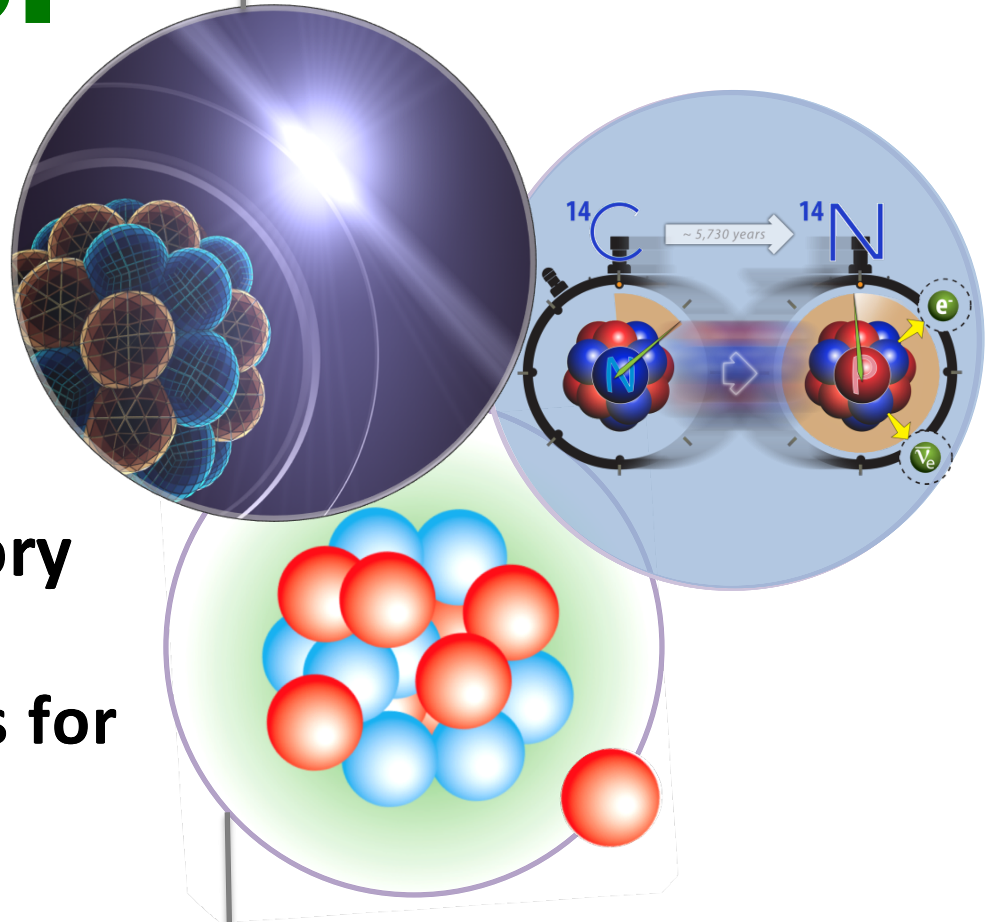
Coupled-cluster calculations of beta decays



Gaute Hagen
Oak Ridge National Laboratory

Precise beta decay calculations for searches for new physics

ECT, April 11th, 2019

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

OAK RIDGE NATIONAL LABORATORY
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nature physics

LETTERS

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

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

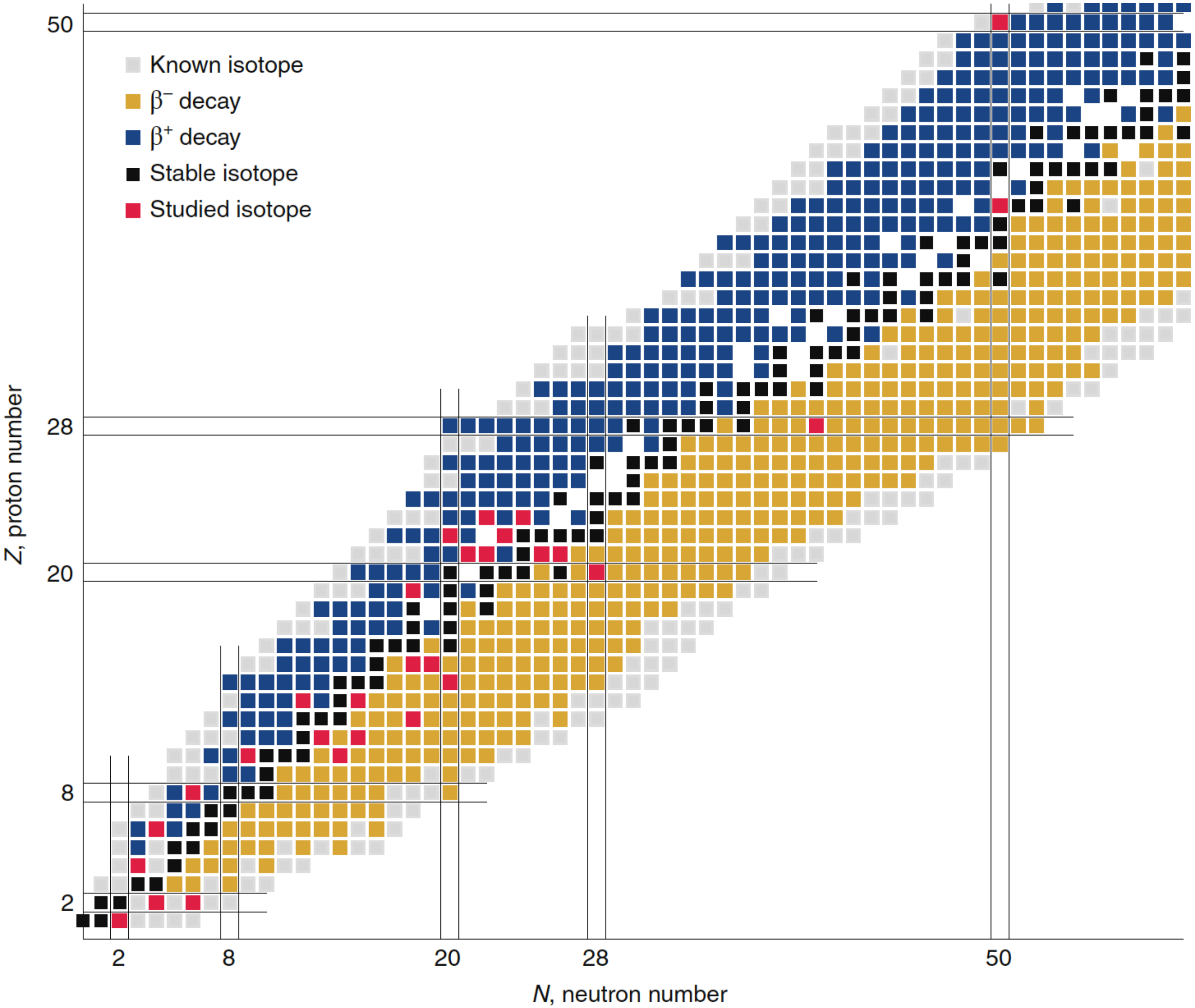
P. Gysbers[1,2], G. Hagen[3,4]*, J. D. Holt[1], G. R. Jansen[3,5], T. D. Morris[3,4,6], P. Navrátil[1], T. Papenbrock[3,4], S. Quaglioni[7], A. Schwenk[8,9,10], S. R. Stroberg[1,11,12] and K. A. Wendt[7]

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

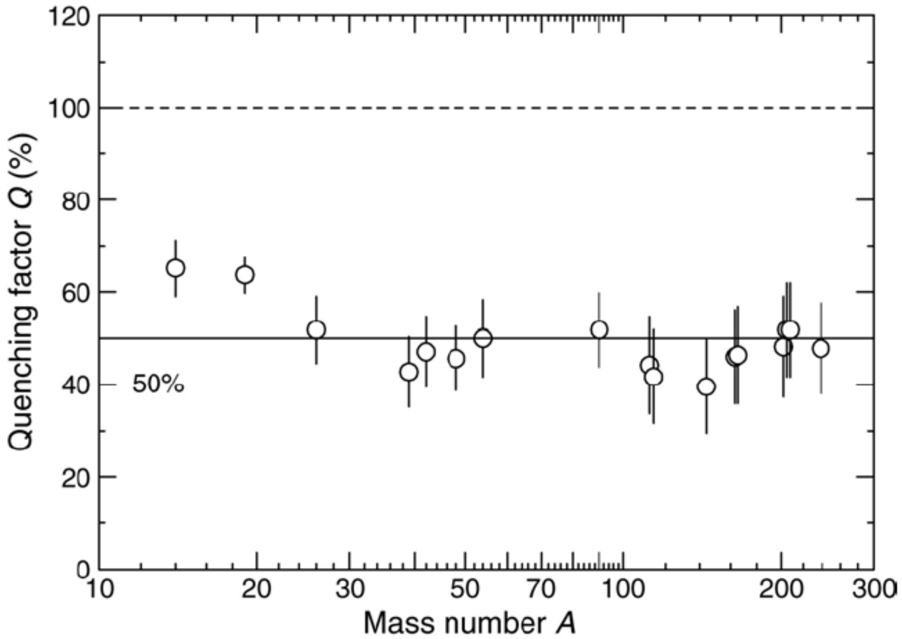
Isotopes studied in this work



Arnau Rios, Nature News & Views (2019)

DOI: 10.1038/s41567-019-0483-y

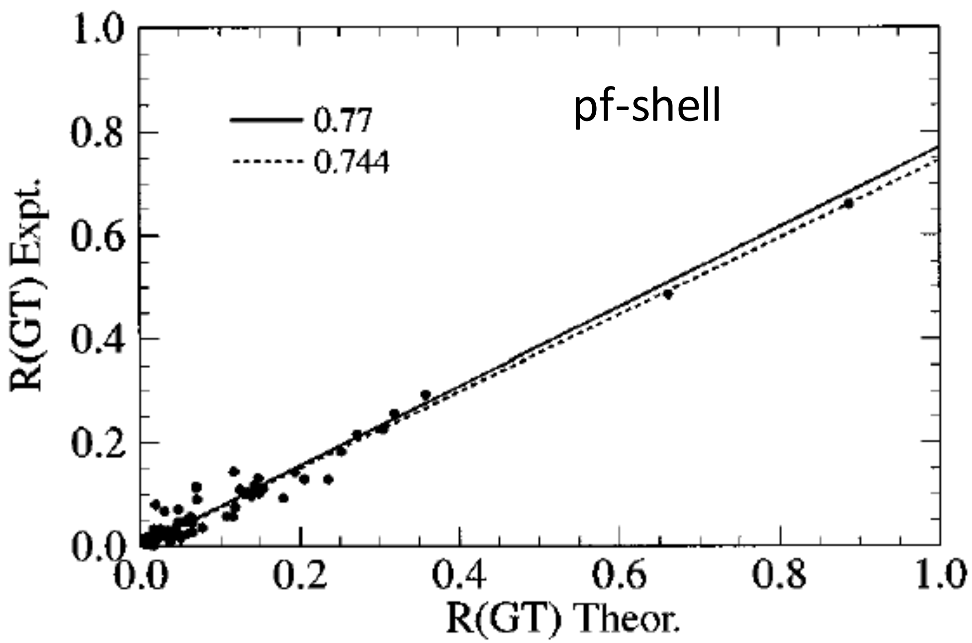
A 50 year old problem:
The puzzle of quenched of beta decays



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

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

Discussion points for the workshop:

- Current experiments aim at a few 0.01% to a few 0.1% precision that needs to be reached.
- What are achievable systematic theoretical uncertainties in ab-initio approaches for calculations of ground-state properties and transitions (Gamow-Teller, M1, E2, etc)?

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

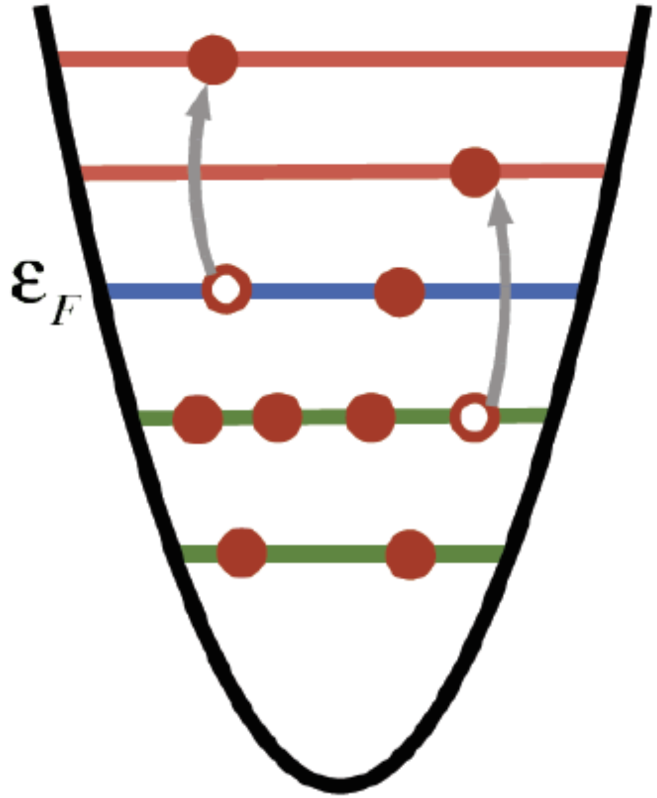
Ab-initio Method: Solve A-nucleon problem with controlled approximations and systematically improvable**:**

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

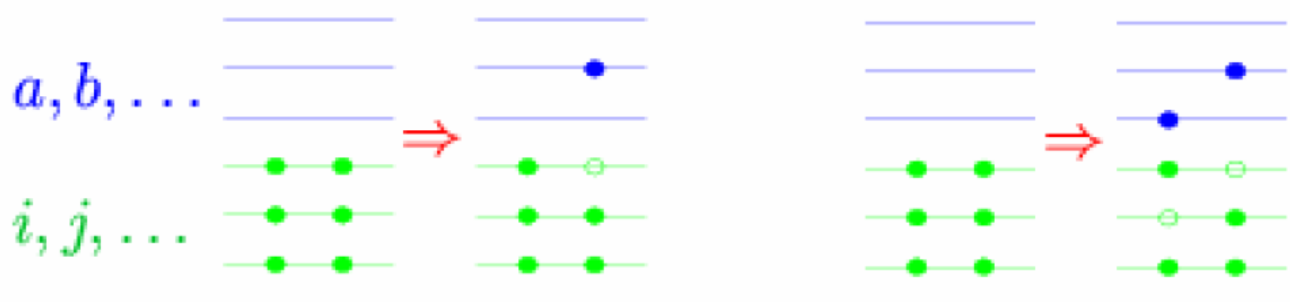
Coupled-cluster method (CCSD approximation)

