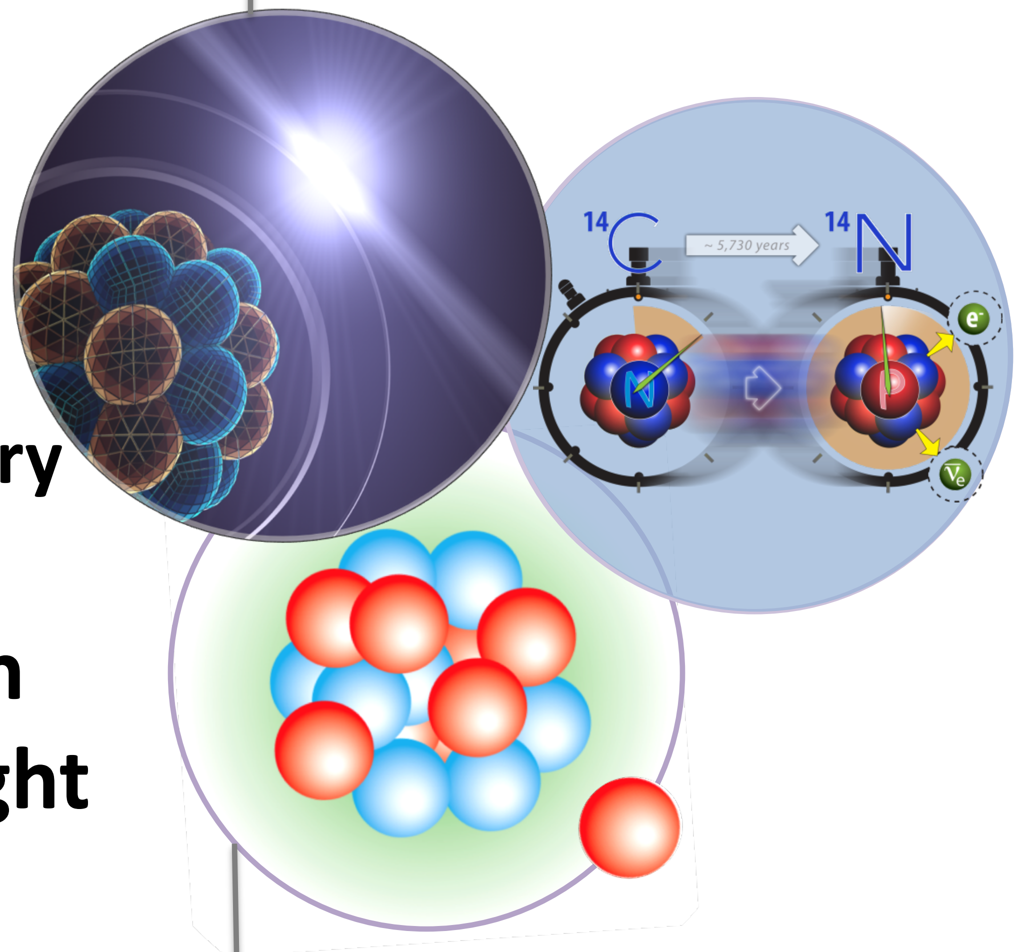
Electroweak decays from coupled-cluster computations

Gaute Hagen
Oak Ridge National Laboratory



Fundamental Physics with Electroweak Probes of Light Nuclei

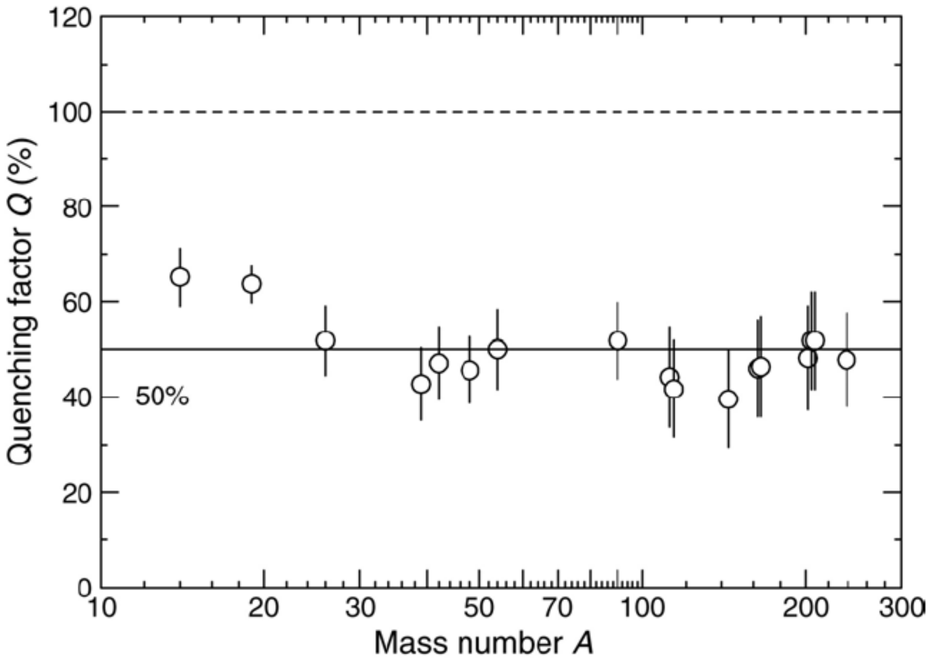
INT, Seattle June 13th, 2018

U.S. DEPARTMENT OF ENERGY

NUCLEI
Nuclear Computational Low-Energy Initiative

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

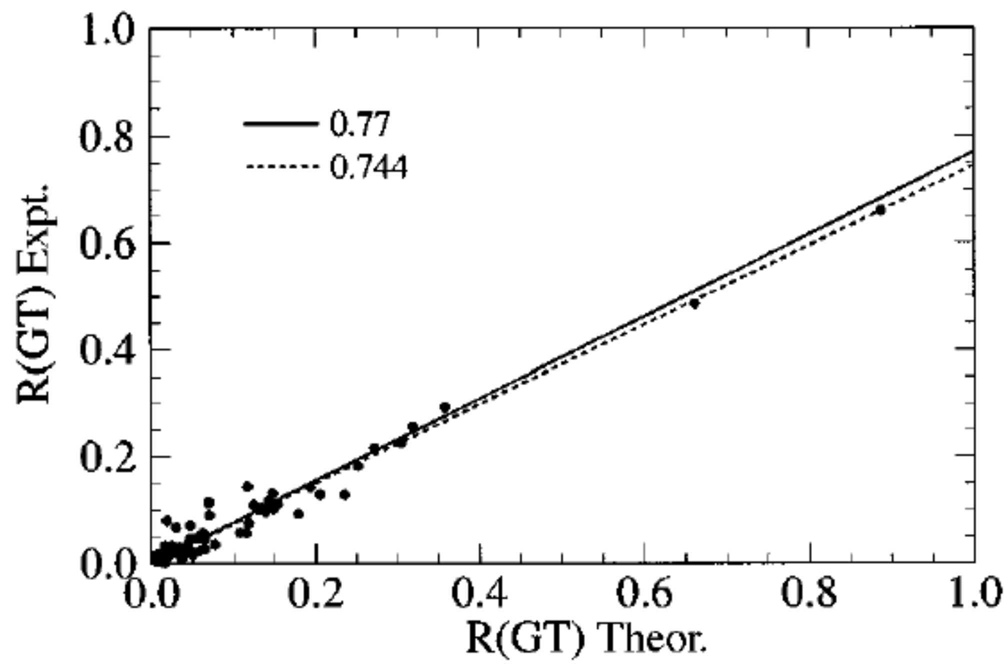
A 50 year old problem: The puzzle of quenched of beta decays



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)?

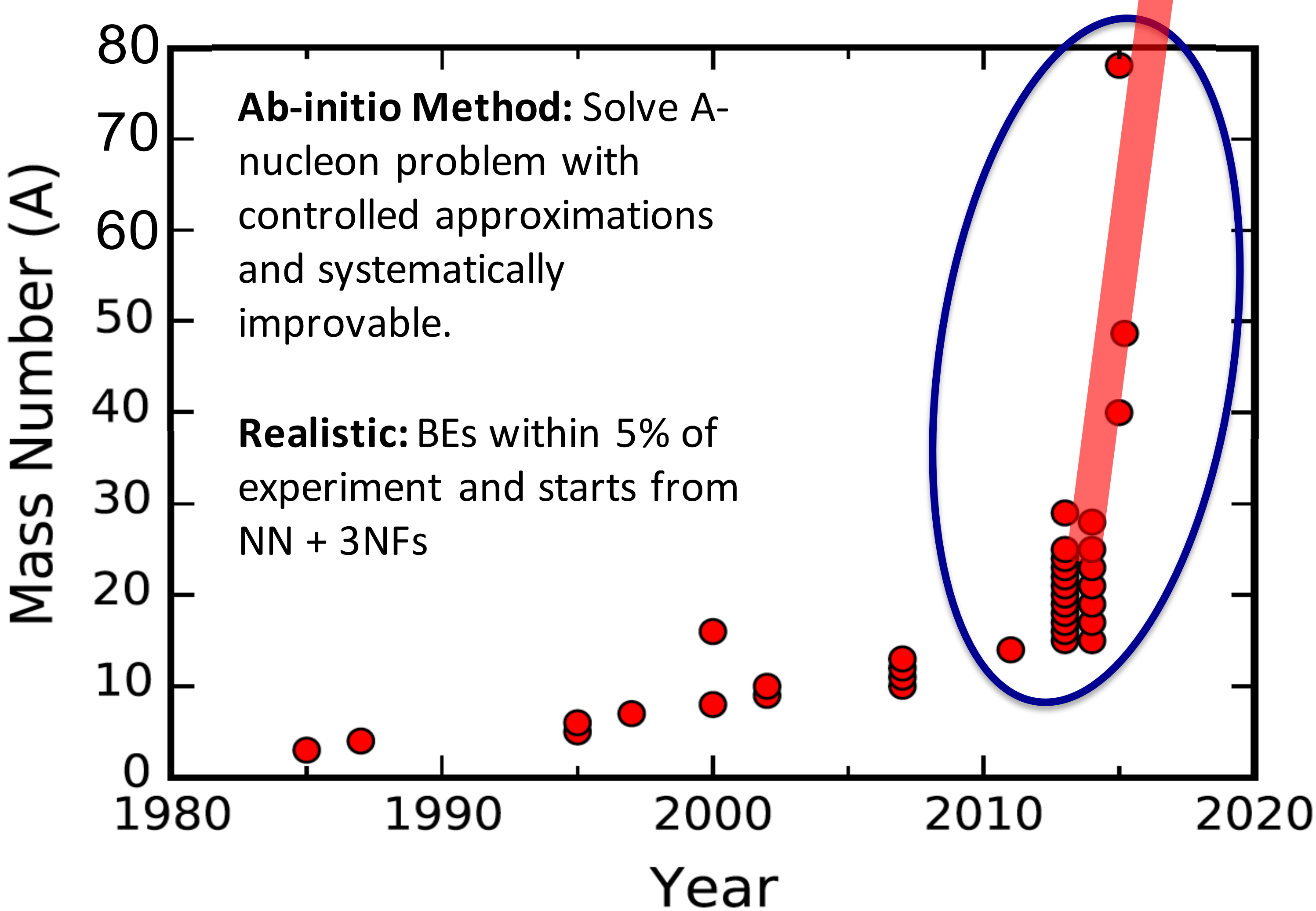
G. Martinez-Pinedo et al, PRC **53**, R2602 (1996)



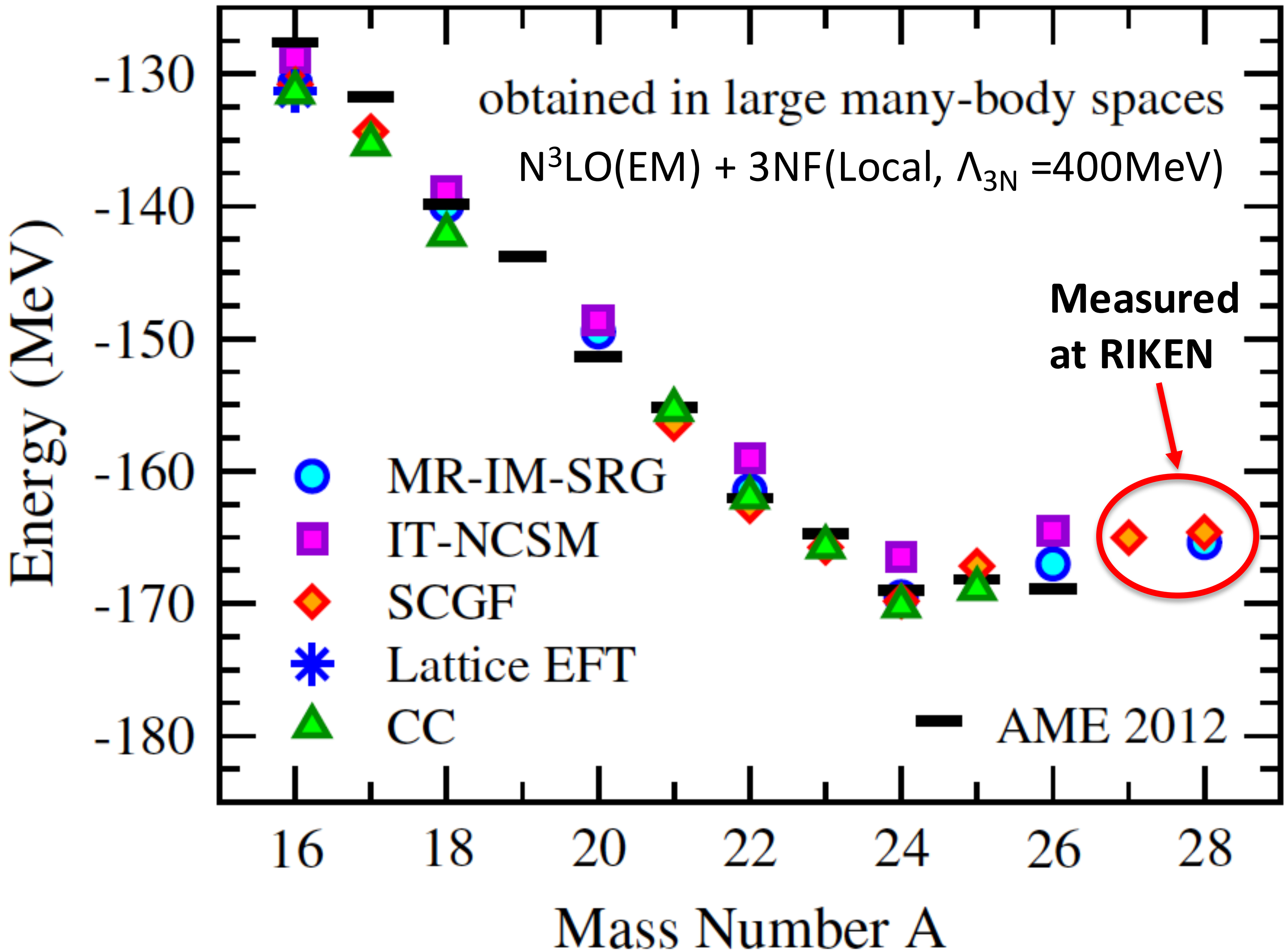
Trend in realistic ab-initio calculations

