'Q'})^{-1} \overline{H}_{Q'P} R_\mu | \Phi_0 \rangle$$

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:

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

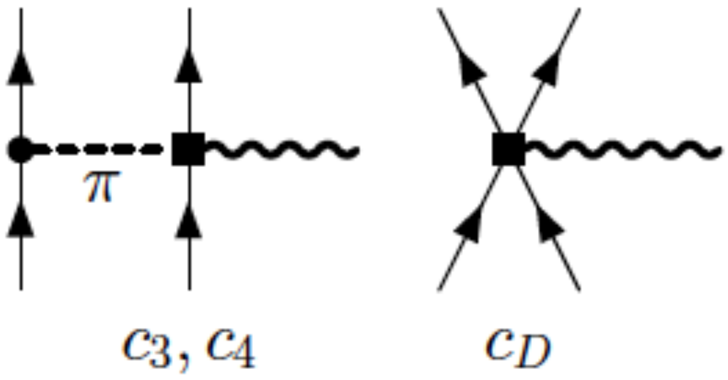
Benchmark between NCSM and CC using NN-N^{4}LO 3N$_{\mathrm{lnl}}$ in ^{8}He:

$$^8\mathrm{He}_0 \rightarrow {}^8\mathrm{Li}_1$$

Method	$\lvert M_{\mathrm{GT}}(\boldsymbol{\sigma\tau})\rvert$	$\lvert M_{\mathrm{GT}}\rvert$
EOM-CCSD	0.45	0.48
EOM-CCSDT-1	0.42	0.45
NCSM	0.41(3)	0.46(3)

Normal ordered one- and two-body current

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



Normal ordered operator:

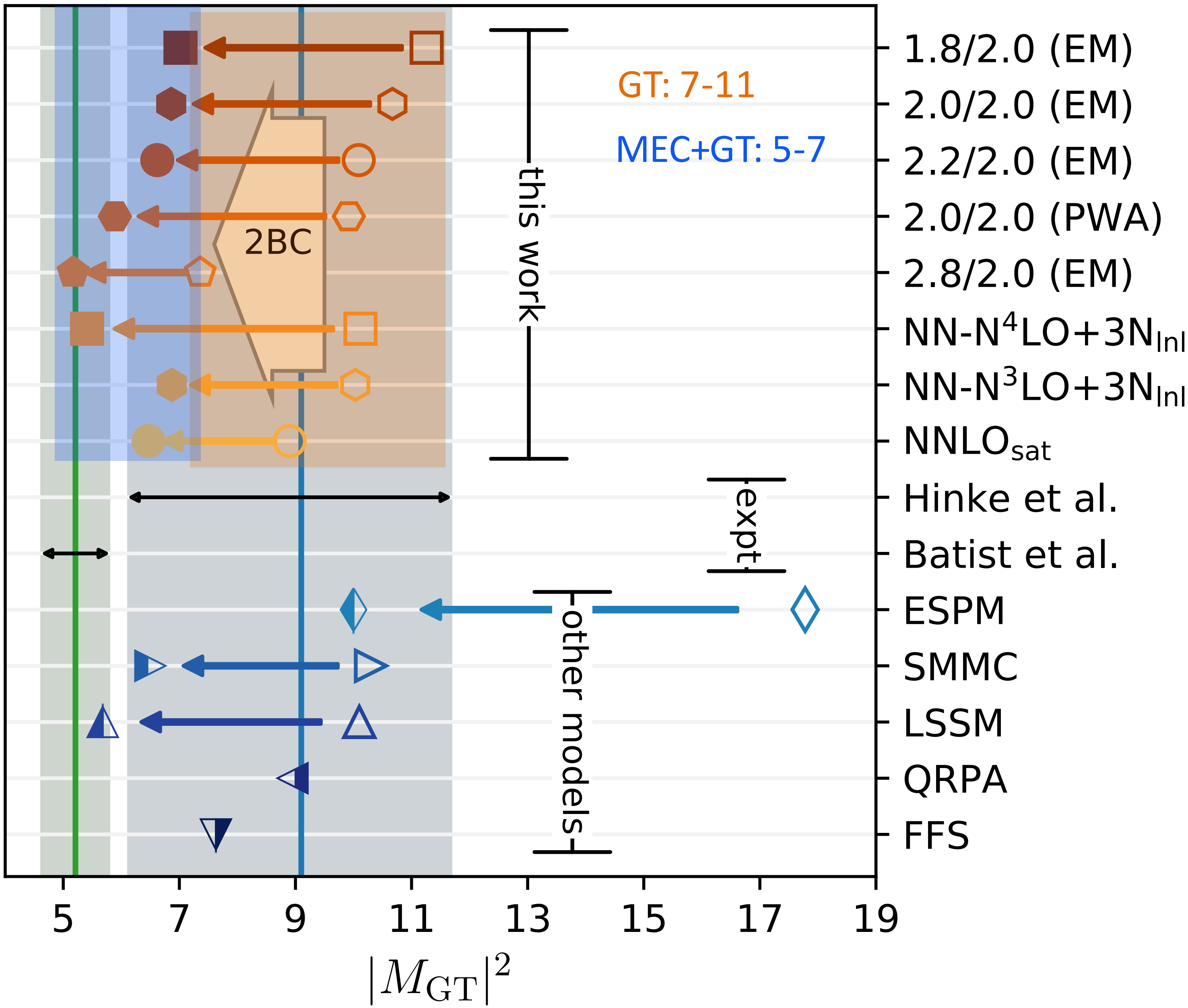
$$\hat{O}_{\rm GT} = O^1_N + O^2_N$$

Benchmark between NCSM and CC using NN-N^{4}LO 3N$_{\rm lnl}$ and NNLO$_{\rm sat}$:

$$^{14}{\rm O}_0 \rightarrow {}^{14}{\rm N}$$

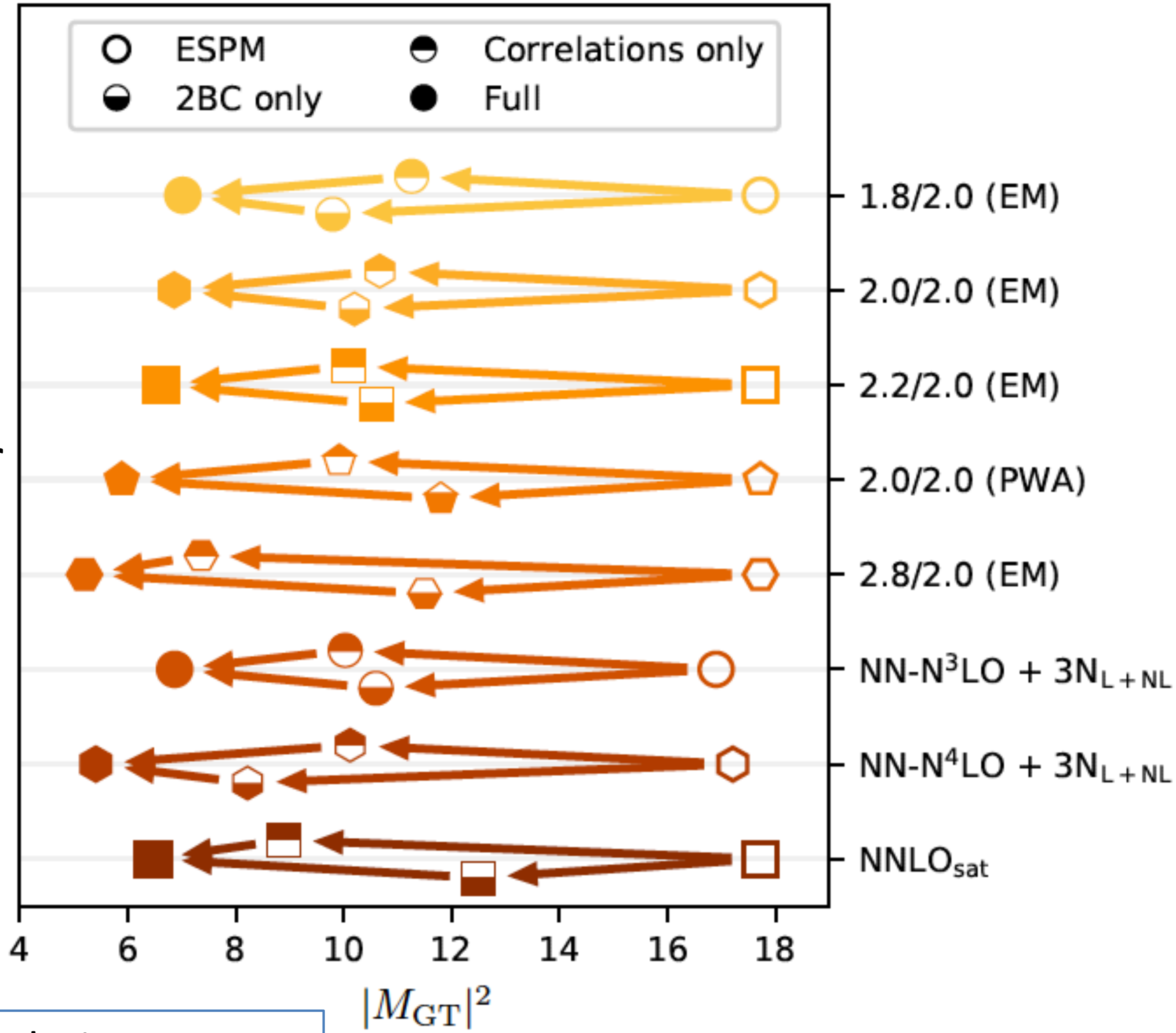
	$\lvert M_{\rm GT}(\boldsymbol{\sigma\tau})\rvert$		$\lvert M_{\rm GT}\rvert$	
Method	NNLO$_{\rm sat}$	NN-N^{4}LO +3N$_{\rm lnl}$	NNLO$_{\rm sat}$	NN-N^{4}LO +3N$_{\rm lnl}$
EOM-CCSD	2.15	2.0	2.08	2.0
EOM-CCSDT-1	1.77	1.97	1.69	1.86
NCSM	1.80(3)	1.86(3)	1.69(3)	1.78(3)

