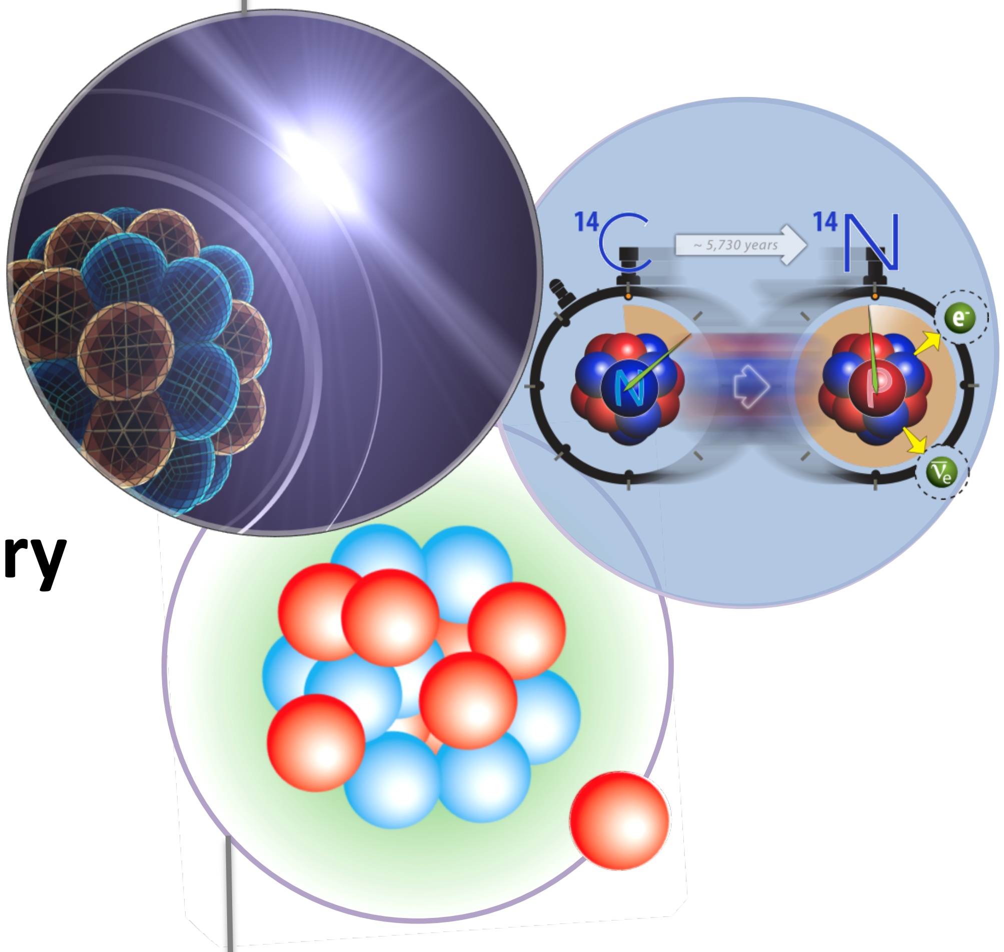
Coupled cluster computations with two-body currents

Gaute Hagen
Oak Ridge National Laboratory



SFB1044 workshop:
Electromagnetic observables for low-energy nuclear physics

Mainz, October 2nd, 2018

U.S. DEPARTMENT OF ENERGY

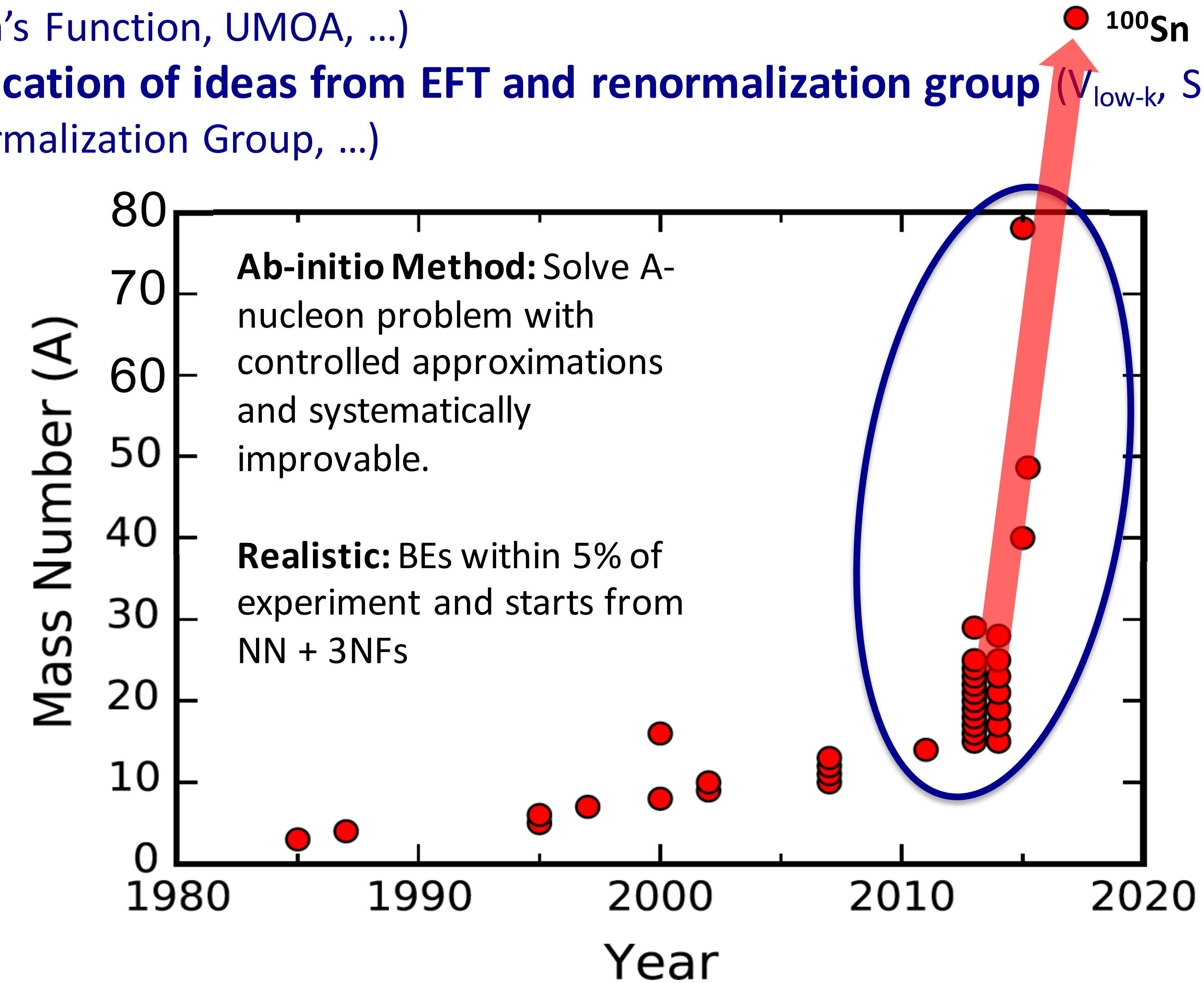
NUCLEI
Nuclear Computational Low-Energy Initiative

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 ($V_{low\text{-}k}$, Similarity Renormalization Group, …)



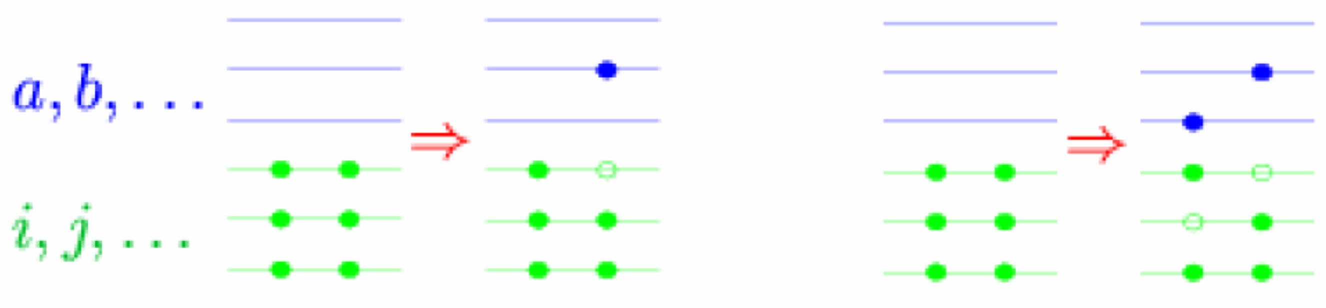
Coupled-cluster method (CCSD approximation)

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!

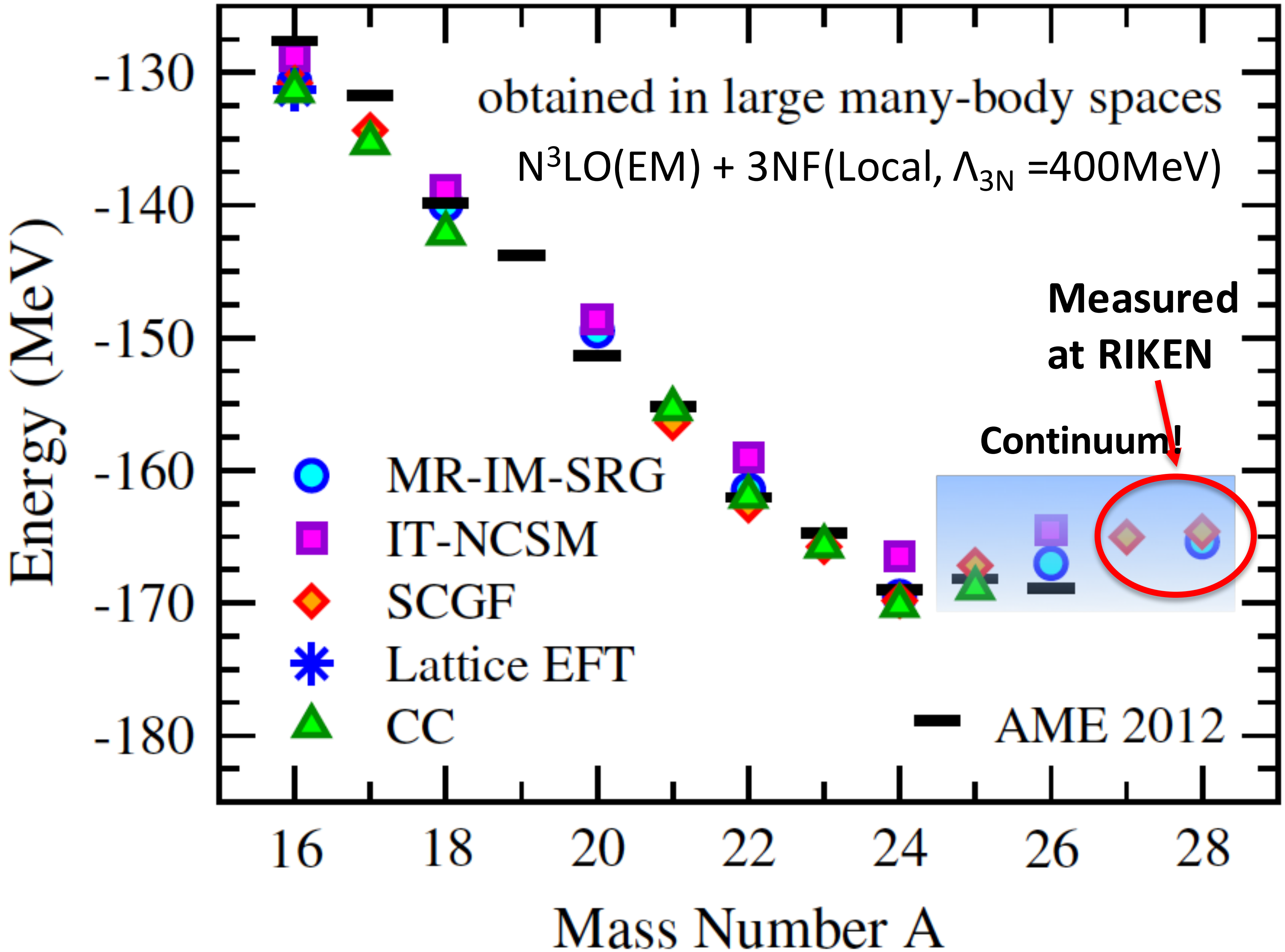


Coupled cluster equations

$$
\begin{aligned}
E &= \langle\Phi|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_i^a|\overline{H}|\Phi\rangle \\
0 &= \langle\Phi_{ij}^{ab}|\overline{H}|\Phi\rangle \\
\overline{H} &\equiv e^{-T}He^{T} = \left(He^{T}\right)_c = \left(H + HT_1 + HT_2 + \frac{1}{2}HT_1^2 + \ldots\right)_c
\end{aligned}
$$

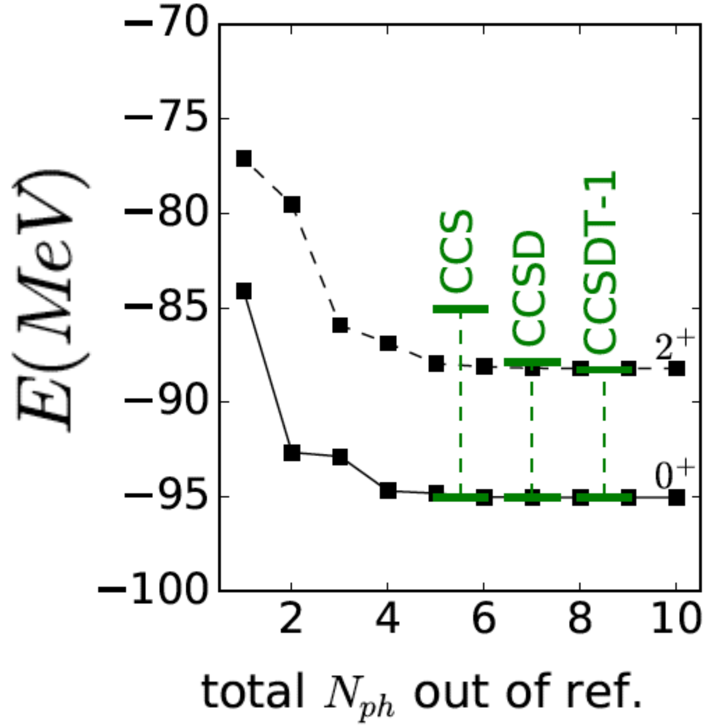
Alternative view: CCSD generates similarity transformed Hamiltonian with no 1p-1h and no 2p-2h excitations.