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, …)



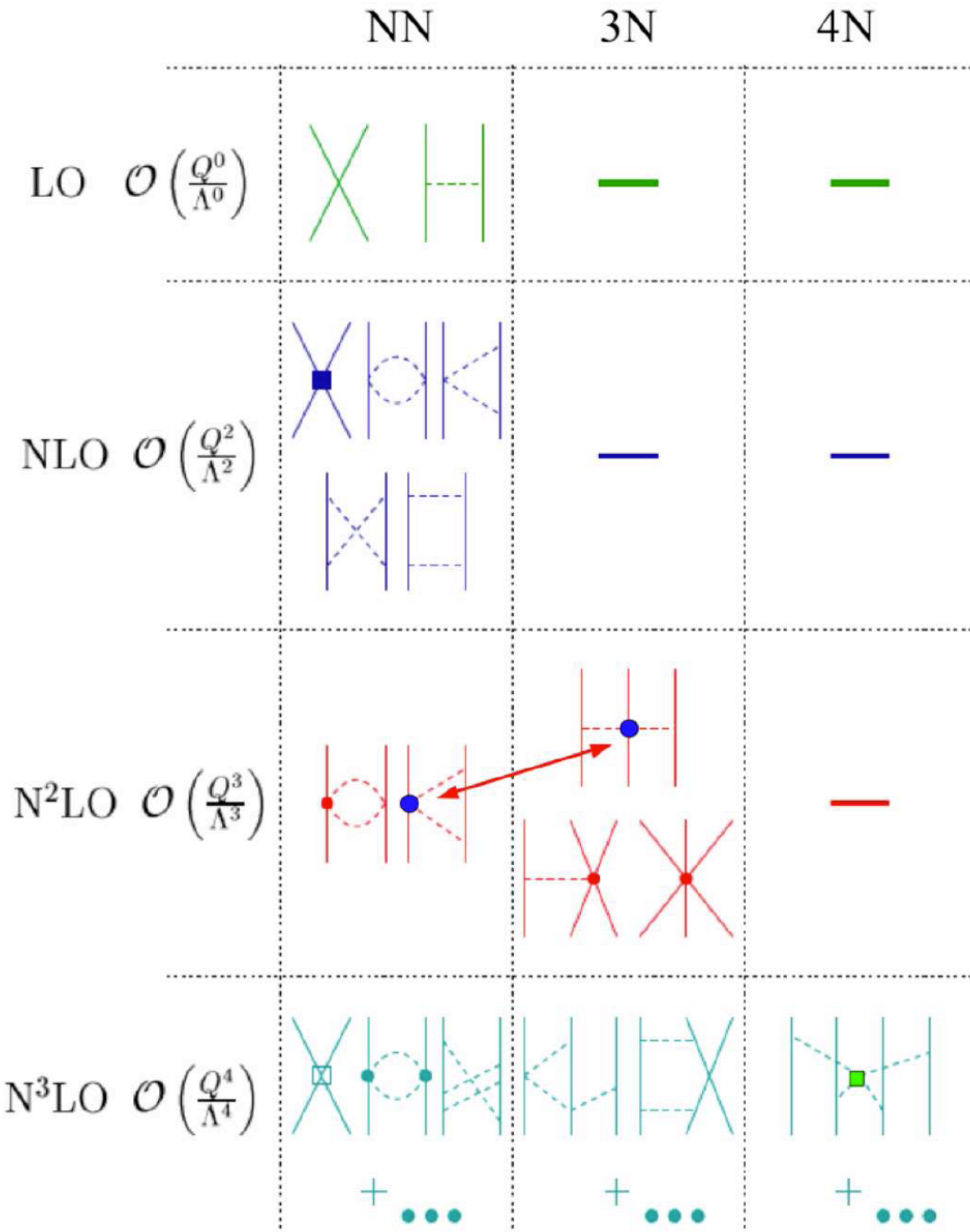
Oxgyen chain with interactions from chiral EFT



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

Nuclear forces from chiral effective field theory

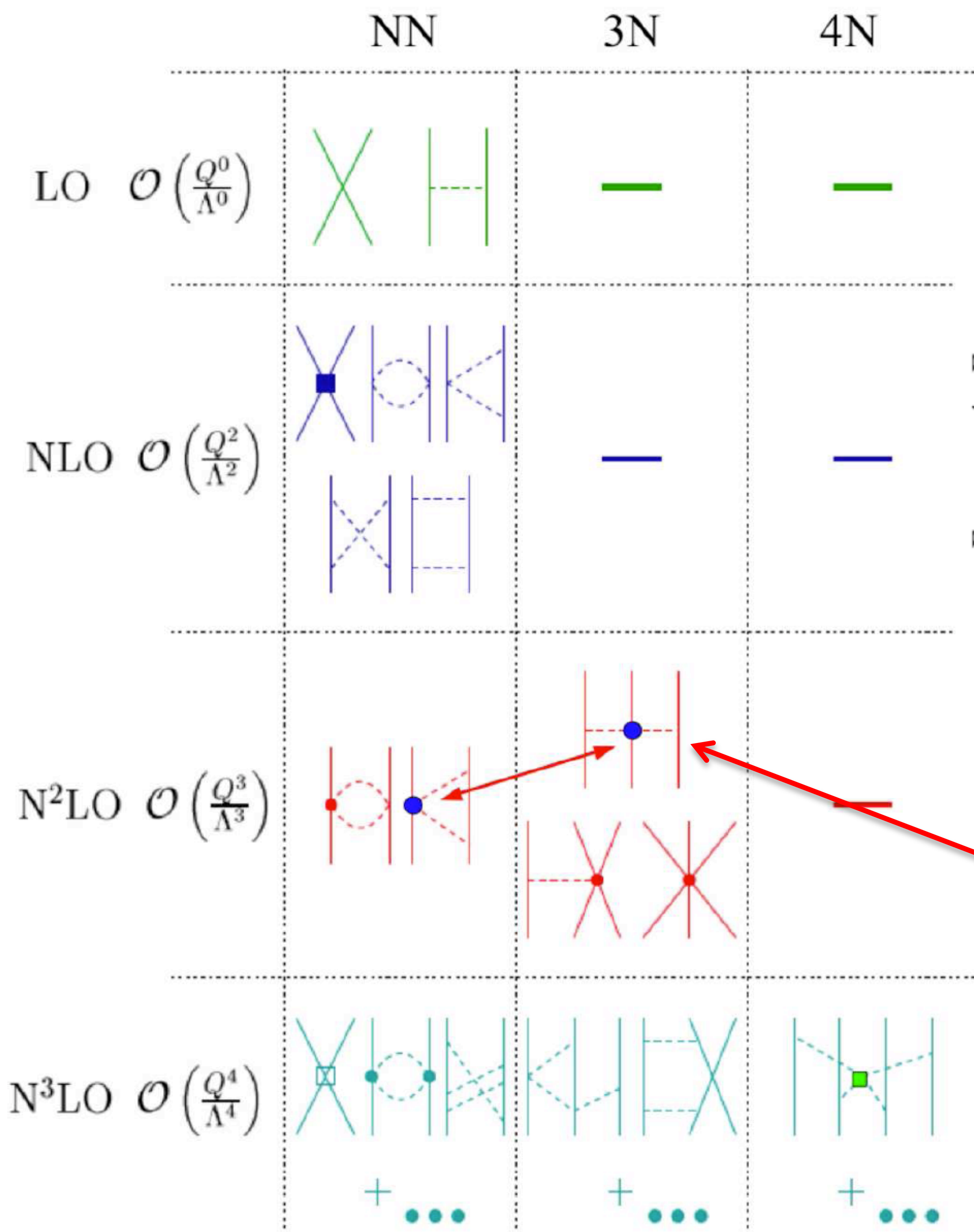
[Weinberg; van Kolck; Epelbaum *et al*.; Entem & Machleidt; …]



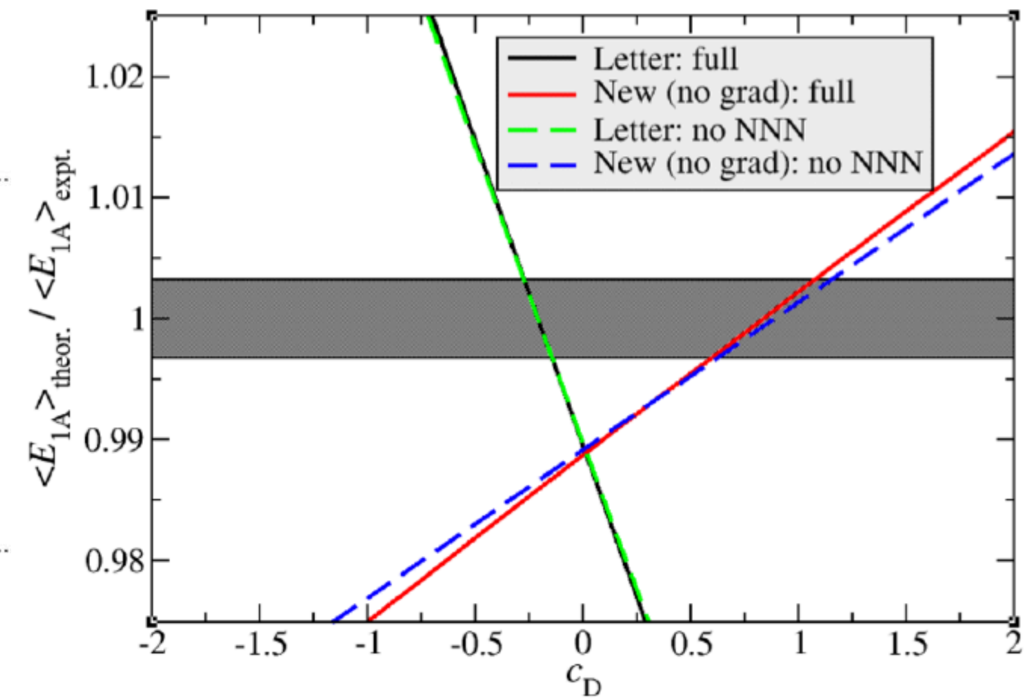
- Developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; Entem et al 2017, Reinert et al 2018…]
- Propagation of uncertainties on the horizon [Navarro Perez 2014, Carlsson et al 2015]
- Different optimization protocols [Ekström et 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, Reinert et al 2018]
- Chiral EFT's with explicit Delta isobars [Krebs et al 2018, Piarulli et al 2017, Ekstrom et al 2017]

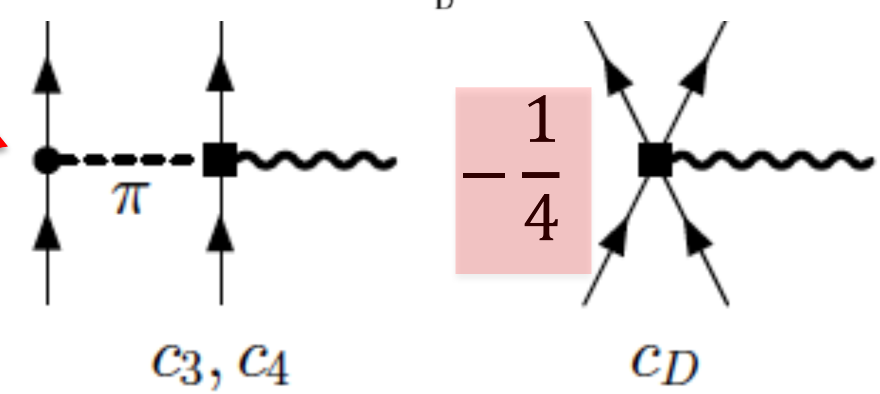
Nuclear forces from chiral effective field theory

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

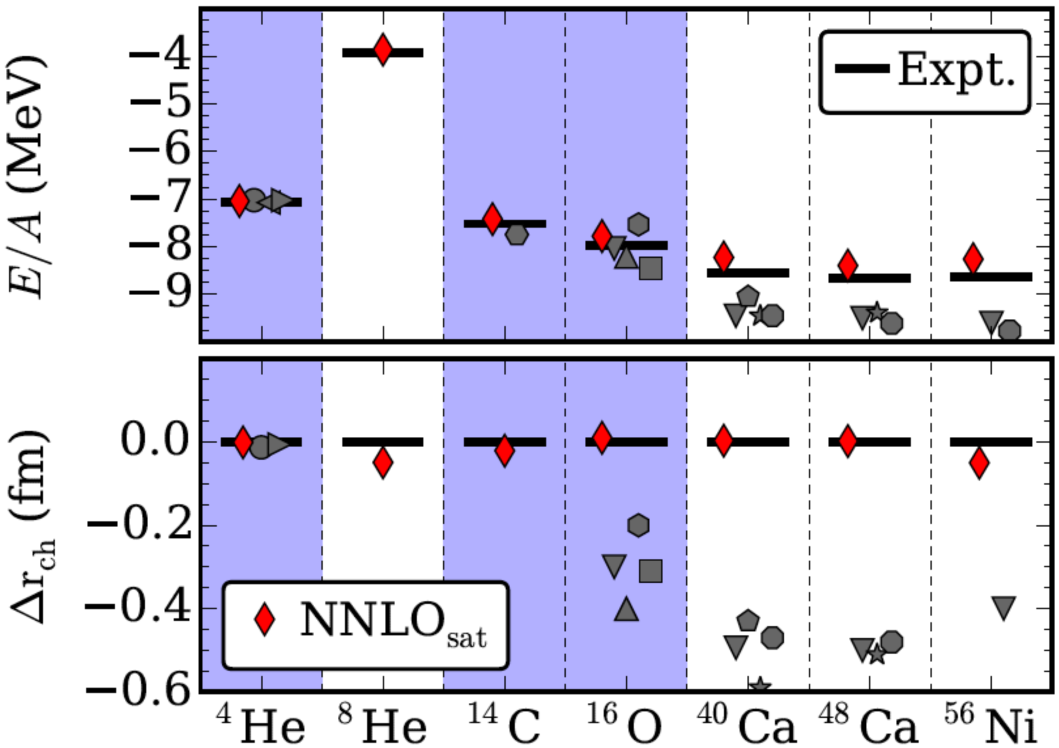


From Sofia Quaglioni and Kyle Wendt





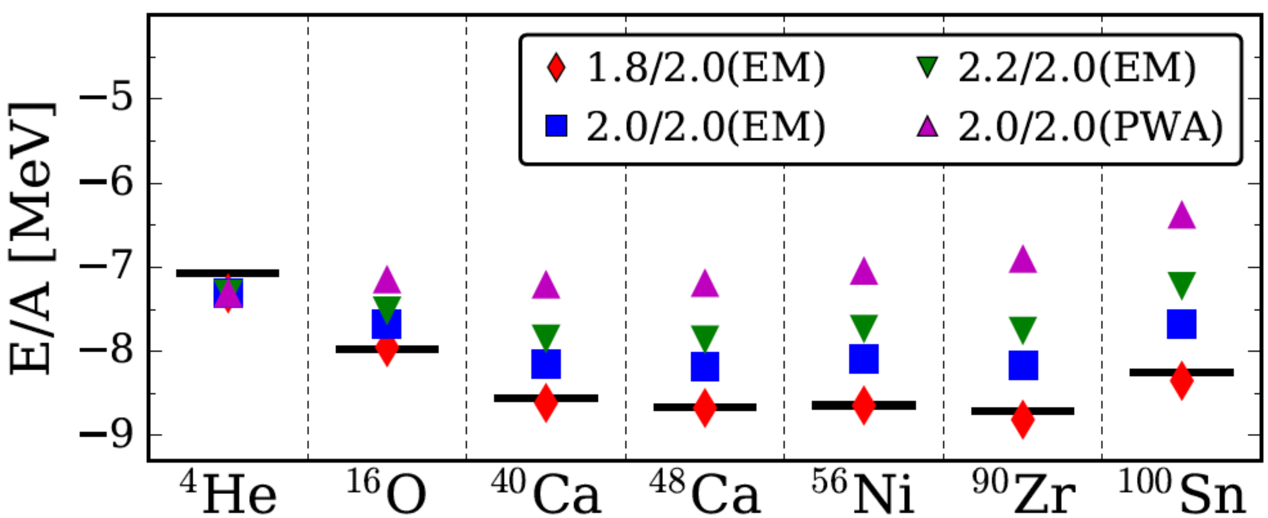
A family of interactions from chiral EFT