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



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

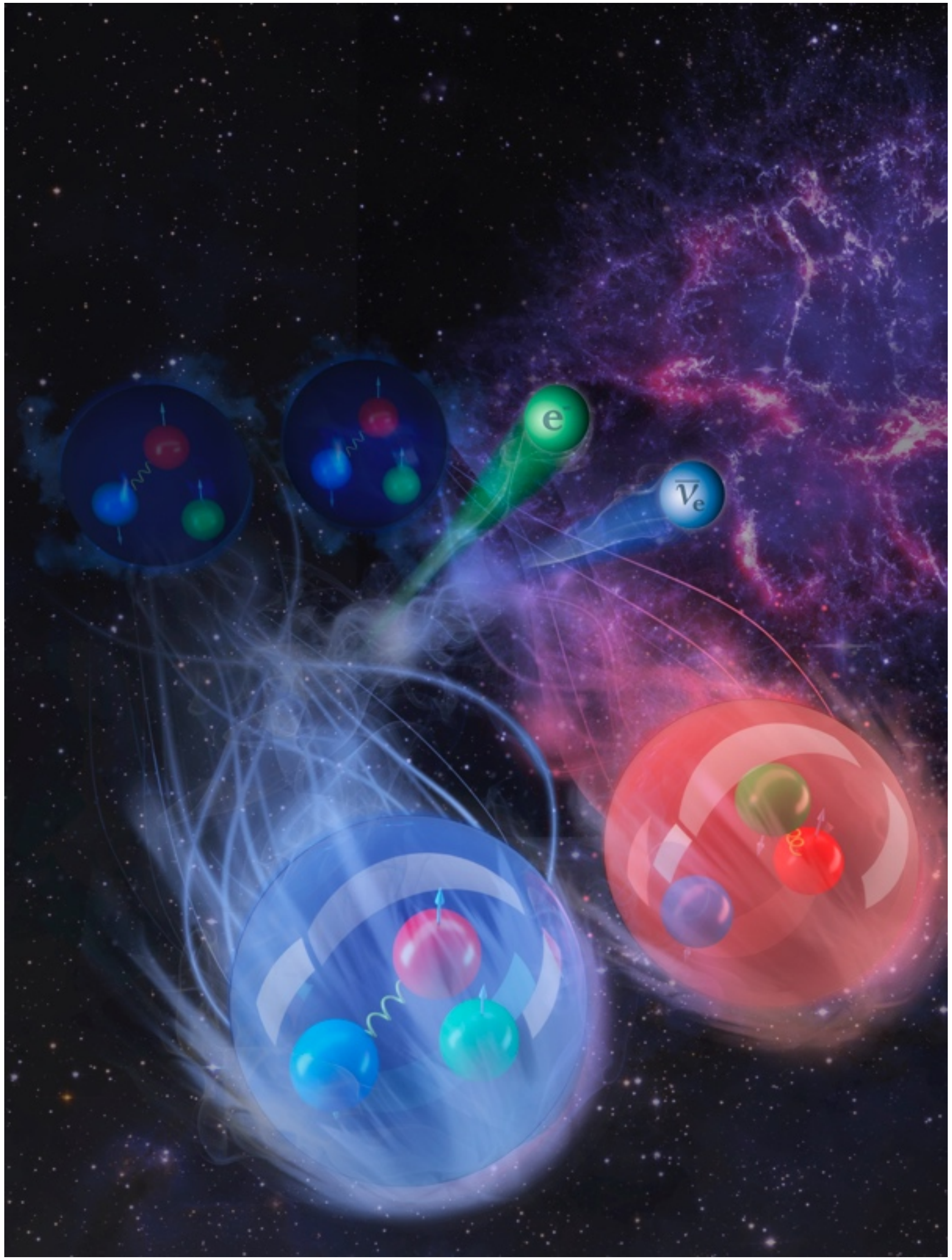
- Subtle interplay between correlations and 2BCs
- Role of correlations (2BC) increase (decrease) for larger cutoffs
- Only sum of correlations and 2BC is observable



Upper path: ESPM -> Correlations -> 2BC
Lower path: ESPM -> 2BC -> Correlations

Conclusions part 1

It is the combination of a proper treatment of strong nuclear correlations and two-body currents that to a large extent solves the beta decay quenching problem

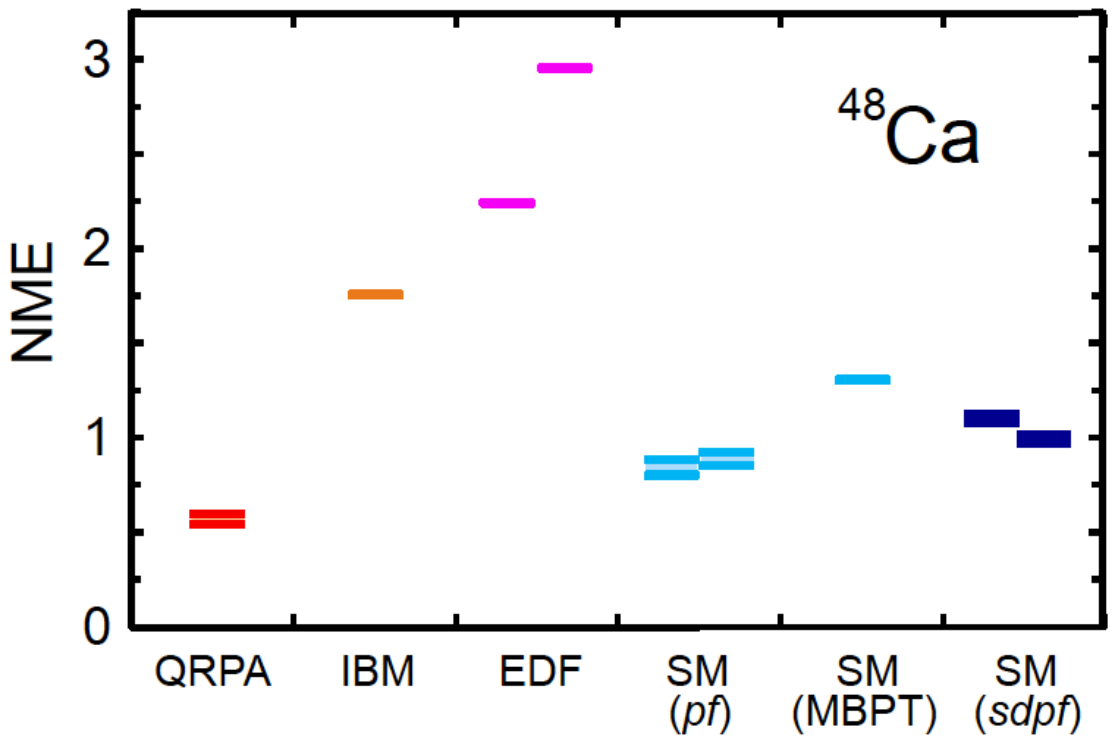


<u>For more details:</u>
P. Gysbers, G. Hagen, *et al*, Nature Physics,
https://www.nature.com/articles/s41567-019-0450-7

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 to six depending on the method
- Need to determine the NME more precisely with quantified uncertainties
- What does ab-initio calculations add to this picture?