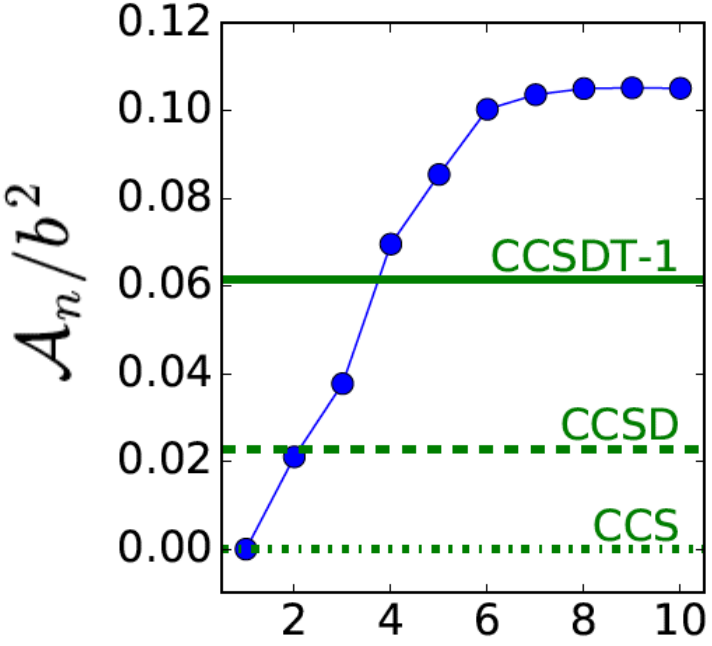
Oxgyen chain with interactions from chiral EFT

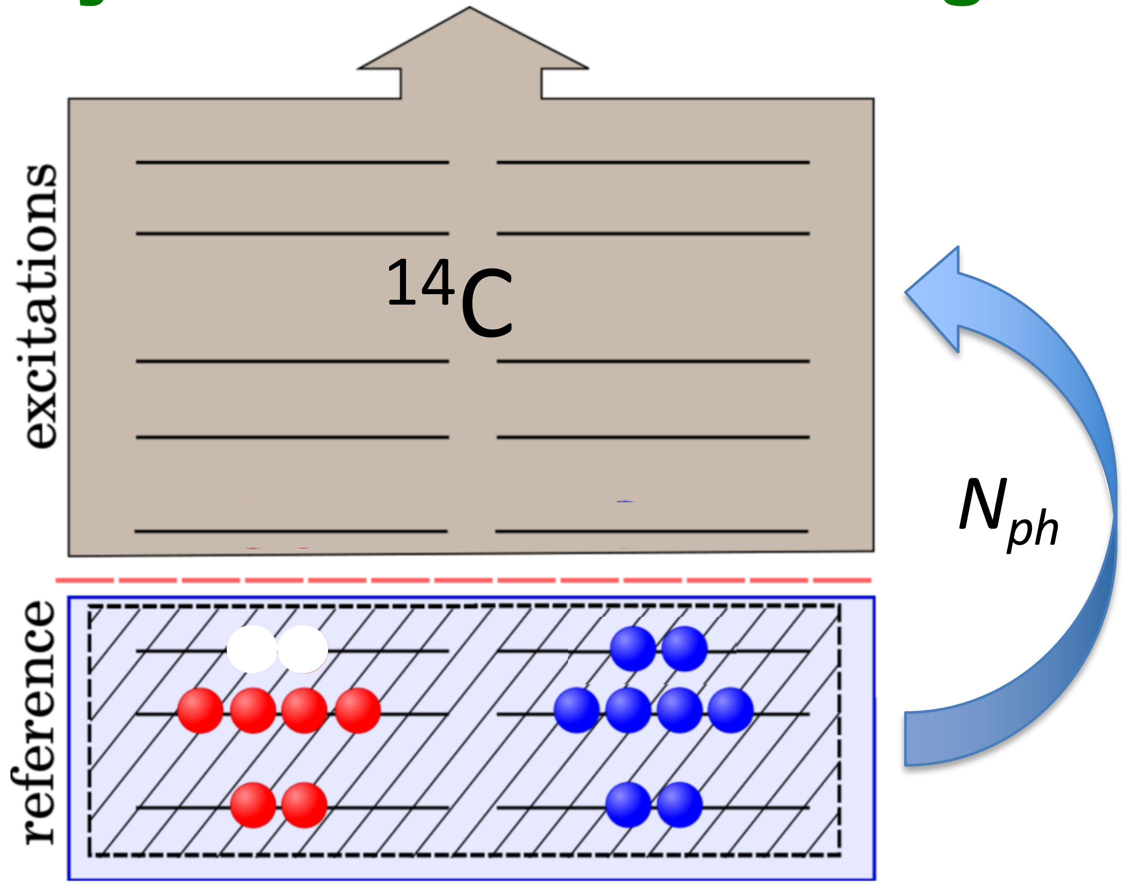


Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

Challenge: Collectivity and transition strengths

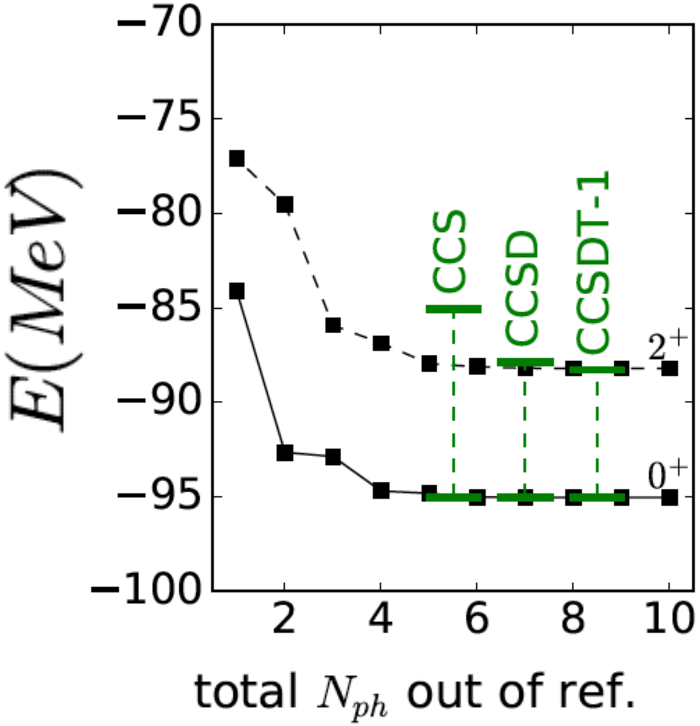


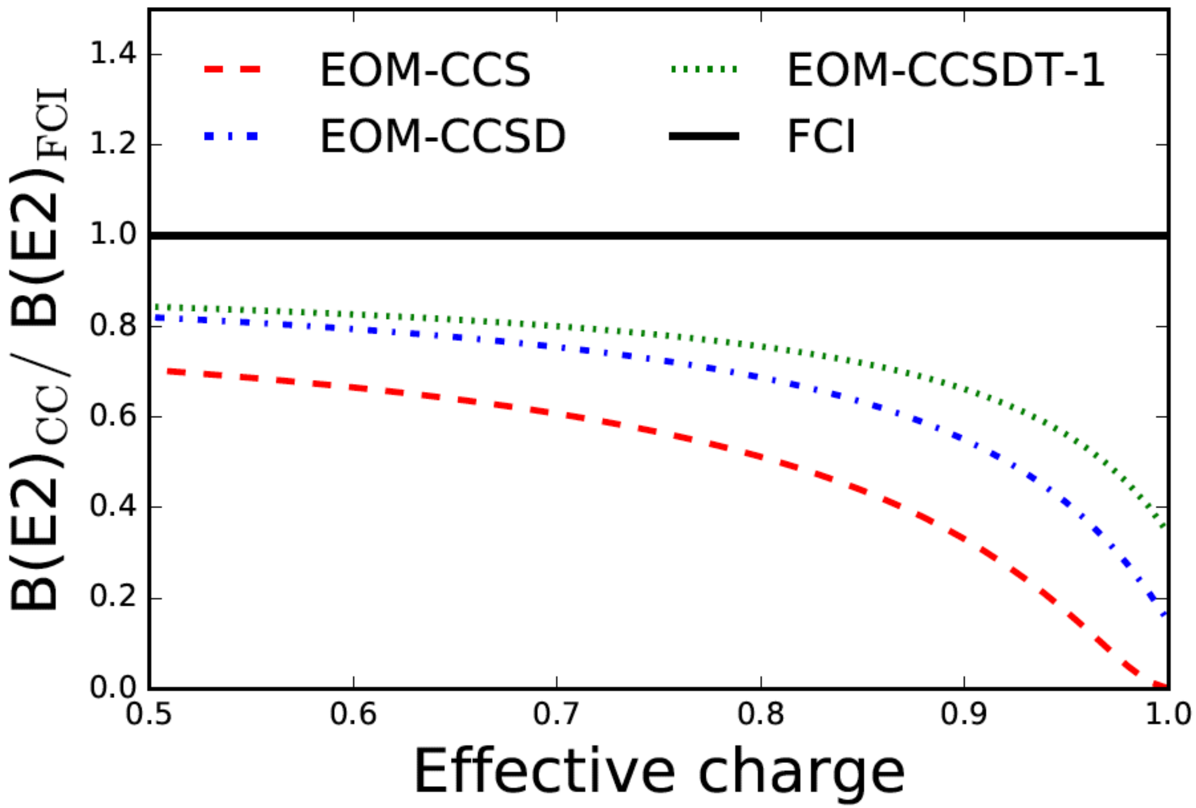


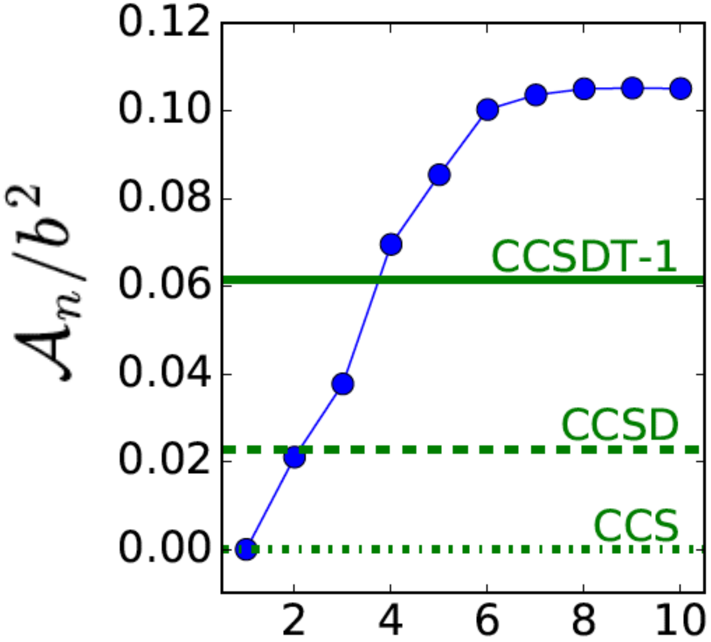


- ^{14}C computed in FCI and CC with psd effective interaction
- Neutron effective charge of charge = 1
- Need excitations beyond 4p4h to describe B(E2) even if 2+ energy is reproduced

Challenge: Collectivity and transition strengths







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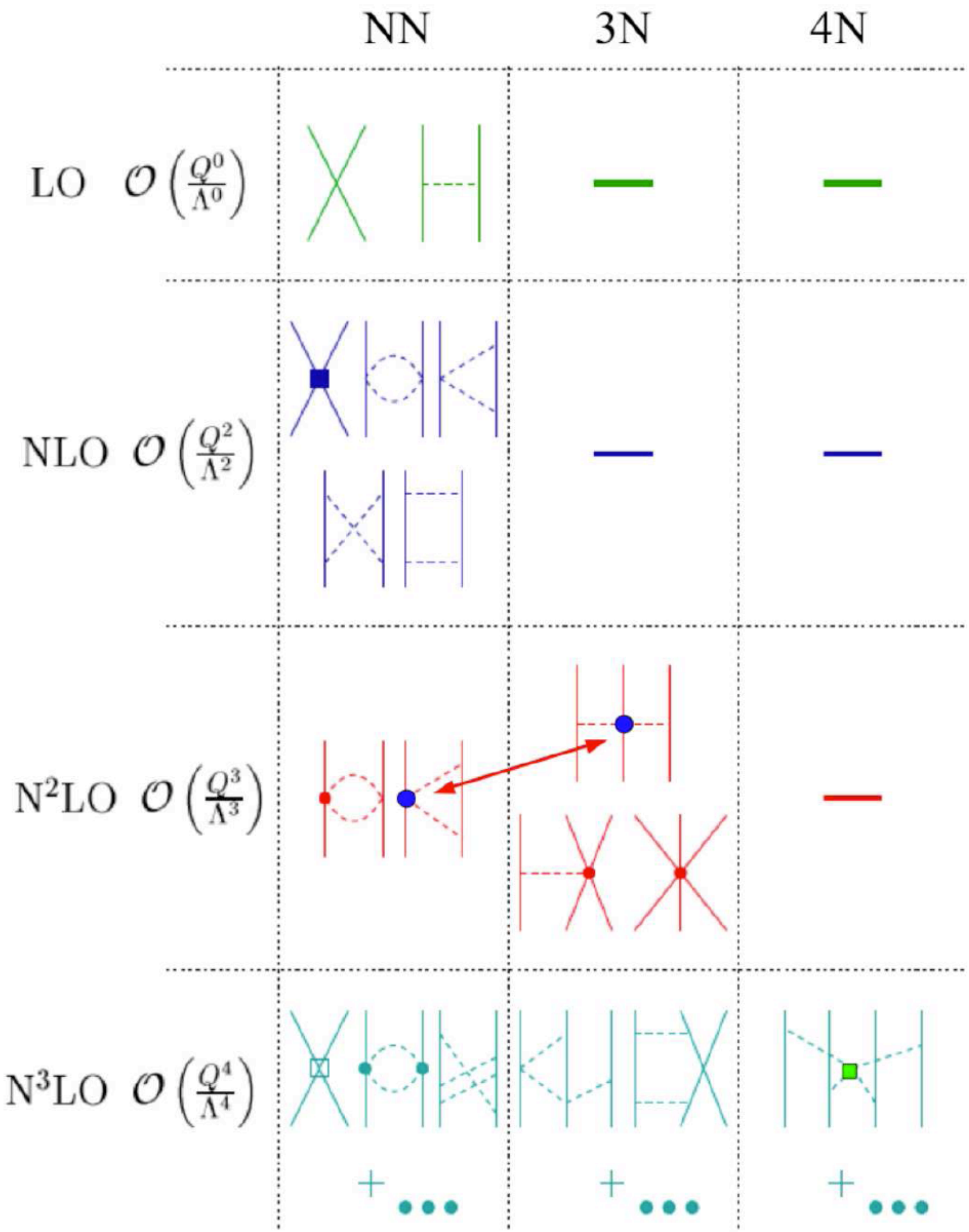
Nuclear forces from chiral effective field theory

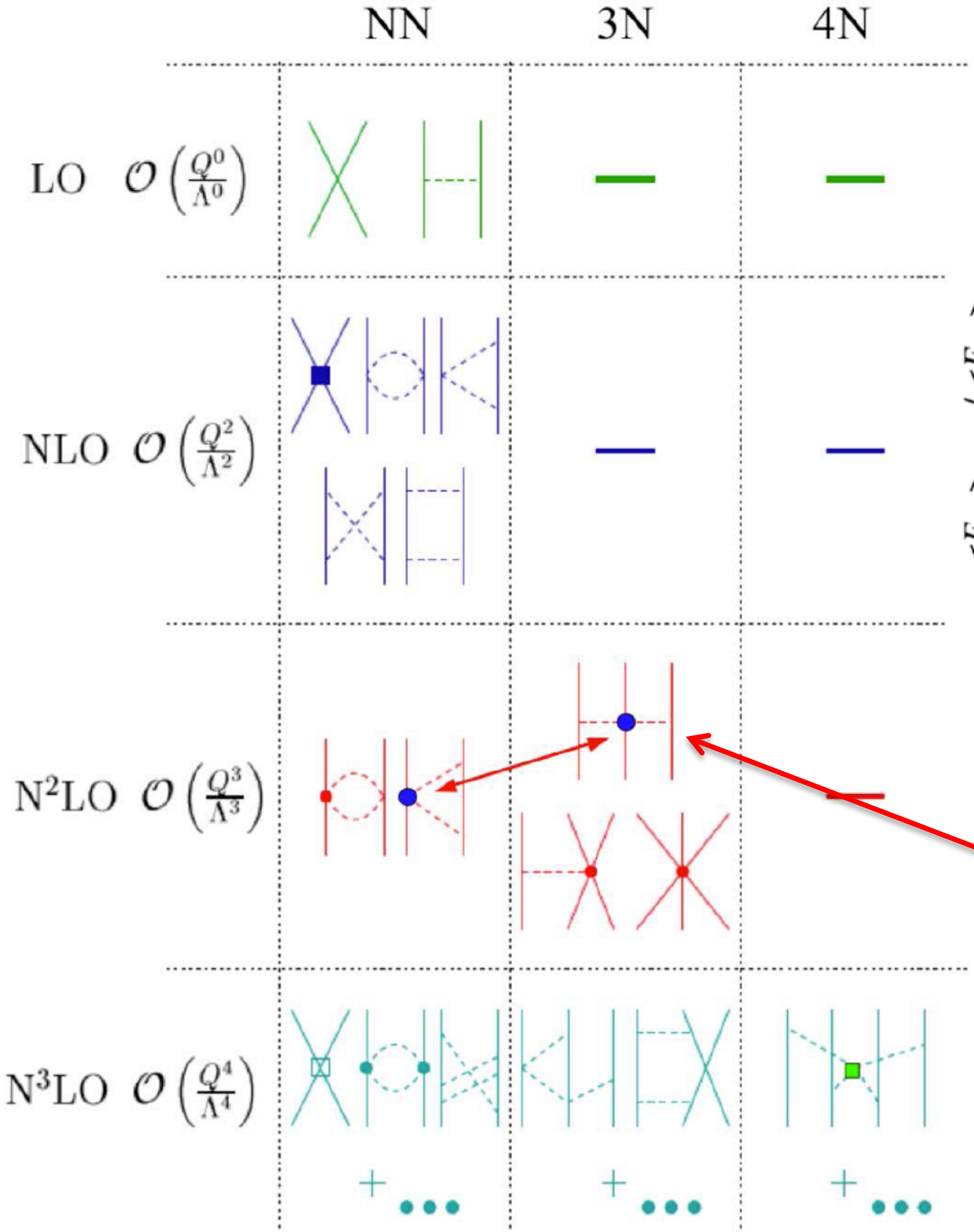
[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]