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

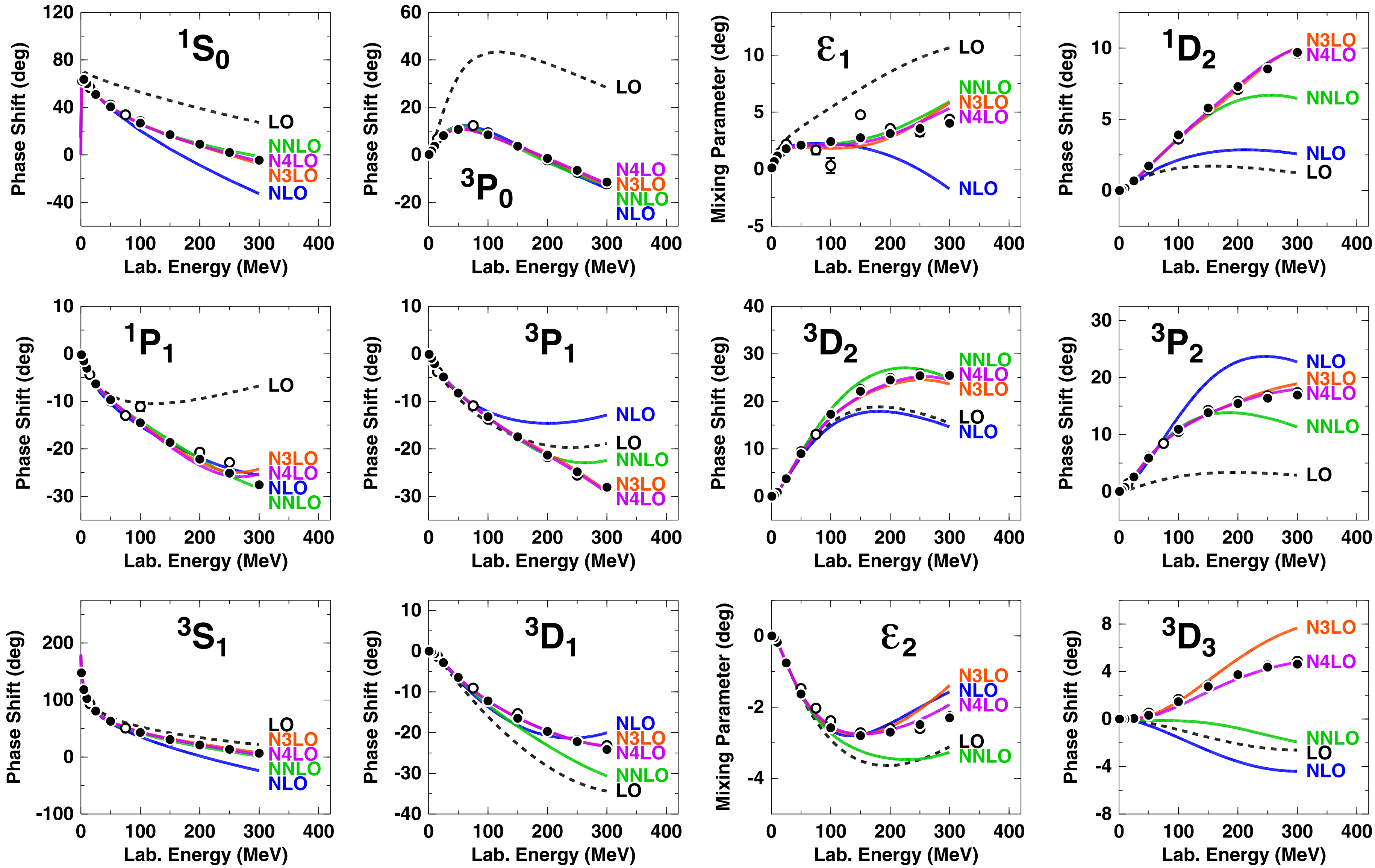
K. Hebeler *et al* PRC (2011).

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

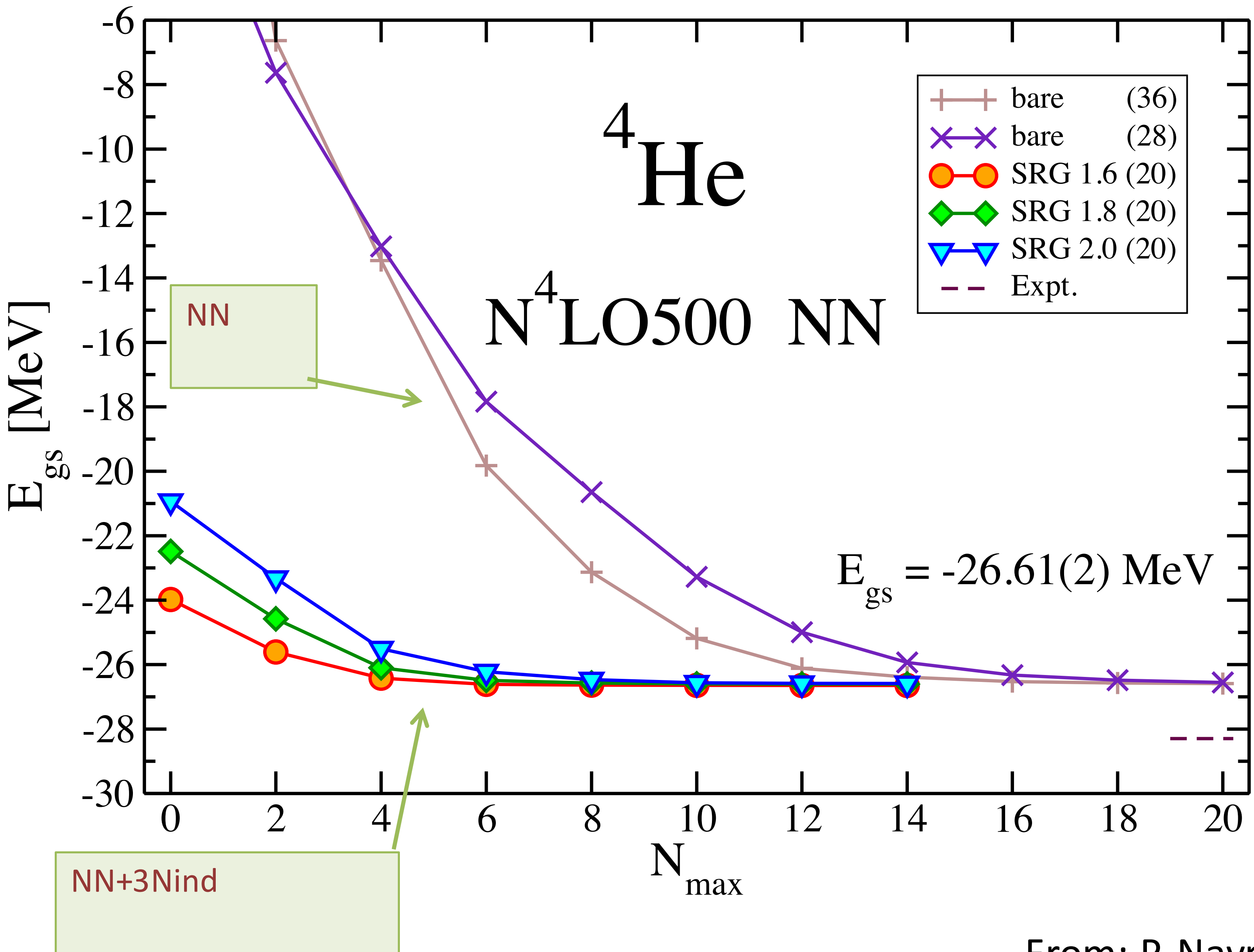
PHYSICAL REVIEW C **96**, 024004 (2017)

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

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



NCSM results for 4He with N4LO (NN-only)



From: P. Navratil

Fit 3N and 2BC contacts to triton half-life

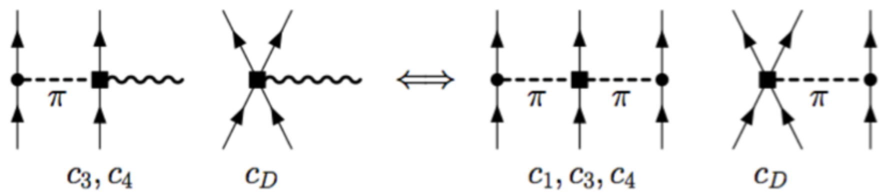
$$\hat{O} = GT^{(1)} + MEC^{(2)} \rightarrow \hat{O}_\alpha = GT^{(1)} + GT^{(2)}_\alpha + MEC^{(2)}_\alpha + \dots$$

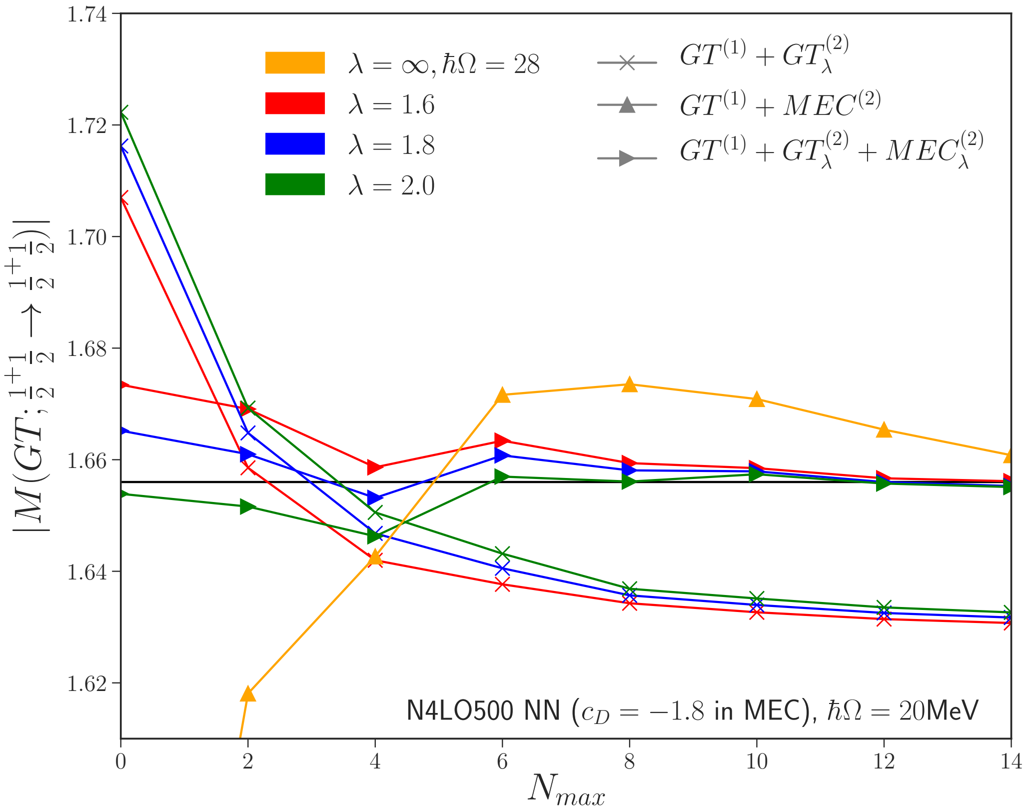
Operator:

Gamow-Teller (1-body) + chiral meson exchange current (2-body) Park (2003)

Potential: "N^{4}LO NN"

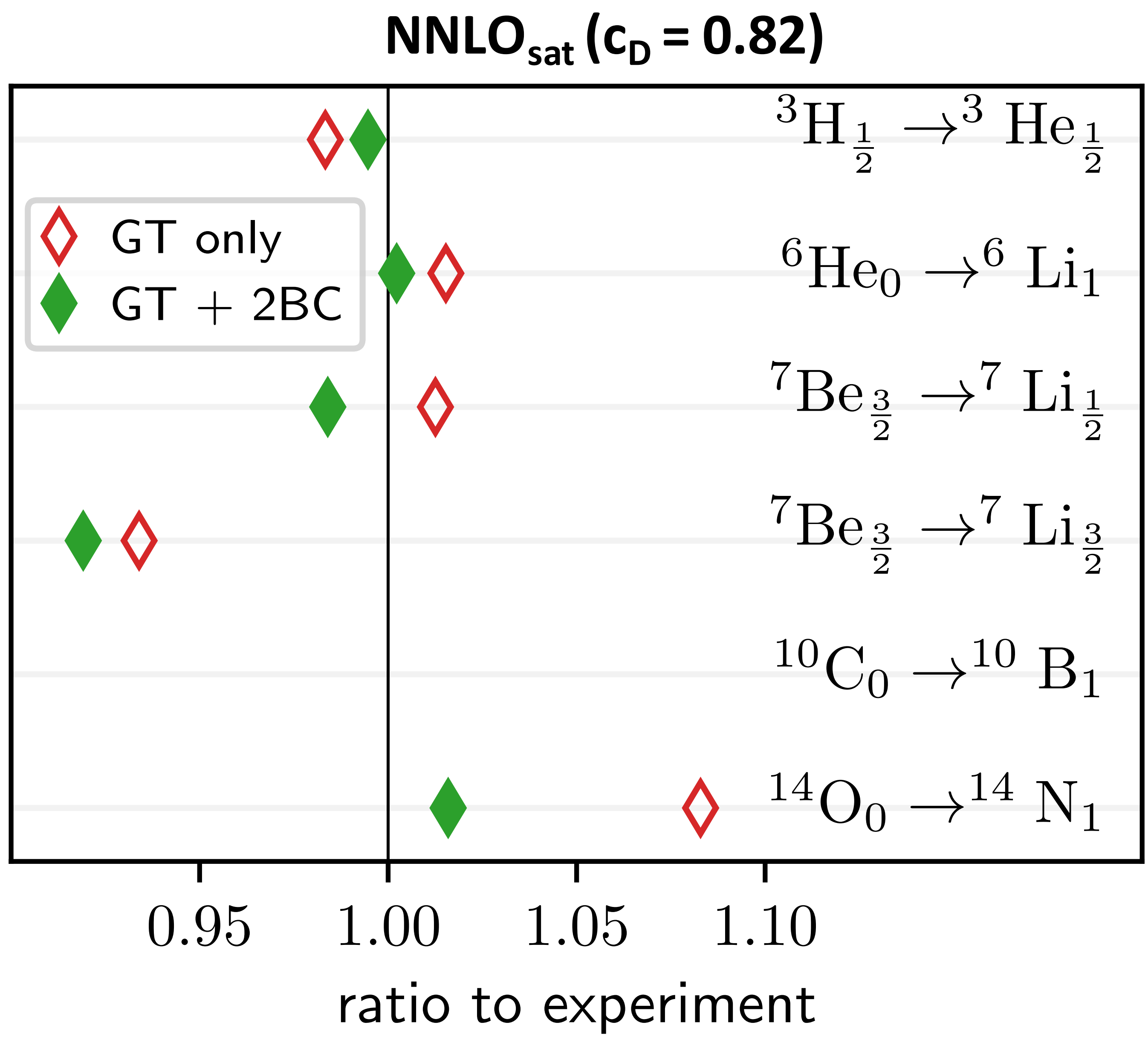
- chiral NN @ N^{4}LO, Machleidt PRC96 (2017), 500MeV cutoff
- LEC $c_D = -1.8$ determined





