Coupled-cluster computations of weak decays in nuclei

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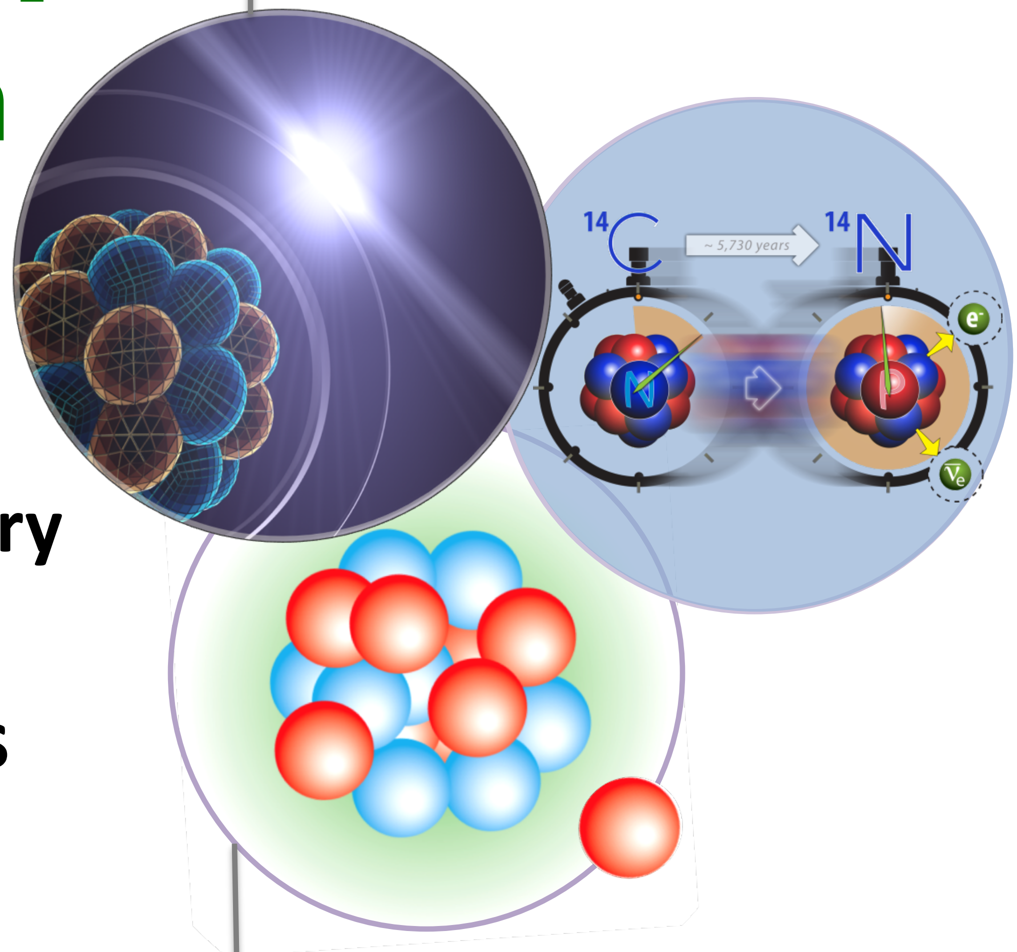