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Editors' Suggestion Featured in Physics

New Leading Contribution to Neutrinoless Double-β Decay

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Within the framework of chiral effective field theory, we discuss the leading contributions to the neutrinoless double-beta decay transition operator induced by light Majorana neutrinos. Based on renormalization arguments in both dimensional regularization with minimal subtraction and a coordinate-space cutoff scheme, we show the need to introduce a leading-order short-range operator, missing in all current calculations. We discuss strategies to determine the finite part of the short-range coupling by matching to lattice QCD or by relating it via chiral symmetry to isospin-breaking observables in the two-nucleon sector. Finally, we speculate on the impact of this new contribution on nuclear matrix elements of relevance to experiment.

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Conclusion.—The above arguments suggest that the new leading-order short-range $\Delta L = 2$ potential identified in this Letter can affect the $0\nu\beta\beta$ amplitude and, consequently, the quantitative implications of experiments on $m_{\beta\beta}$ at the $\mathcal{O}(1)$ level. (At subleading orders, a similar analysis of the

Neutrinoless ββ-decay of ^{48}Ca

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

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

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

$$M^{0\nu}_{GT} + M^{0\nu}_{F} + M^{0\nu}_{T}$$

Compute ^{48}Ti using a double charge exchange equation of motion method: $\overline{H}_N R_\mu|\Phi_0\rangle = E_\mu R_\mu|\Phi_0\rangle$

$$R_\mu = \frac{1}{4}\sum_{ijab} r^{ab}_{ij} p^\dagger_a p^\dagger_b n_i n_j + \frac{1}{36}\sum_{ijkabc} r^{abc}_{ijk} p^\dagger_a p^\dagger_b N^\dagger_c N_k n_i n_j$$

$$L_\mu = \frac{1}{4}\sum_{ijab} l^{ij}_{ab} p_b p_a n^\dagger_i n^\dagger_j + \frac{1}{36}\sum_{ijkabc} l^{ijj}_{abc} p_a p_b N_c N^\dagger_k n^\dagger_i n^\dagger_j$$

ββ-decay of ^{48}Ca

$$M^{2\nu} = \sum_{\mu} \frac{\langle 0_f^+ | O_{\mathrm{GT}} | 1_\mu^+ \rangle \langle 1_\mu^+ | O_{\mathrm{GT}} | 0_i^+ \rangle}{E_\mu - E_i + Q_{\beta\beta}/2}$$

$$= \langle 0_f^+ | O_{\mathrm{GT}} \frac{1}{H - E_i + Q_{\beta\beta}/2} O_{\mathrm{GT}} | 0_i^+ \rangle$$

$$= \langle \Phi_0 | L_0 \overline{O}_{\mathrm{GT}} \frac{1}{\overline{H} - E_i + Q_{\beta\beta}/2} \overline{O}_{\mathrm{GT}} | \Phi_0 \rangle$$

Lanczos continued fraction method

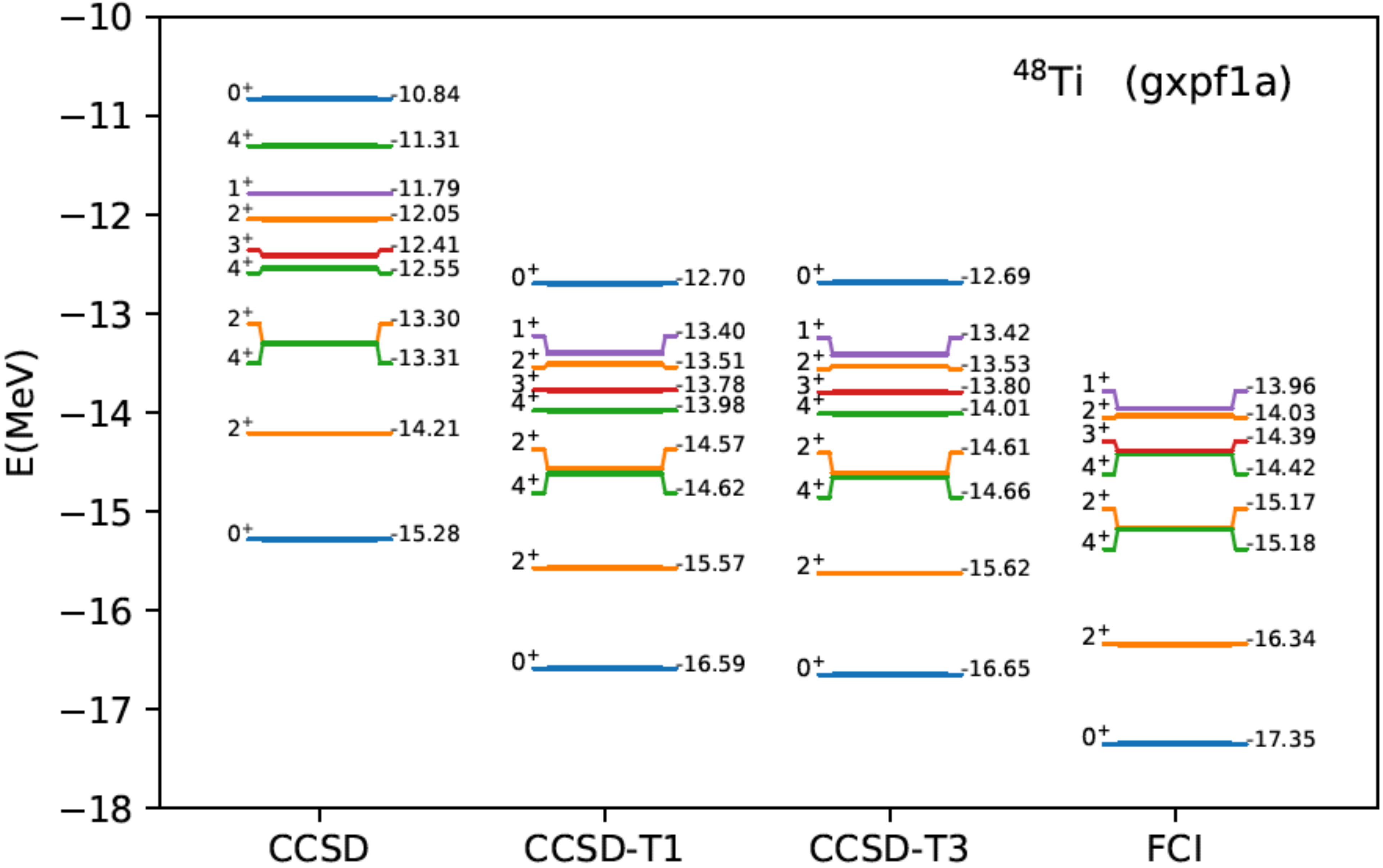
$$M^{2\nu} = \langle \Phi_0 | L_0 \overline{O}_{\mathrm{GT}} \frac{1}{\overline{H} - E_i + Q_{\beta\beta}/2} \overline{O}_{\mathrm{GT}} | \Phi_0 \rangle$$