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

$$B_1 = T_1$$

$$B_2 = T_2 + \frac{1}{2} T_1^2$$

$$B_3 = T_3 + T_2 T_1 + \frac{1}{6} T_1^3$$

$$B_4 = T_4 + T_3 T_1 + \frac{1}{2} T_2^2 + \frac{1}{2} T_2 T_1^2 + \frac{1}{24} T_1^4$$

$$\ldots$$

CCSD

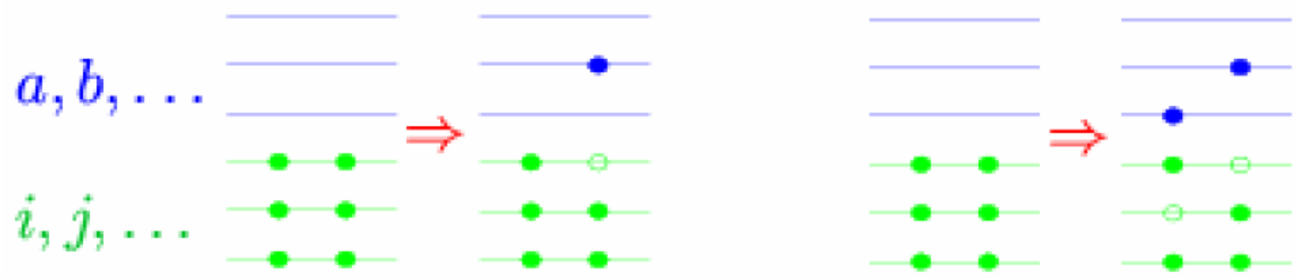
CCSDT

Disconnected quadruples

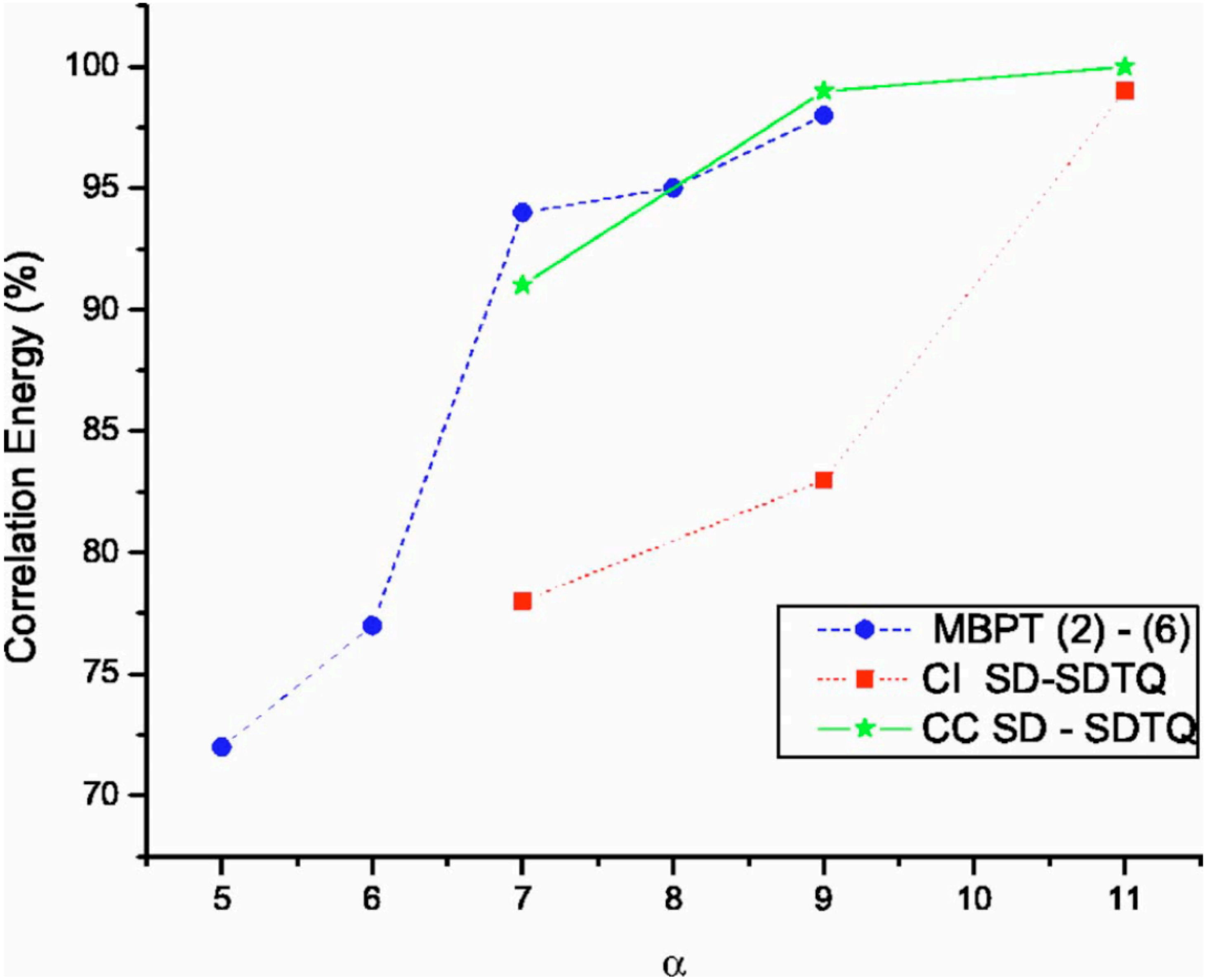
Connected quadruples

- 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)

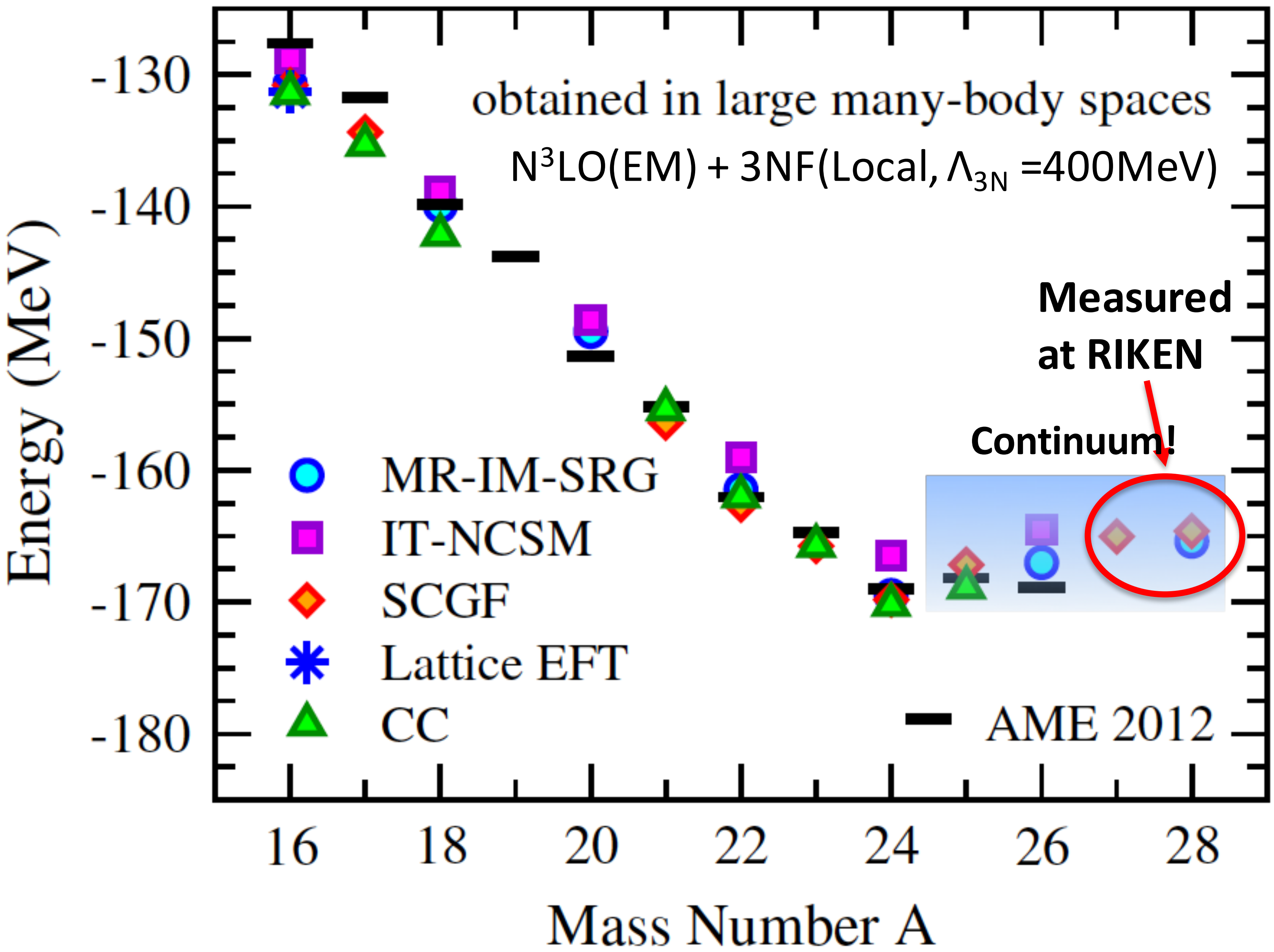
Coupled-cluster method

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).

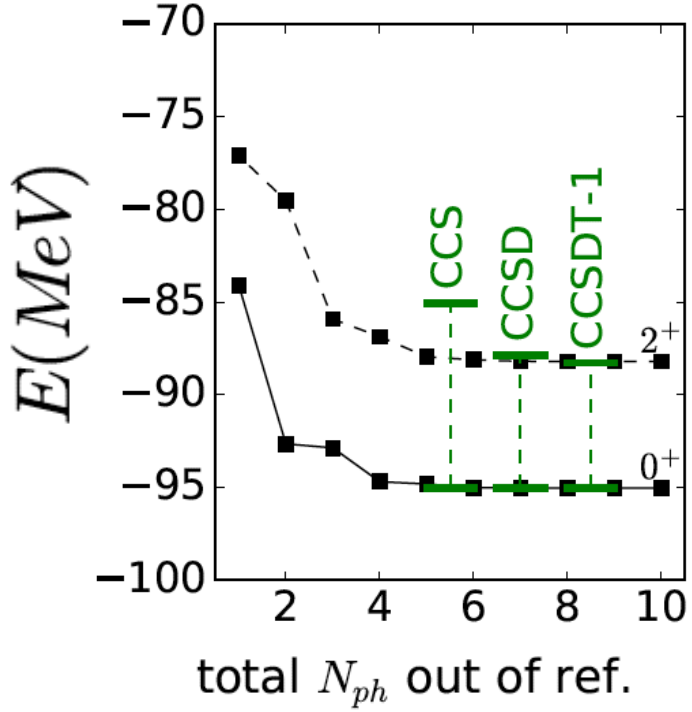
$\Delta E_3 \sim 10 - 13\%$

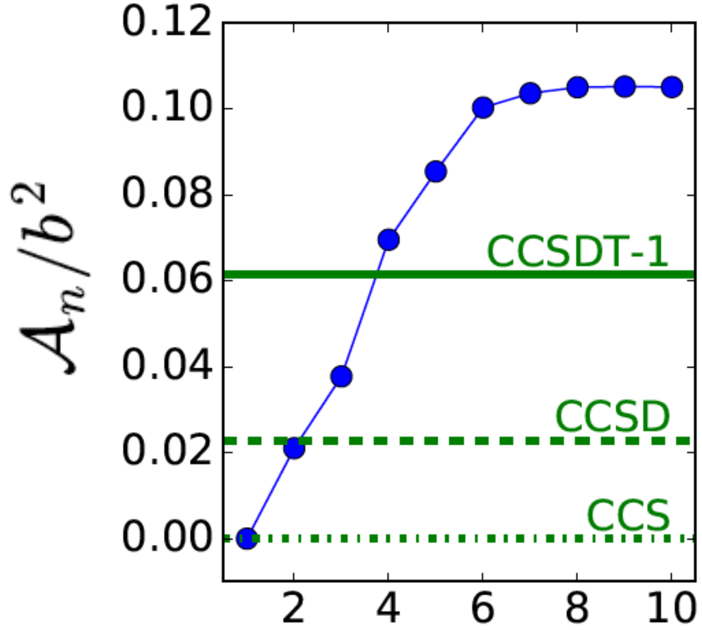
Oxgyen chain with interactions from chiral EFT