Nuclear ab initio Theories and Neutrino Physics

INT, March 6th, 2018

U.S. DEPARTMENT OF ENERGY
NUCLEI
Nuclear Computational Low-Energy Initiative
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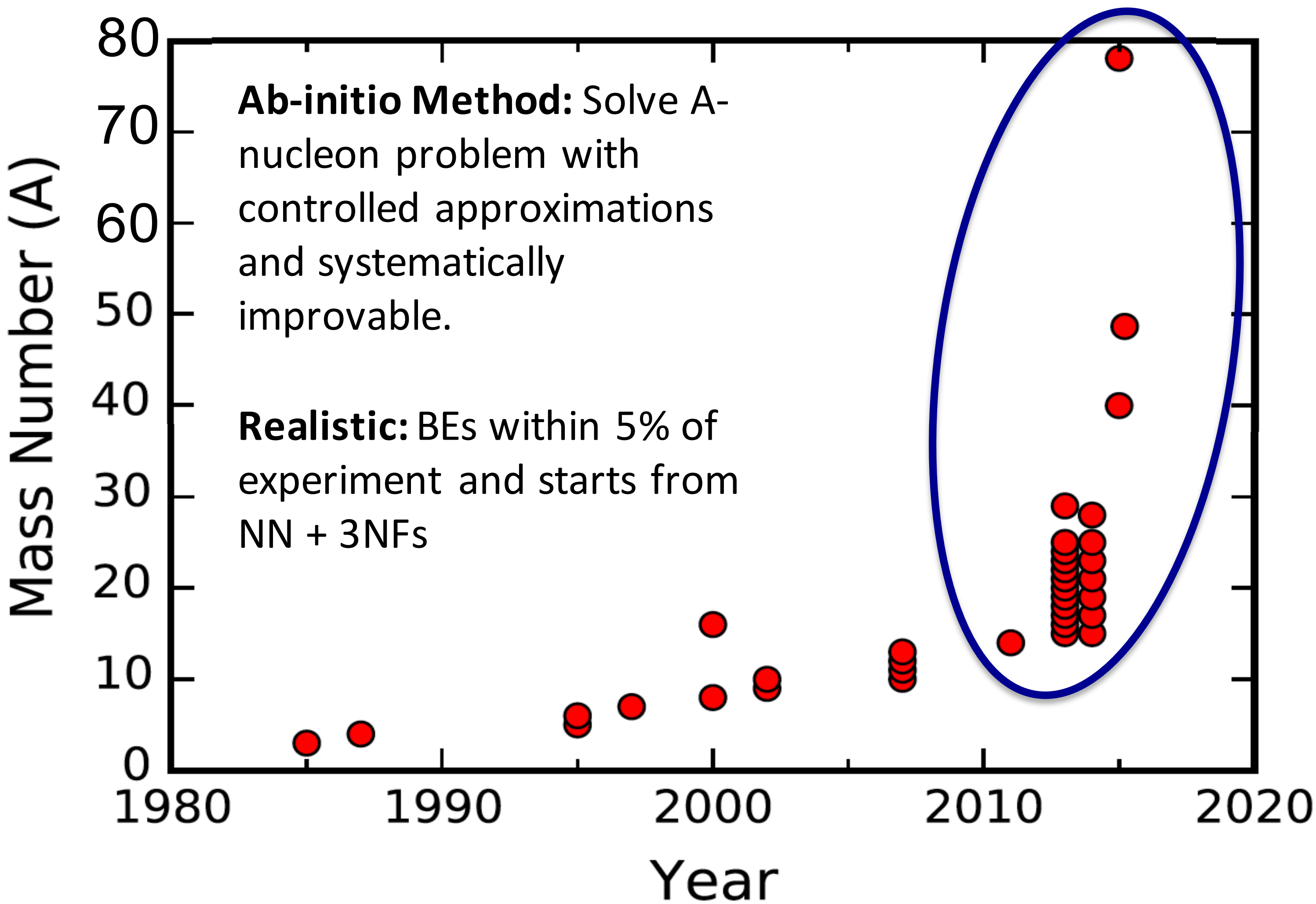
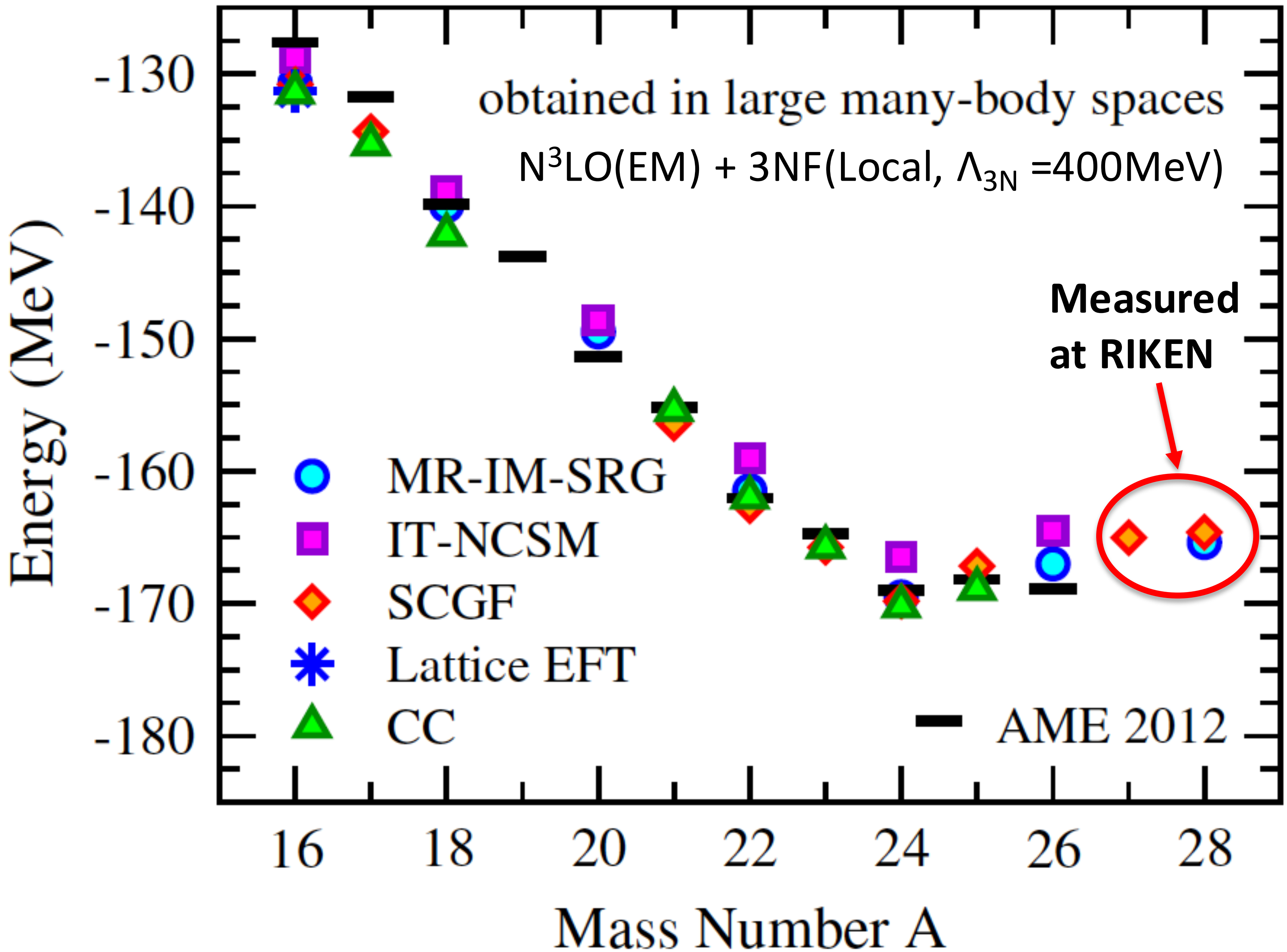
Trend in realistic ab-initio calculations

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

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



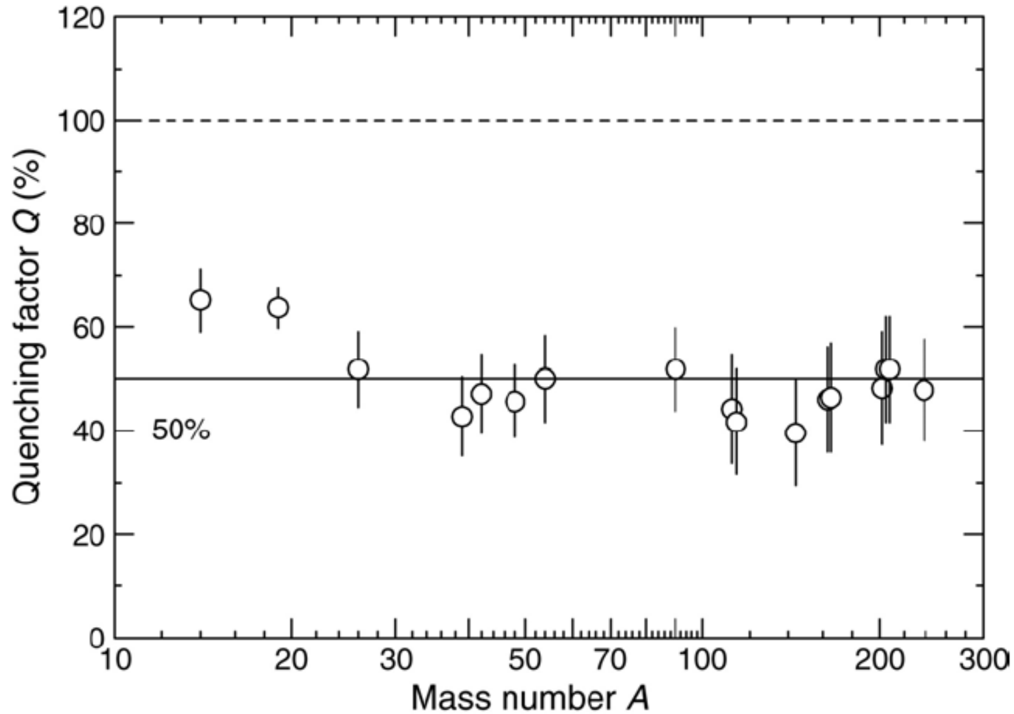
Oxgyen chain with interactions from chiral EFT