Define left/right Lanczos pivots: $\langle \tilde{\nu}_0 | = \langle \Phi_0 | L_0 \overline{O}_{\mathrm{GT}} \quad | \nu_0 \rangle = \overline{O}_{\mathrm{GT}} | \Phi_0 \rangle$

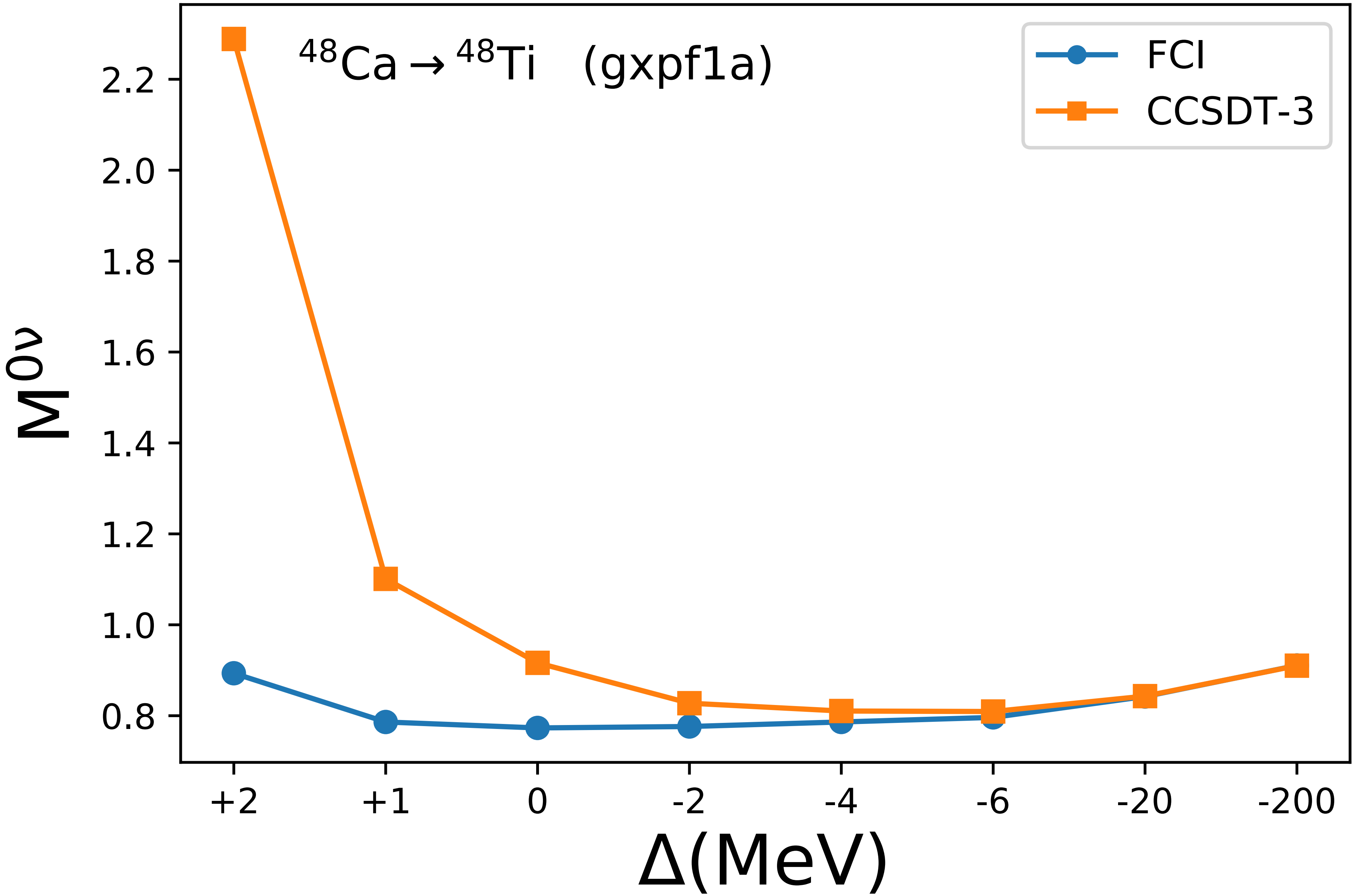
$$M^{2\nu} = \langle \tilde{\nu}_0 | \nu_0 \rangle \left\{ \frac{1}{(a_0 - Q_{\beta\beta}/2) - \frac{b_0^2}{(a_1 - Q_{\beta\beta}/2) - \frac{b_1^2}{(a_2 - Q_{\beta\beta}/2) \; - \cdots}}} \right\}$$

- Lanczos continued fraction method, see e.g. Engel, Haxton, Vogel PRC (1992), Haxton, Nollett, Zurek PRC (2005), Miorelli et al PRC (2016).
- Matrix element is converged to machine precision after ~10-20 iterations.
- Need more than 50 1^+ states converged in ^{48}Sc (300-400 Lanczos iterations) if we sum explicitly over intermediate states