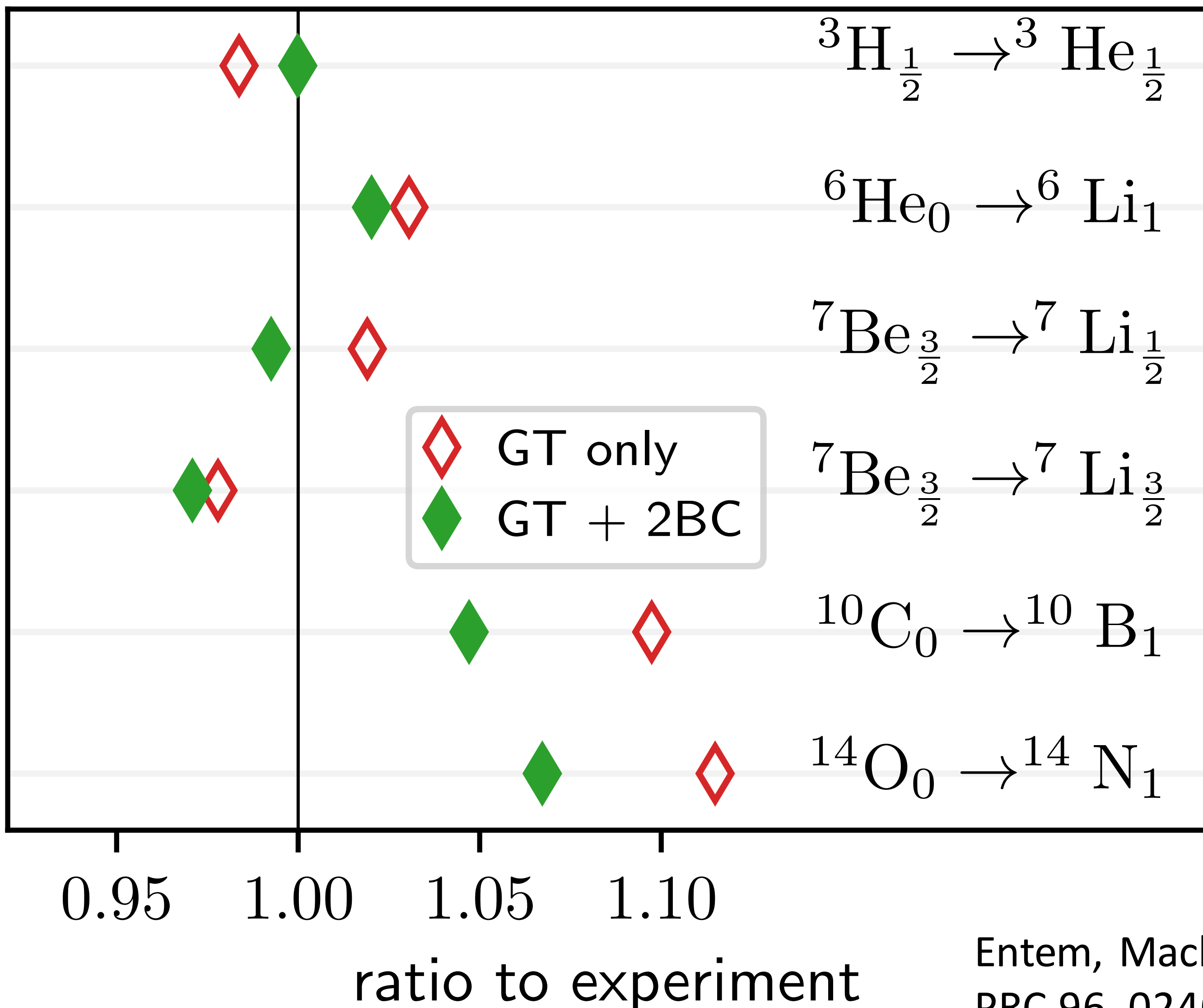
From: P. Gysbers, P. Navratil, S. Quaglioni

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



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

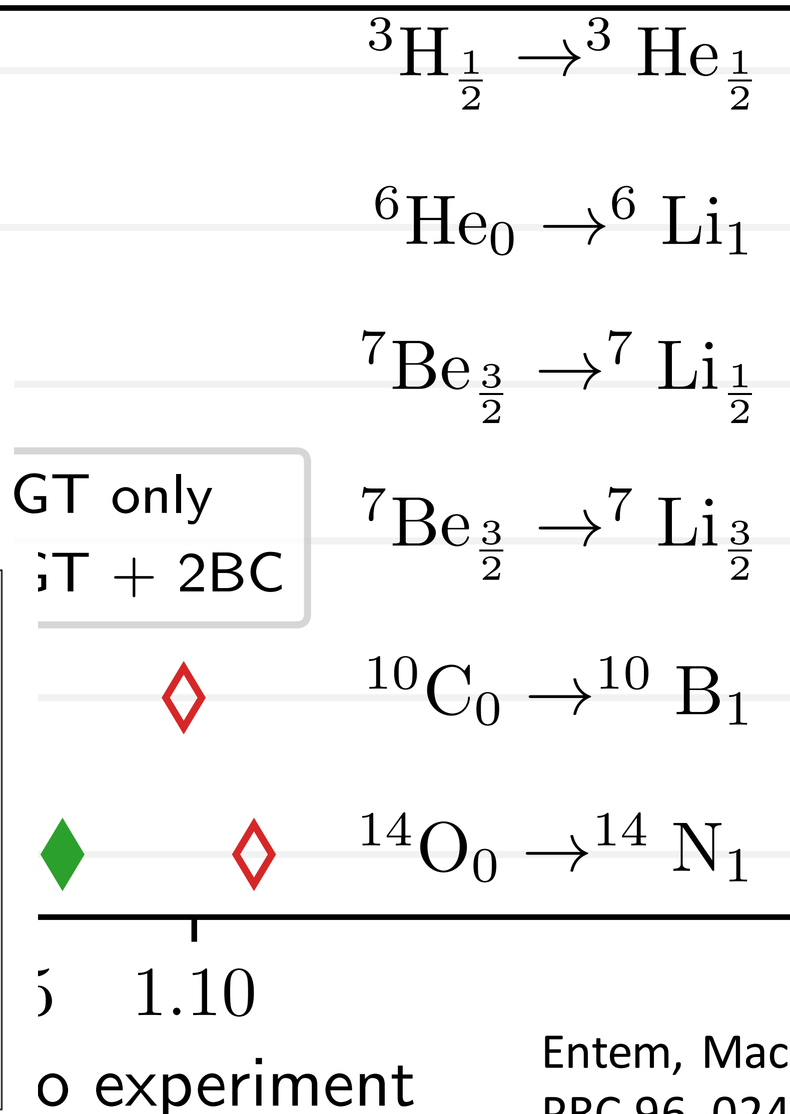
N4LO(EM) + $3N_{lnl}$ SRG-evolved to 2.0fm^{-1} (c_D = -1.8)



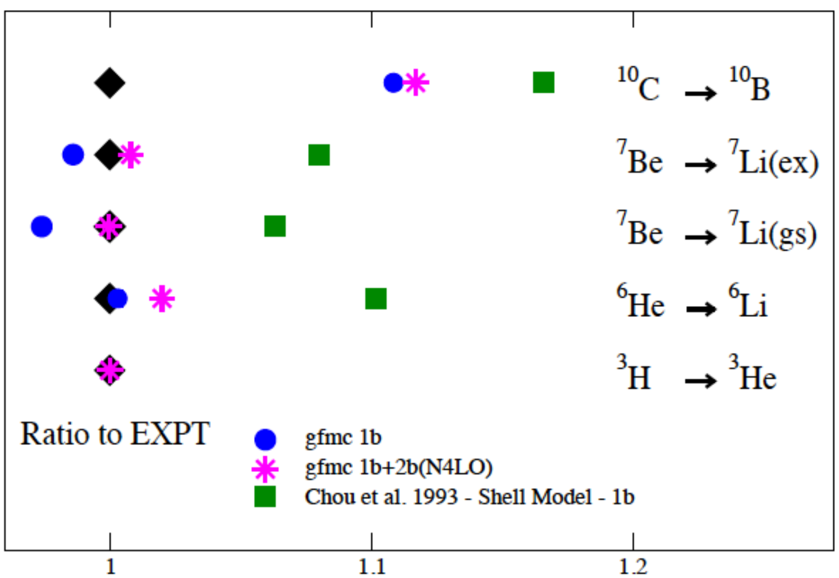
Entem, Machleidt & Nosyk,
PRC 96, 024004 (2017)

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)

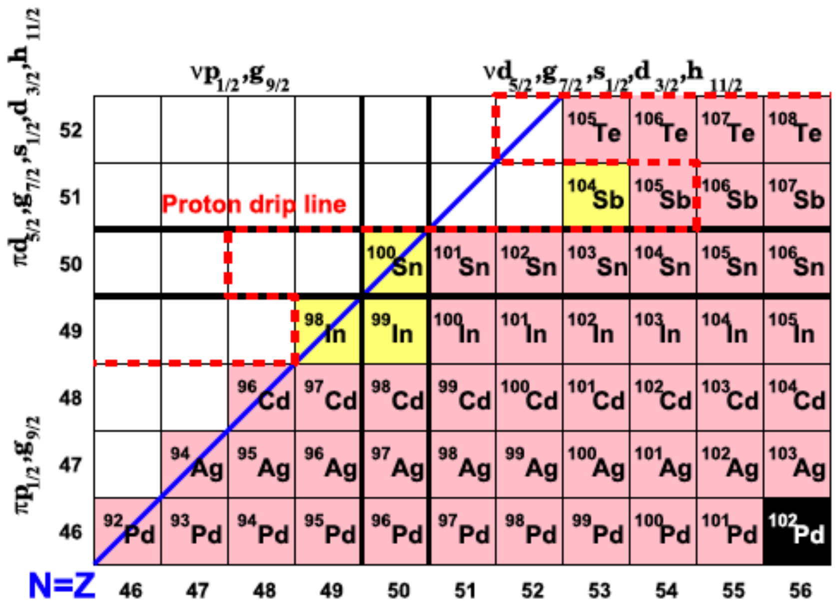


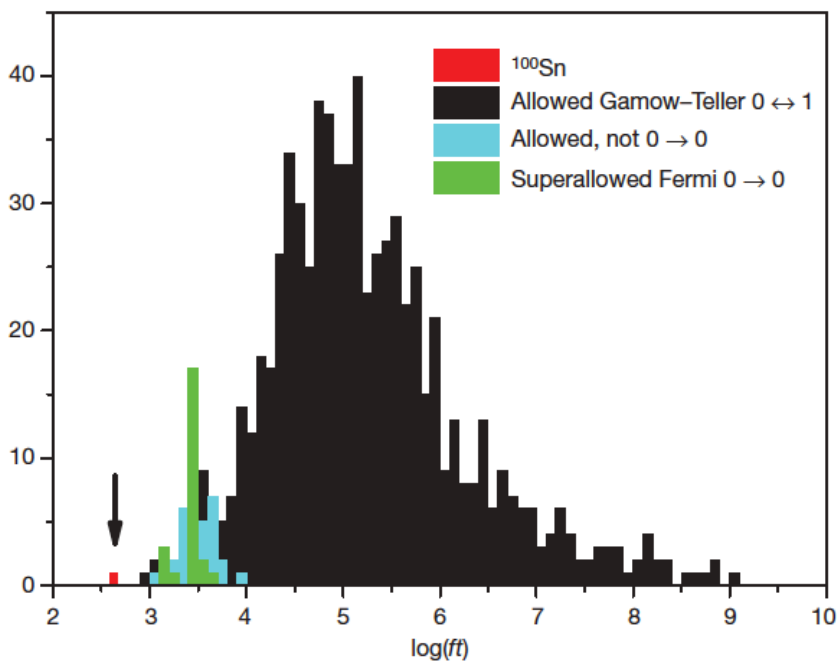
In QMC calculations of beta-decays 2BC increase the GT strength by 2-3%
S. Pastore et al, PRC 97, 022501 (2018).