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

The puzzle of quenched of beta decays

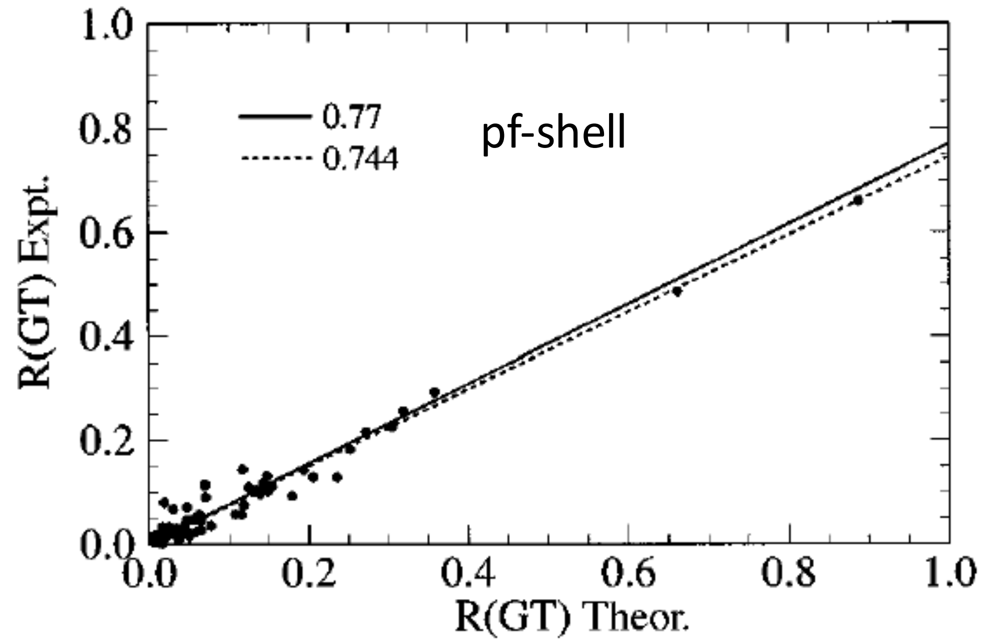
Long-standing problem: Experimental beta-decay strengths quenched compared to theoretical results.



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

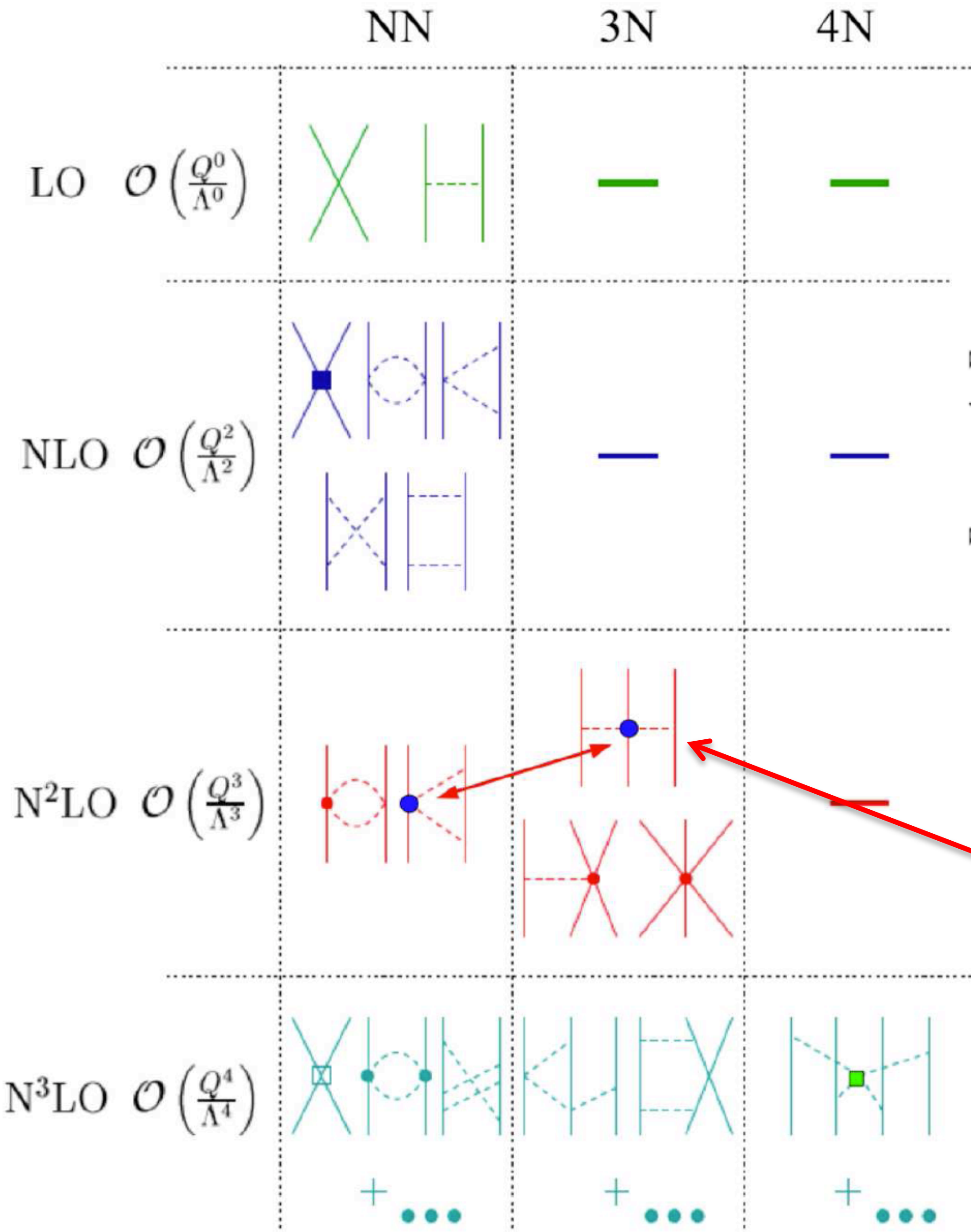
- Renormalizations of the Gamow-Teller operator?
- Missing correlations in nuclear wave functions?
- Model-space truncations?
- Two-body currents (2BCs)?