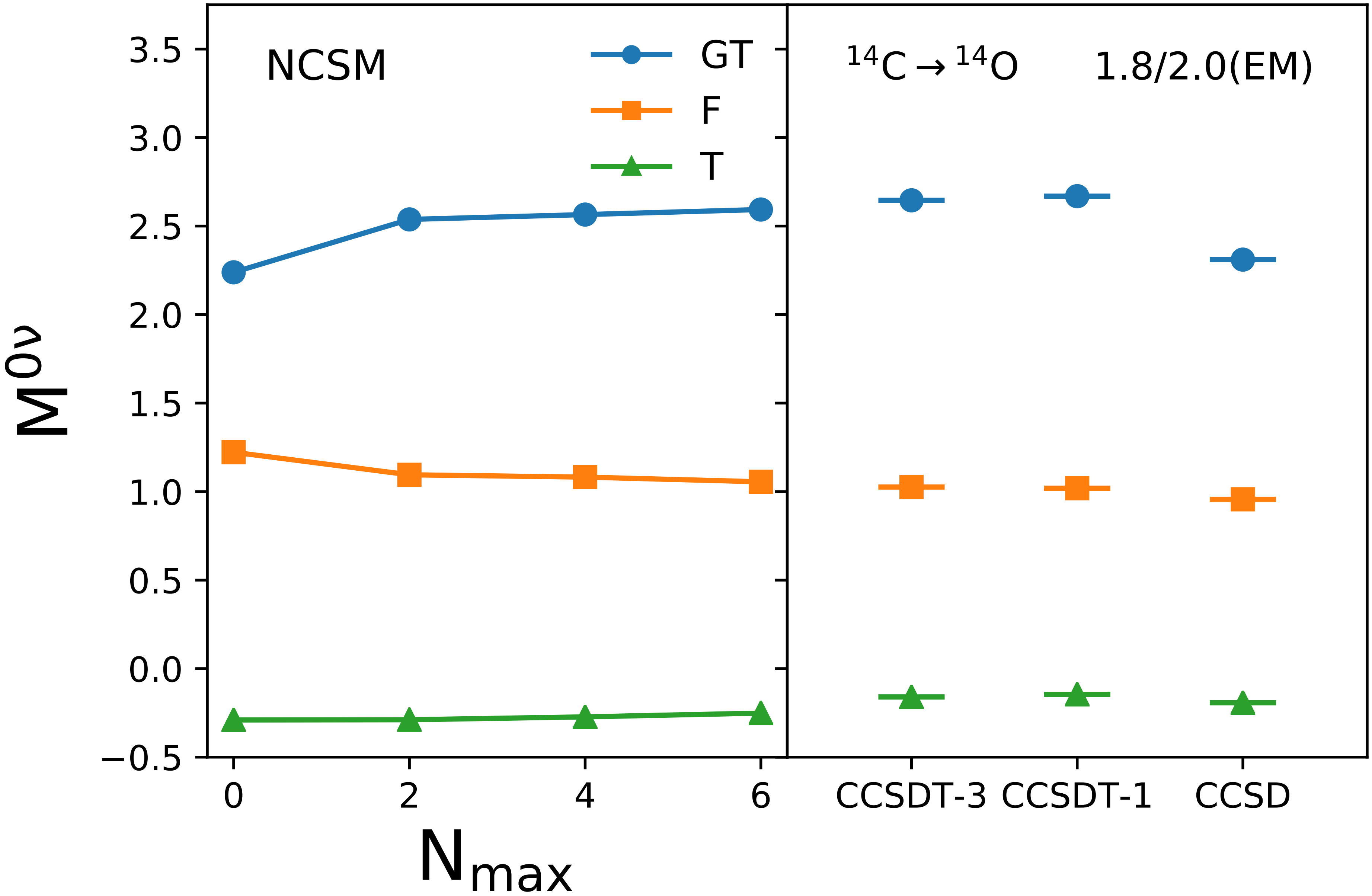
Benchmarking CC with FCI in ^{48}Ti



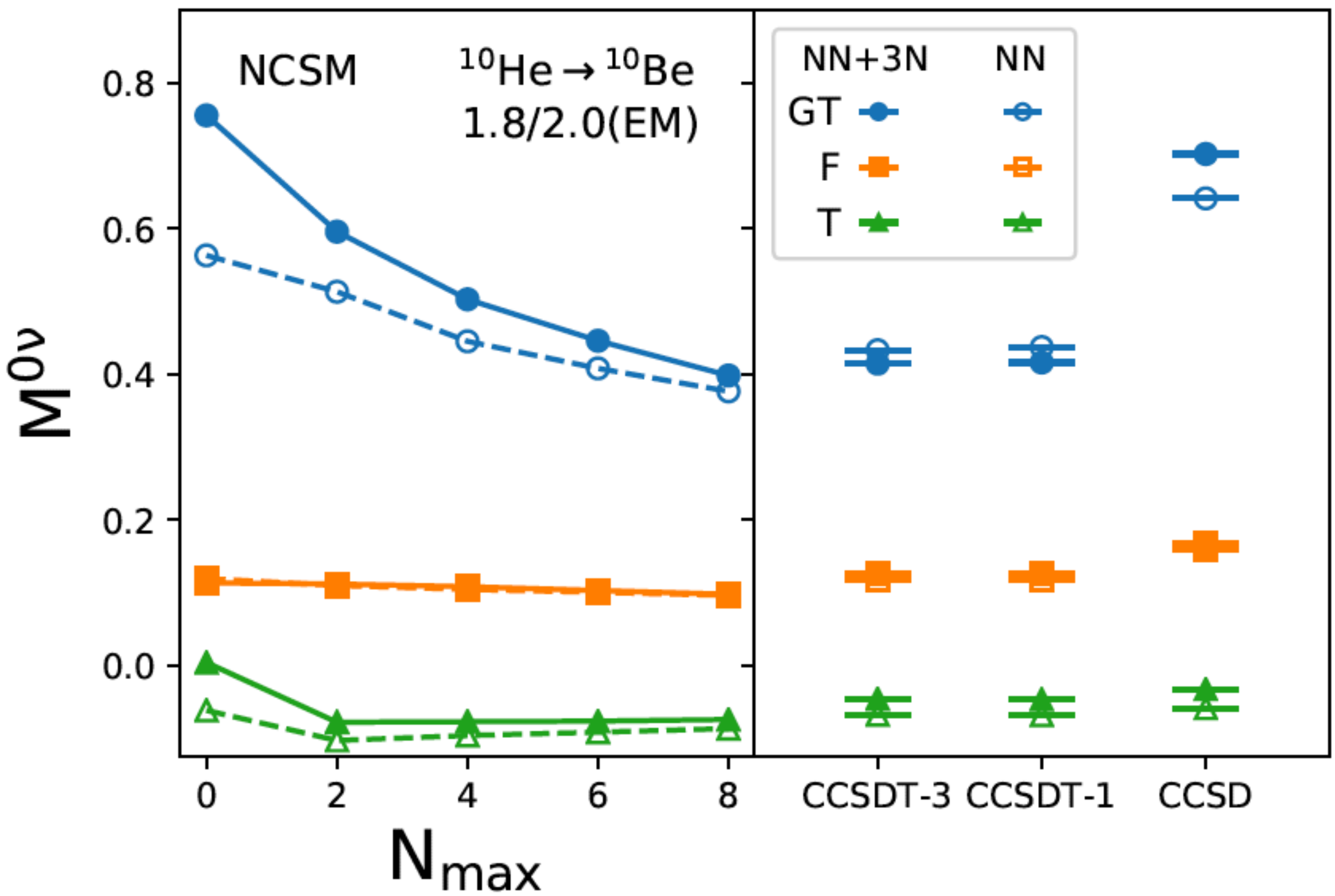
Benchmarking CC with FCI in ^{48}Ca



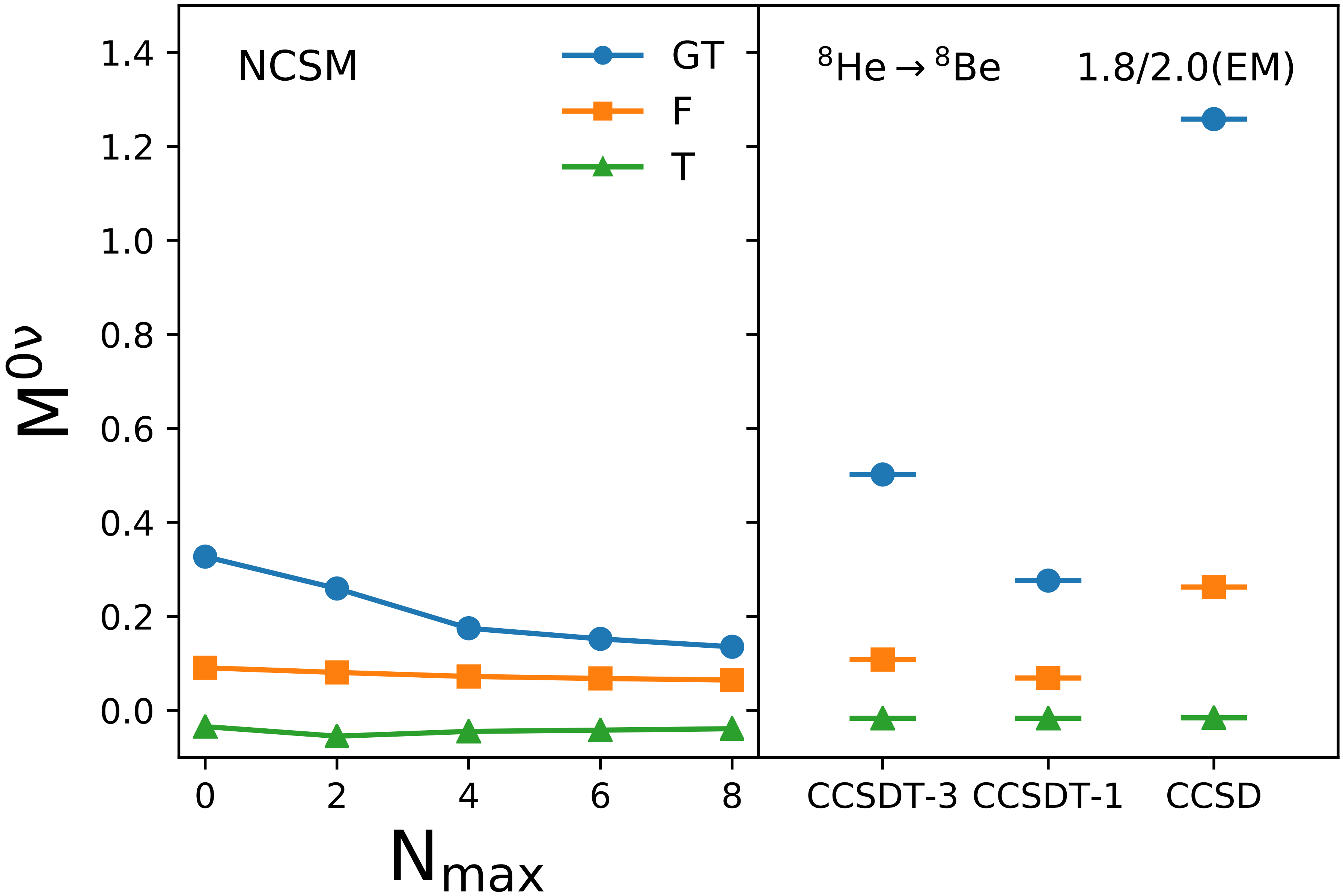
Benchmark between CC and NCSM in light nuclei