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

^{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

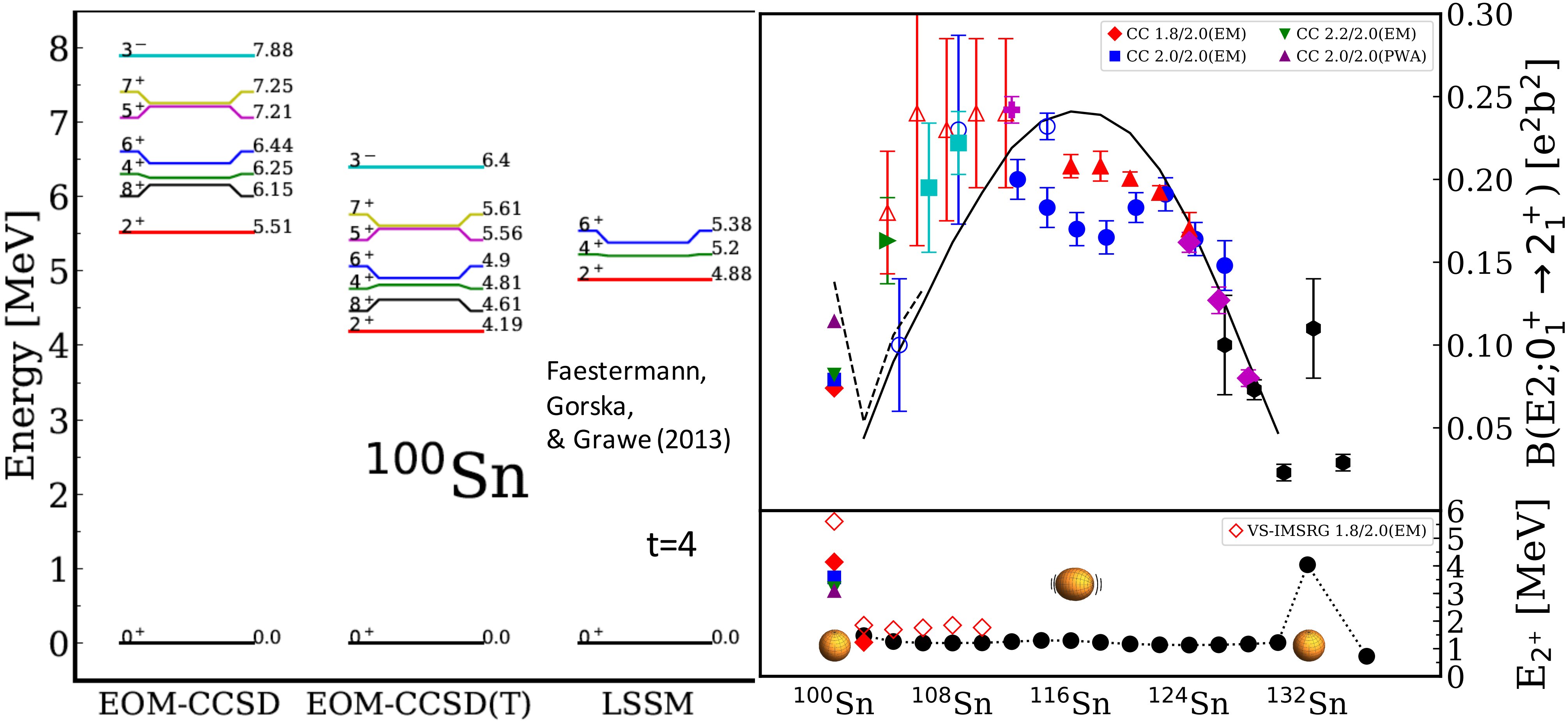
Quantify the effect of quenching from correlations and 2BCs

PHYSICAL REVIEW LETTERS 120, 152503 (2018)

Editors' Suggestion

Structure of the Lightest Tin Isotopes

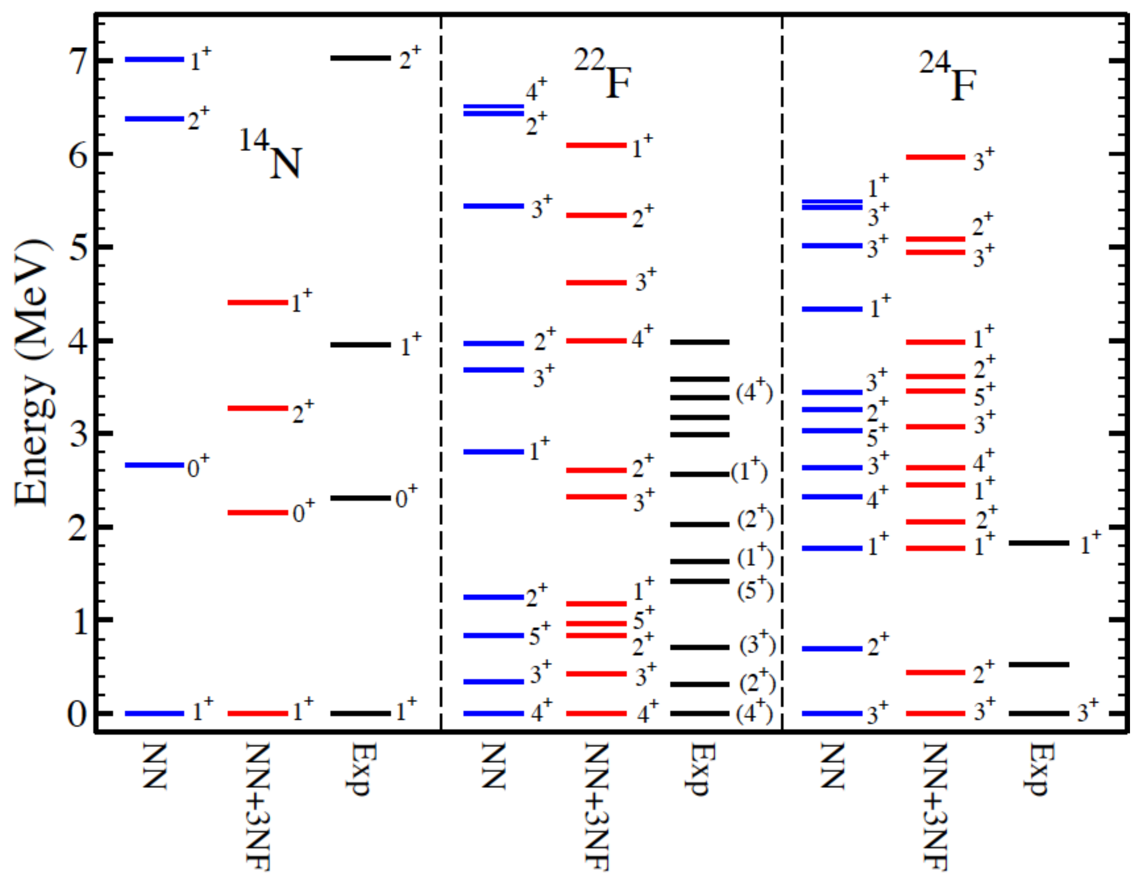
T. D. Morris,[1,2] J. Simonis,[3,4] S. R. Stroberg,[5,6] C. Stumpf,[3] G. Hagen,[2,1] J. D. Holt,[5] G. R. Jansen,[7,2]
T. Papenbrock,[1,2] R. Roth,[3] and A. Schwenk[3,4,8]

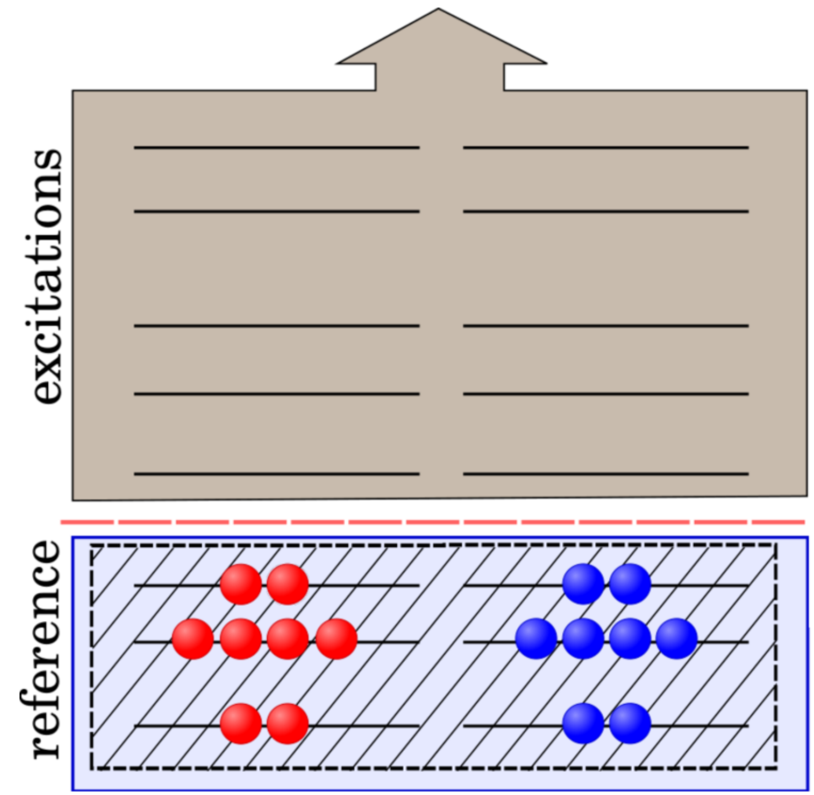


Coupled cluster calculations of beta-decay partners

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

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



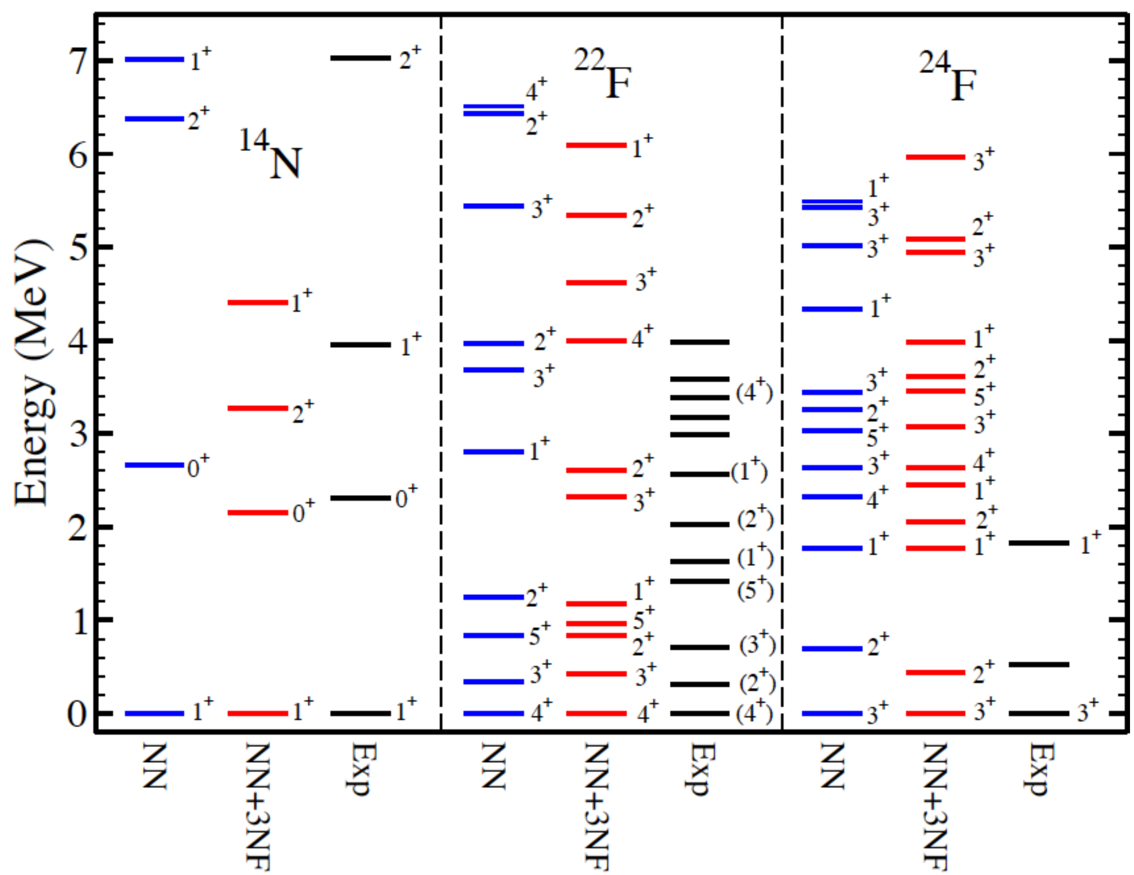


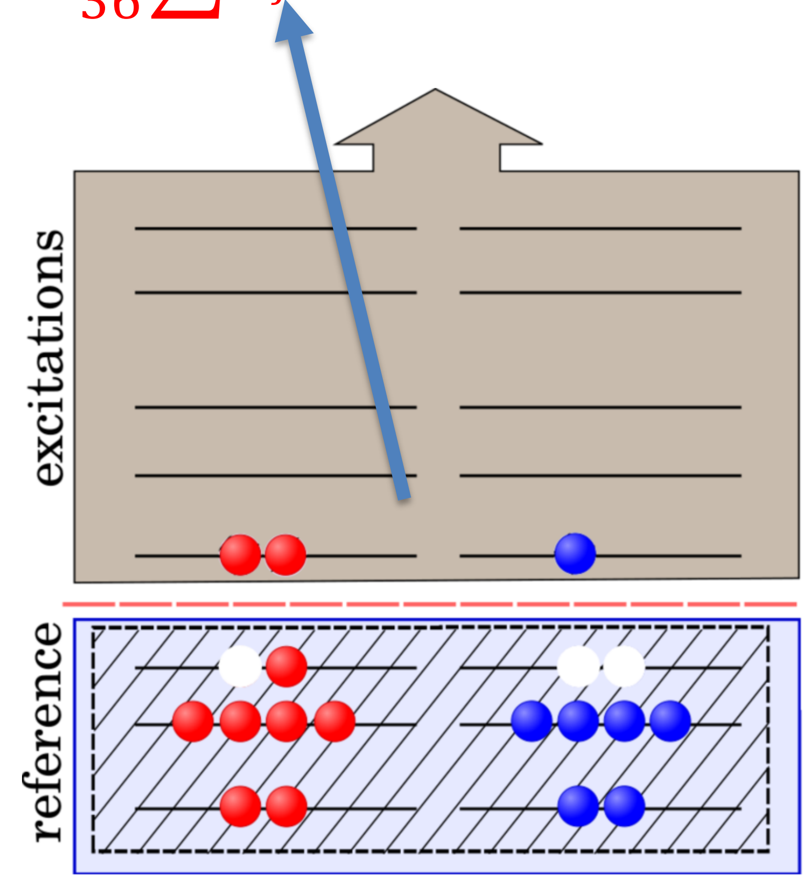
A. Ekström, G. Jansen, K. Wendt et al, PRL 113 262504 (2014)

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)

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.