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

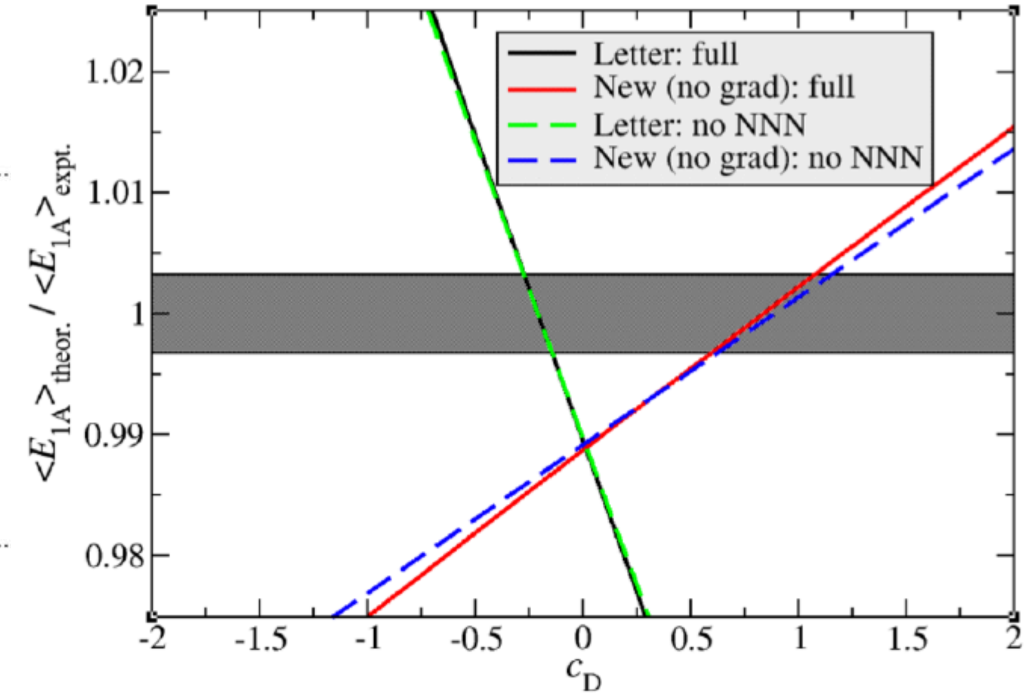


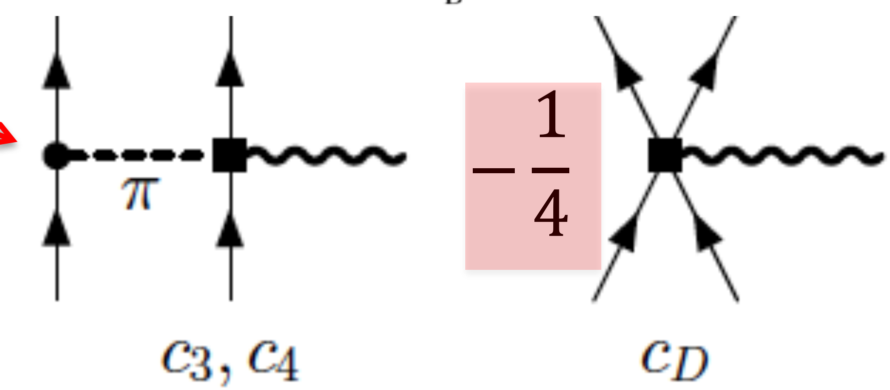
Nuclear forces from chiral effective field theory