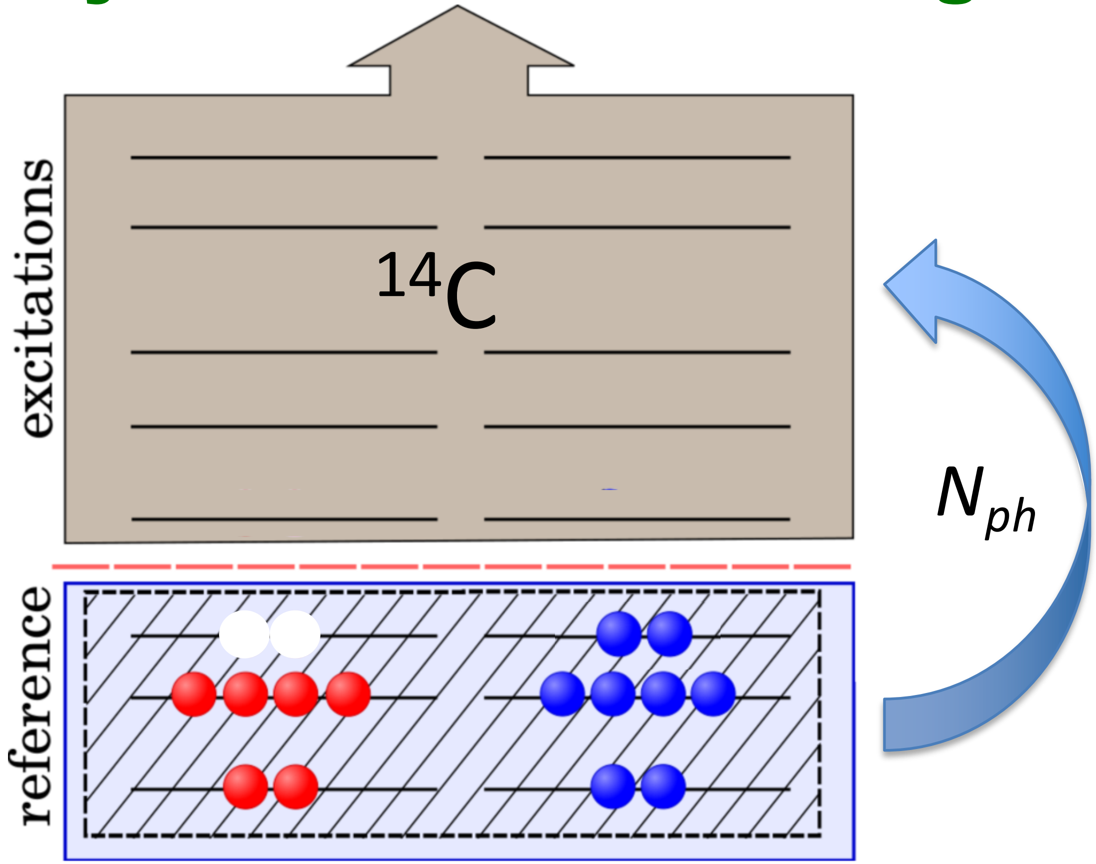


Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

Challenge: Collectivity and transition strengths

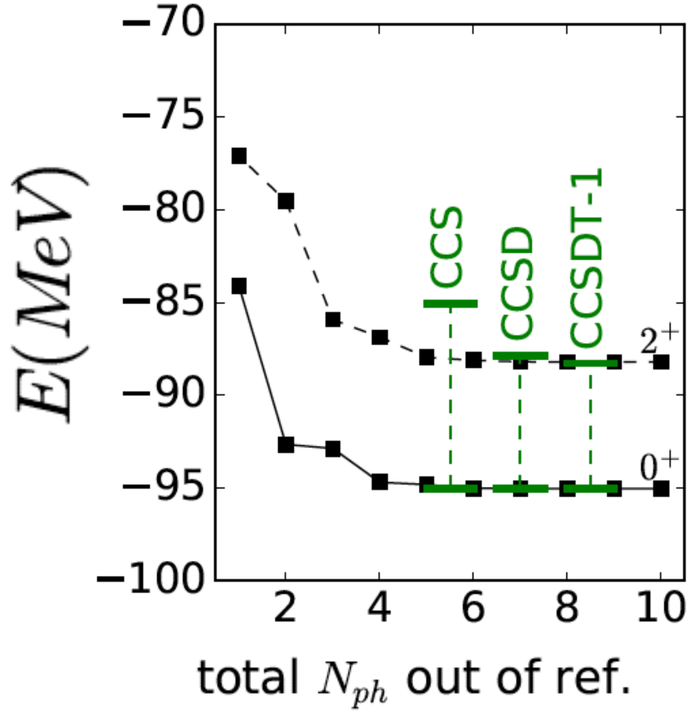


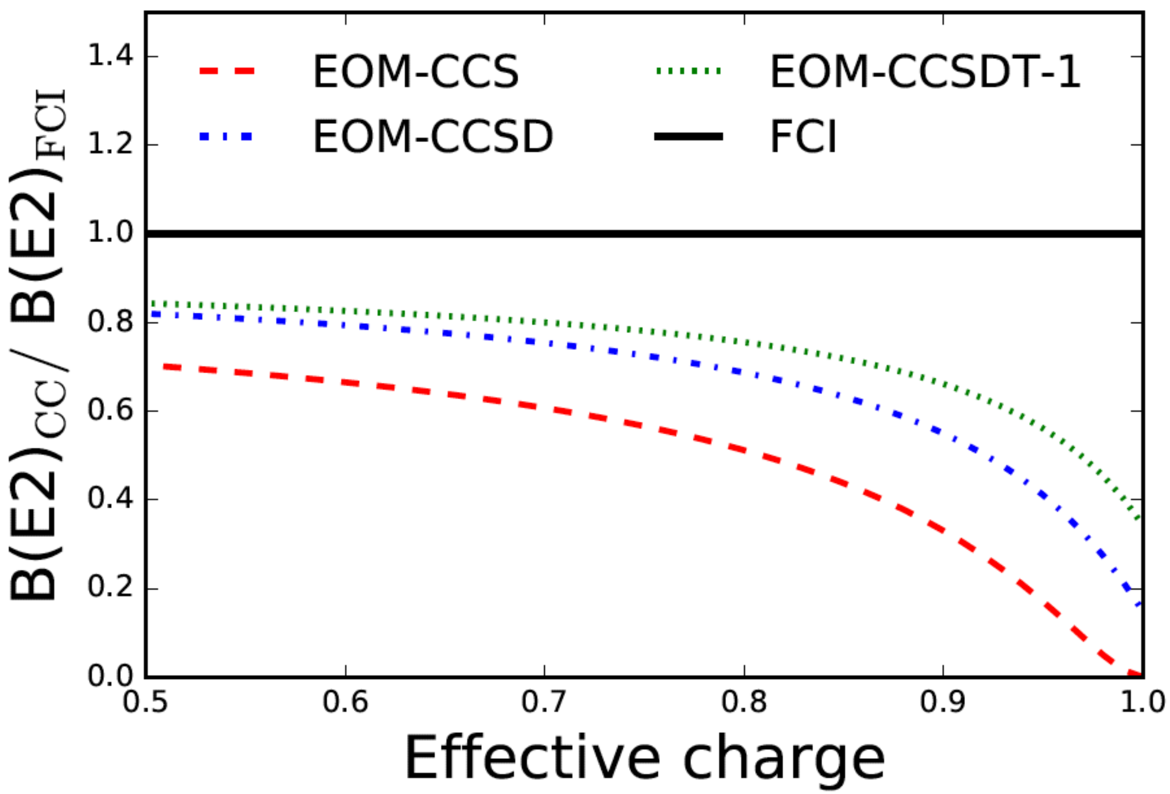


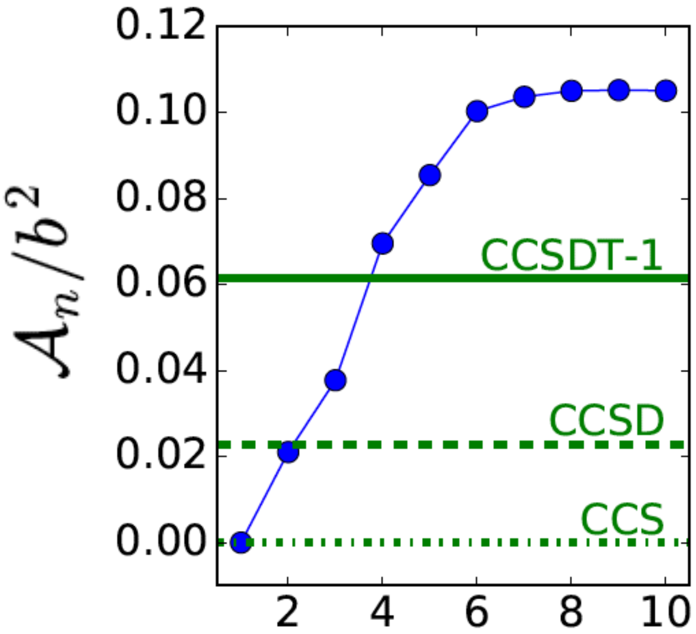


- ^{14}C computed in FCI and CC with psd effective interaction
- Neutron effective charge of charge = 1
- Need excitations beyond 4p4h to describe B(E2) even if 2+ energy is reproduced

Challenge: Collectivity and transition strengths



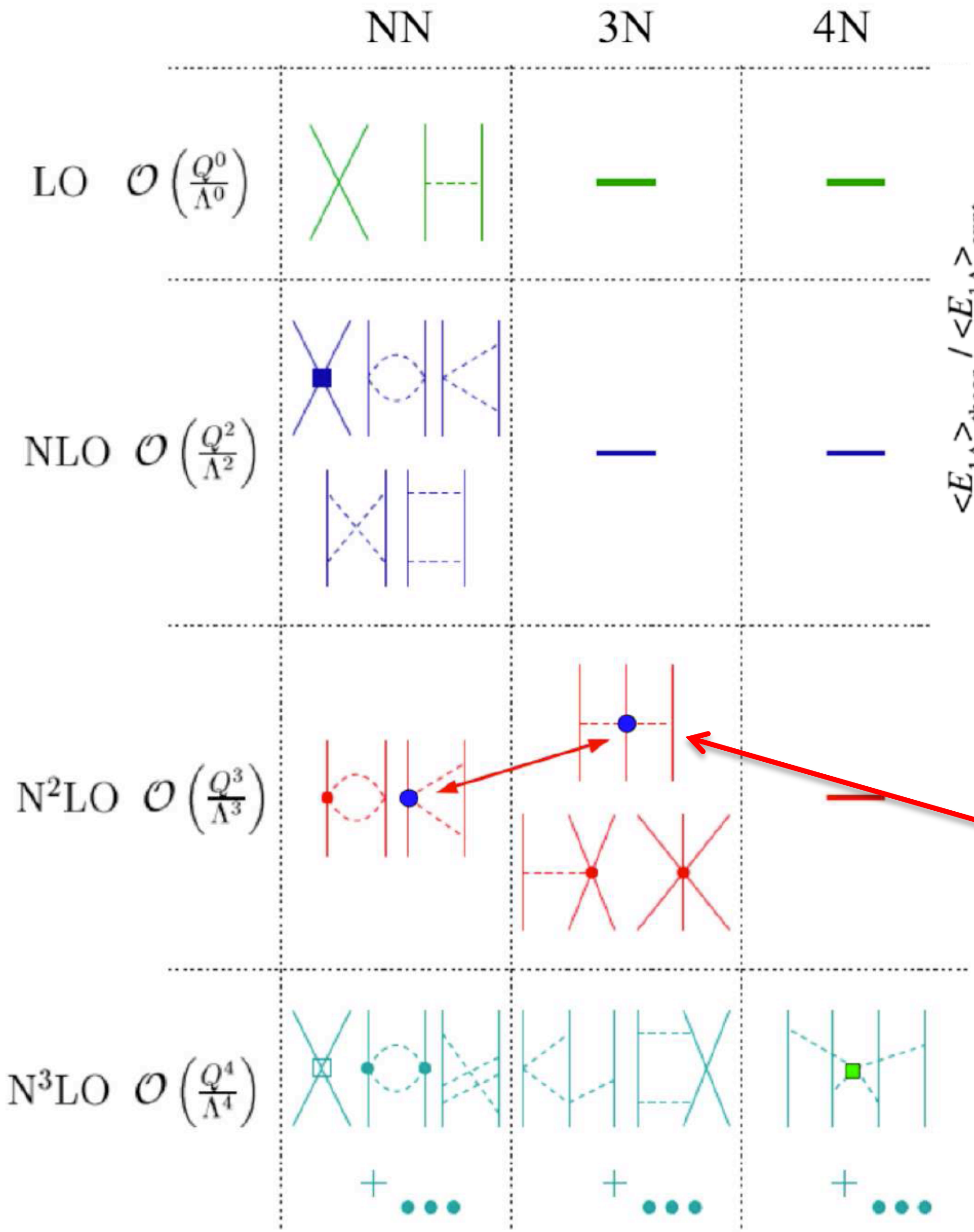




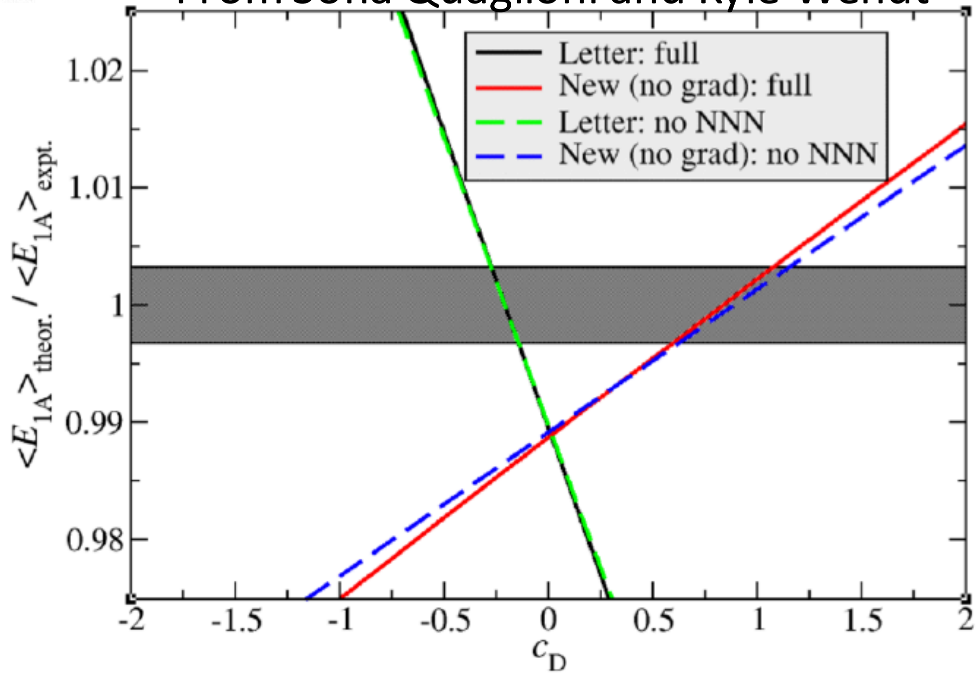
- ^{14}C computed in FCI and CC with psd effective interaction
- Neutron effective charge of charge = 1
- Need excitations beyond 4p4h to describe B(E2) even if 2+ energy is reproduced

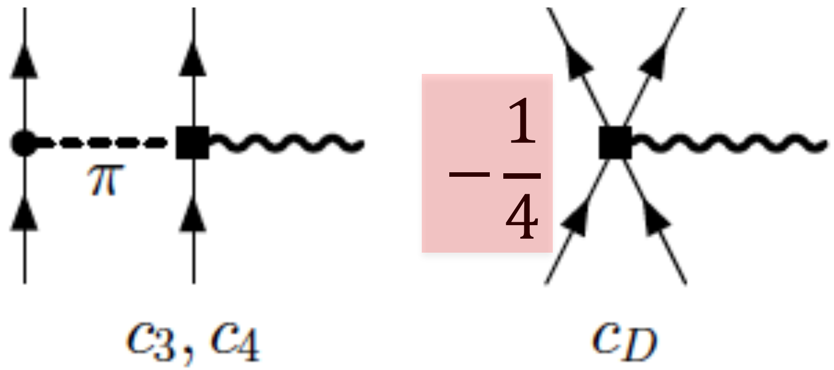
Nuclear forces from chiral effective field theory