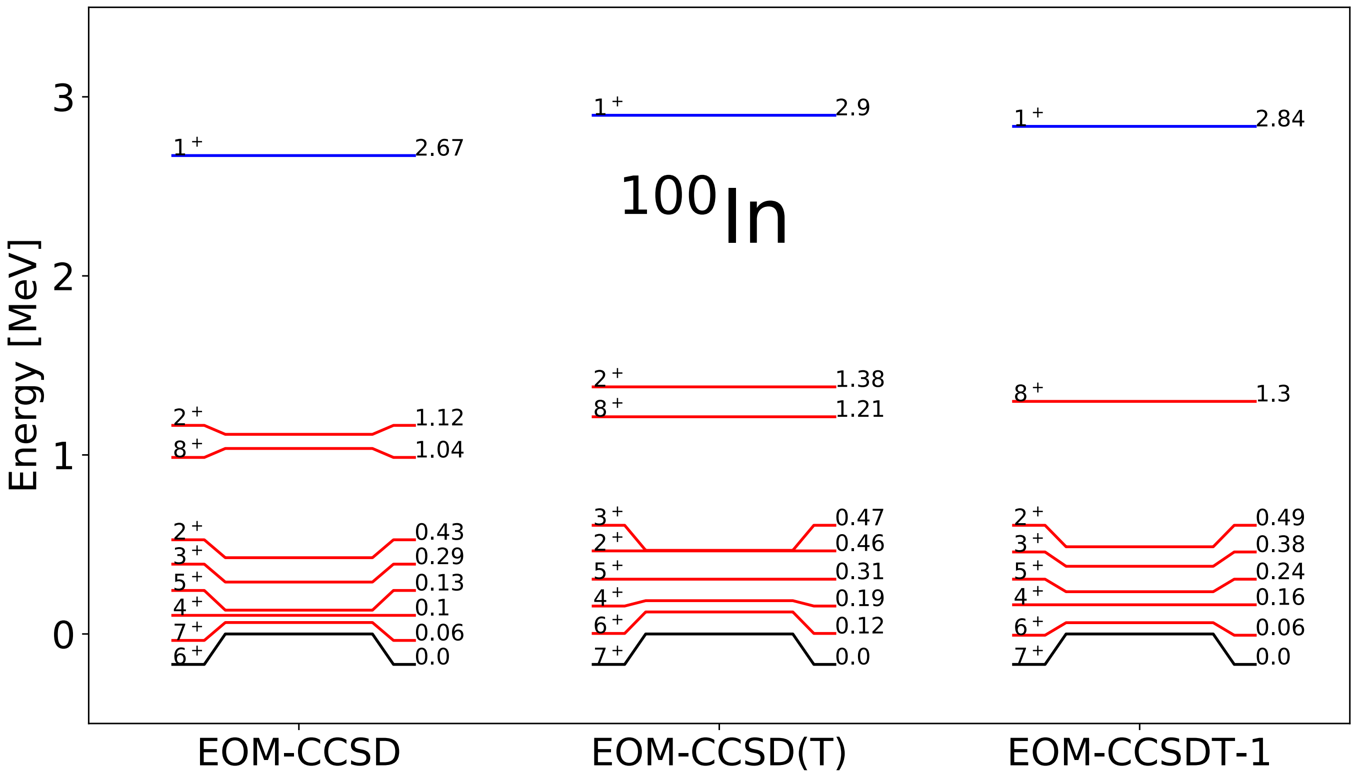
$$\overline{H}_{PP}R_P + \overline{H}_{PQ}(\omega - \overline{H}_{QQ})^{-1}\overline{H}_{QP}R_P = \omega R_P$$

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

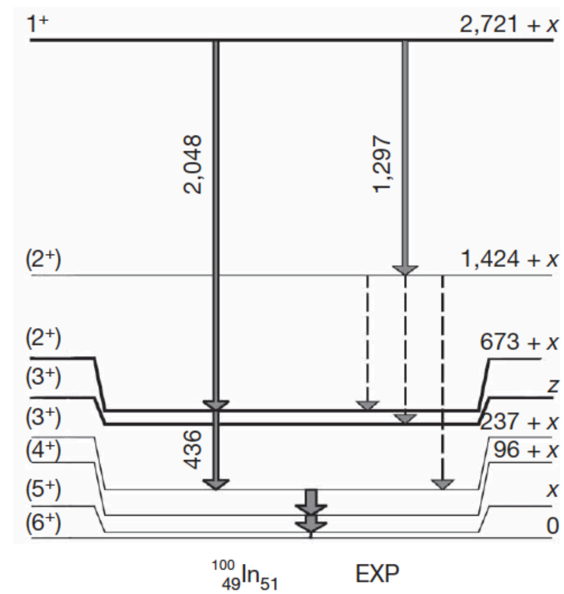
W. C. Haxton and C.-L. Song Phys. Rev. Lett. **84** (2000); W. C. Haxton Phys. Rev. C **77**, 034005 (2008)
C. E. Smith, J. Chem. Phys. **122**, 054110 (2005)

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

1.8/2.0 (EM)



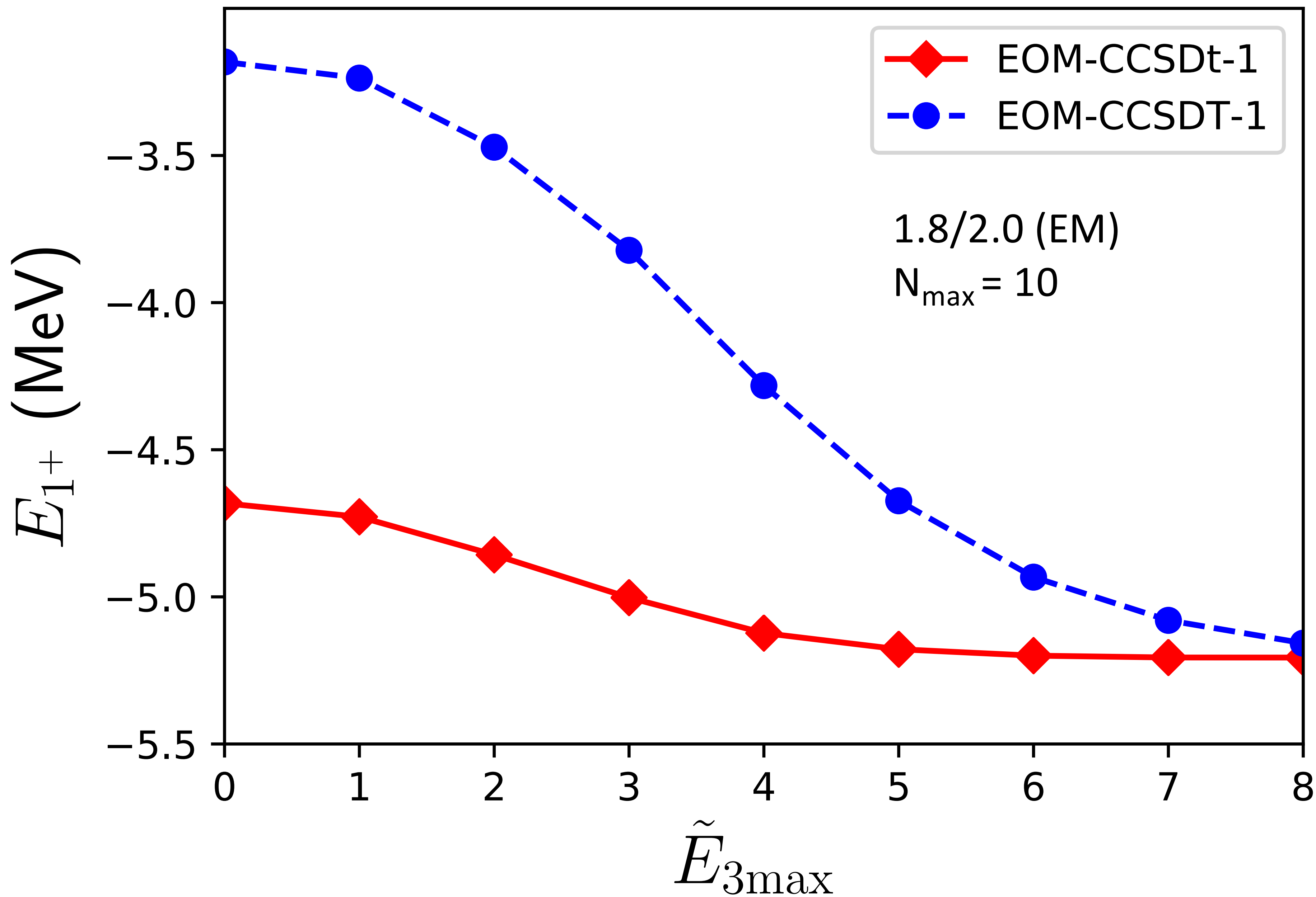
Hinke et al, Nature (2012)



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

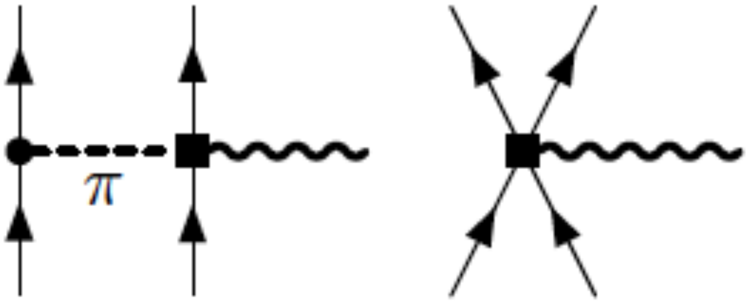
$$\Delta\omega_\mu = \langle\Phi_0|L_\mu \overline{H}_{PQ'}(\omega_\mu - \overline{H}_{Q'Q'})^{-1}\overline{H}_{Q'P}R_\mu|\Phi_0\rangle$$

Convergence of excited states in ^{100}In



Normal ordered one- and two-body current

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



c_3, c_4 c_D

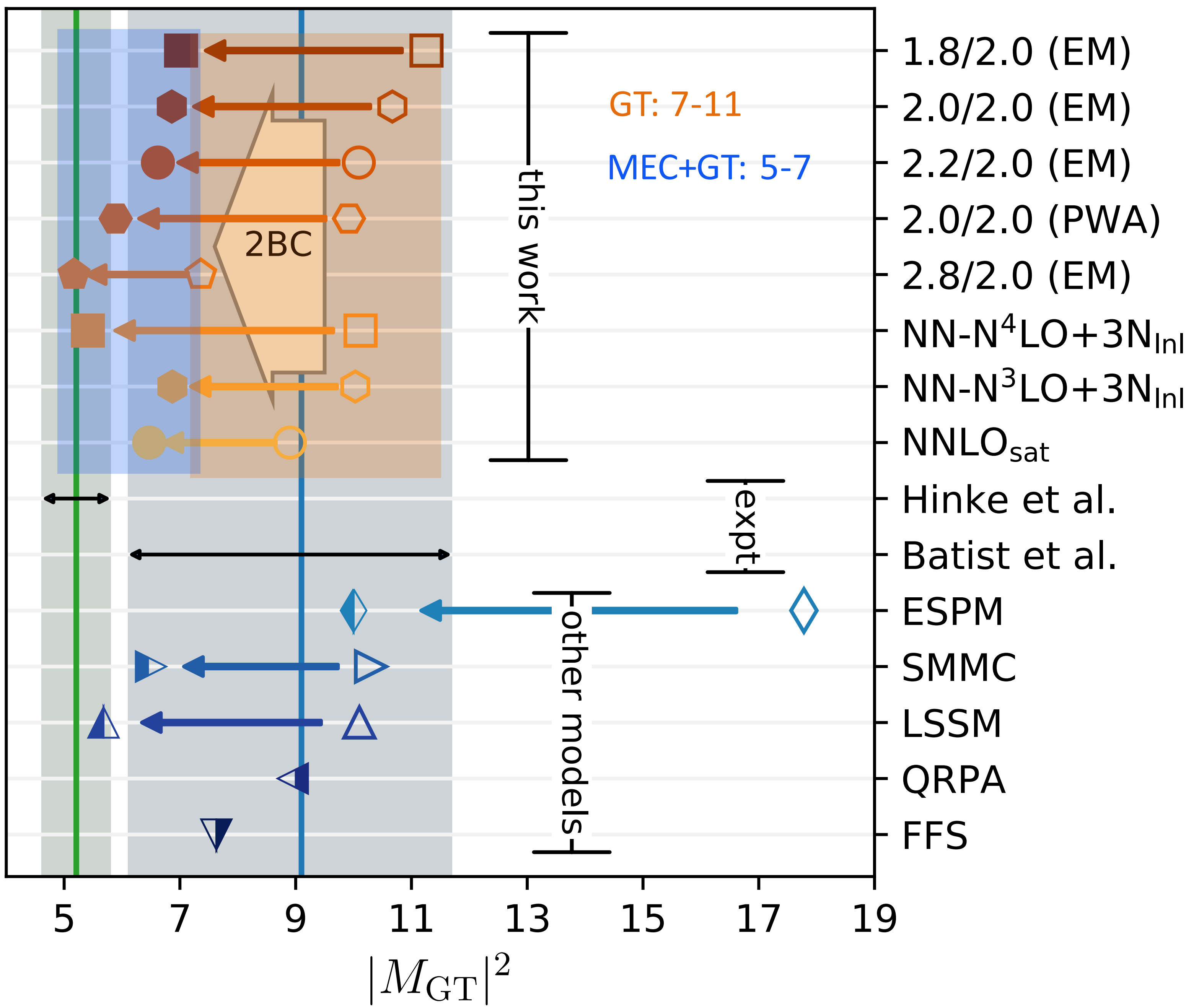
Normal ordered operator:

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

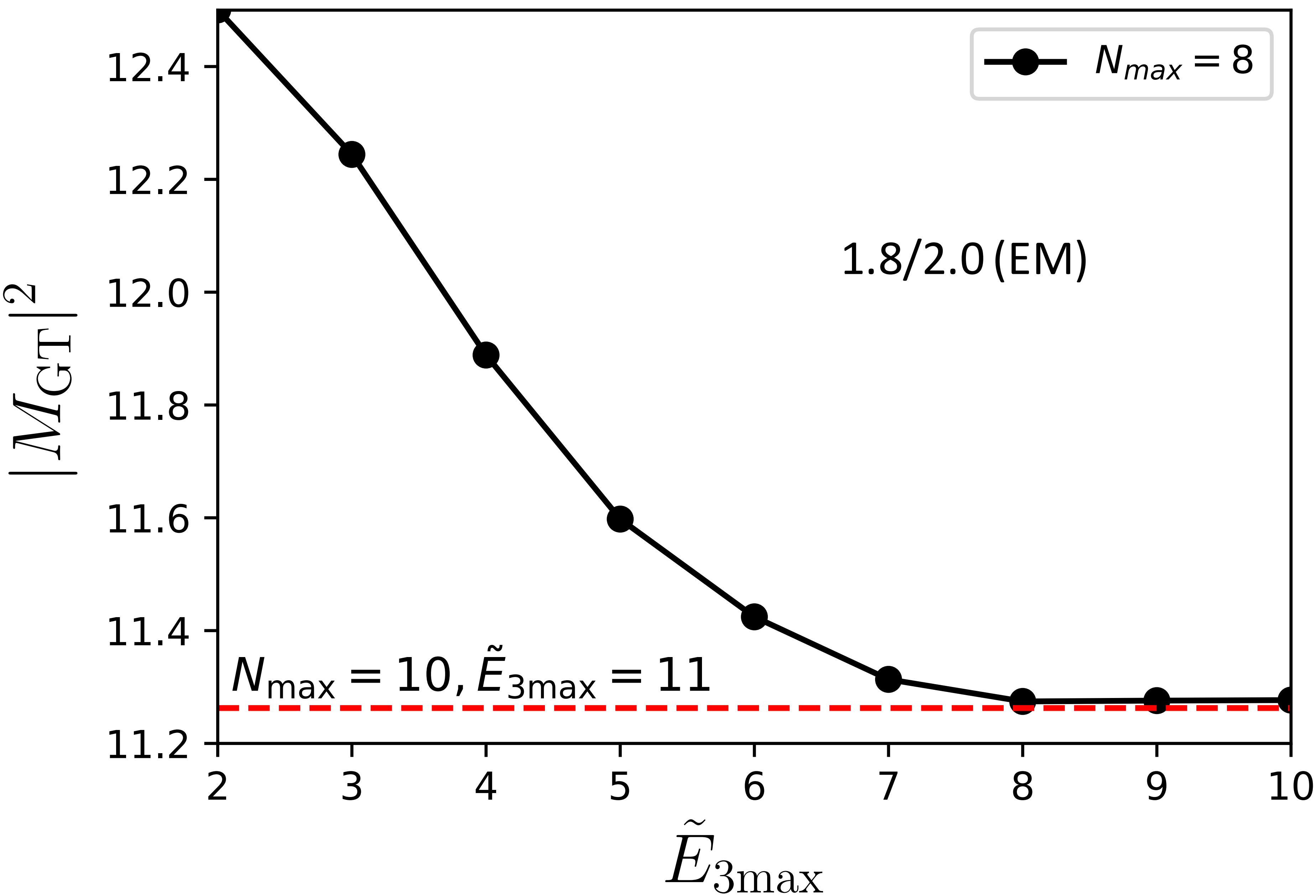
Benchmark between NCSM and CC for the large transition in ^{14}O using NNLO$_{\mathrm{sat}}$