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

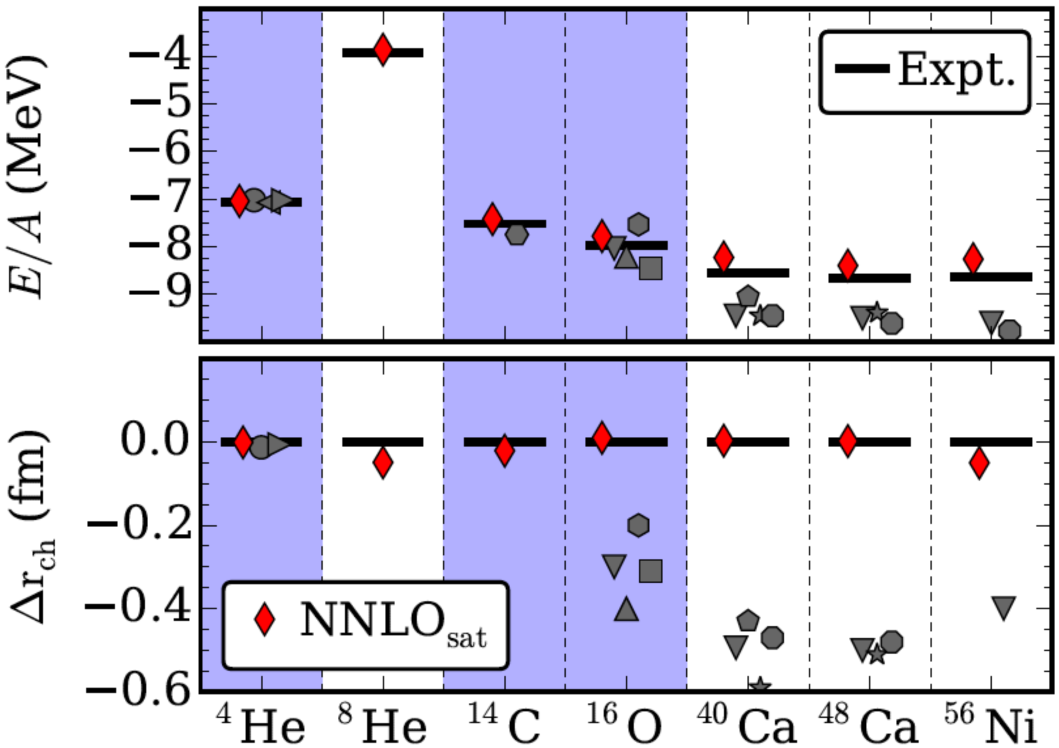


From Sofia Quaglioni and Kyle Wendt





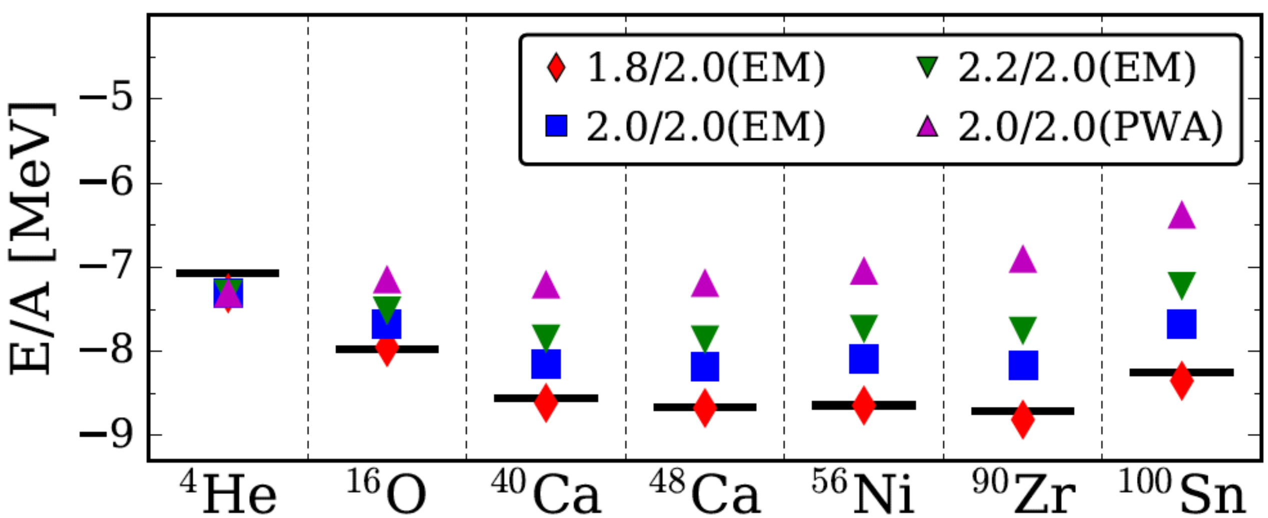
A family of interactions from chiral EFT