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



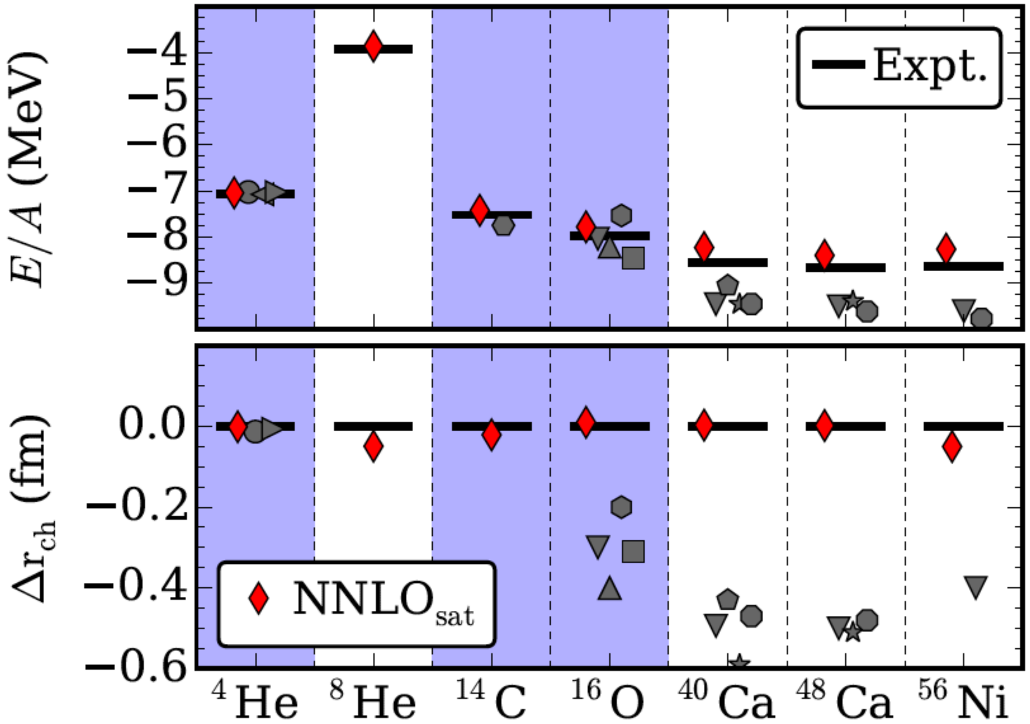
From Sofia Quaglioni and Kyle Wendt





Chiral EFT offers consistency between forces and currents

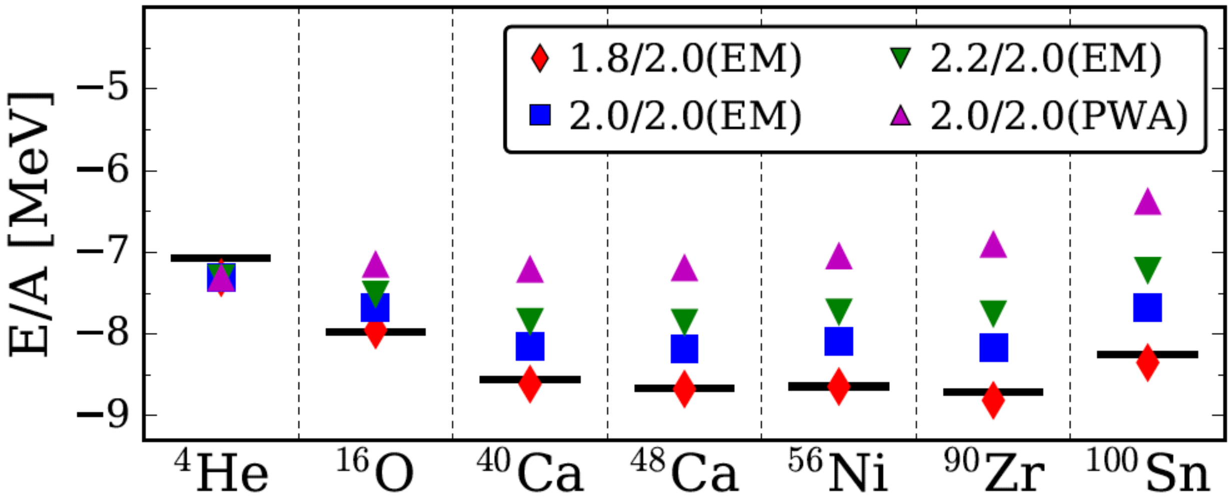
A family of interactions from chiral EFT



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

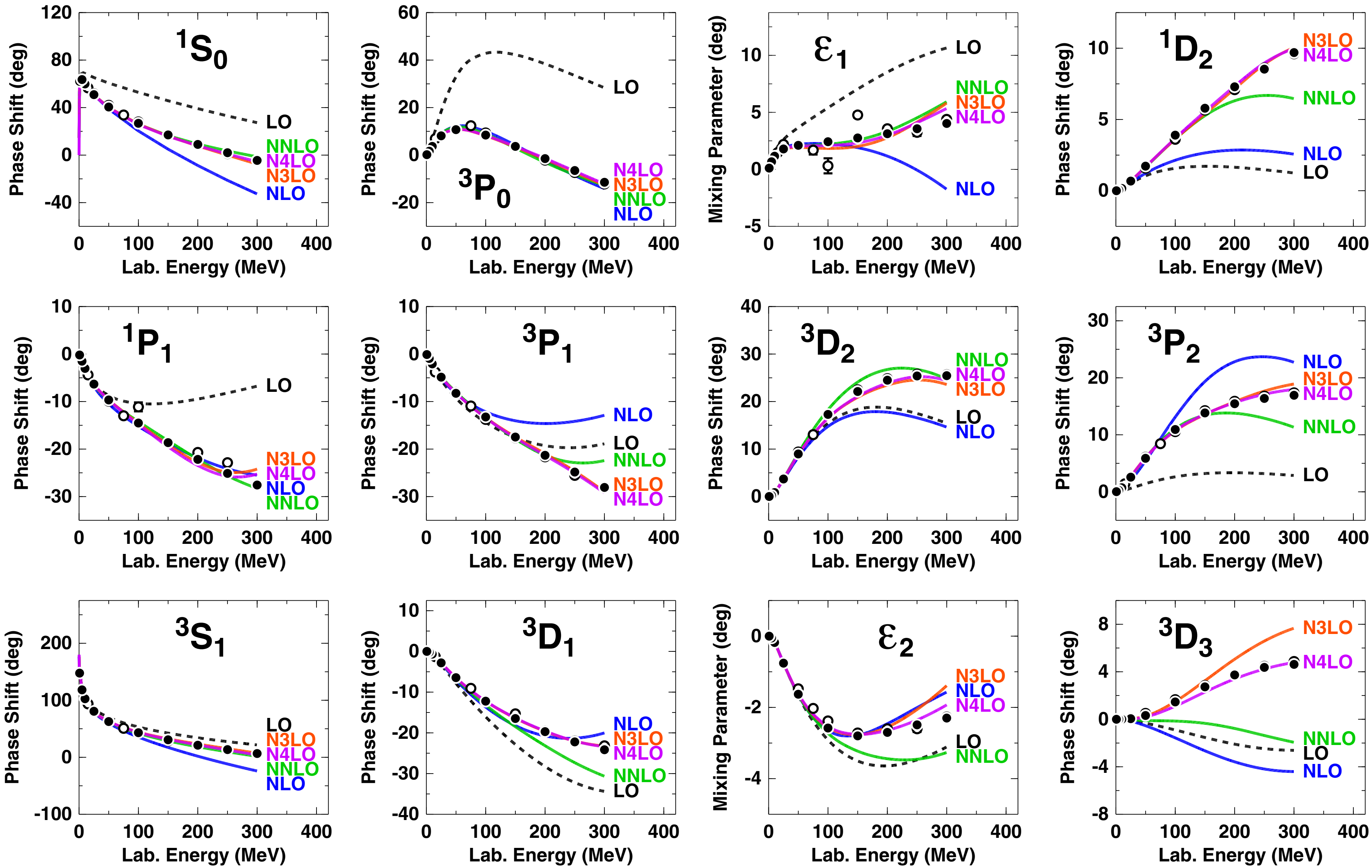
K. Hebeler *et al* PRC (2011).

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

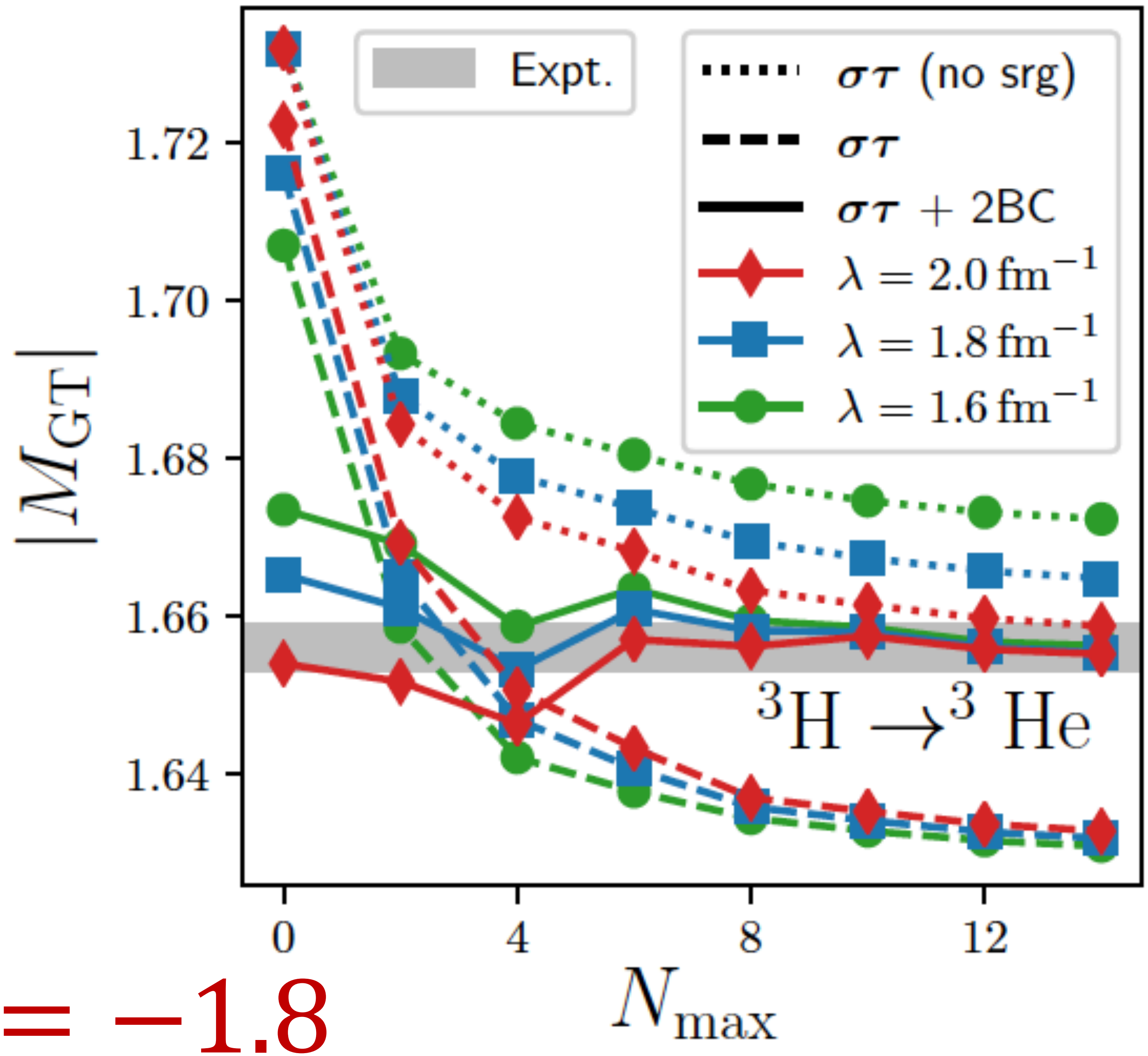
PHYSICAL REVIEW C **96**, 024004 (2017)

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

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



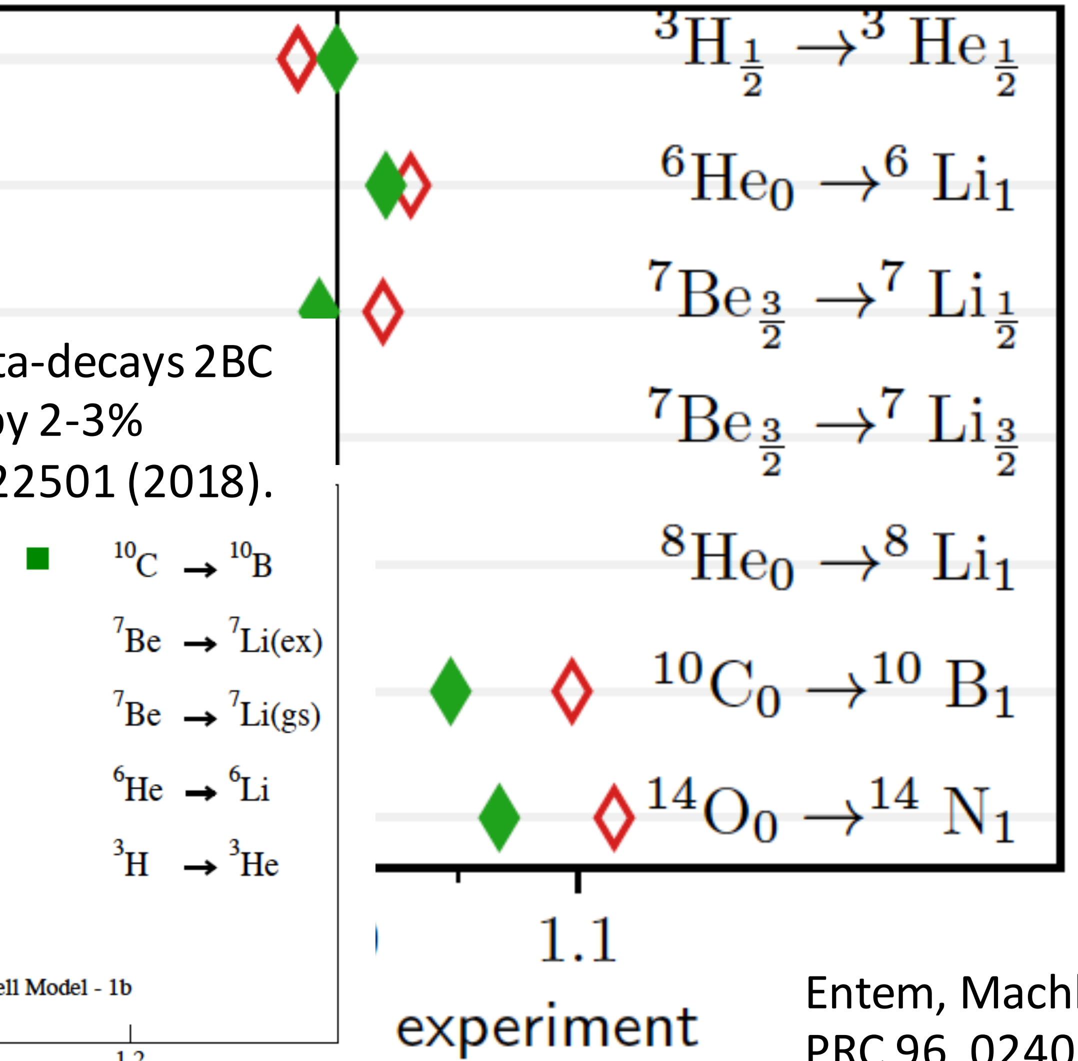
SRG and convergence in NCSM



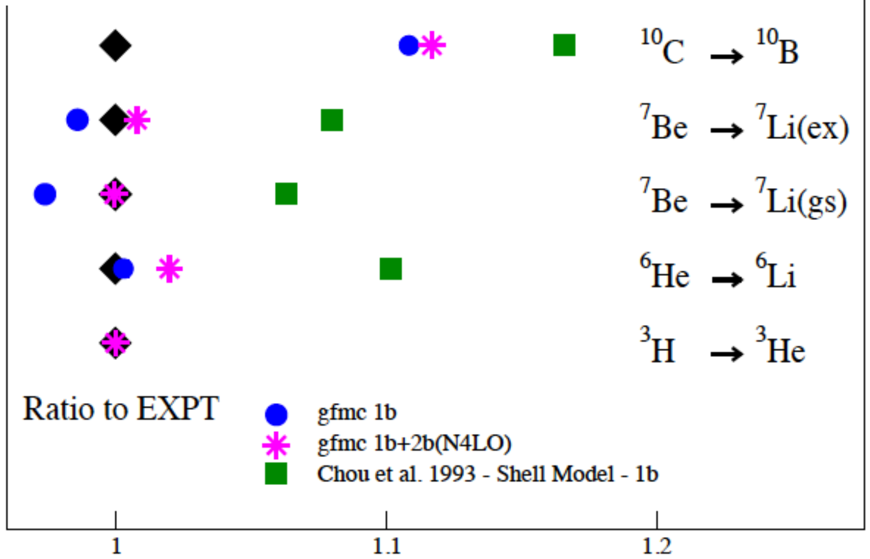
$c_D = -1.8$

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)