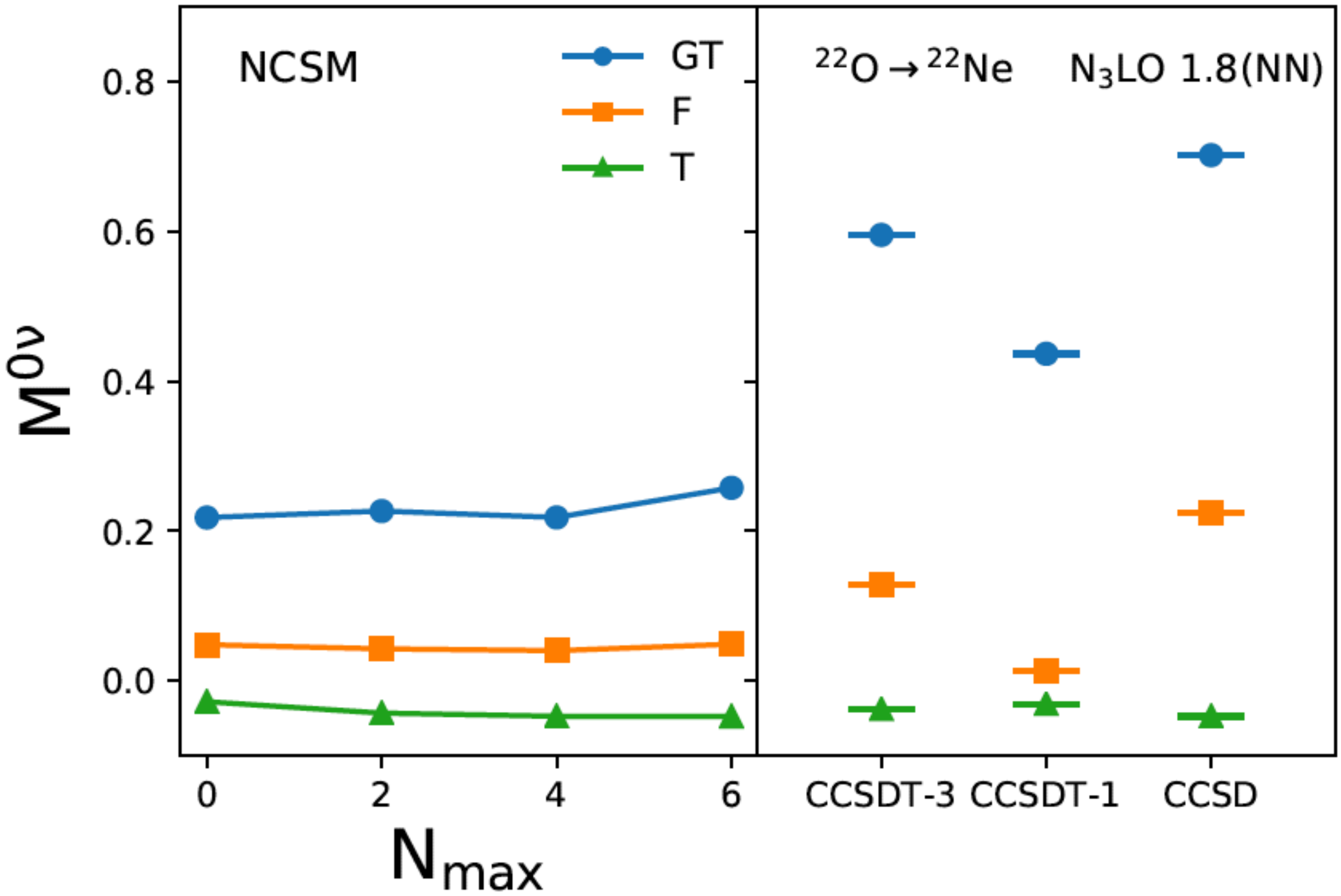
Benchmark between CC and NCSM in light nuclei



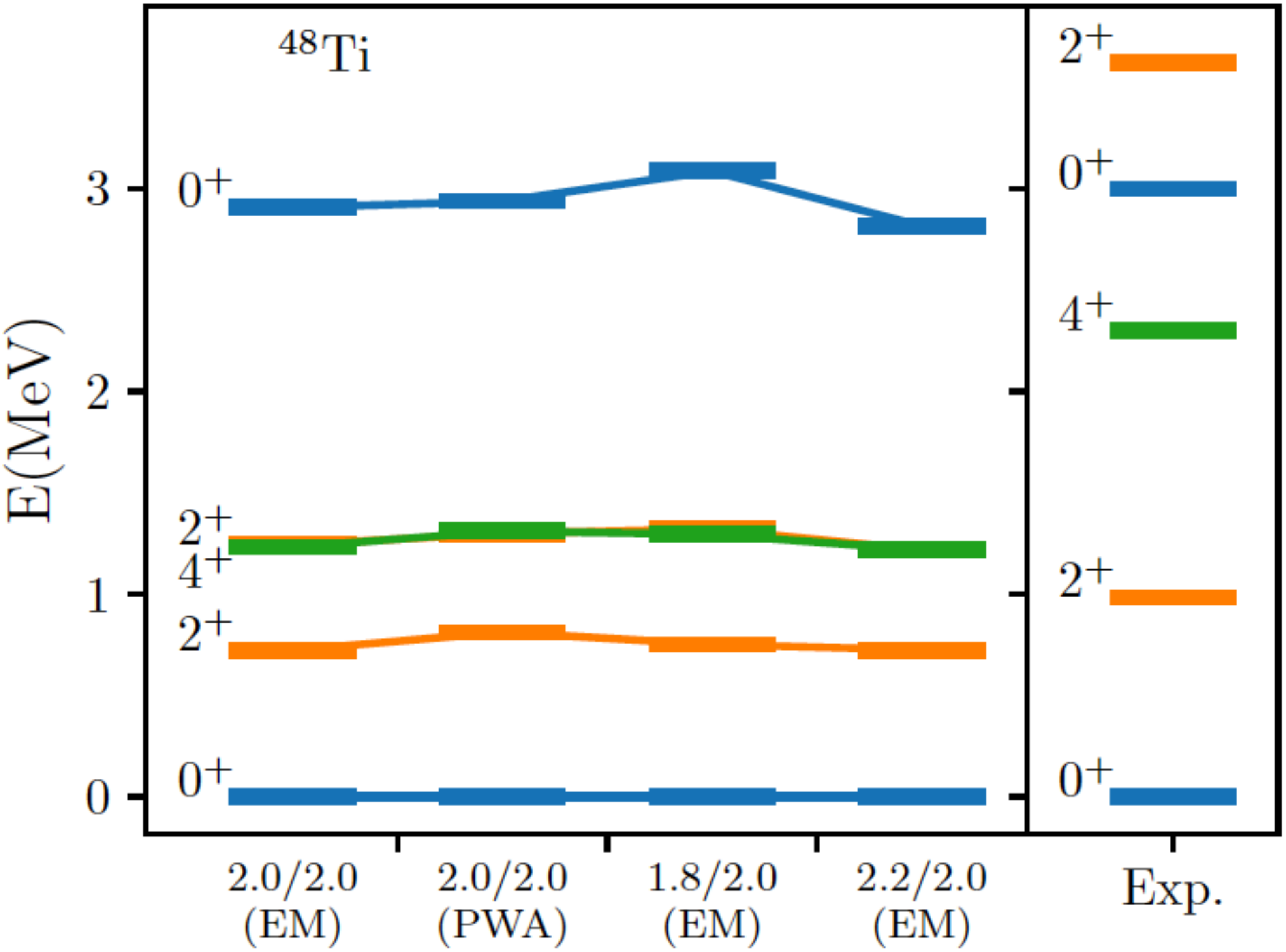
Benchmark between CC and NCSM in light nuclei