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

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

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



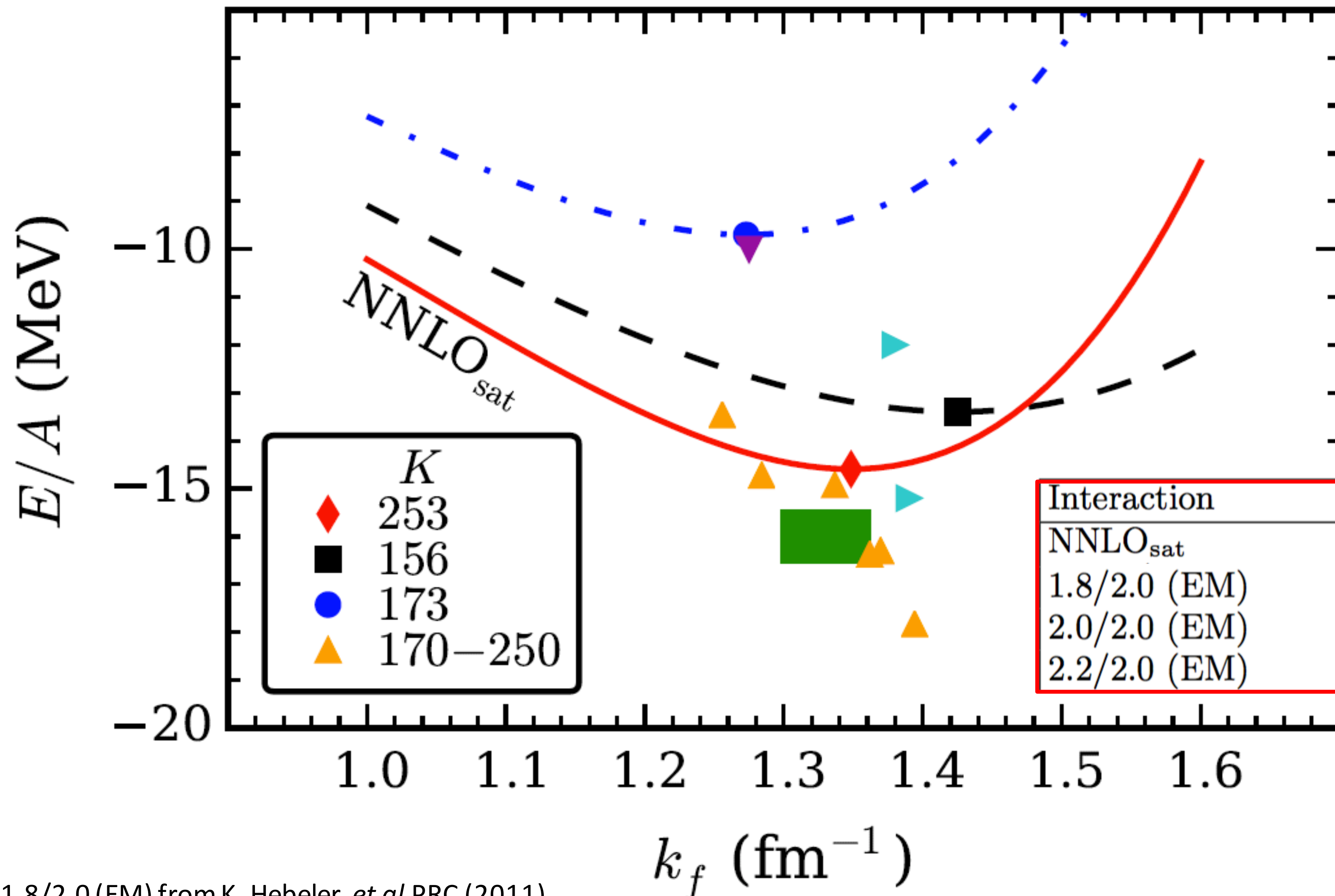
1.8/2.0(EM): Accurate BEs

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

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

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

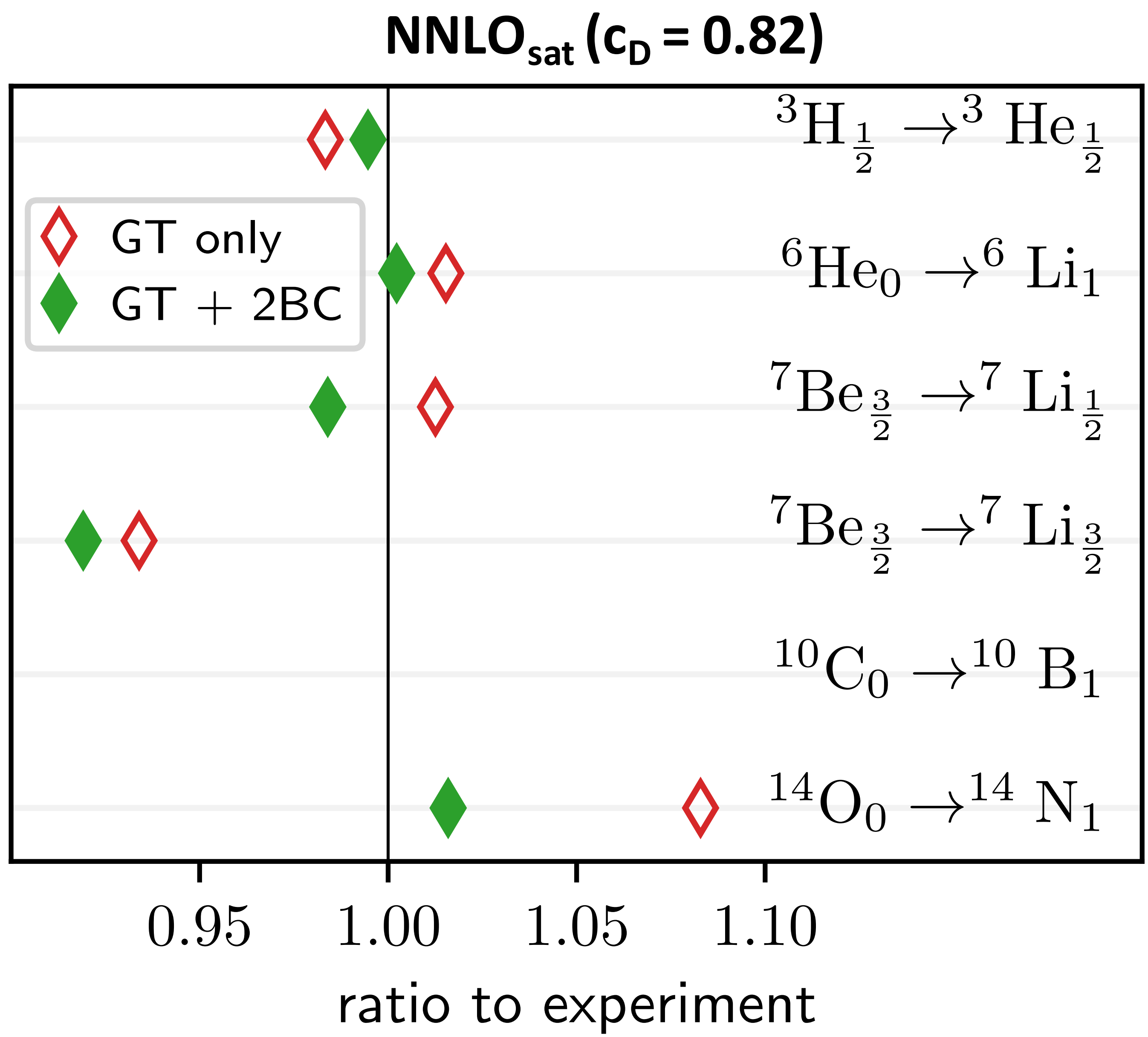
Saturation in nuclear matter from chiral interactions



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

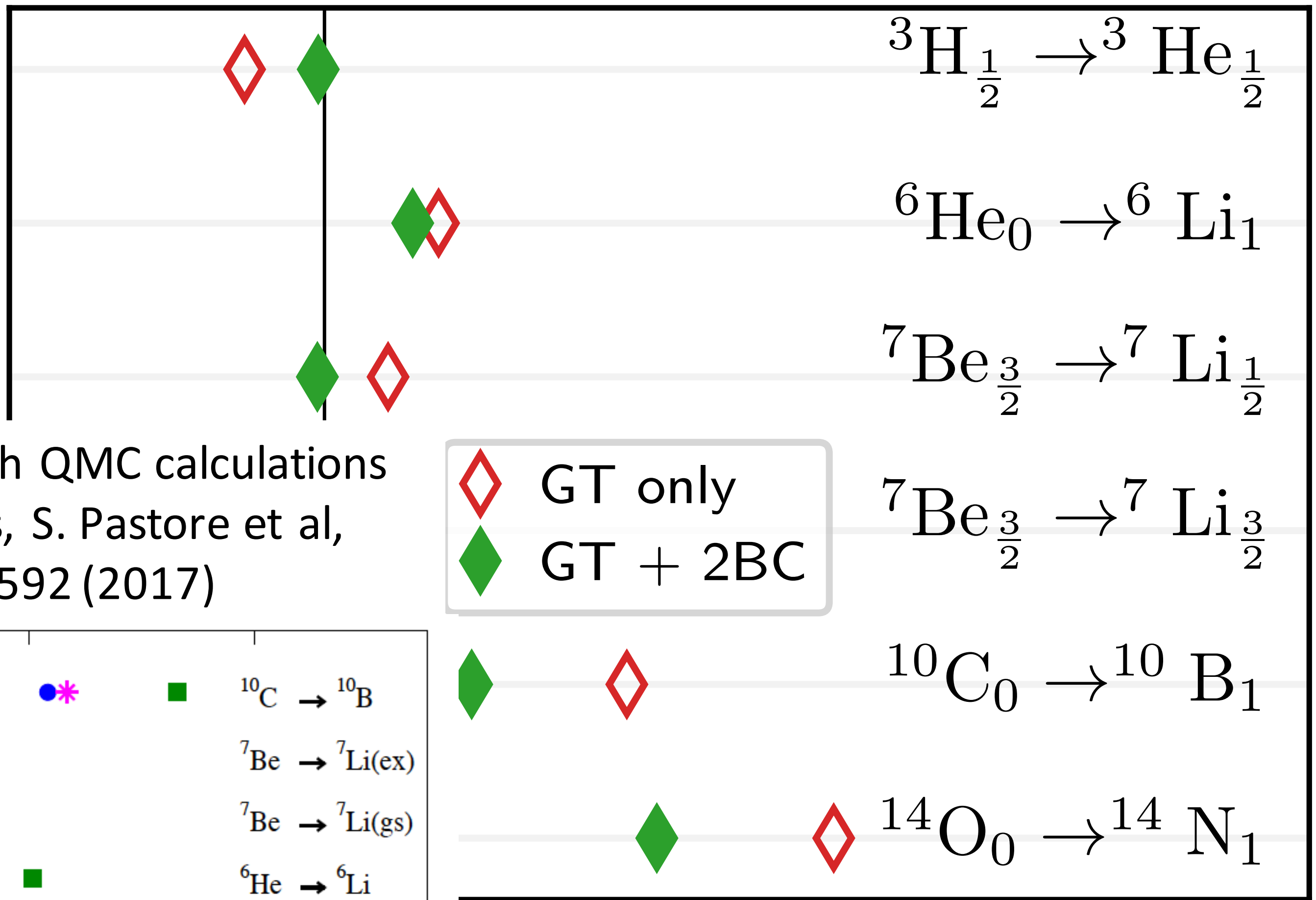
1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