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)

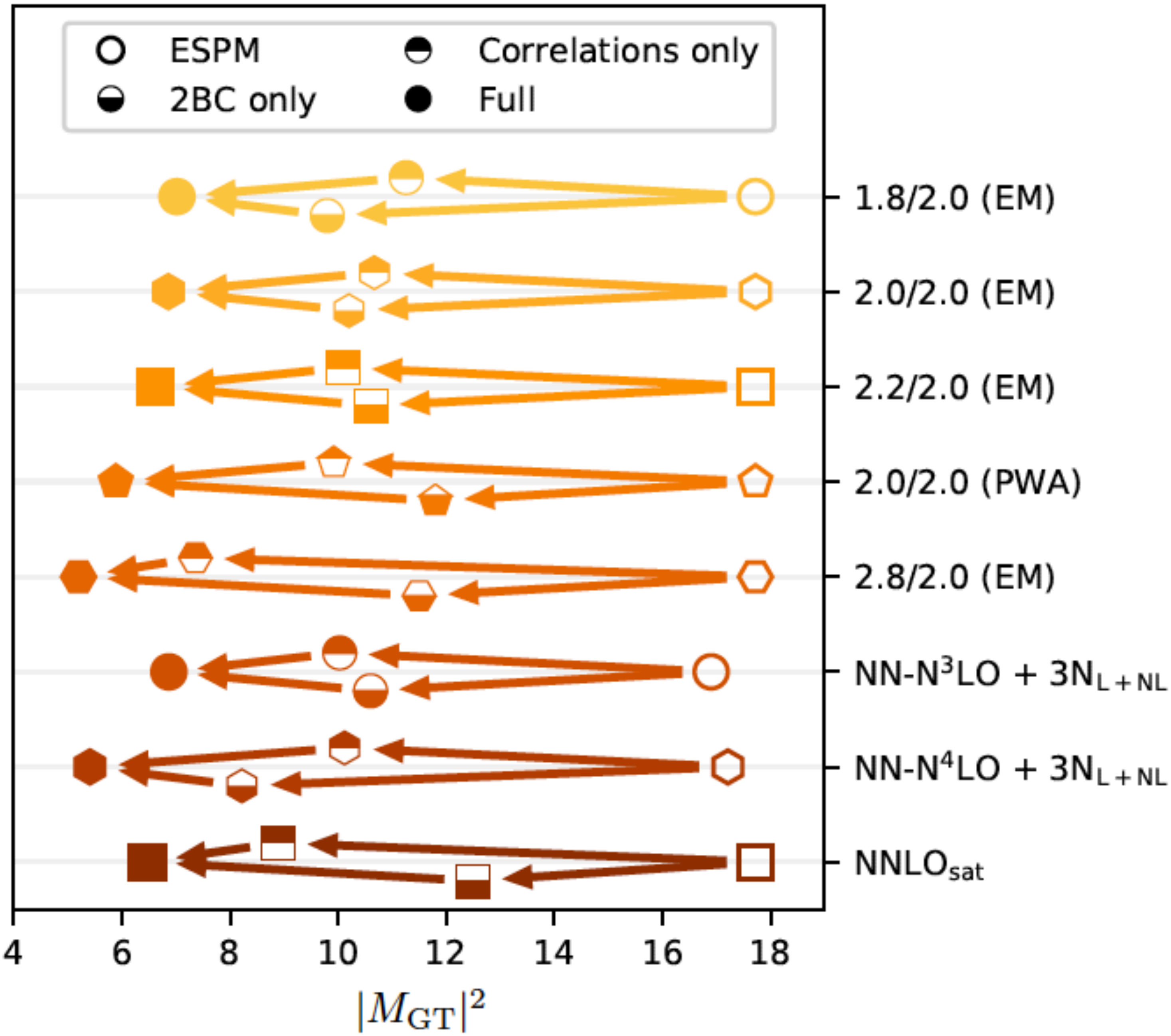
Super allowed Gamow-Teller decay of ^{100}Sn



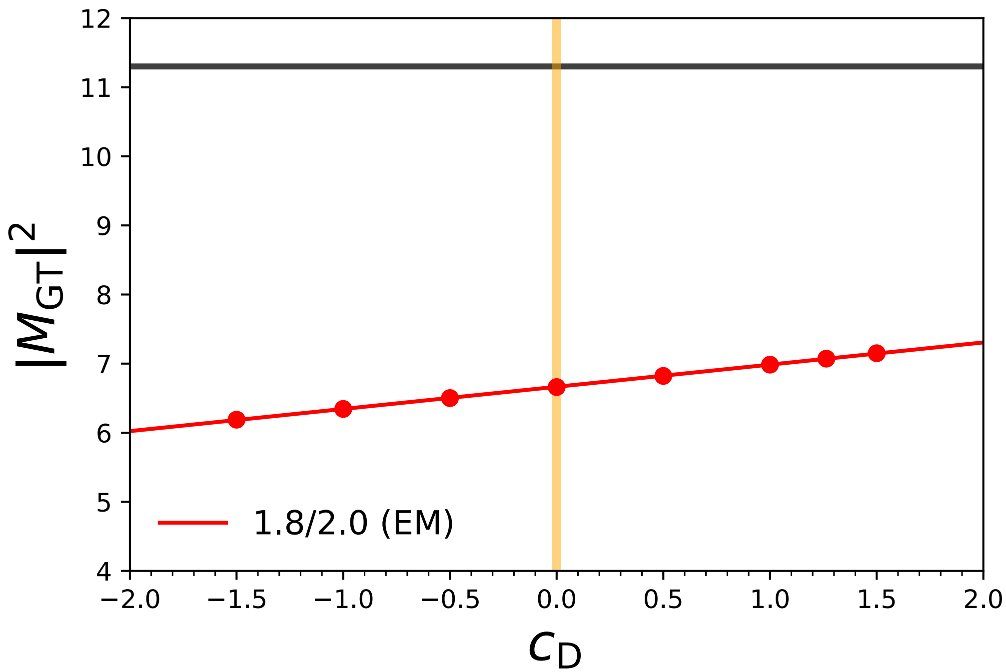
Convergence of GT transition in ^{100}Sn

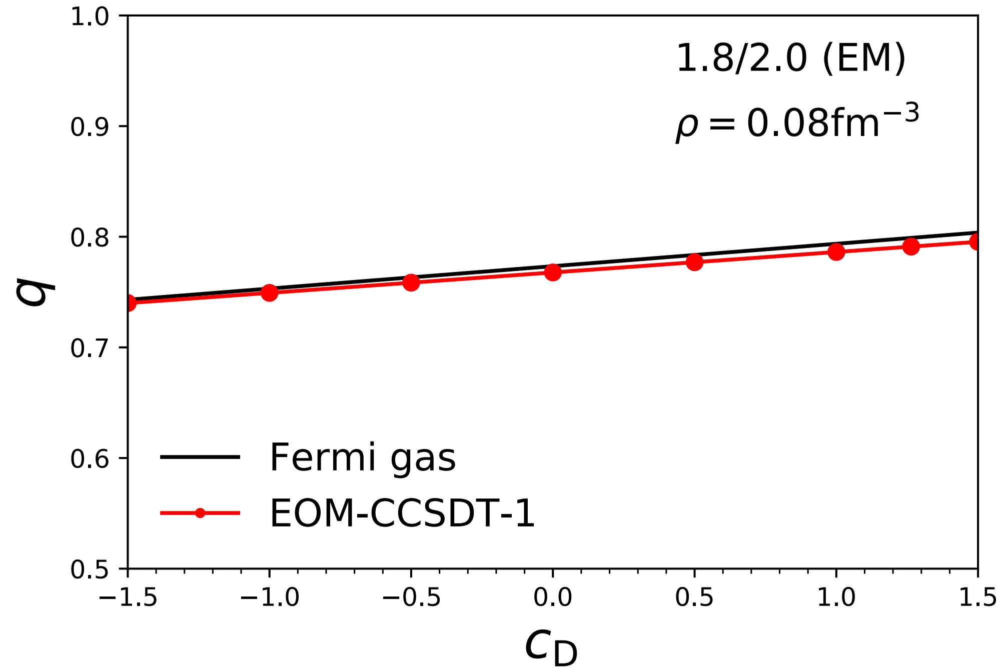


Role of 2BC and correlations in ^{100}Sn



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



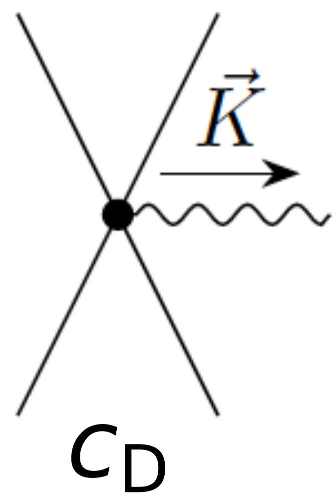


J. Menéndez, D. Gazit, A. Schwenk

PRL 107, 062501 (2011)

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

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

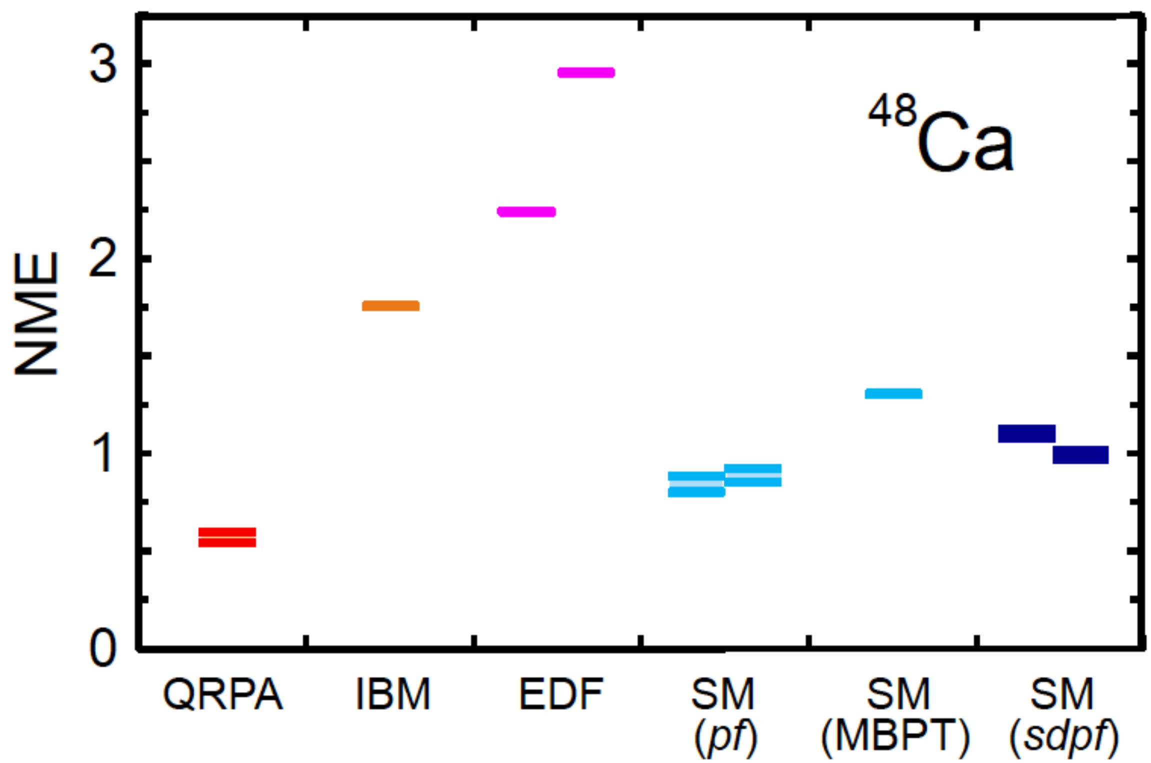


Short-ranged contact term of 2BC (heavy meson exchange)

Neutrinoless ββ-decay of ^{48}Ca

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

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?