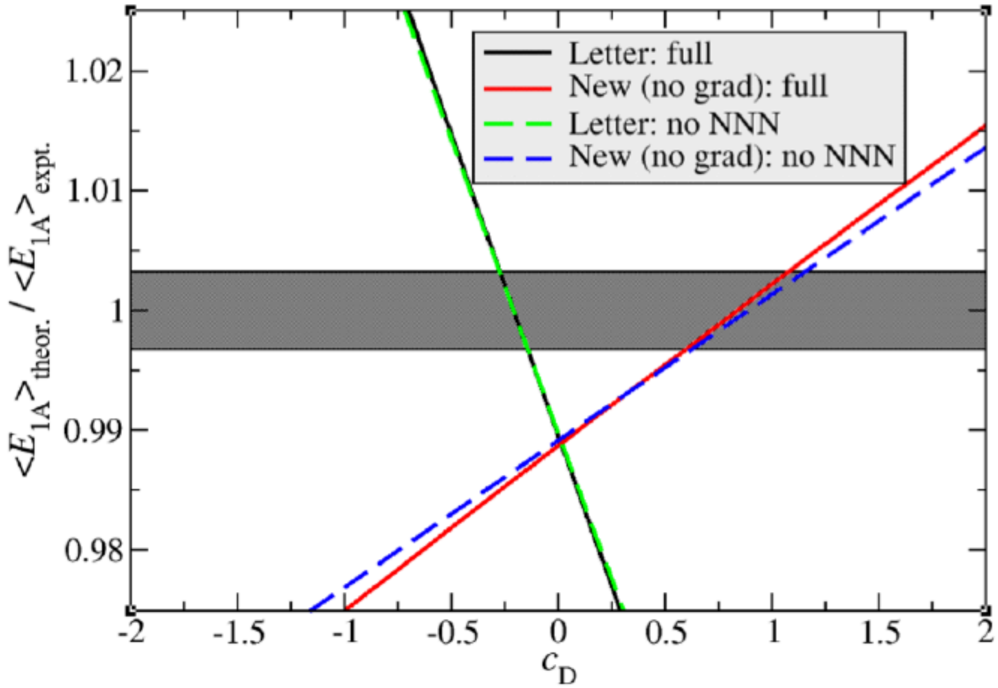
- Developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; Entem et al 2017, Reinert et al 2017…]
- Propagation of uncertainties on the horizon [Navarro Perez 2014, Carlsson et al 2015]
- Different optimization protocols [Ekström et al 2013, Carlsson et al 2016]
- Improved understanding/handling via SRG [Bogner et al 2003; Bogner et al 2007]
- local / semi-local / non-local formulations [Epelbaum et al 2015, Gezerlis et al 2013/2014]
- Chiral EFT's with explicit Delta isobars [Krebs et al 2018, Piarulli et al 2017, Ekstrom et al 2017]

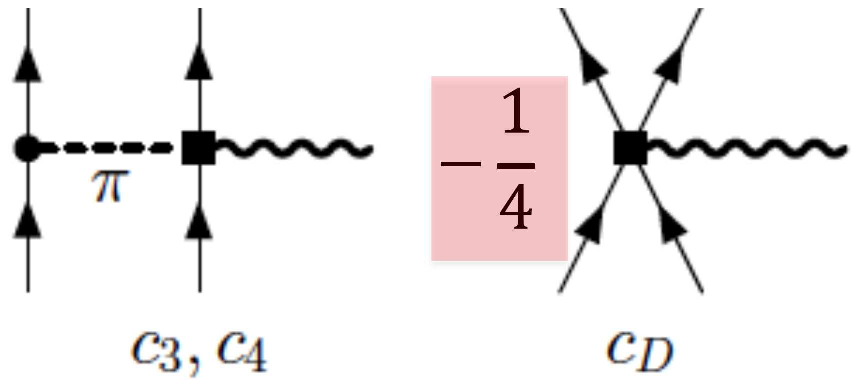
Nuclear forces from chiral effective field theory

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

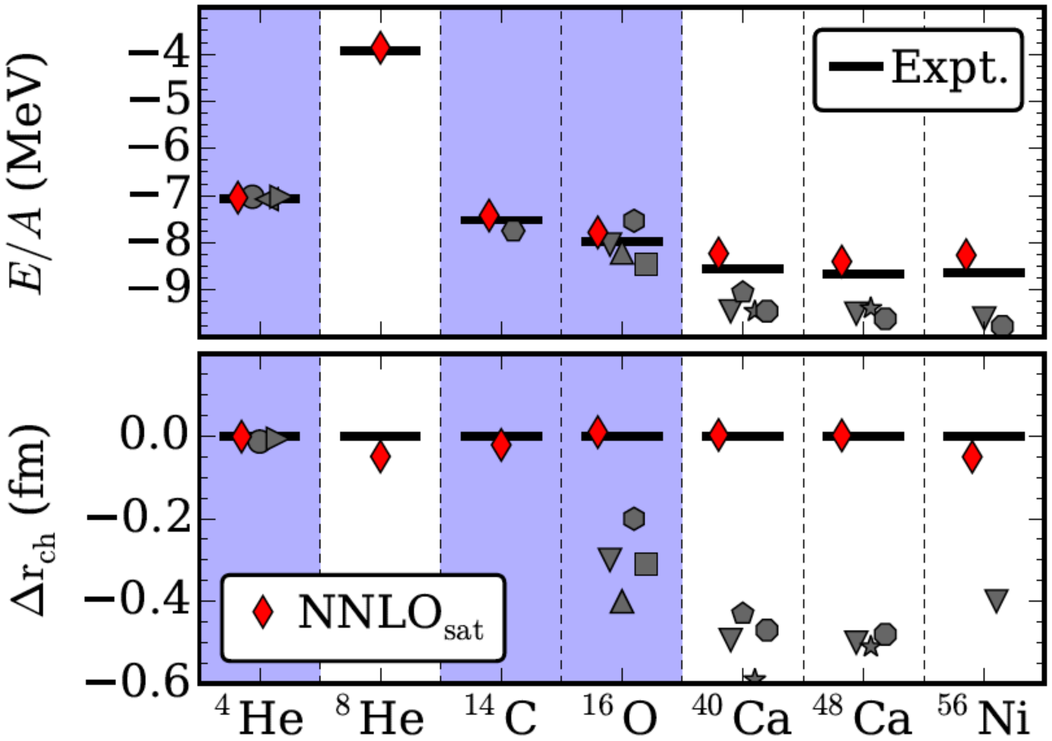


From Sofia Quaglioni and Kyle Wendt





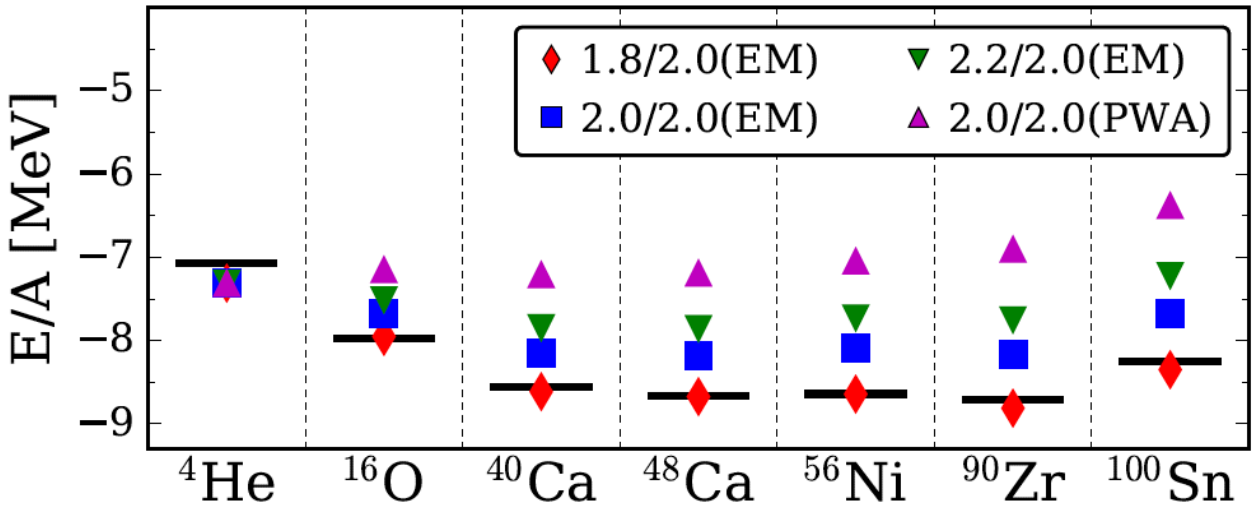
A family of interactions from chiral EFT



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).

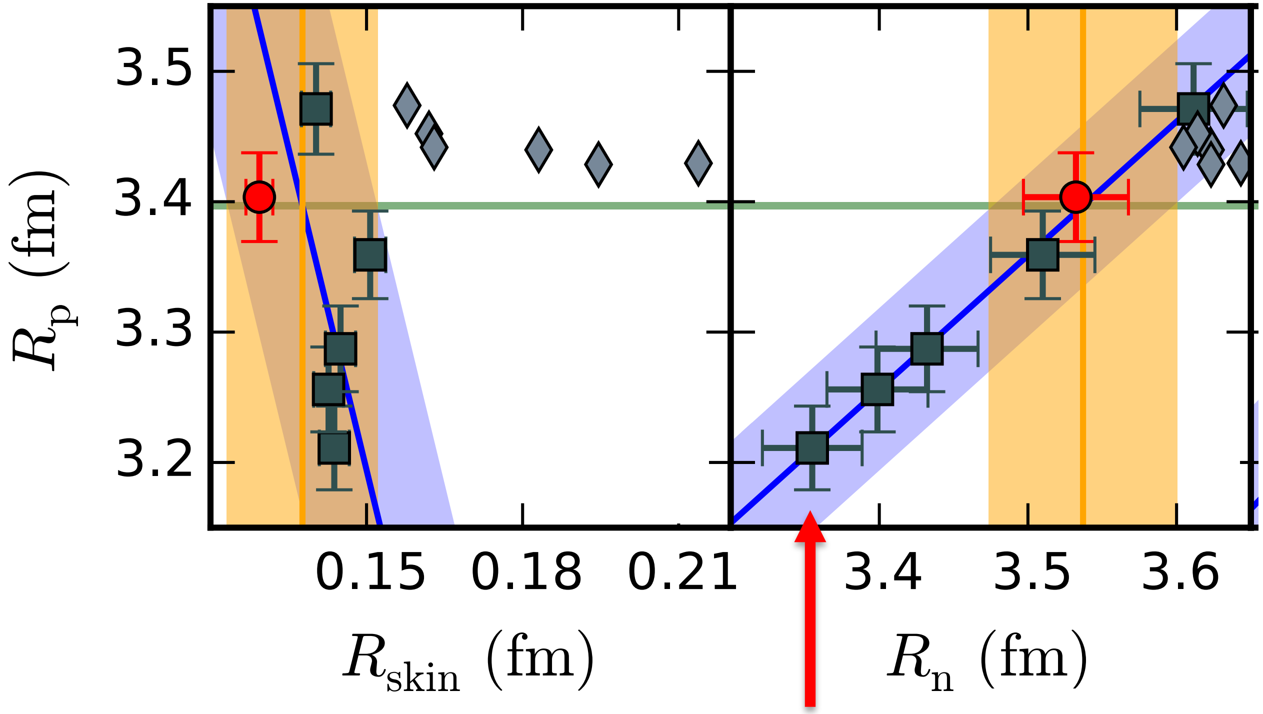


1.8/2.0(EM): Accurate BEs

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).

Neutron radius and skin of ^{48}Ca



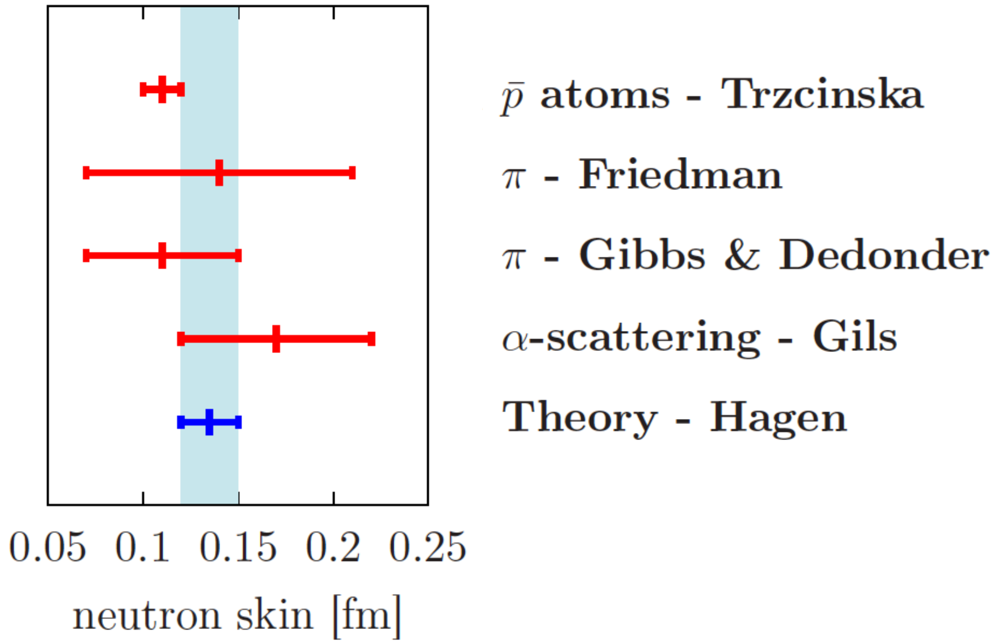
1.8/2.0 (EM)