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

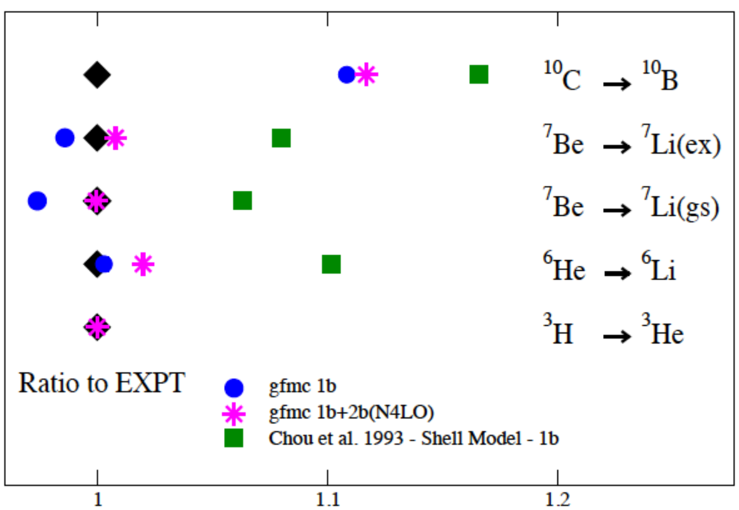


Theory to experiment ratios for beta decays in light nuclei from NCSM

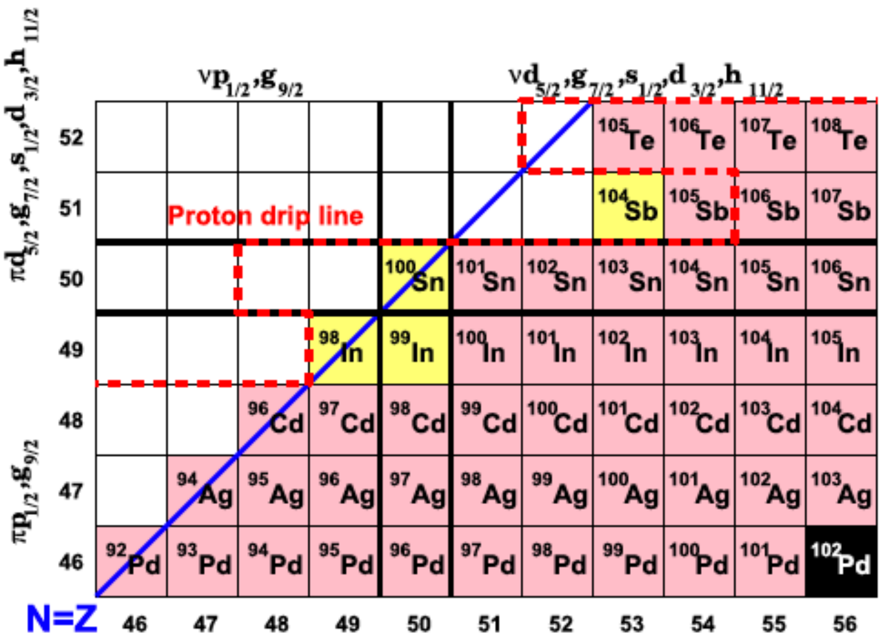
N3LO(EM) + $3N_{lnl}$ SRG-evolved to 2.0fm^{-1} ($c_D = 0.7$)



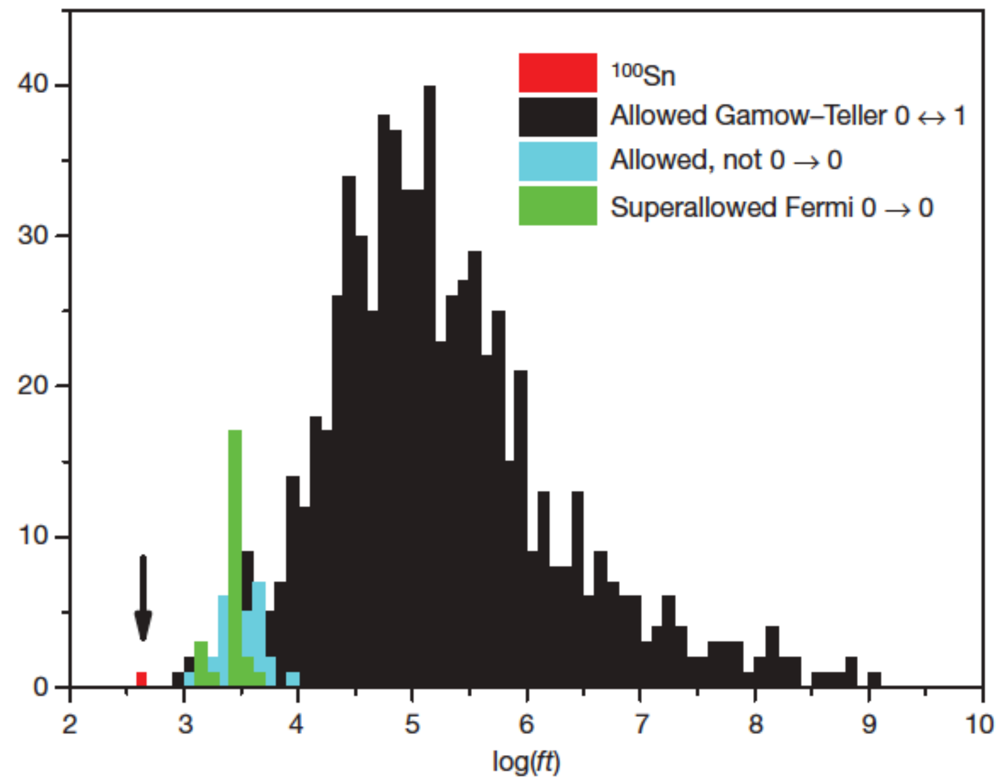
Consistent with QMC calculations of beta-decays, S. Pastore et al, arXiv:1709.03592 (2017)