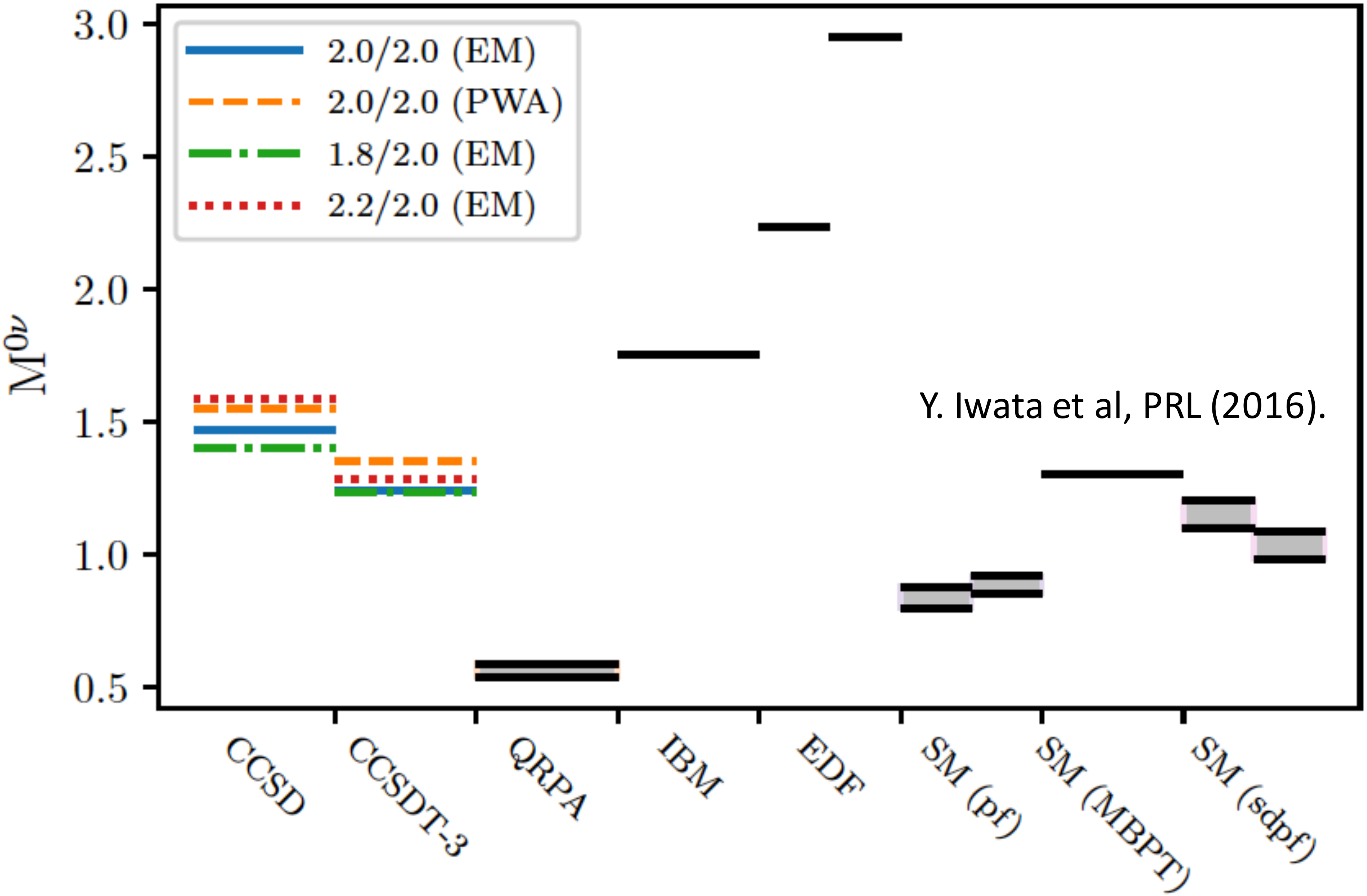
Benchmark between CC and NCSM in light nuclei