G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

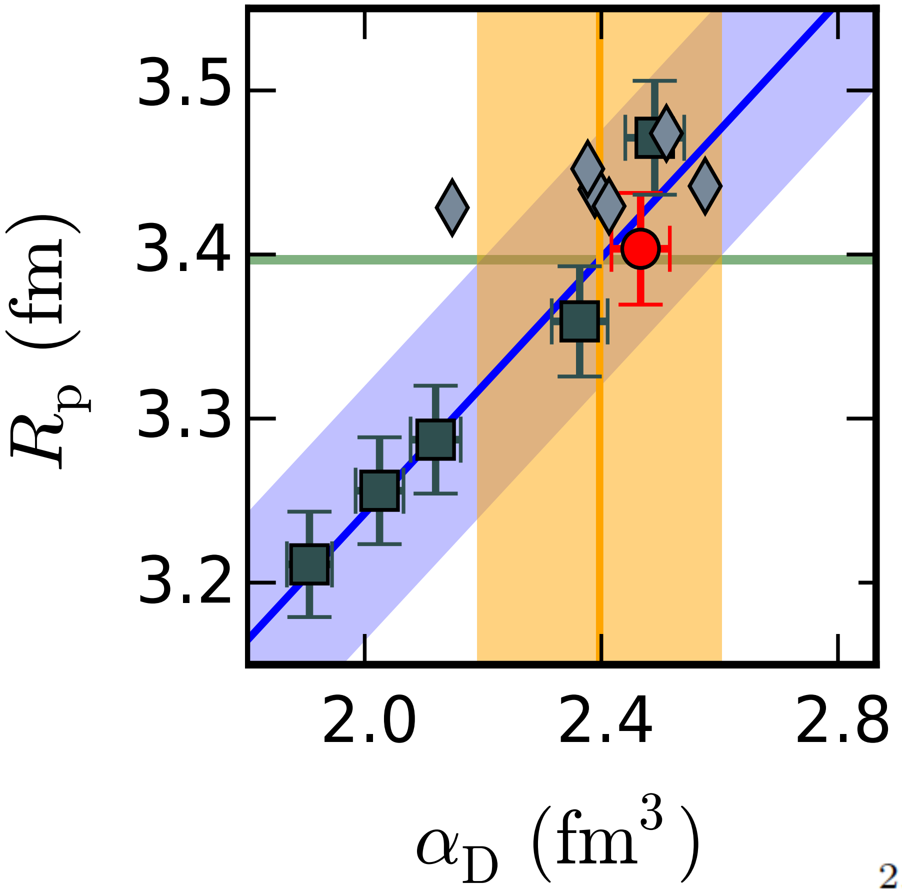
Uncertainty estimates from family of chiral interactions: K. Hebeler *et al* PRC (2011)

DFT:
SkM*, SkP, Sly4, SV-min, UNEDF0, and UNEDF1

- Neutron skin significantly smaller than in DFT
- Neutron skin almost independent of the employed Hamiltonian
- Our predictions for ^{48}Ca are consistent with existing data



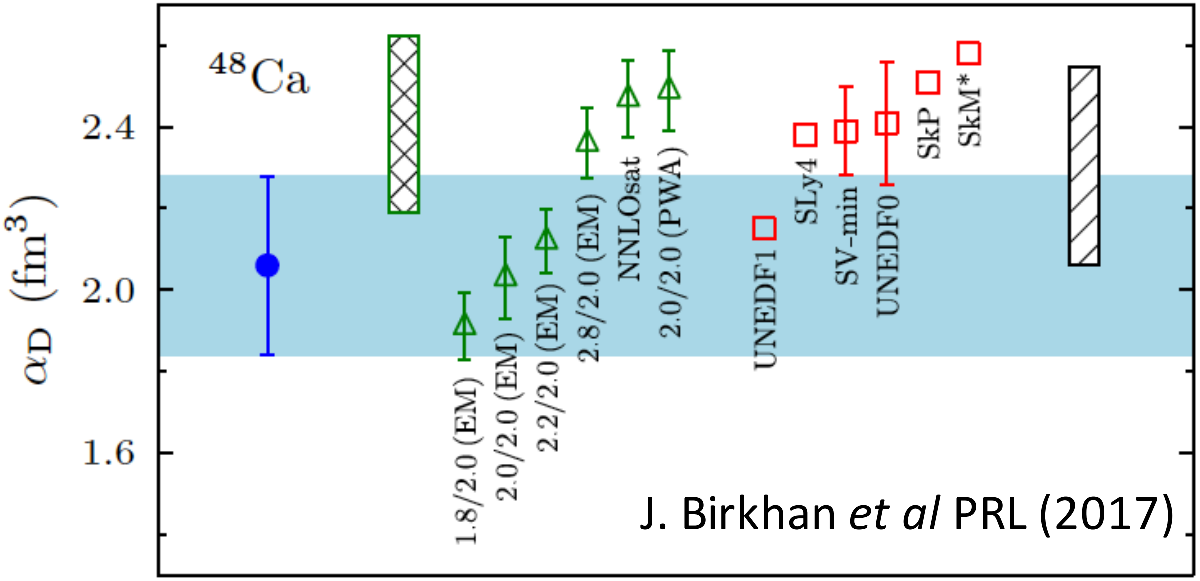
Dipole polarizability of ^{48}Ca



- DFT results are consistent and within band of ab-initio results
- α_D meausred by the Osaka-Darmstadt collaboration
- Ab-initio prediction overlaps with experimental uncertainty
- α_D constrains the neutron skin to 0.14 – 0.20fm

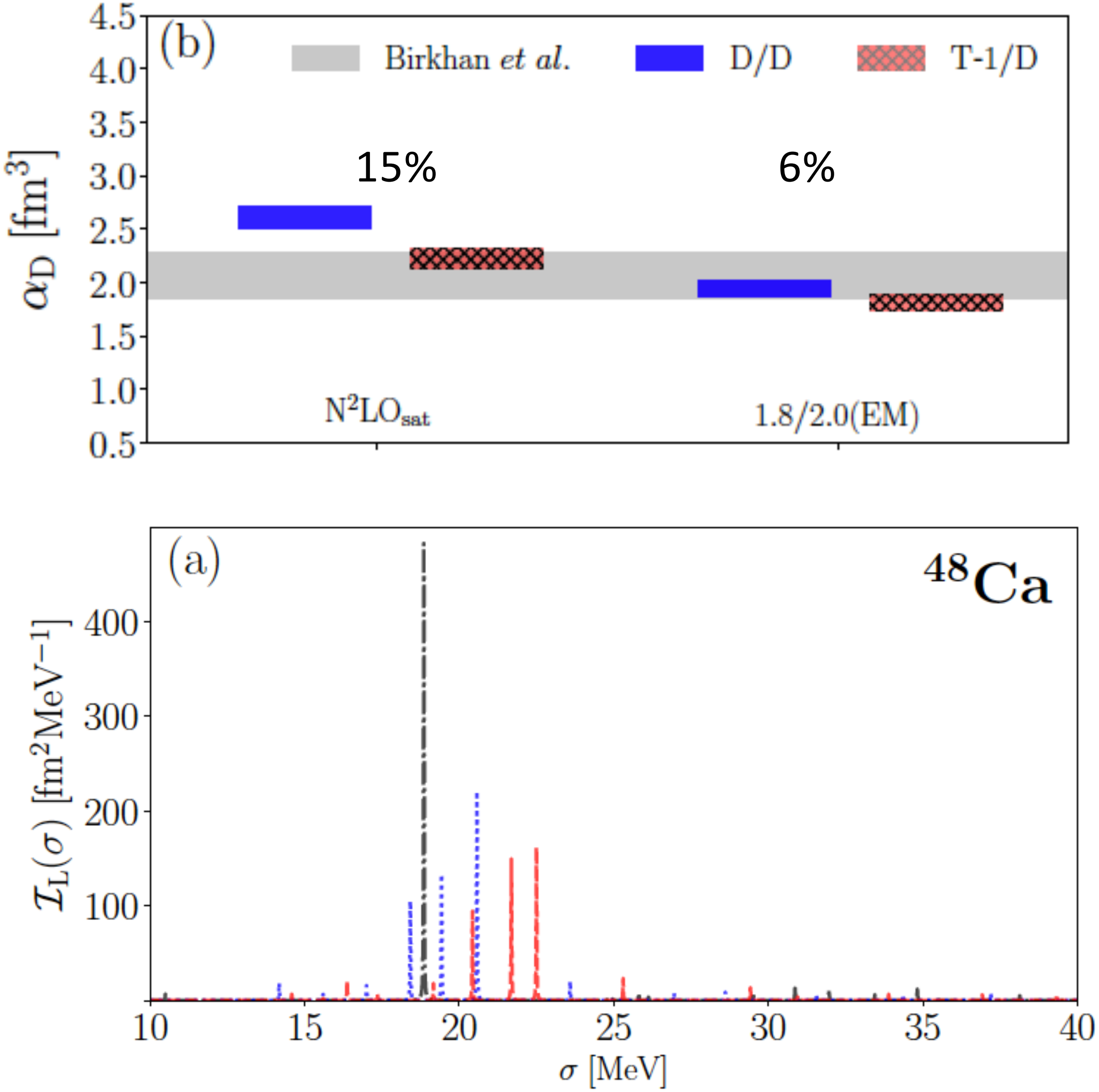
G. Hagen *et al*, Nature Physics **12**, 186–190 (2016)

Ab-initio prediction from correlation with R_p:
$2.19 \lesssim \alpha_D \lesssim 2.60$ fm^3



J. Birkhan *et al* PRL (2017)

Compute the dipole polarizability of ^{48}Ca with increased precision



- Triples impacts α_D
- Less than 1% effect from triples on radii
- The inclusion of triples fragments the strength and increases strength at higher energies
- Triples impacts the running sum for α_D

Higher order corrleations are important!

M. Miorelli et al,
Phys. Rev. C 98, 014324 (2018)

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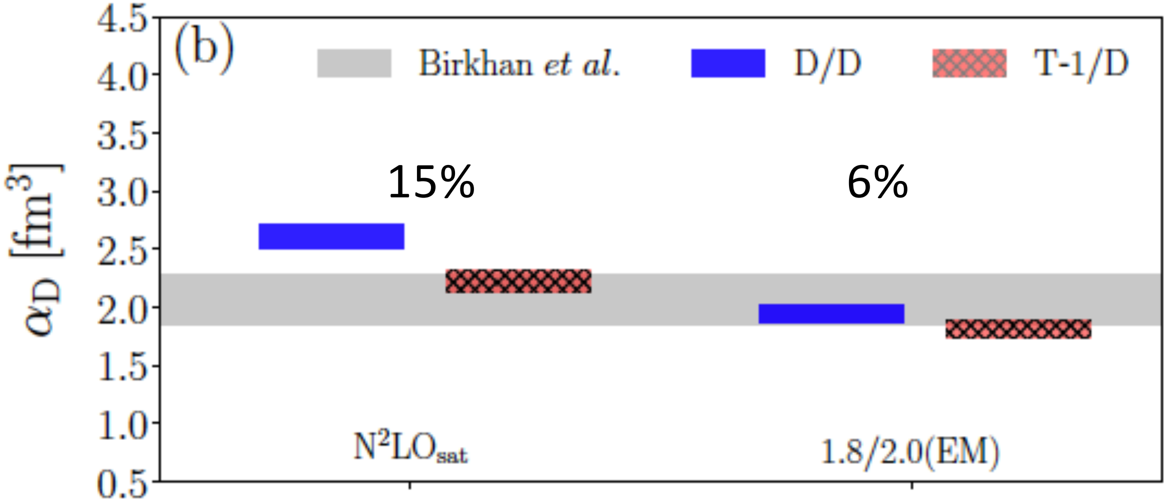

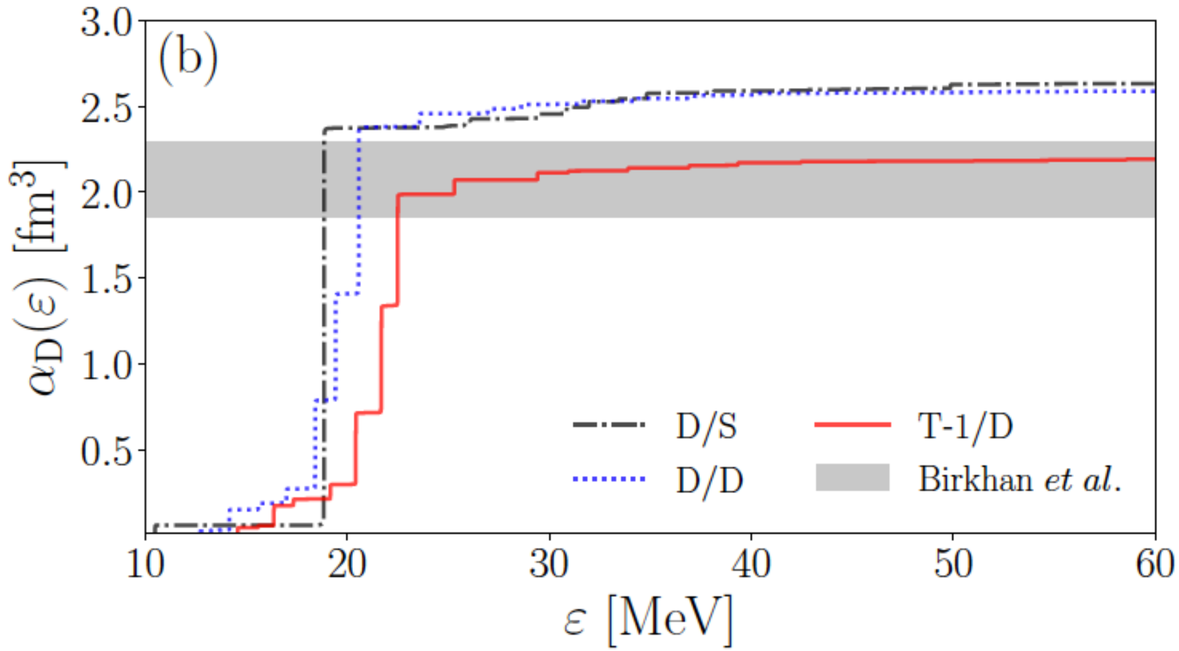

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Inclusive electron scattering and the Coulomb sum rule

Towards ν-scattering/response of ^{16}O and ^{40}Ar:
Electron scattering off ^{16}O and ^{40}Ca

The CSR is the total integerated strength of inelastic longitudinal response function

$$CSR(q) = \int d\omega \; R_L^{in}(\omega, \mathbf{q}) / G_p^2(Q^2)$$

$$R_L^{in}(\omega, \mathbf{q}) = \sum_f |\langle f | \rho(\mathbf{q}) | \mathbf{0} \rangle|^2 \delta(\omega - \mathbf{E_f} + \mathbf{E_0})$$

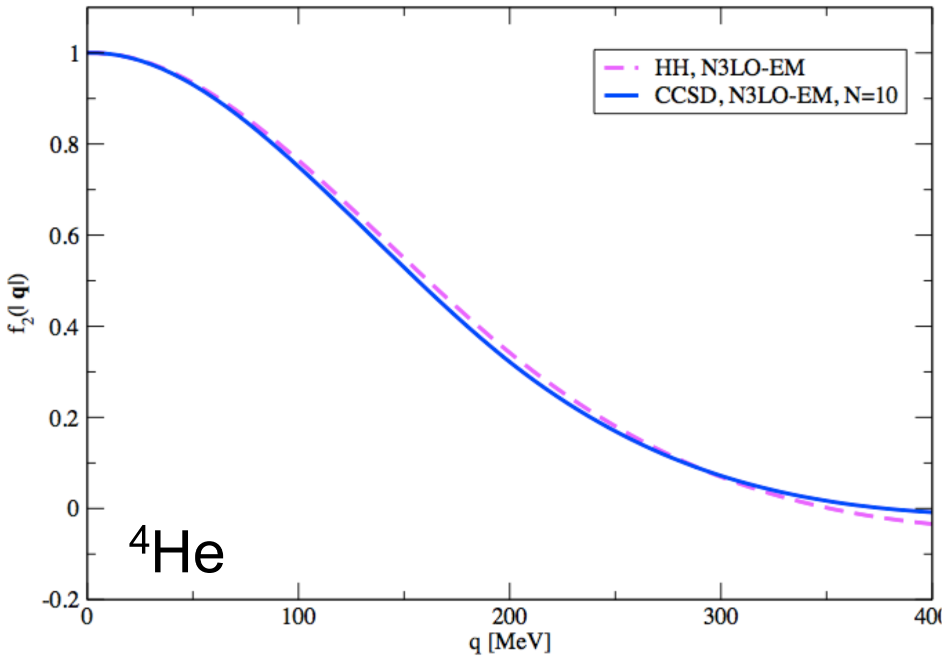
Here $\rho(q)$ is the nuclear charge operator
Final state different from g.s. since we want the inelastic response

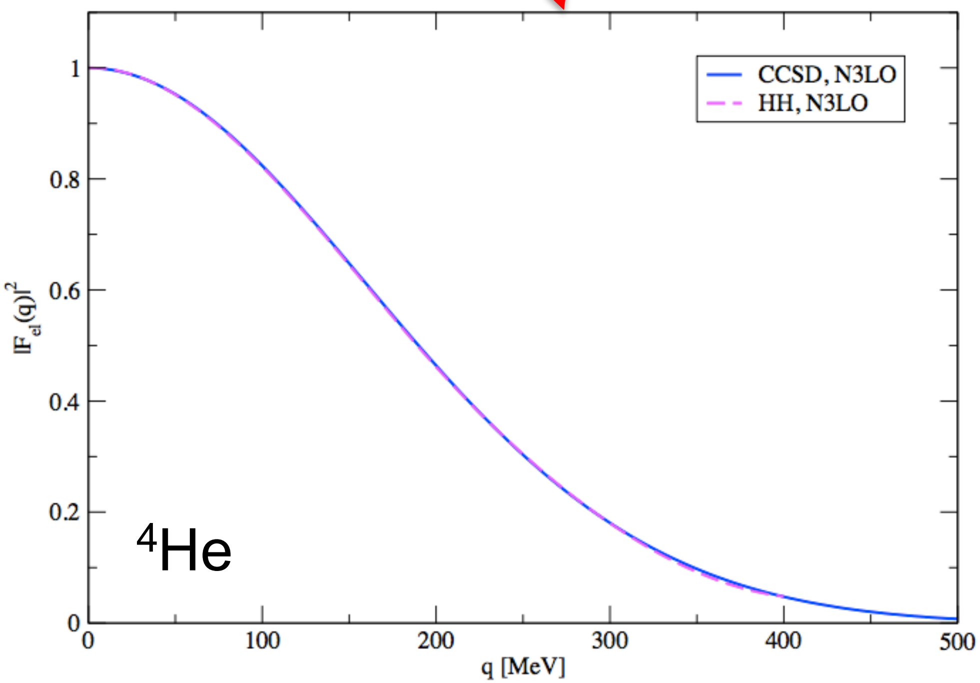
We approached the problem as we do for the calculation of the total strength of the dipole response function in PRL **111**, 122502 (2013).