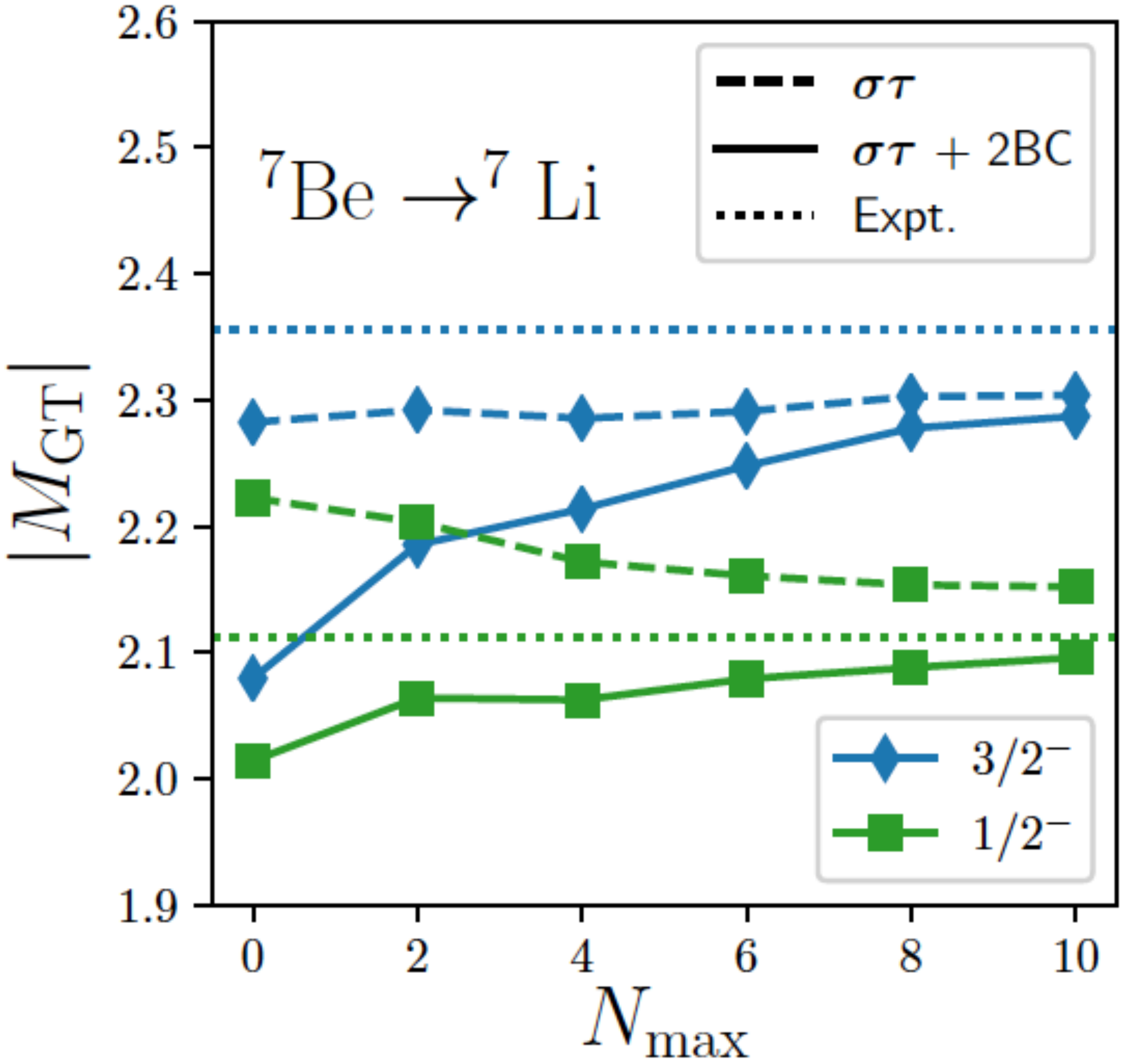


In QMC calculations of beta-decays 2BC increase the GT strength by 2-3%
S. Pastore et al, PRC 97, 022501 (2018).

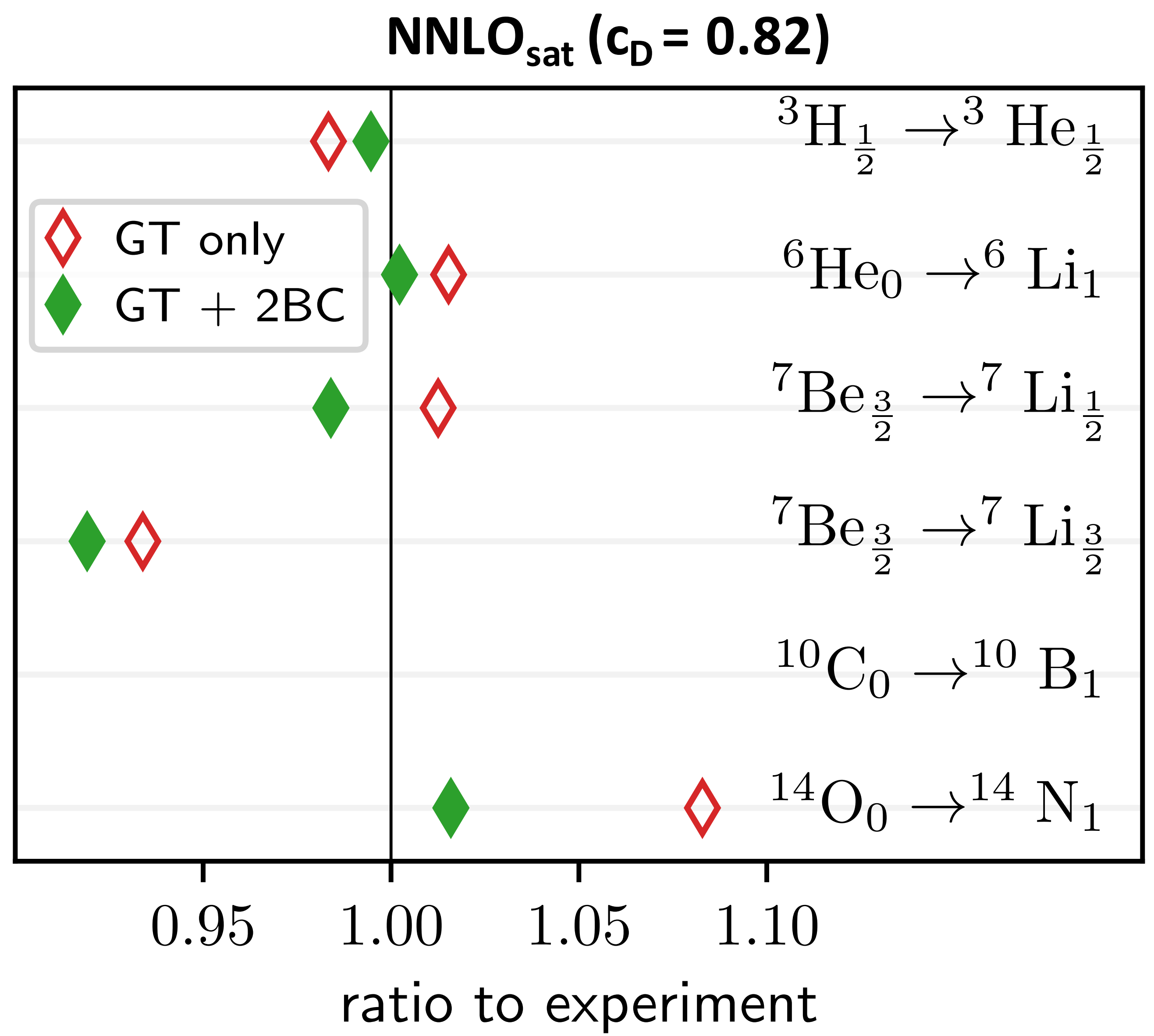


Entem, Machleidt & Nosyk, PRC 96, 024004 (2017)

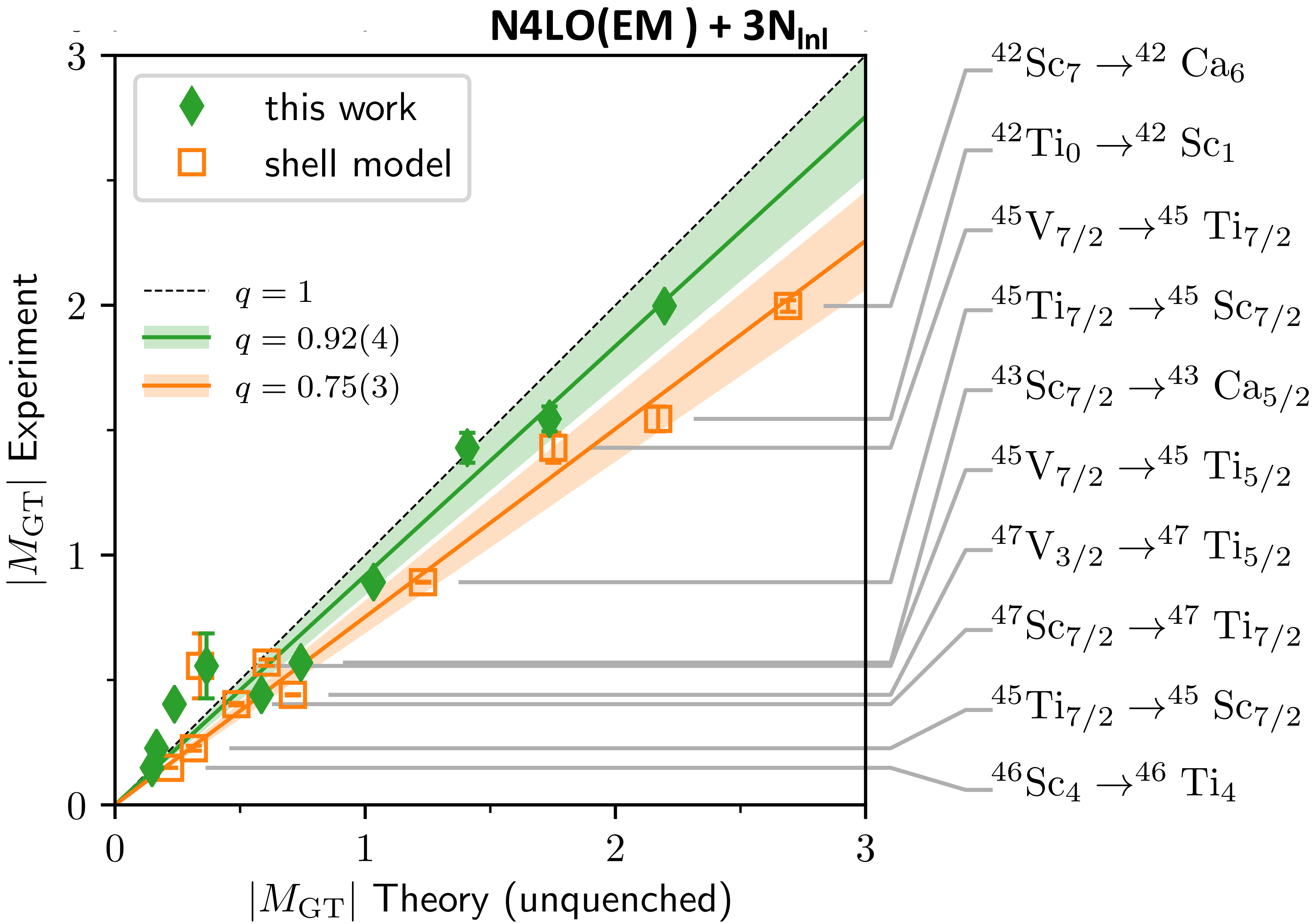
SRG and convergence in NCSM



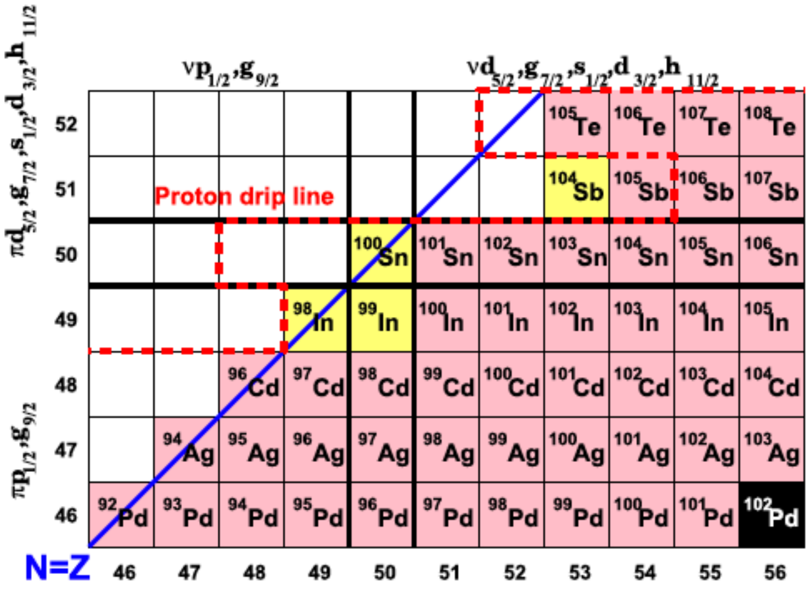
Theory to experiment ratios for beta decays in light nuclei from NCSM