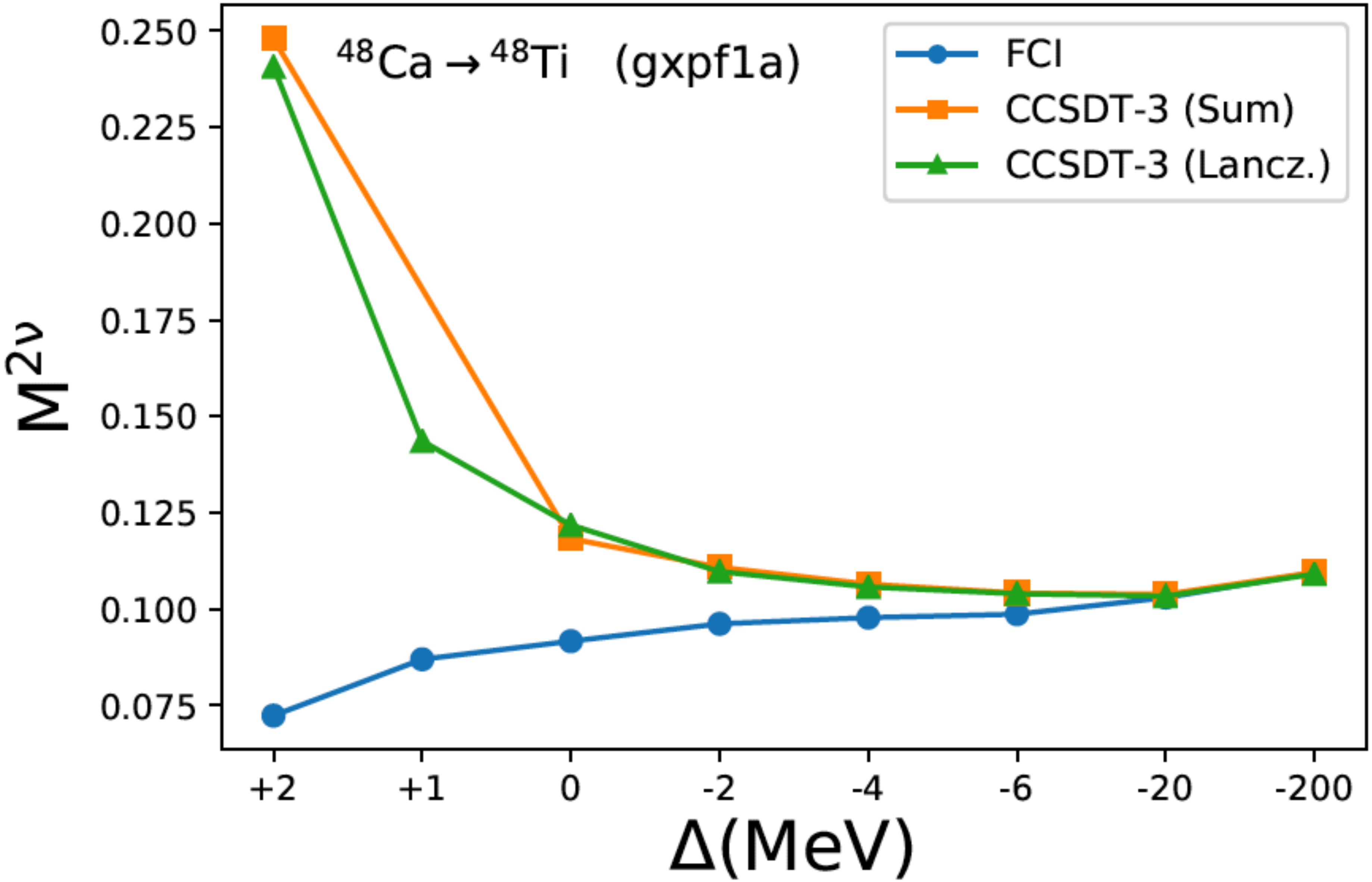
Spectra of ^{48}Ti from EOM-CC



Neutrinoless double beta-decay of ^{48}Ca

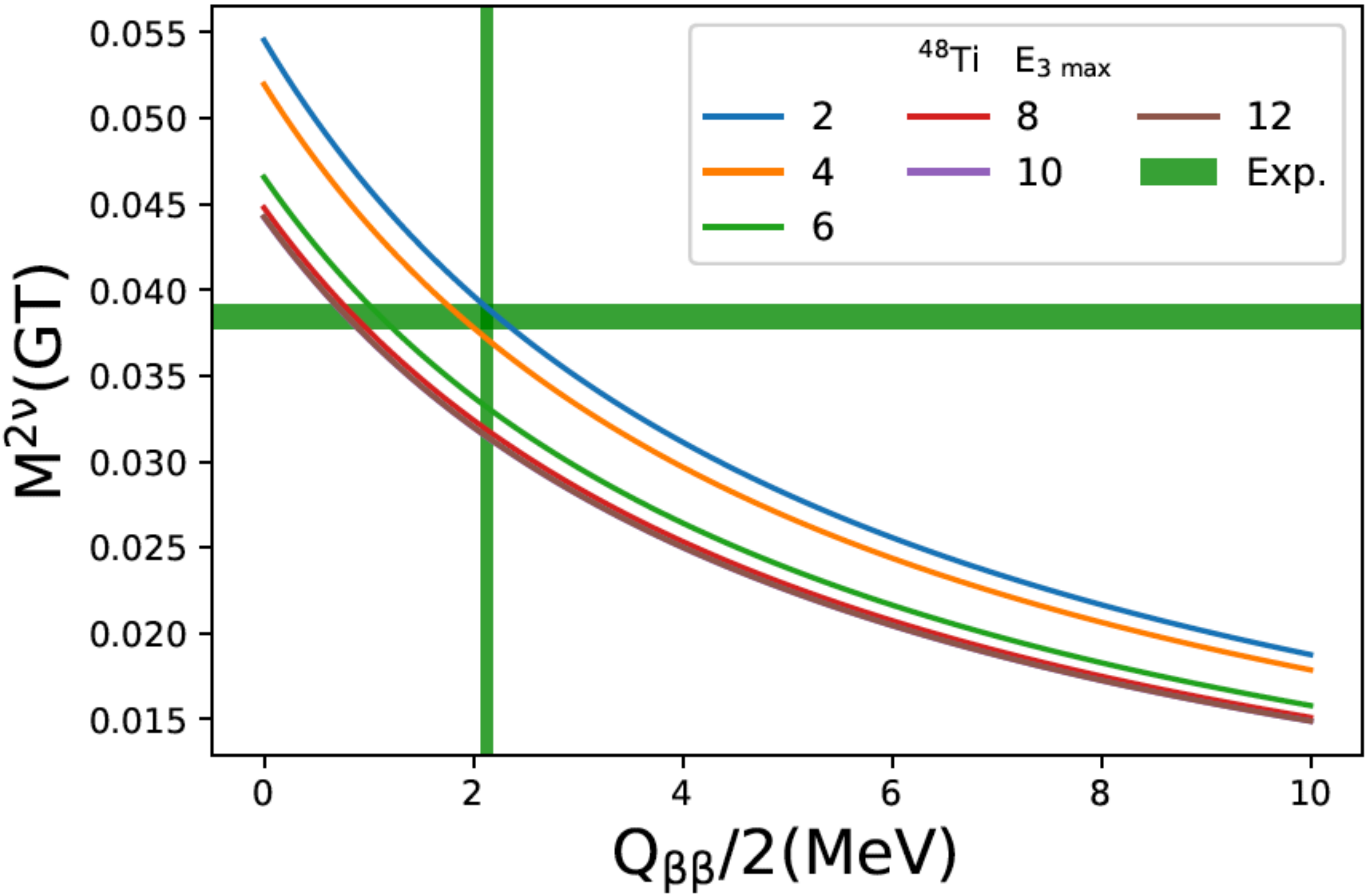


Double beta-decay of ^{48}Ca: Benchmark EOM-CC with FCI



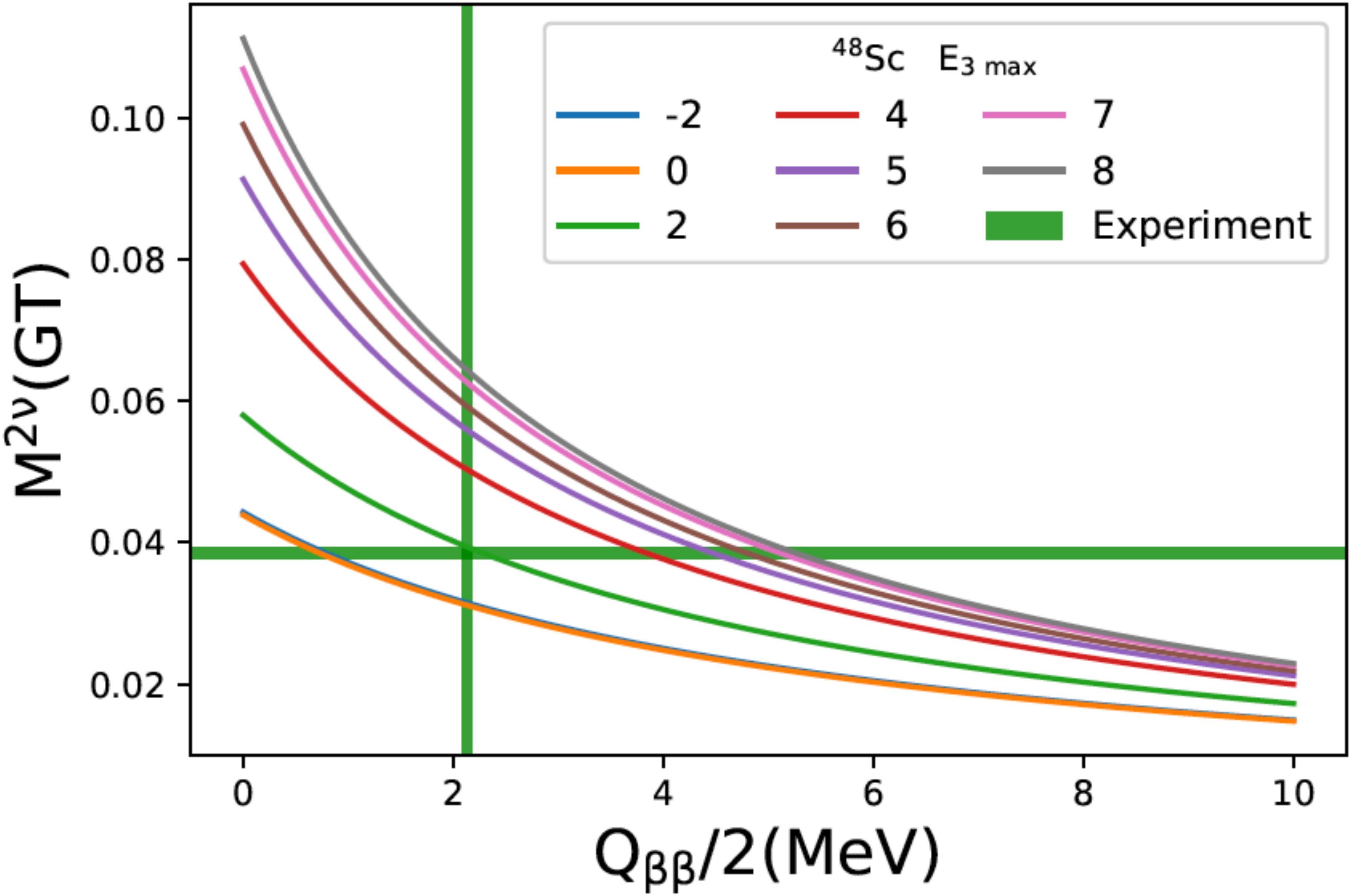
Double beta-decay of ^{48}Ca

The role of 3p3h excitations in the ground-state of ^{48}Ti



Double beta-decay of ^{48}Ca

The role of 3p3h excitations in the intermediate 1^+ states of ^{48}Sc



Conclusions part 2

- Double-charge exchange EOM-CC allows for a systematically improvable description of double-beta decay:
  - 0vbb compatible with large-scale shell-model
  - 2vbb is in fair agreement with experiment (2BC missing)
- EOM-CC is in good agreement with exact calculations for states that are not well deformed
- In order to properly describe deformed final states we are working on a deformed m-scheme implementation of EOM-CC

Collaborators

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