Inclusive electron scattering and the Coulomb sum rule

$$\mathrm{CSR}(q) = Z + \langle 0 | \sum_{i \neq j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} | 0 \rangle - |F(\mathbf{q})|^2 Z^2$$

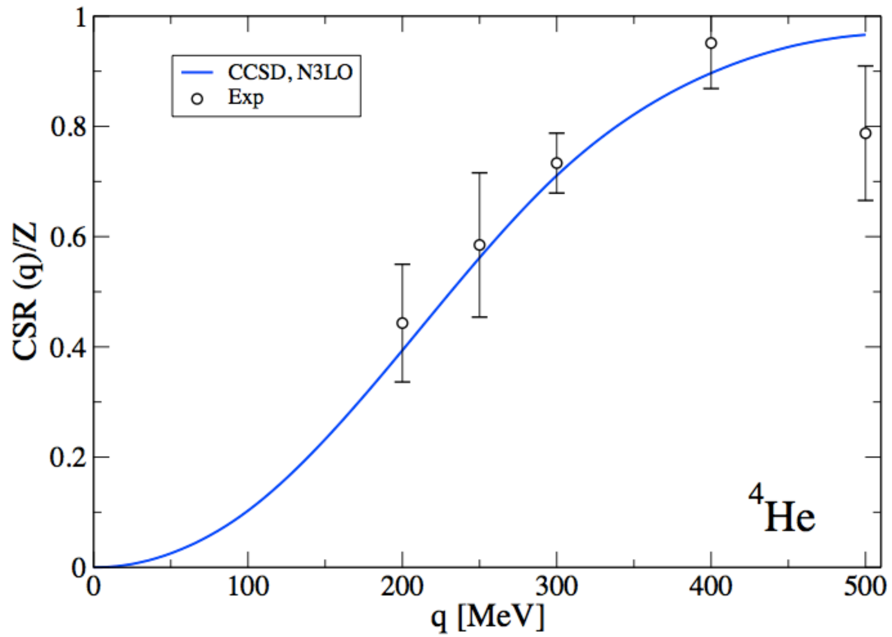
$$\langle 0 | \sum_{i \neq j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} | 0 \rangle = Z(Z-1) f_2(|\mathbf{q}|)$$



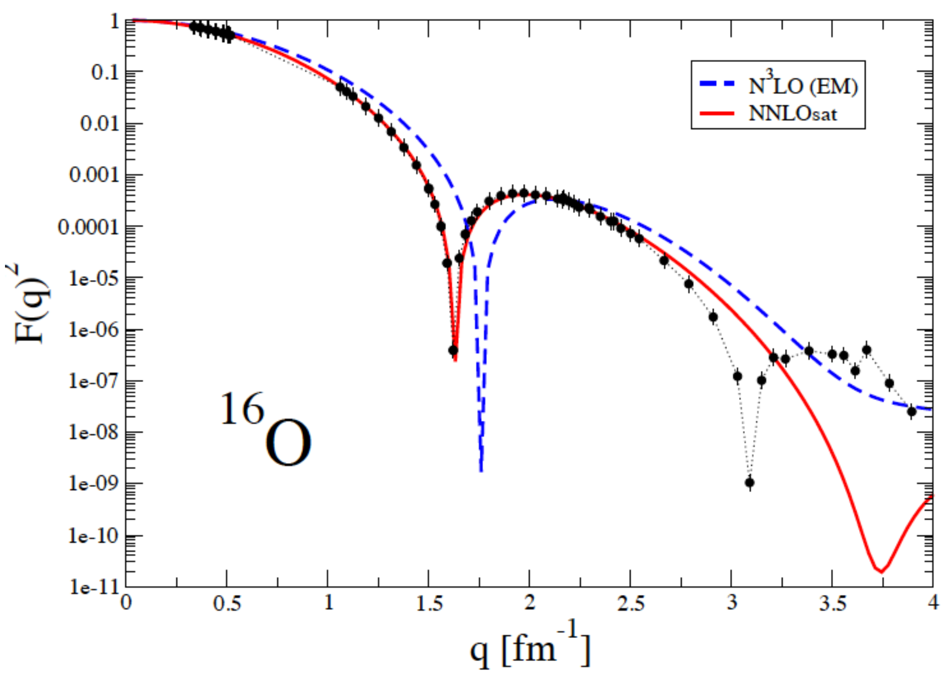


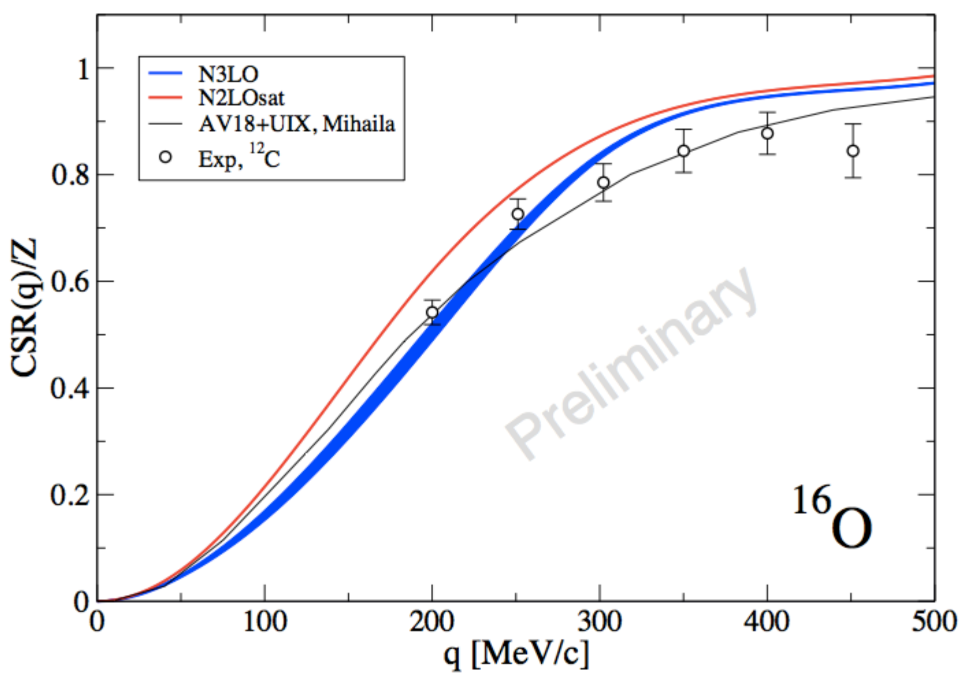
Benchmark with “exact” Hyperspherical Harmonics for ^{4}He

Comparison to data in ^{4}He and ^{16}O

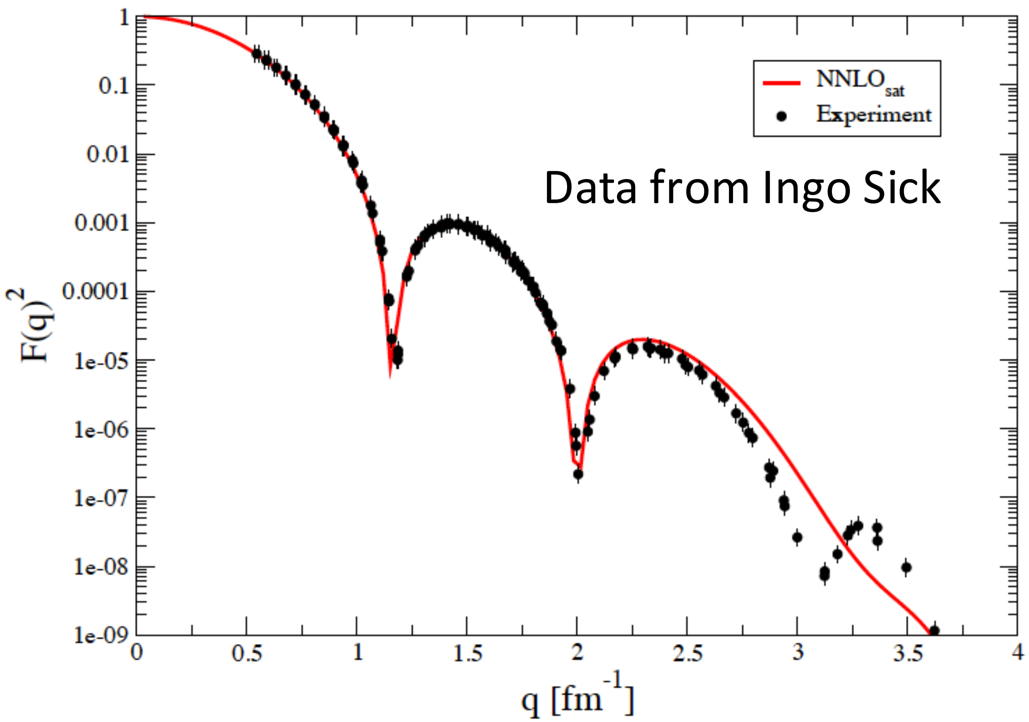


- Good agreement in ^{4}He
- CSR for 16O based on $NNLO_{sat}$ and N3LO(EM)
- Comparison to data in ^{12}C and to Mihaila and Heisenberg (PRL 2000)

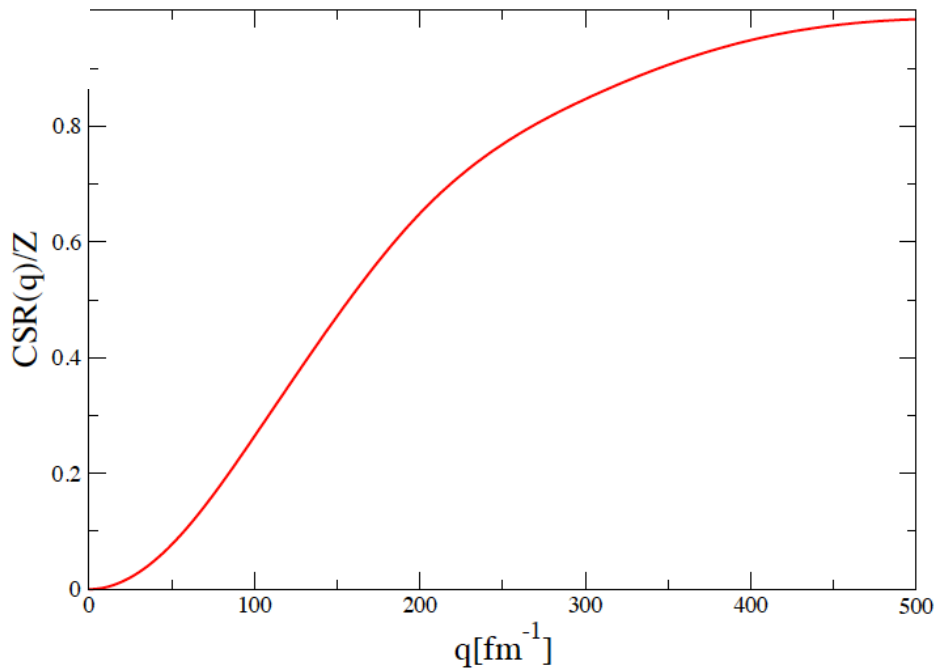




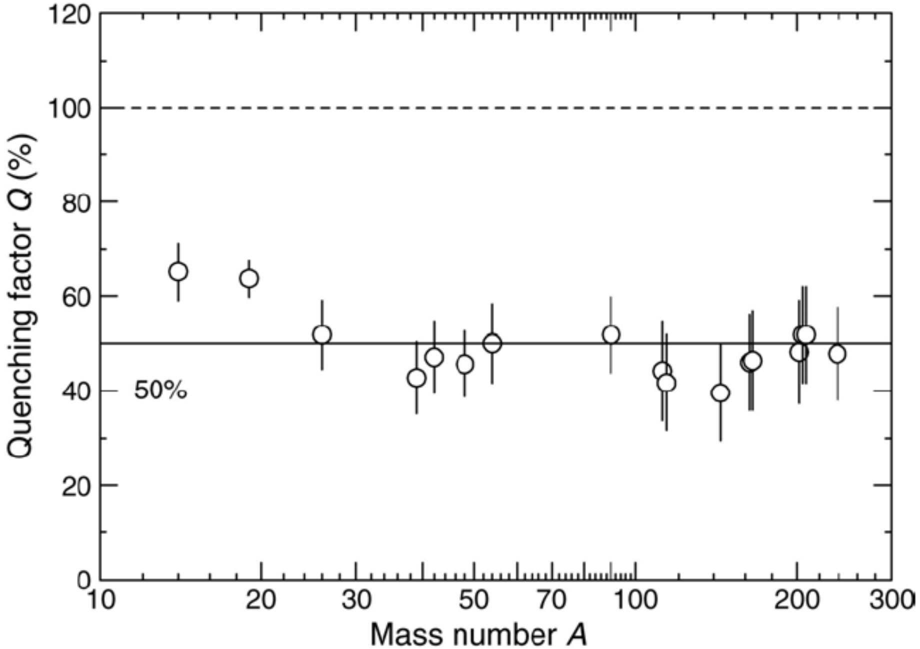
Comparison to data in ^{40}Ca with NNLO$_{sat}$



- Excellent agreement with elastic charge form factor up to momentum transfers of ~500MeV/c
- Very little data for the CSR
- To exhaust the sum rule need to integrate longitudinal response over large energy range