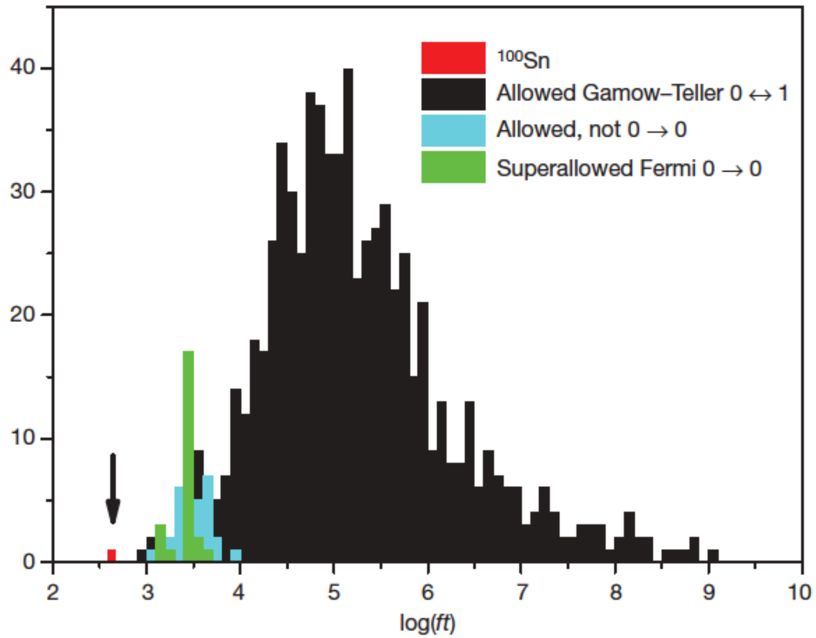


The role of 2BC in the pf-shell



^{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

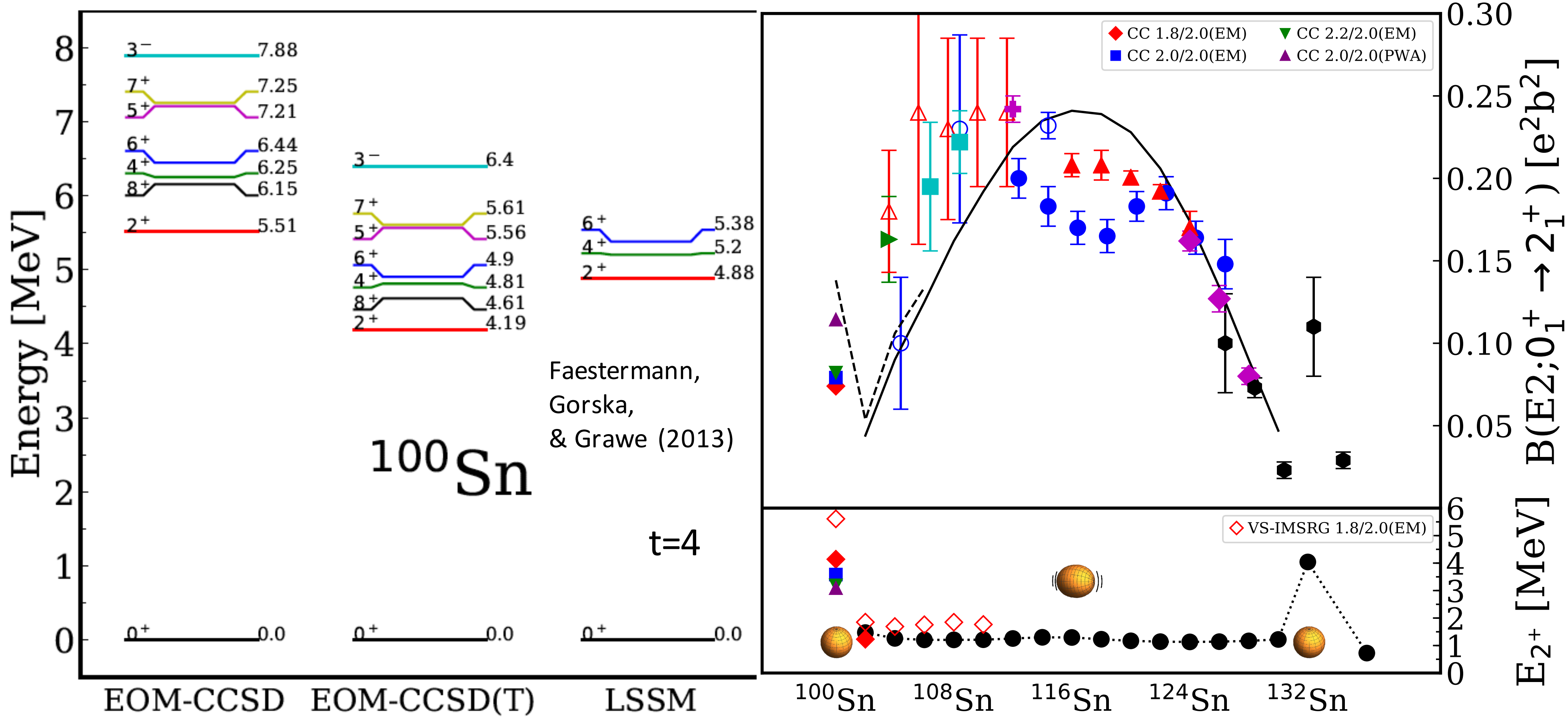
Quantify the effect of quenching from correlations and 2BCs

PHYSICAL REVIEW LETTERS 120, 152503 (2018)

Editors' Suggestion

Structure of the Lightest Tin Isotopes

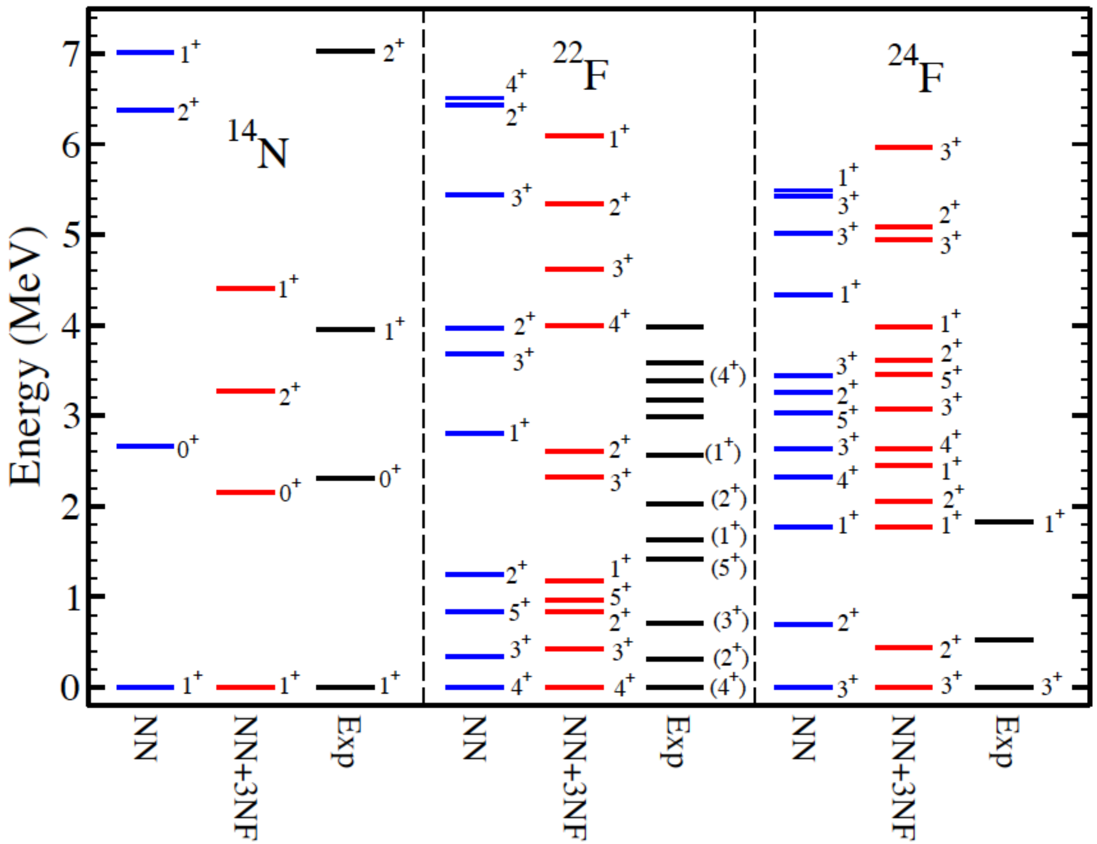
T. D. Morris,[1,2] J. Simonis,[3,4] S. R. Stroberg,[5,6] C. Stumpf,[3] G. Hagen,[2,1] J. D. Holt,[5] G. R. Jansen,[7,2]
T. Papenbrock,[1,2] R. Roth,[3] and A. Schwenk[3,4,8]

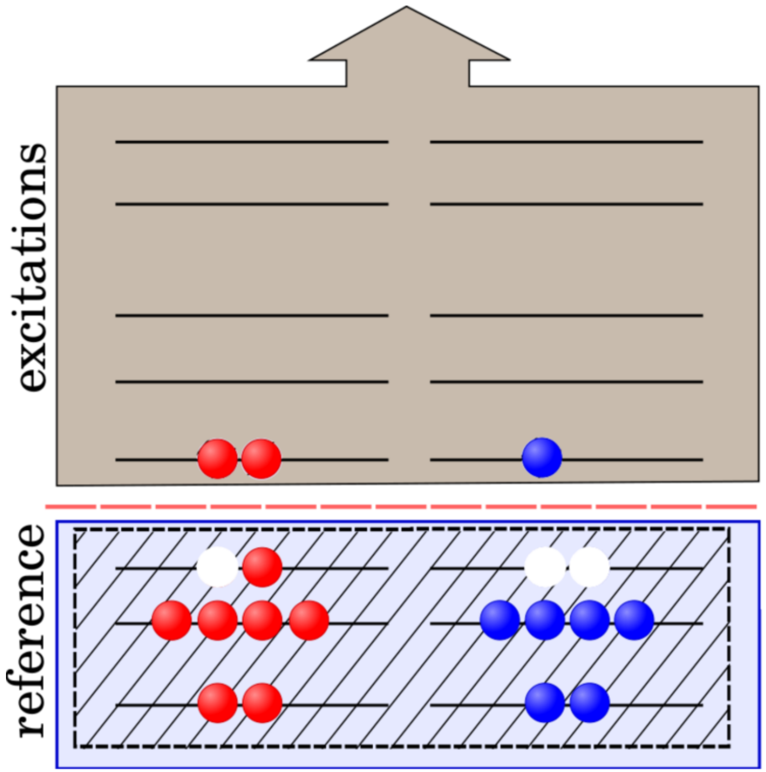


Coupled cluster calculations of beta-decay partners

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

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





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

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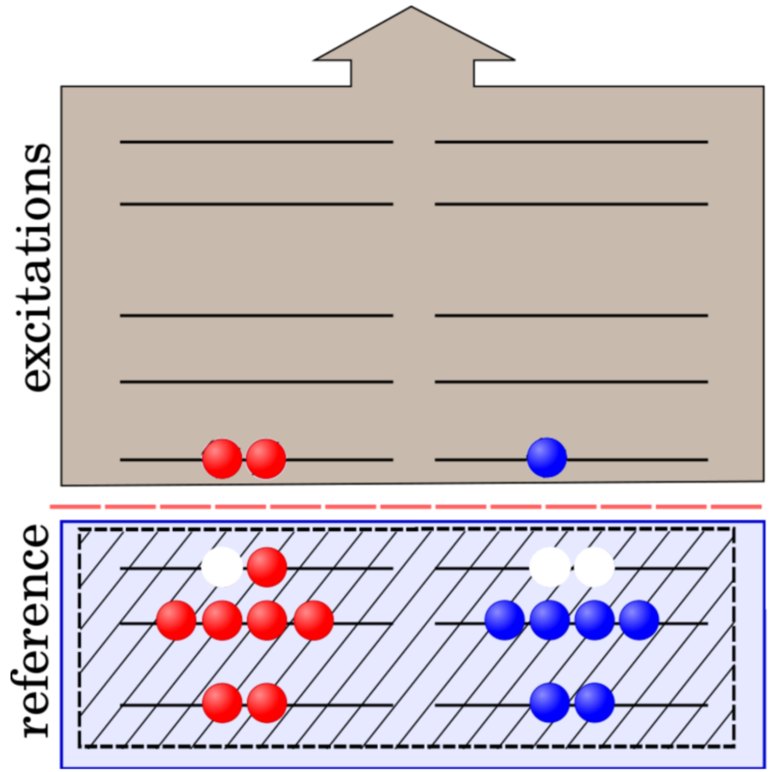
Introduce an energy cut on allowed three-particle three-hole excitations:

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

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

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



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

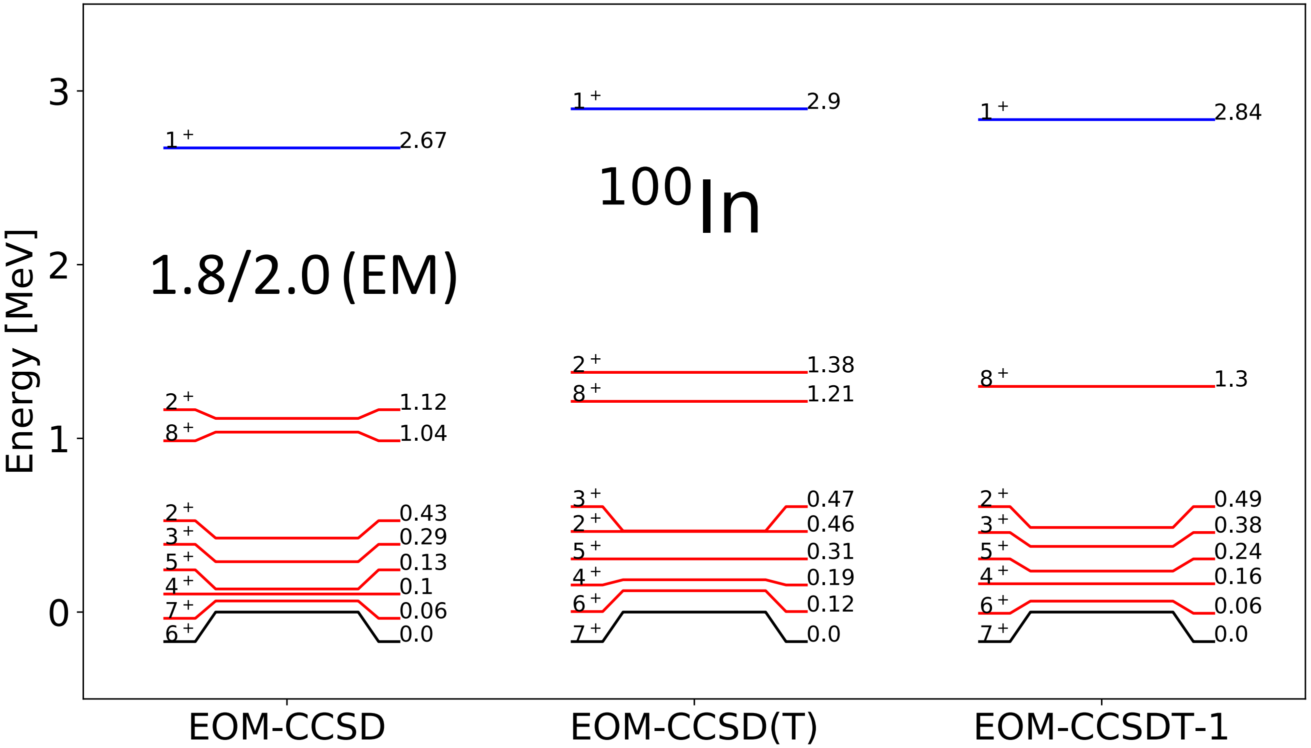
- Bloch-Horowitz is exact; iterative solution poss.