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:

$$M_{GT}^{0\nu} + \left(\frac{g_V}{g_A}\right)^2 M_F^{0\nu} + M_T^{0\nu}$$

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

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

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

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

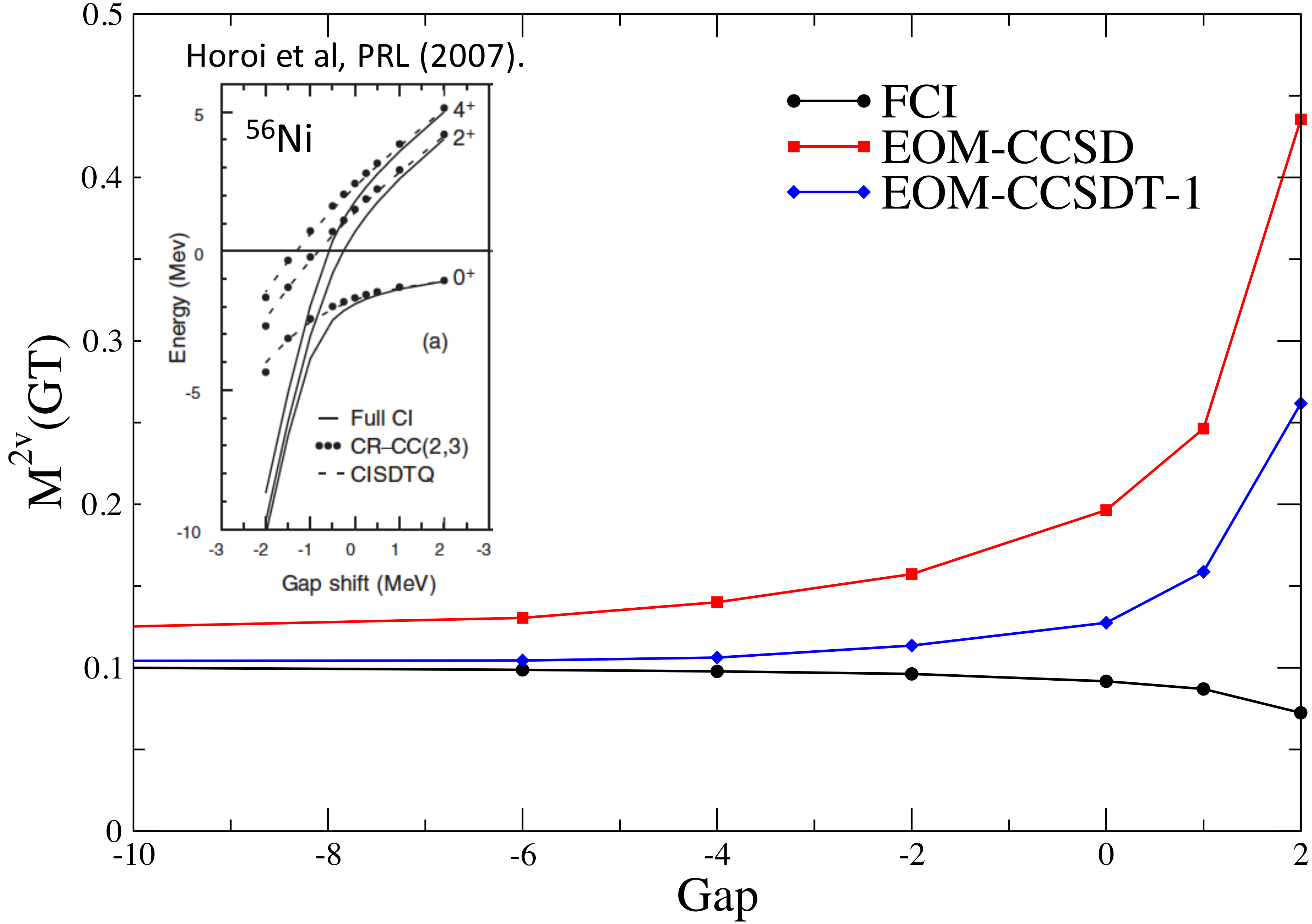
$$M^{2\nu} = \langle \Phi_0 | L_0 \overline{O}_{\mathrm{GT}} \frac{1}{\overline{H} - E_i + Q_{\beta\beta}/2} \overline{O}_{\mathrm{GT}} | \Phi_0 \rangle$$

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

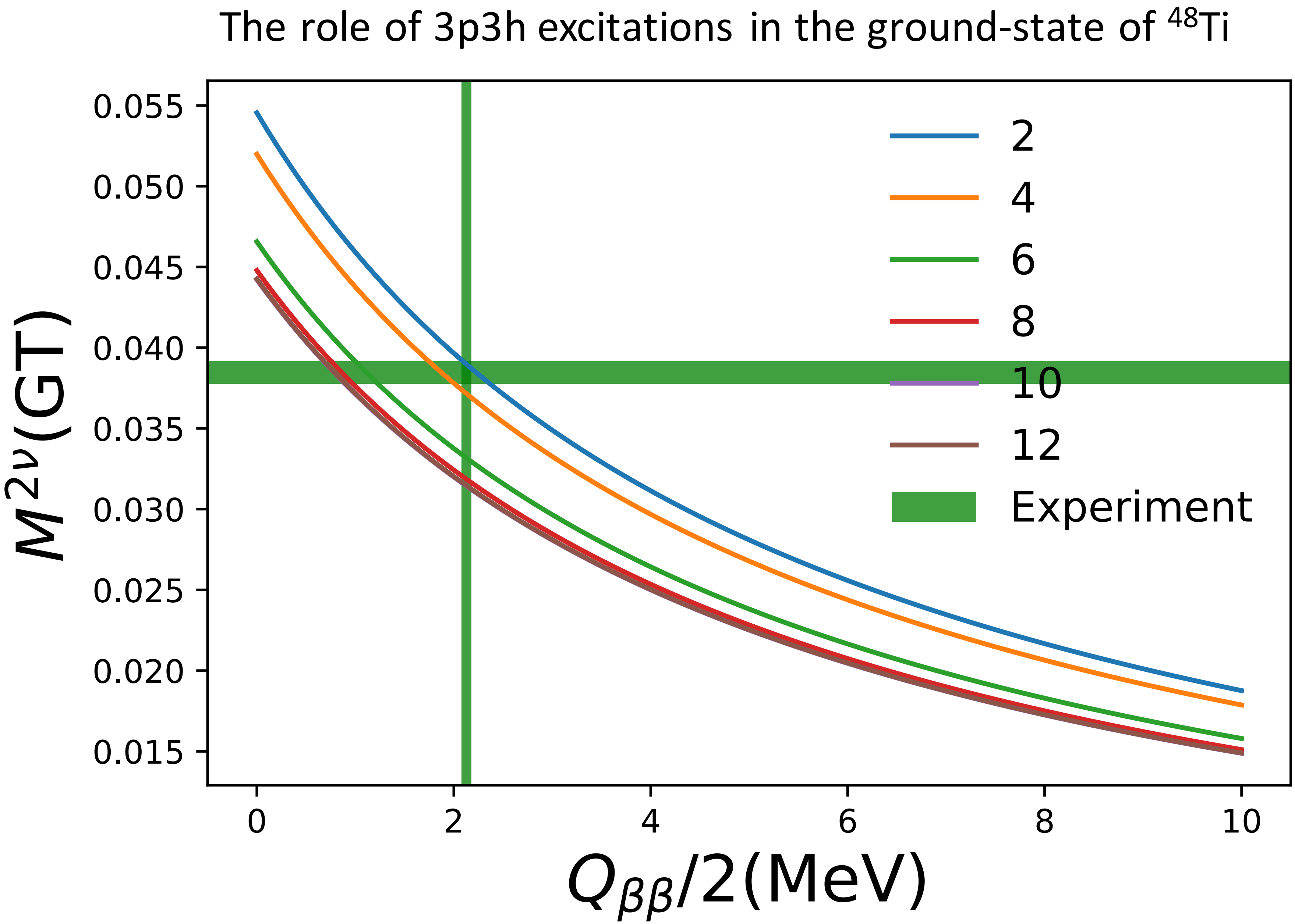
$$M^{2\nu} = \langle \tilde{\nu}_0 | \nu_0 \rangle \left\{ \frac{1}{(a_0 - Q_{\beta\beta}/2) - \frac{b_0^2}{(a_1 - Q_{\beta\beta}/2) - \frac{b_1^2}{(a_2 - Q_{\beta\beta}/2) \quad - \cdots}}} \right\}$$

- 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 iterations.
- Need more than 50 1^+ states converged in ^{48}Sc (300-400 Lanczos iterations) if we sum explicitly over intermediate states

ββ-decay of ^{48}Ca with KB3G shell-model interaction

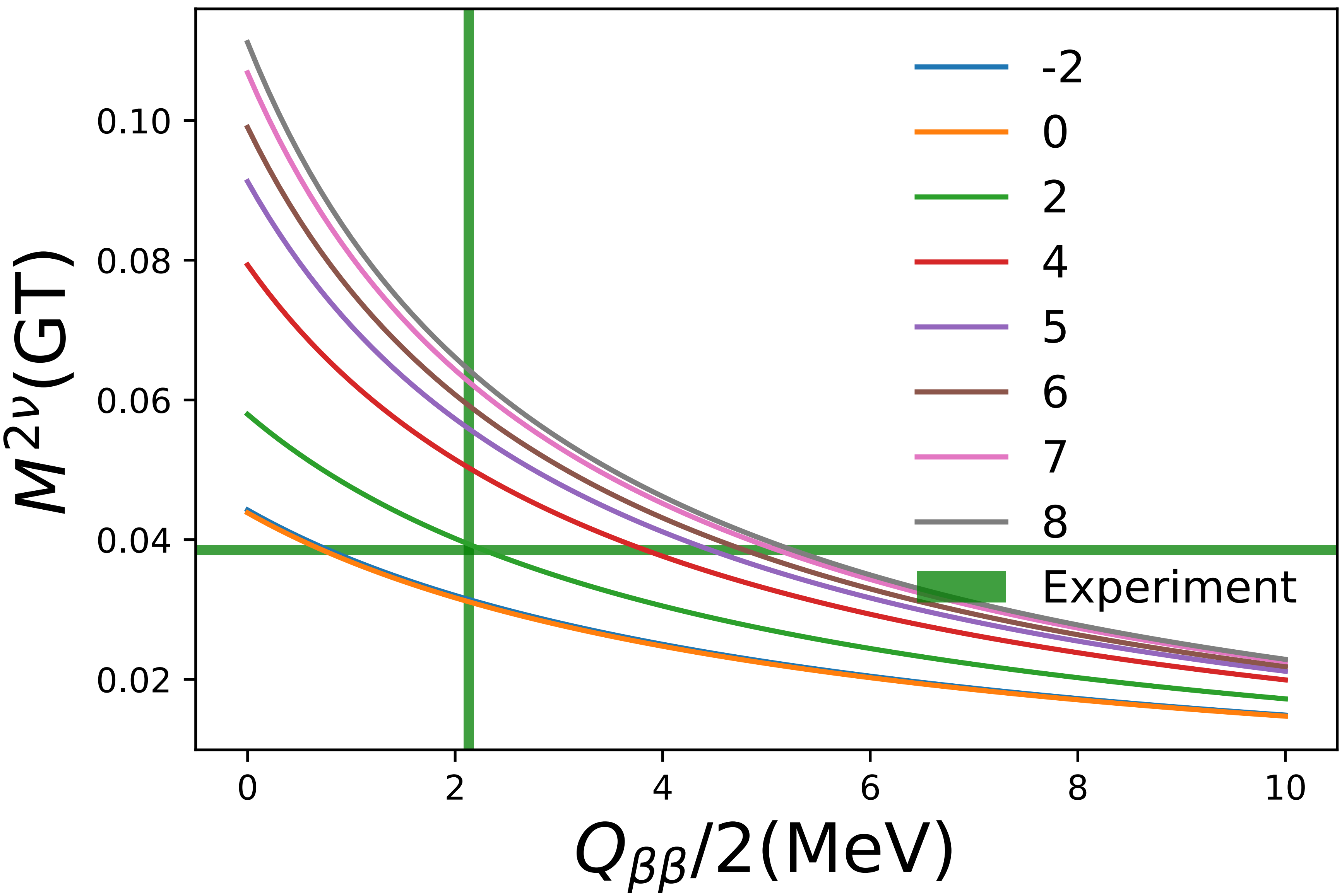


ββ-decay of ^{48}Ca



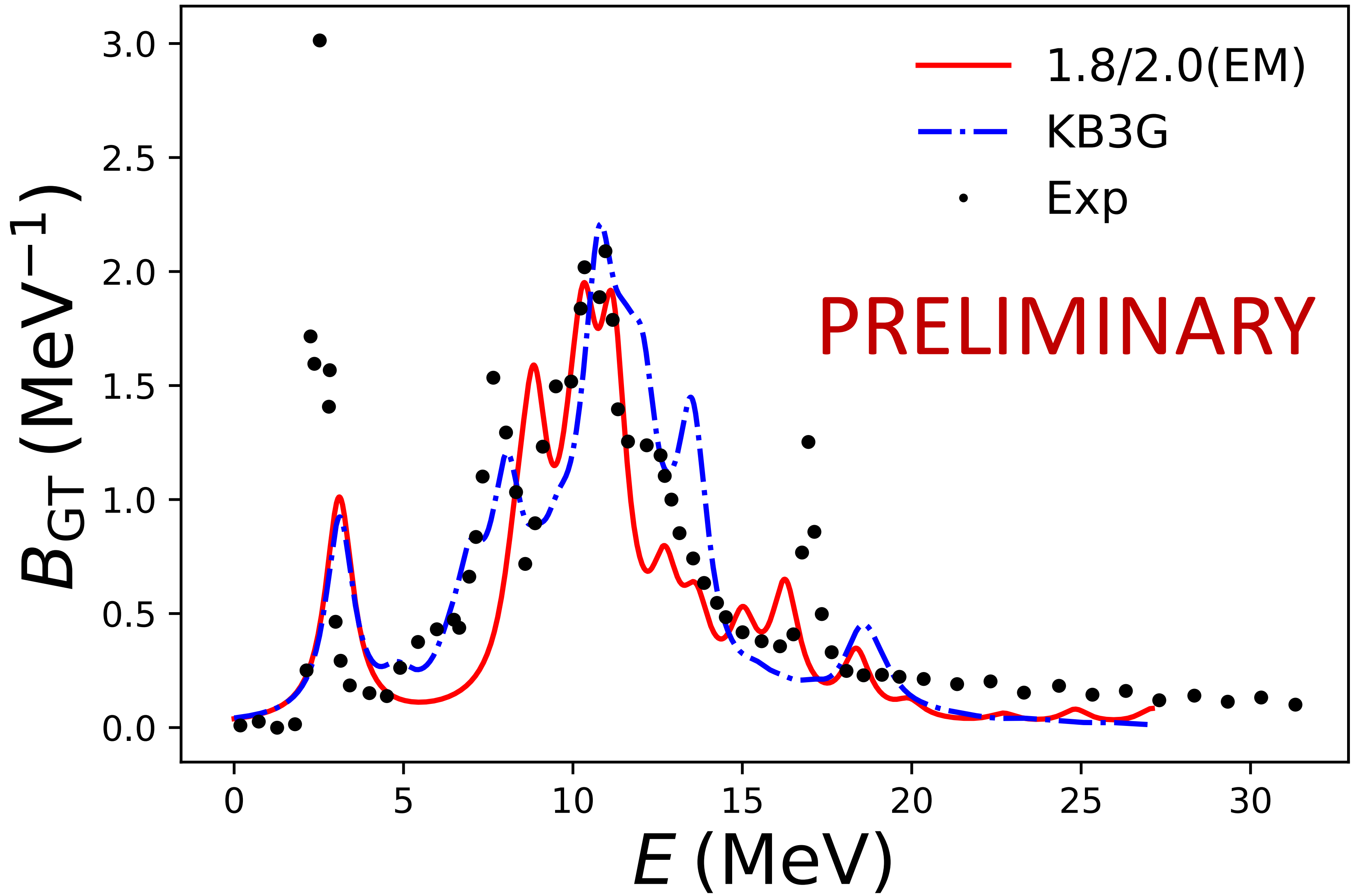
ββ-decay of ^{48}Ca

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



Gamow-Teller strengths in ^{48}Ca

GT-strength computed using the Lanczos method and EOM-CCSDT-1
No 2BCs, strength function folded with a Lorentzian of width 0.5MeV.



Collaborators

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

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

@ LLNL: **K. Wendt**

@ Mainz: S. Bacca

@ TRIUMF: **P. Gysbers**, J. Holt, P. Navratil

@ Reed College: **S. R. Stroberg**