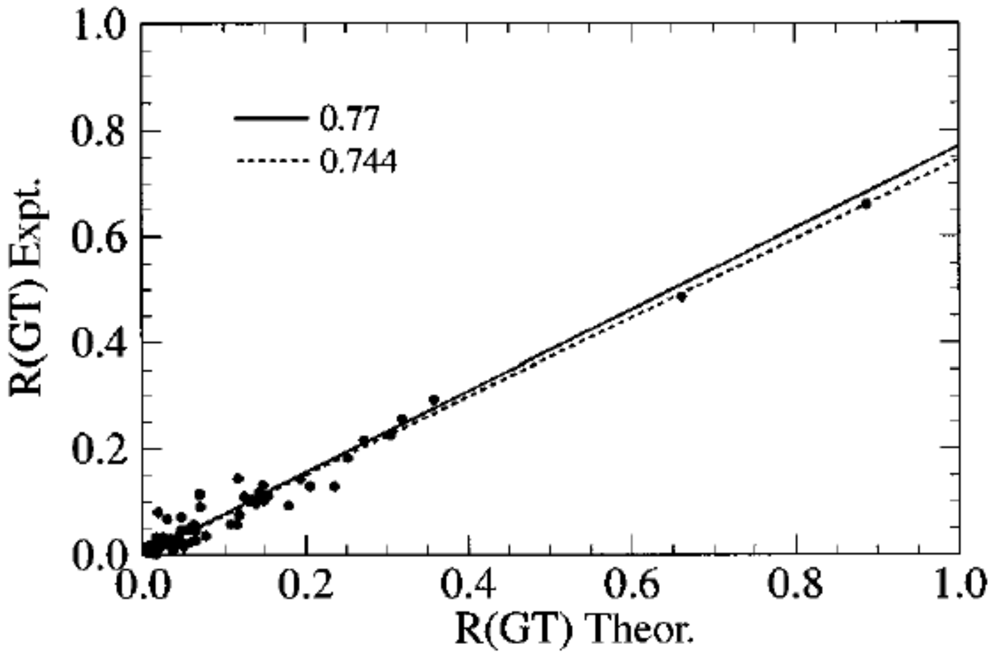
A 50 year old problem:
The puzzle of quenched of beta decays



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

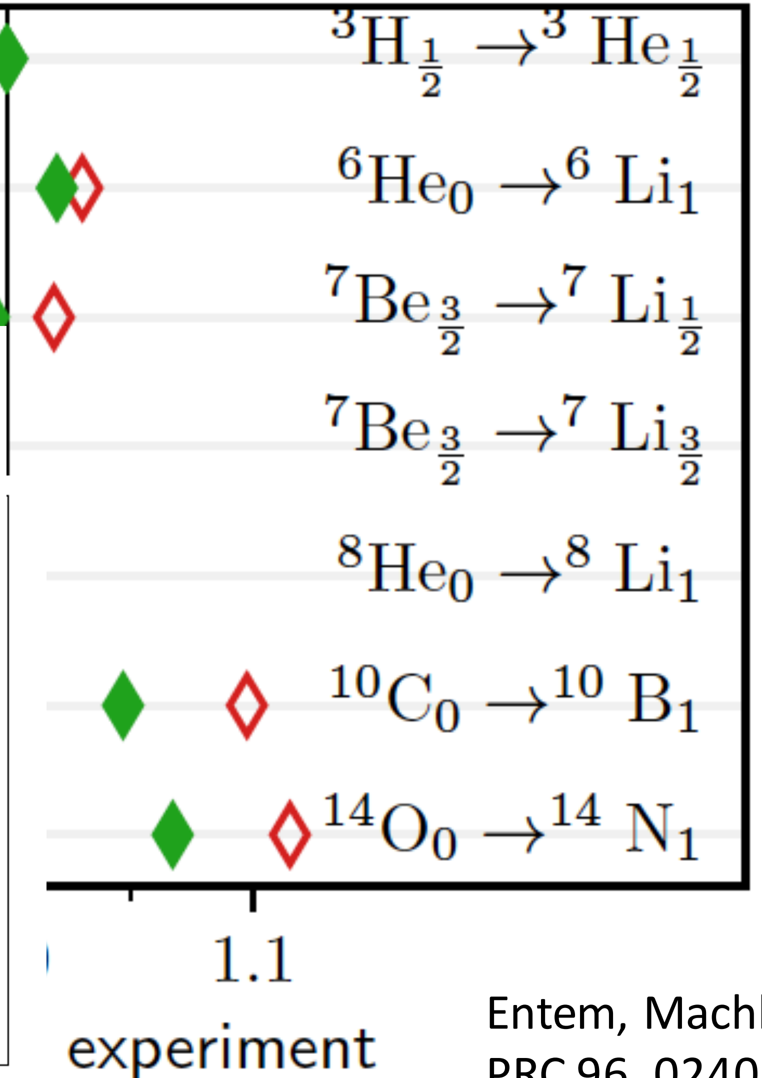
- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?
- Two-body currents (2BCs)?

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

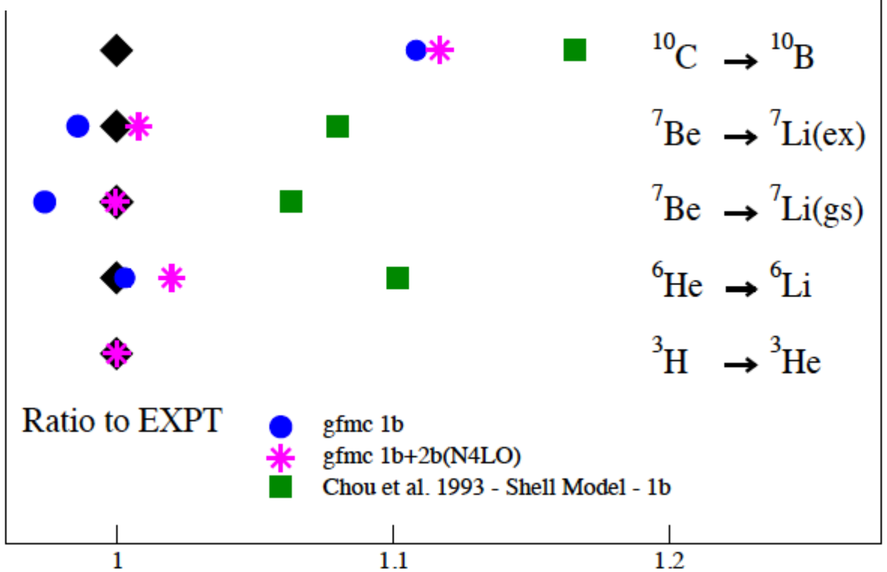


Theory to experiment ratios for beta decays in light nuclei from NCSM

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)

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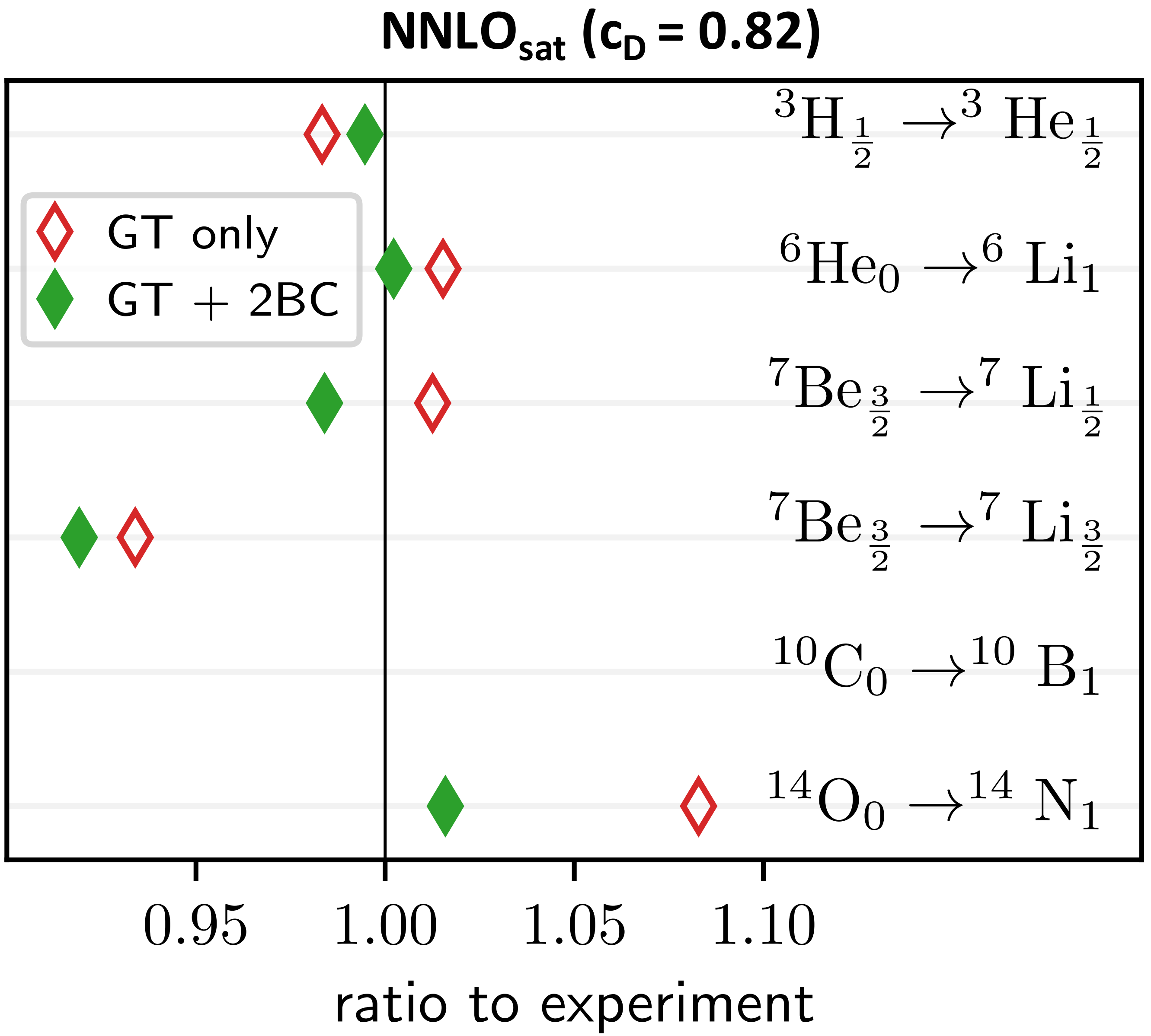
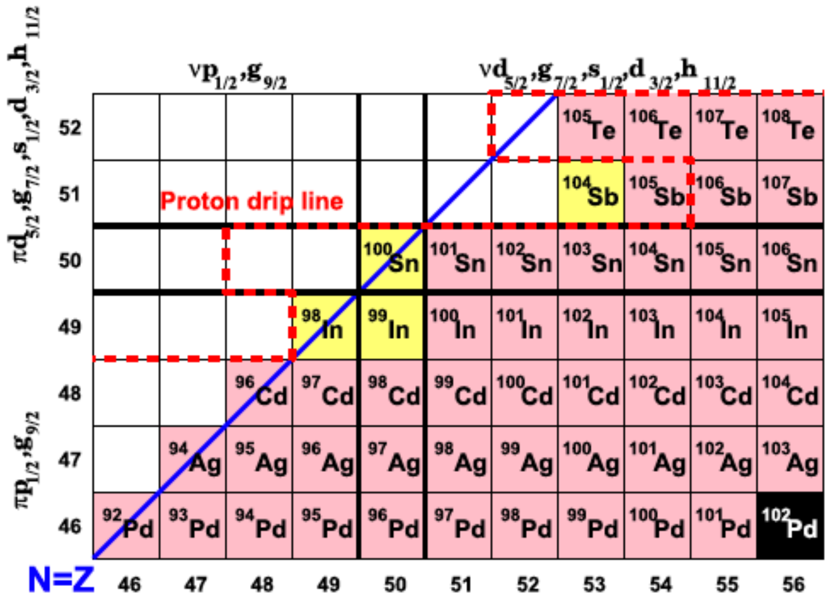
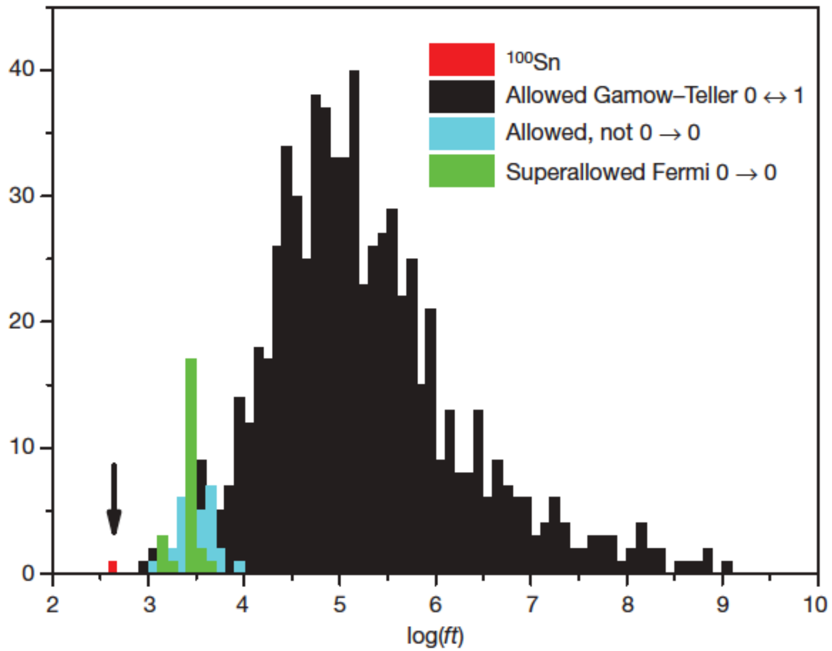


^{100}Sn – a nucleus of superlatives





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

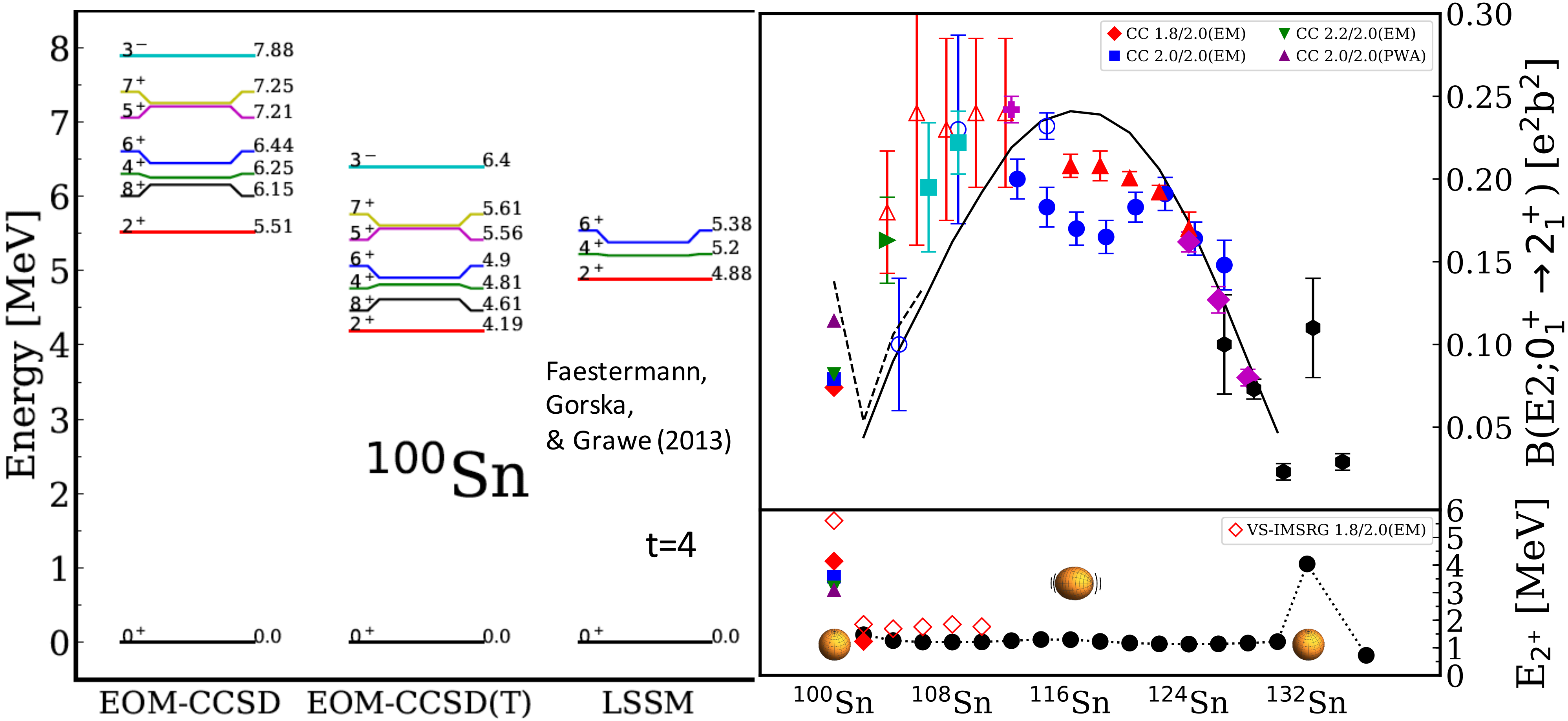
Quantify the effect of quenching from correlations and 2BCs