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

- 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)

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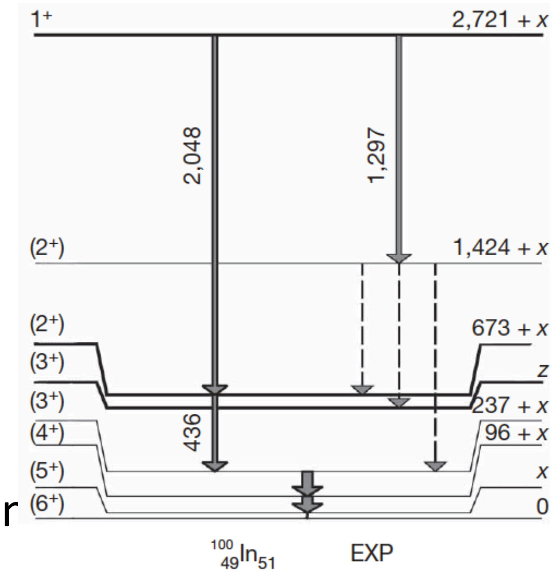


es:

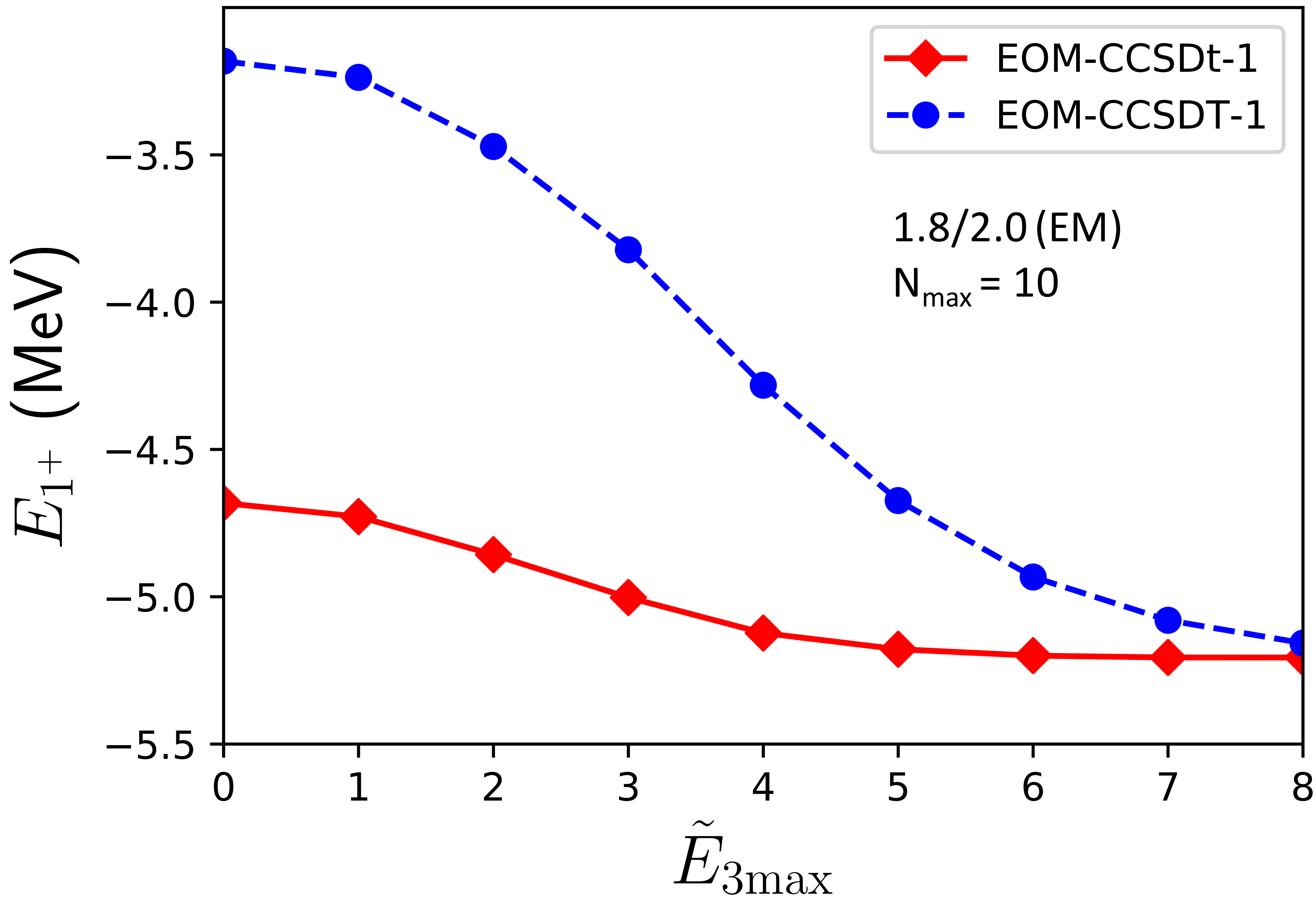
Q-space: $\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\max}$

Everything outside Q we label Q'

Use perturbative approach to calculate contribution from Q':

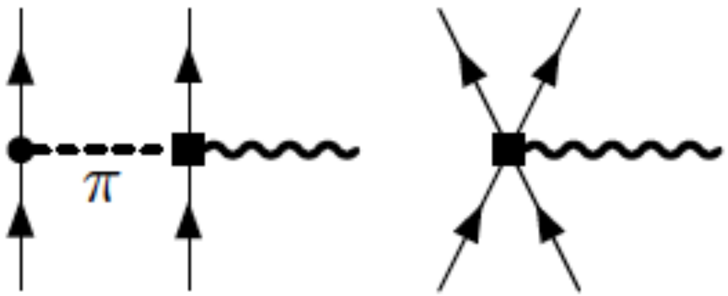
$$\Delta\omega_\mu = \langle \Phi_0 | L_\mu \overline{H}_{PQ'} (\omega_\mu - \overline{H}_{Q'Q'})^{-1} \overline{H}_{Q'P} R_\mu | \Phi_0 \rangle$$

Convergence of excited states in ^{100}In



Normal ordered one- and two-body current

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



c_3, c_4 $\quad$ c_D

Normal ordered operator:

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

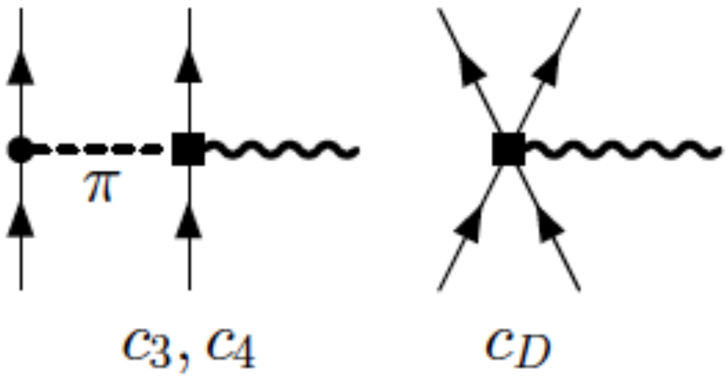
Benchmark between NCSM and CC using NN-N^{4}LO 3N$_{\mathrm{lnl}}$ in ^{8}He:

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

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



Normal ordered operator:

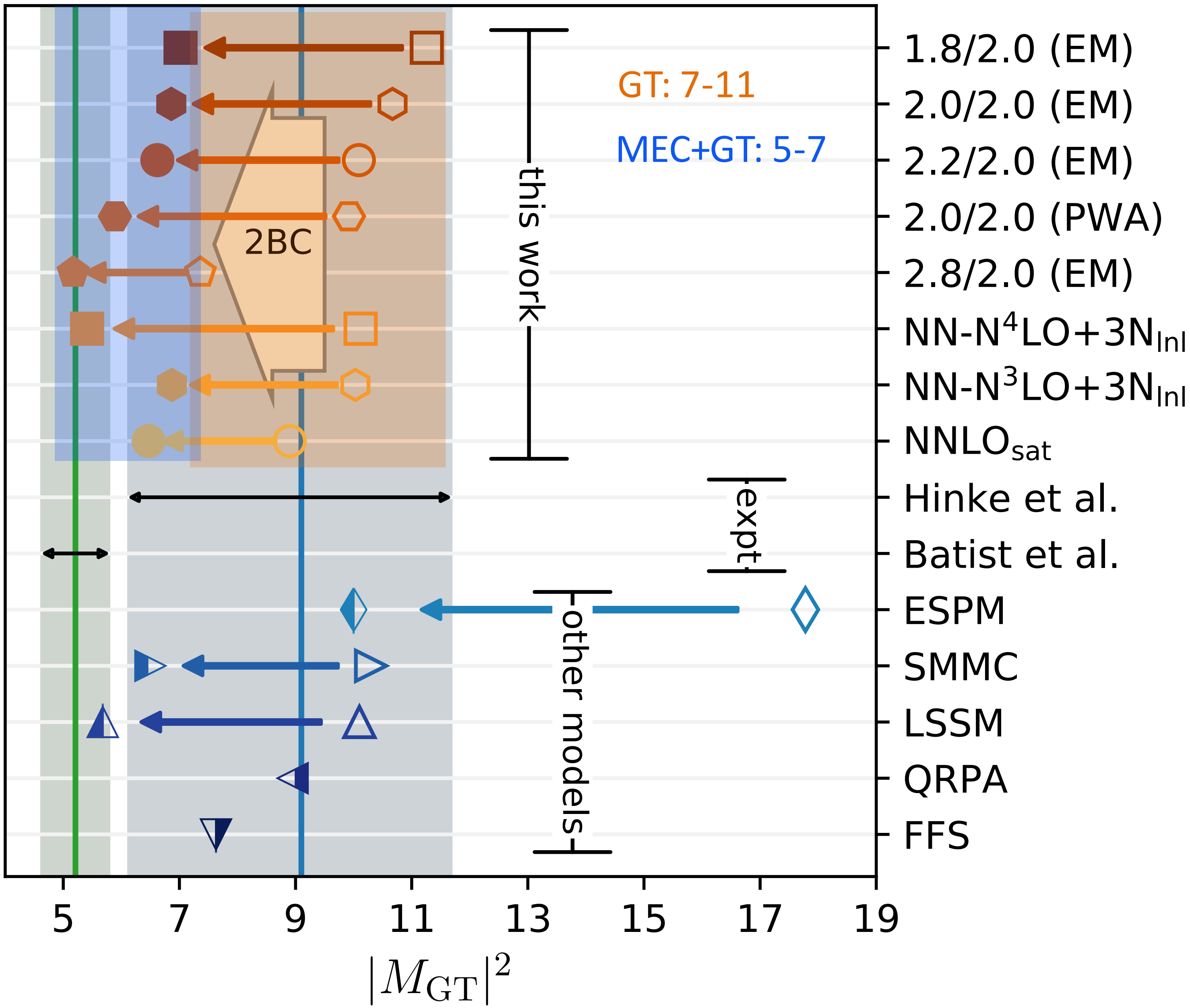
$$\hat{O}_{\mathrm{GT}} = O^1_N + \cancel{O^2_N}$$

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

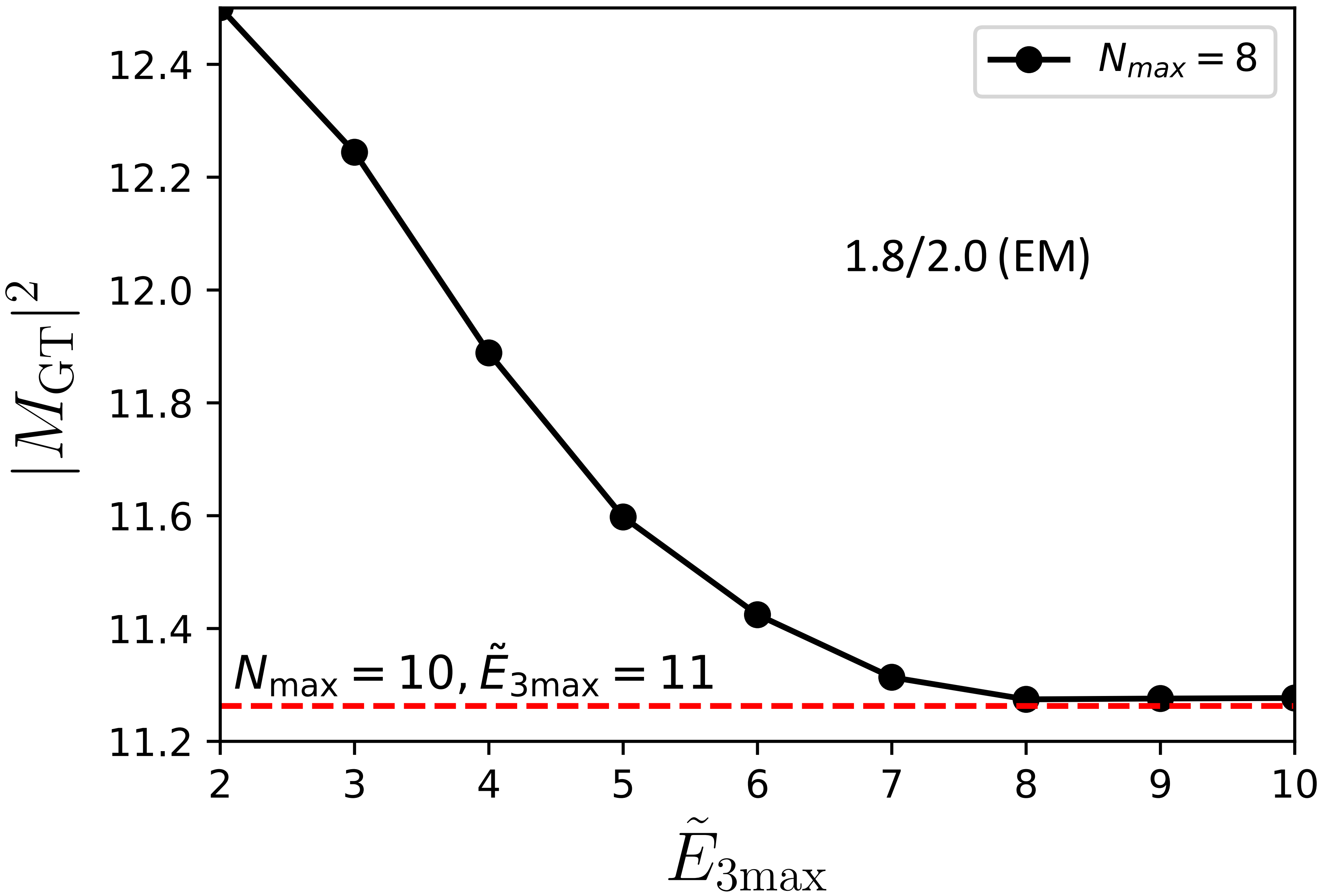
$$^{14}\mathrm{O}_0 \rightarrow {}^{14}\mathrm{N}$$

	$\lvert M_{\mathrm{GT}}(\boldsymbol{\sigma\tau})\rvert$		$\lvert M_{\mathrm{GT}}\rvert$	
Method	NNLO$_{\mathrm{sat}}$	NN-N^{4}LO +3N$_{\mathrm{lnl}}$	NNLO$_{\mathrm{sat}}$	NN-N^{4}LO +3N$_{\mathrm{lnl}}$
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

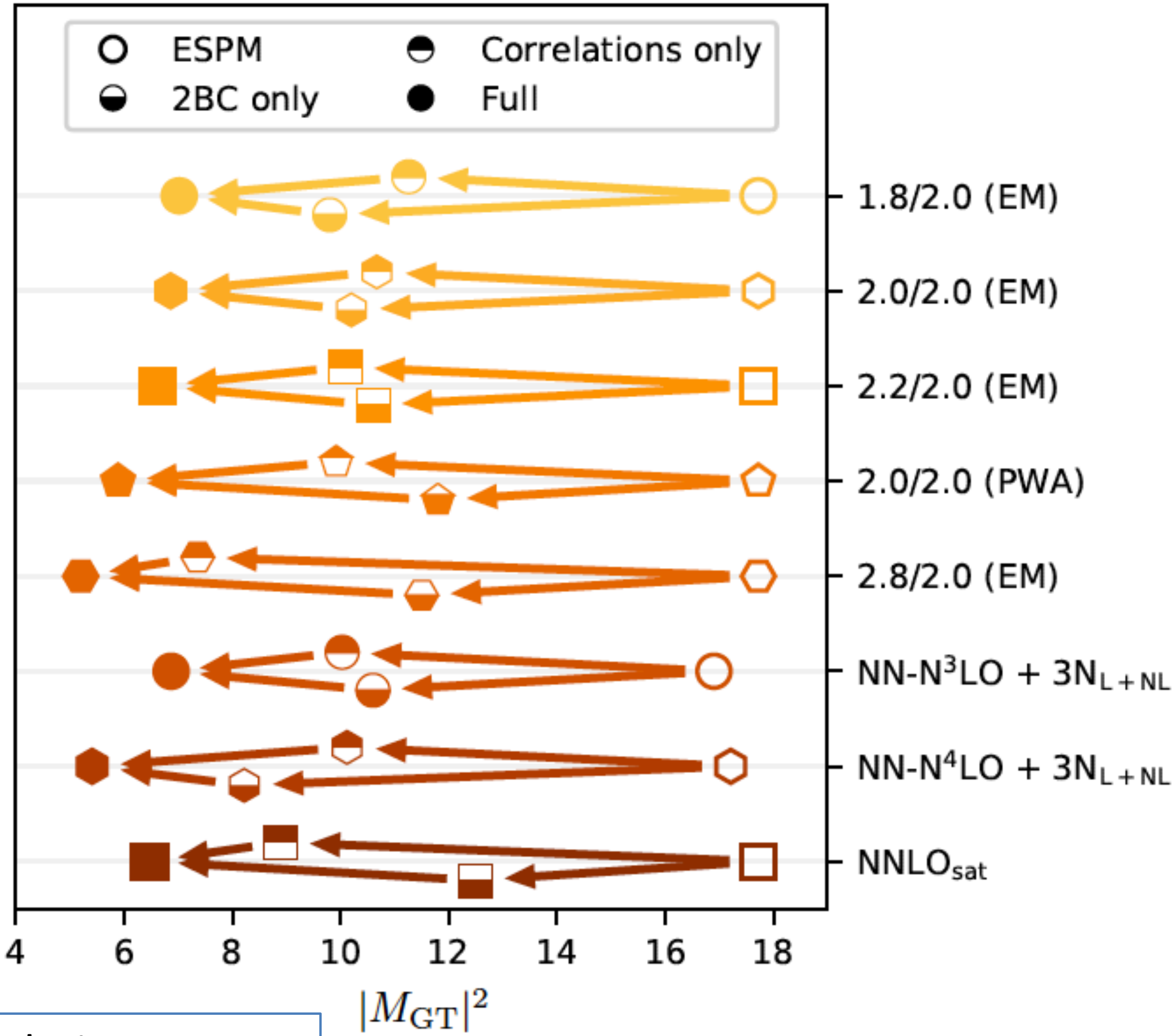


Convergence of GT transition in ^{100}Sn



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

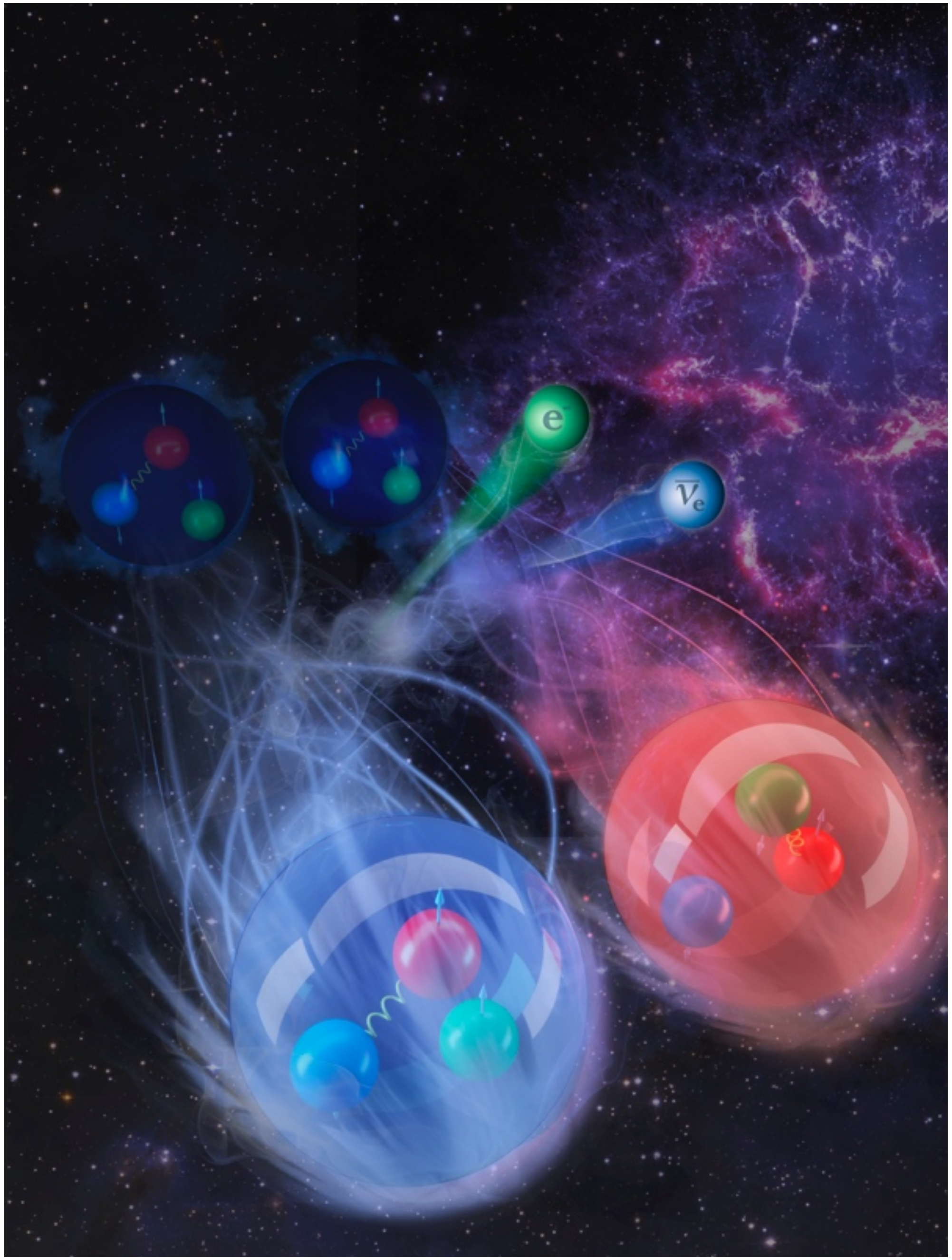
- Subtle interplay between correlations and 2BCs
- Role of correlations (2BC) increase (decrease) for larger cutoffs
- Only sum of correlations and 2BC is observable



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

Conclusions

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



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

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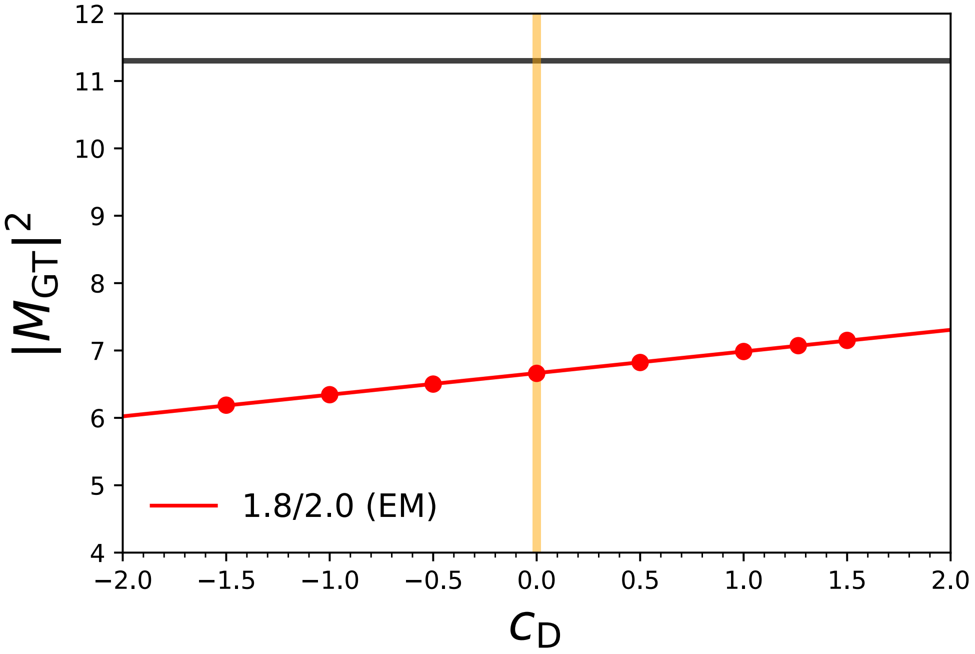
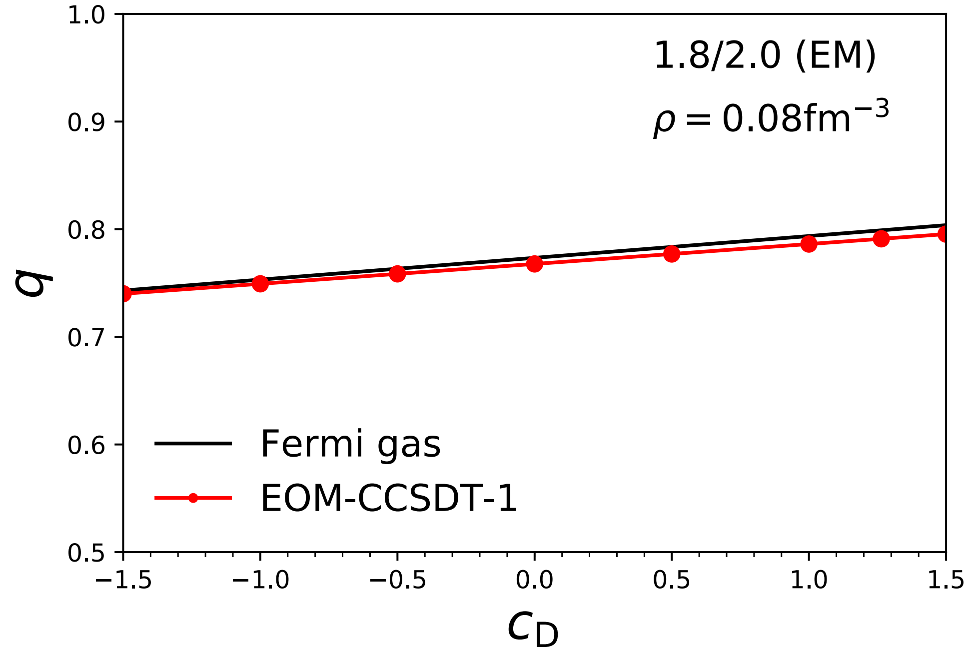
The small role of short-ranged 2BC on GT decay



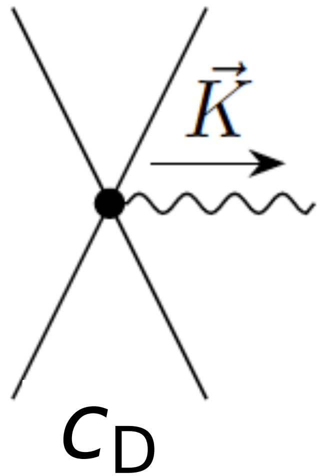


J. Menéndez, D. Gazit, A. Schwenk

PRL 107, 062501 (2011)

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

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



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

Summary of results for ^{100}Sn

Interaction	$\vert m_{\mathrm{GT}}(\boldsymbol{\sigma\tau})\vert^2$	$\vert M_{\mathrm{GT}}(\boldsymbol{\sigma\tau})\vert^2$	$\vert m_{\mathrm{GT}}\vert^2$	$\vert M_{\mathrm{GT}}\vert^2$	log ft	q	q (ESPM)	ΔE [MeV]	BE/A [MeV]
$\mathrm{NNLO_{sat}}$	17.7	8.9	12.5	6.5	2.77	0.85	0.84	7.4	not converged
$\mathrm{NN\text{-}N^3LO{+}3N_{lnl}}$	16.9	10.0	10.6	6.9	2.74	0.83	0.79	6.1	7.6
$\mathrm{NN\text{-}N^4LO{+}3N_{lnl}}$	17.2	10.1	8.2	5.4	2.85	0.73	0.69	5.8	7.1
1.8/2.0 (EM)	17.7	11.3	9.8	7.0	2.73	0.79	0.74	5.1	8.4
2.0/2.0 (EM)	17.7	10.7	10.2	6.9	2.74	0.80	0.76	6.0	7.7
2.0/2.0 (PWA)	17.7	9.9	11.5	5.9	2.81	0.77	0.81	6.8	6.4
2.2/2.0 (EM)	17.7	10.1	10.6	6.6	2.76	0.81	0.77	6.7	7.2
2.8/2.0 (EM)	17.7	7.4	11.8	5.2	2.86	0.84	0.82	8.3	not converged
Batist *et al.* [14]				5.2 ± 0.6				5.11	8.25
Hinke *et al.* [13]				$9.1^{+2.6}_{-3.0}$	$2.62^{+0.13}_{-0.11}$				