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

Editors' Suggestion

Structure of the Lightest Tin Isotopes

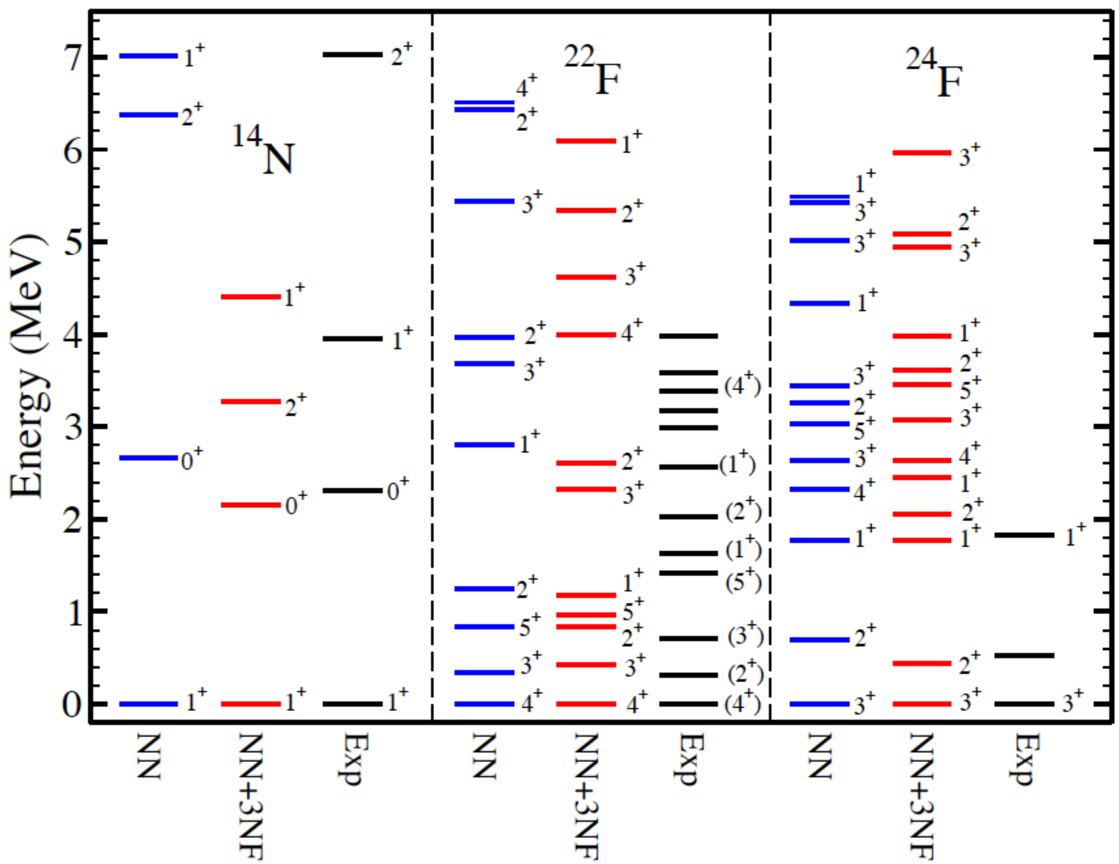
T. D. Morris,[1,2] J. Simonis,[3,4] S. R. Stroberg,[5,6] C. Stumpf,[3] G. Hagen,[2,1] J. D. Holt,[5] G. R. Jansen,[7,2]
T. Papenbrock,[1,2] R. Roth,[3] and A. Schwenk[3,4,8]

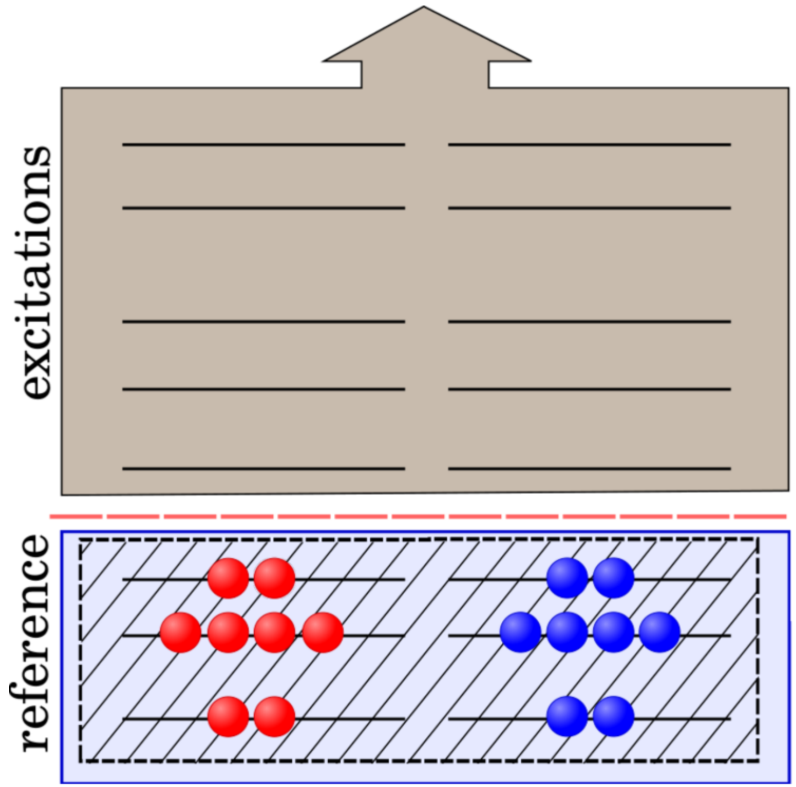


Coupled cluster calculations of beta-decay partners

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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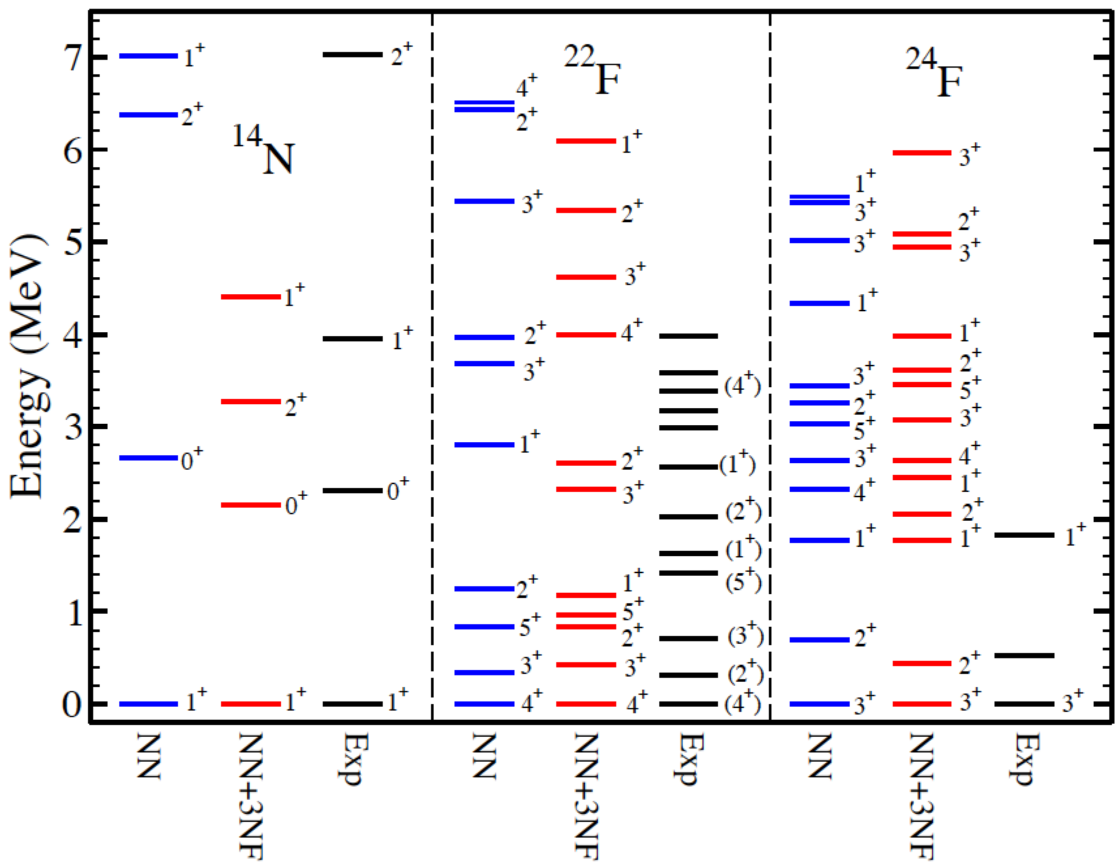
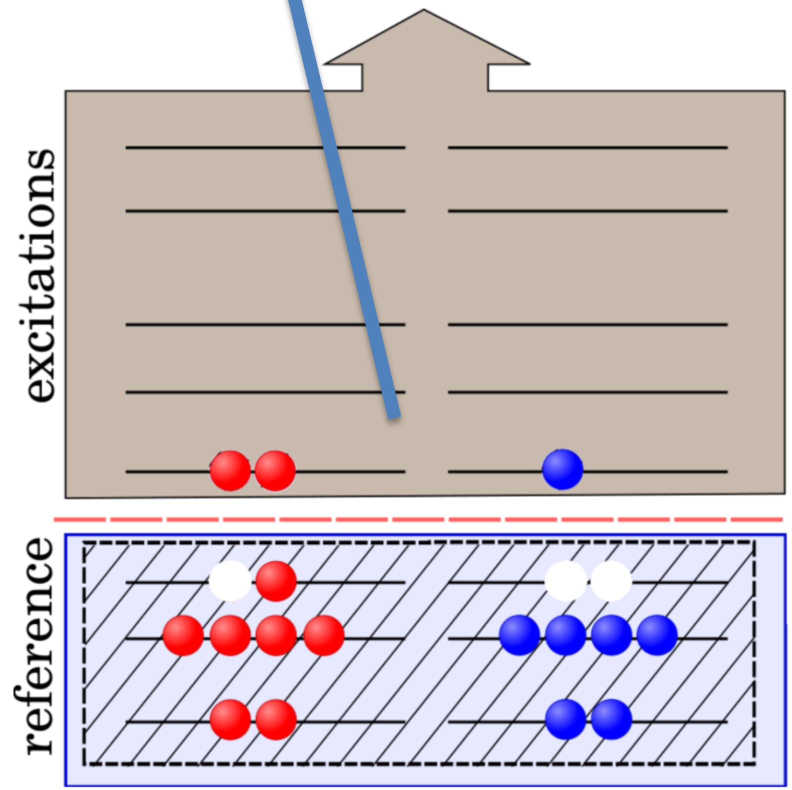




A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

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

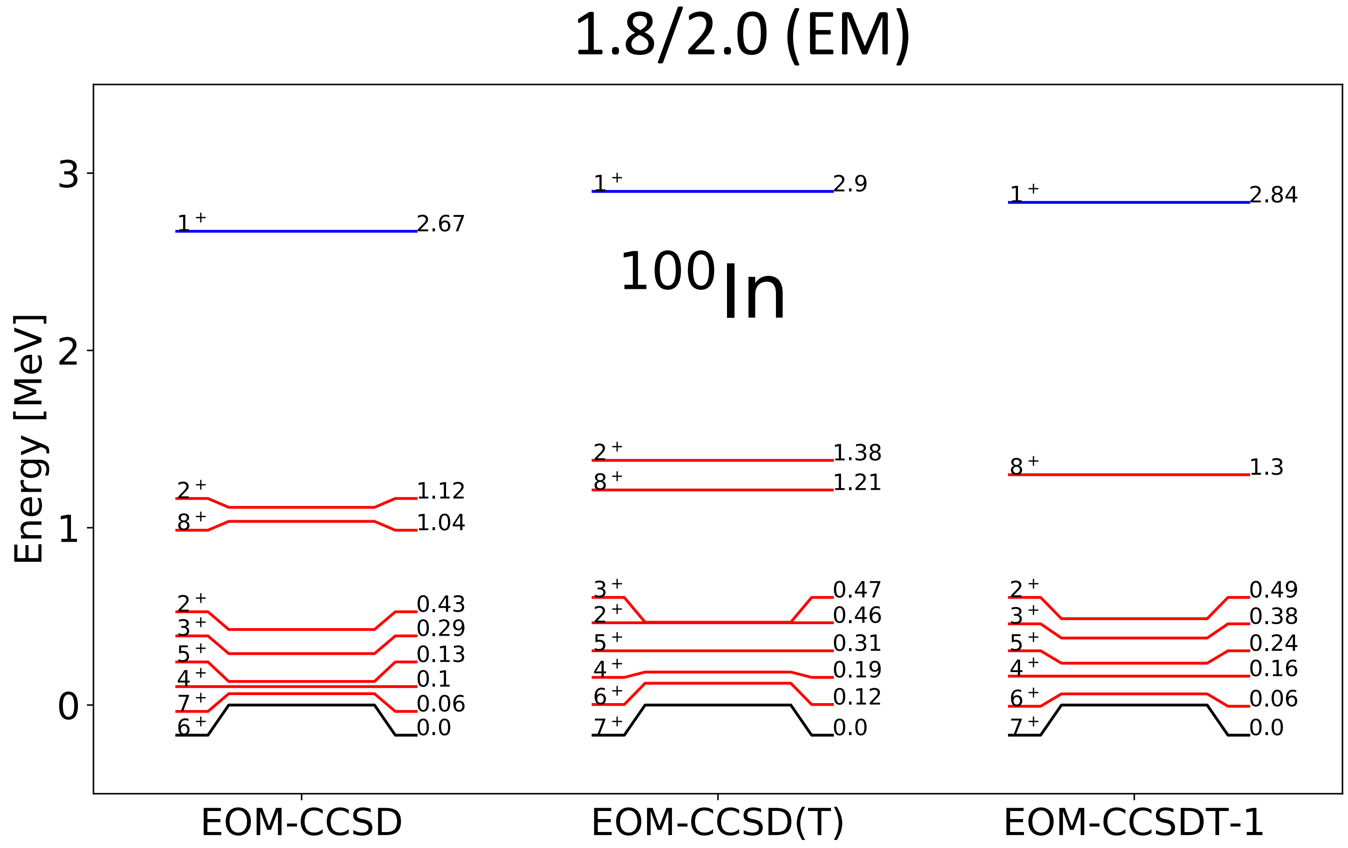
- Bloch-Horowitz is exact; iterative solution poss.

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

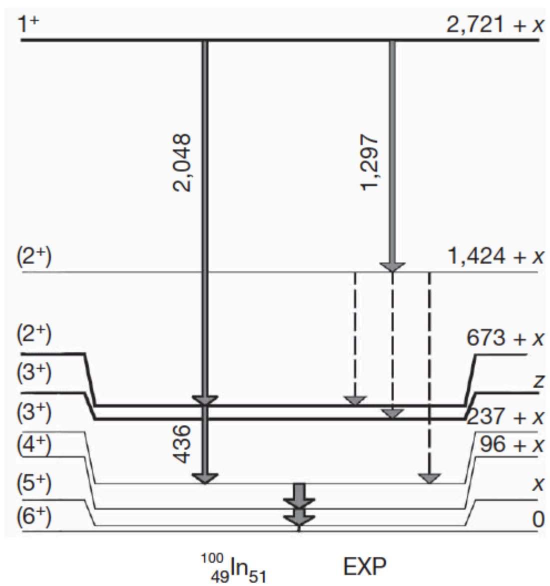
- Q-space is restricted to: $\tilde{E}_{pqr} = \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\max}$
- No large memory required for lanczos vectors
- Can only solve for one state at a time
- Reduces matrix dimension from ~10^9 to ~10^6

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)

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



Hinke et al, Nature (2012)

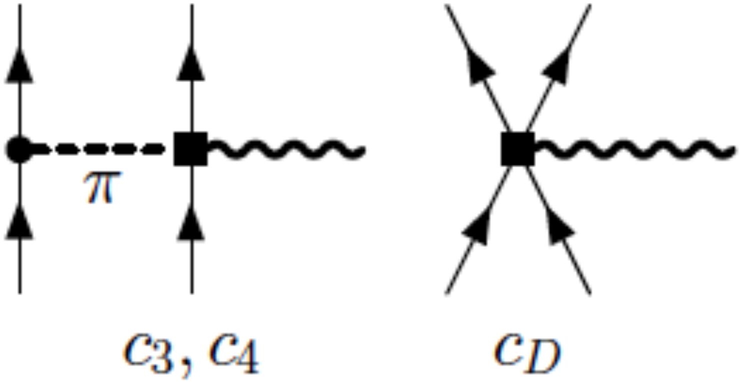


Charge-exchange EOM-CC with perturbative corrections accounting for excluded 3p3h states:

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

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:

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

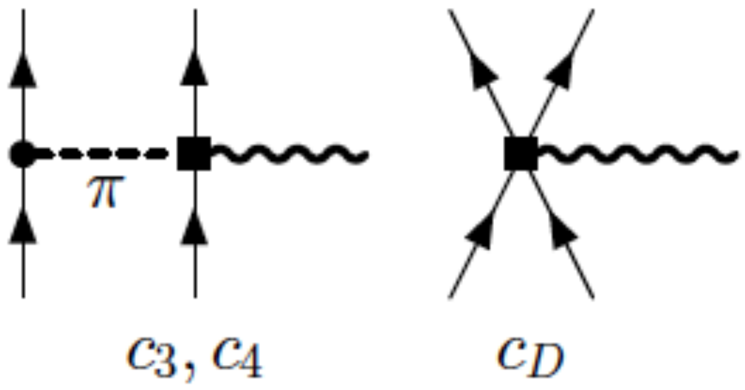
Benchmark between NCSM and CC using NN-N^{4}LO 3N$_{\mathrm{lnl}}$ in ^{8}He:

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

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:

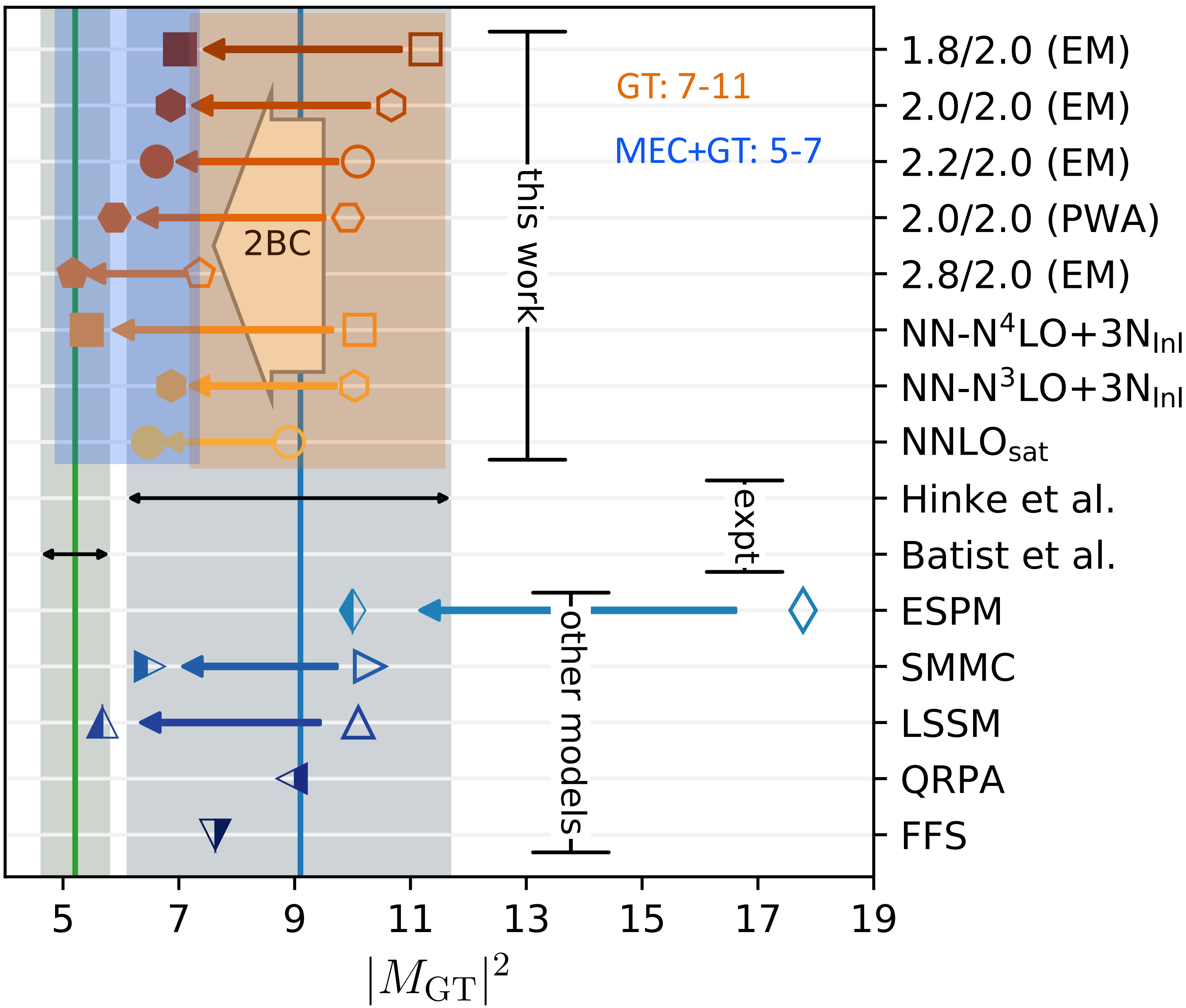
$$\hat{O}_{\mathrm{GT}} = O_N^1 + \cancel{O_N^2}$$

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

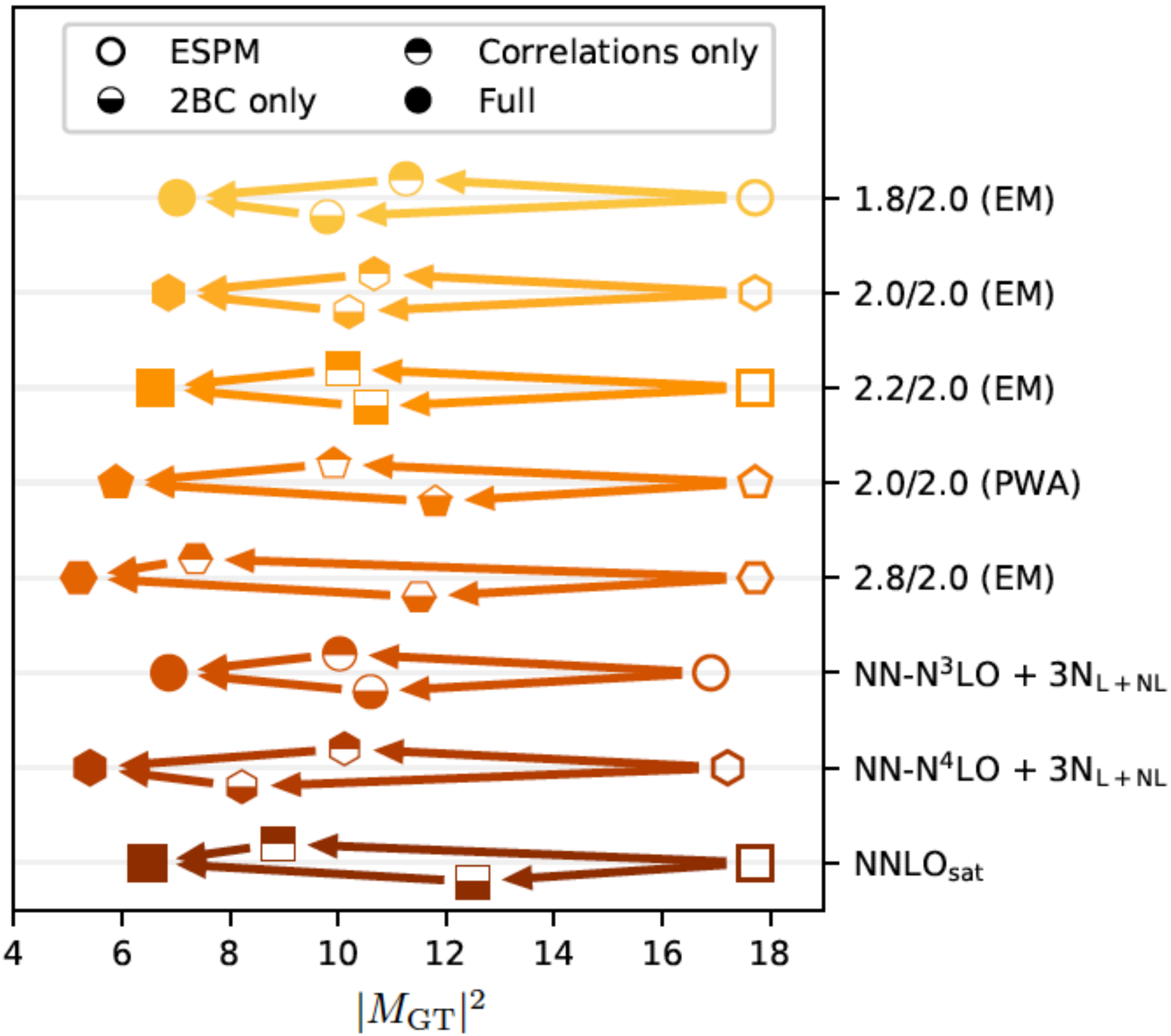
$$^{14}\mathrm{O}_0 \rightarrow {}^{14}\mathrm{N}$$

	$\lvert M_{\mathrm{GT}}(\boldsymbol{\sigma\tau})\rvert$		$\lvert M_{\mathrm{GT}}\rvert$	
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)

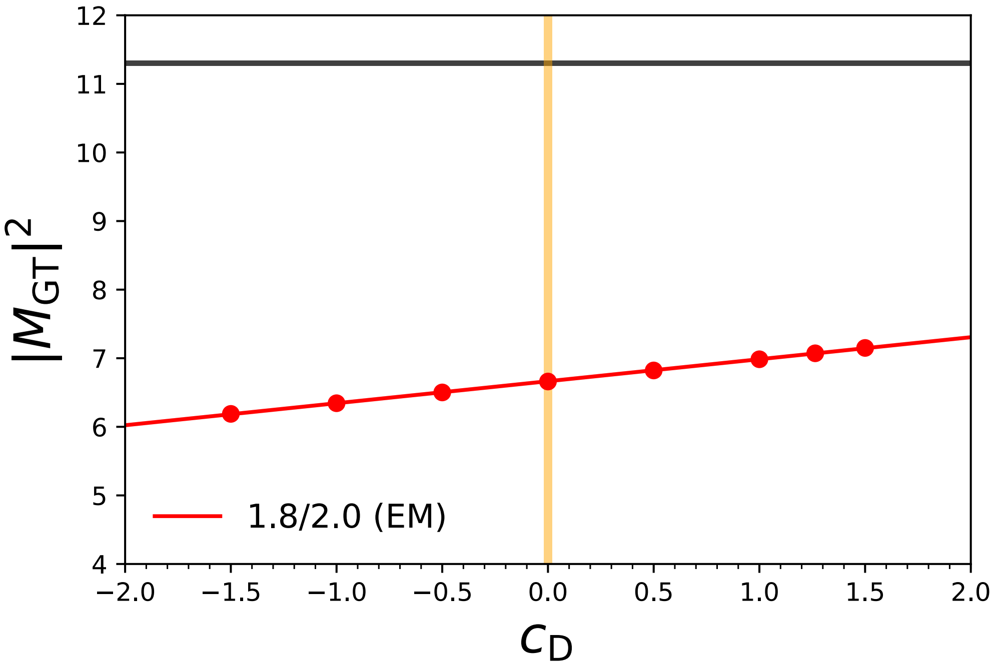
Super allowed Gamow-Teller decay of ^{100}Sn

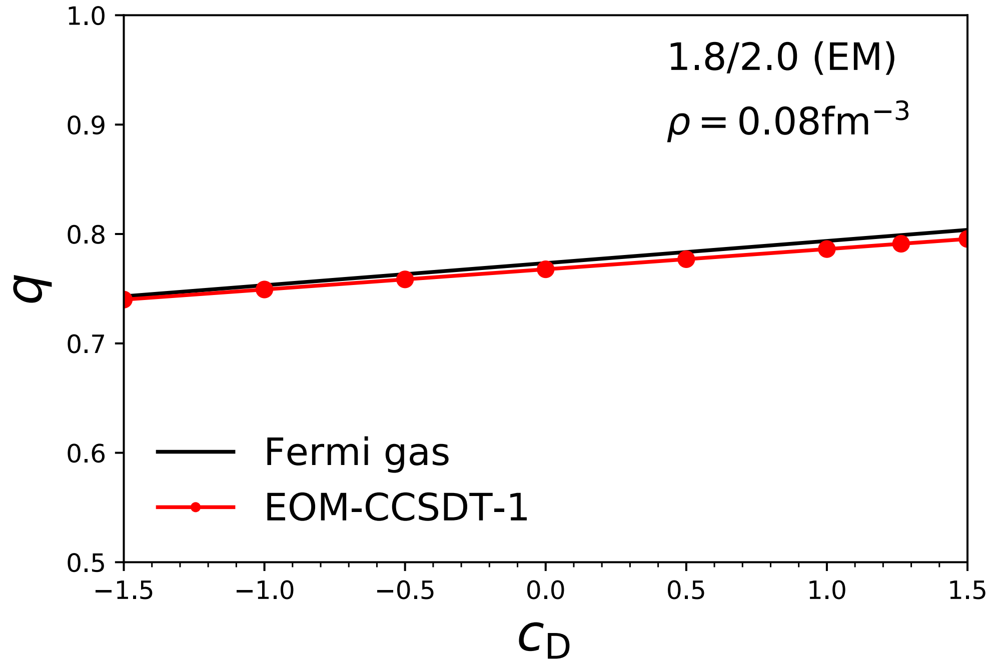


Role of 2BC and correlations in ^{100}Sn



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





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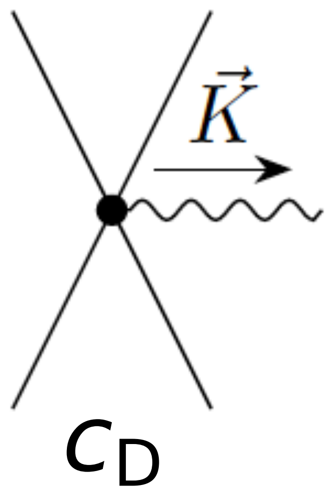
One-body normal ordering of 2BC in free Fermi gas

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



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

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