Gamow-Teller transition in ^{100}Sn



Hinke et al, Nature (2012)

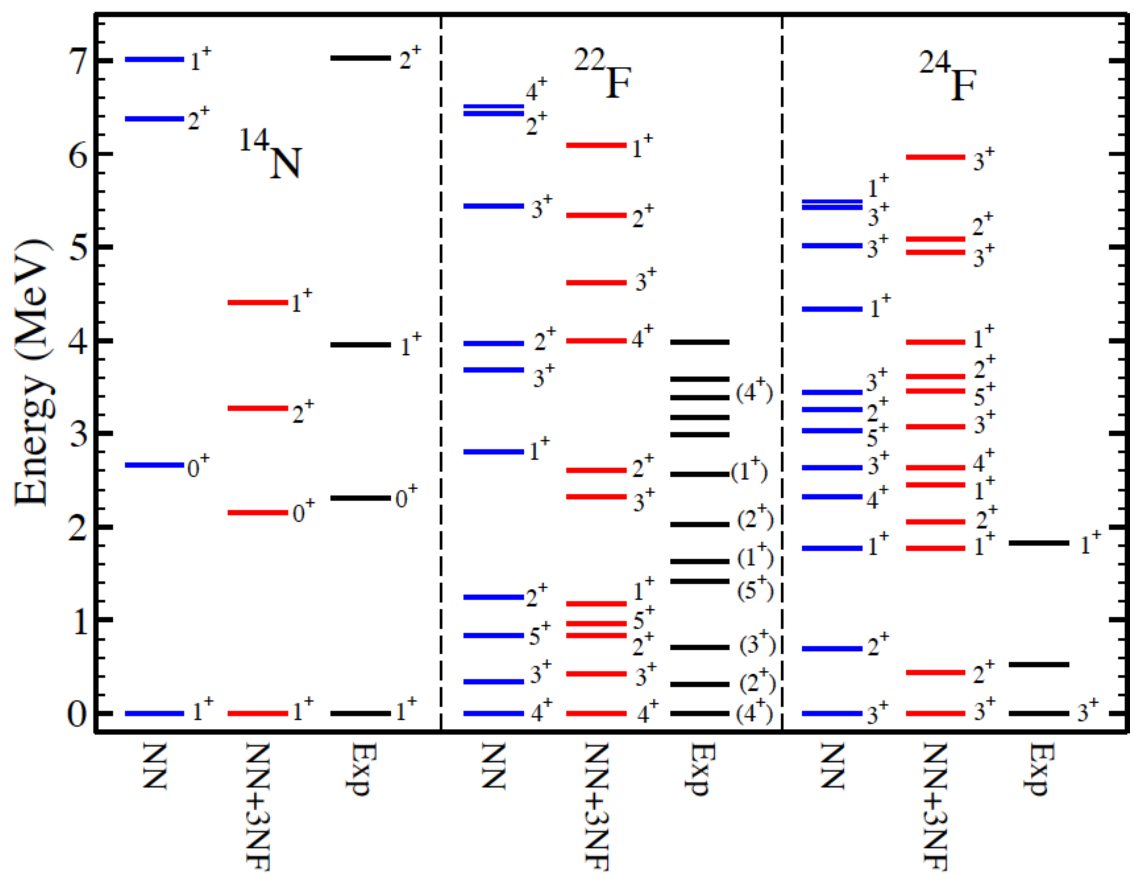


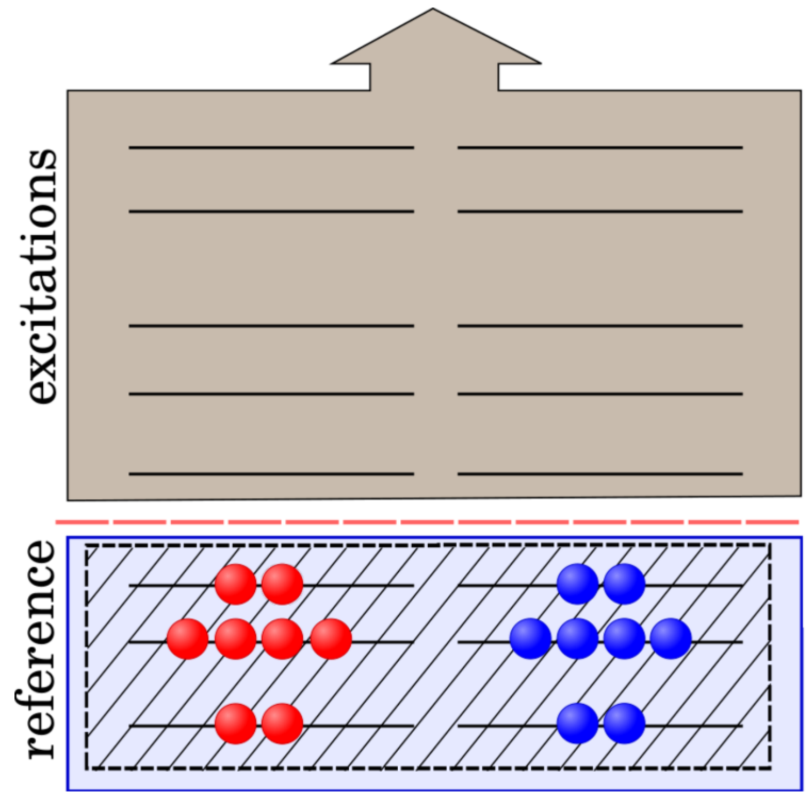
- ^{100}Sn is doubly magic and in the closest proximity to the proton dripline
- ^{100}Sn is ideally suited for first principles approaches
- Largest known strength in allowed nuclear β-decay

Coupled cluster calculations of beta-decay partners

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

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





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

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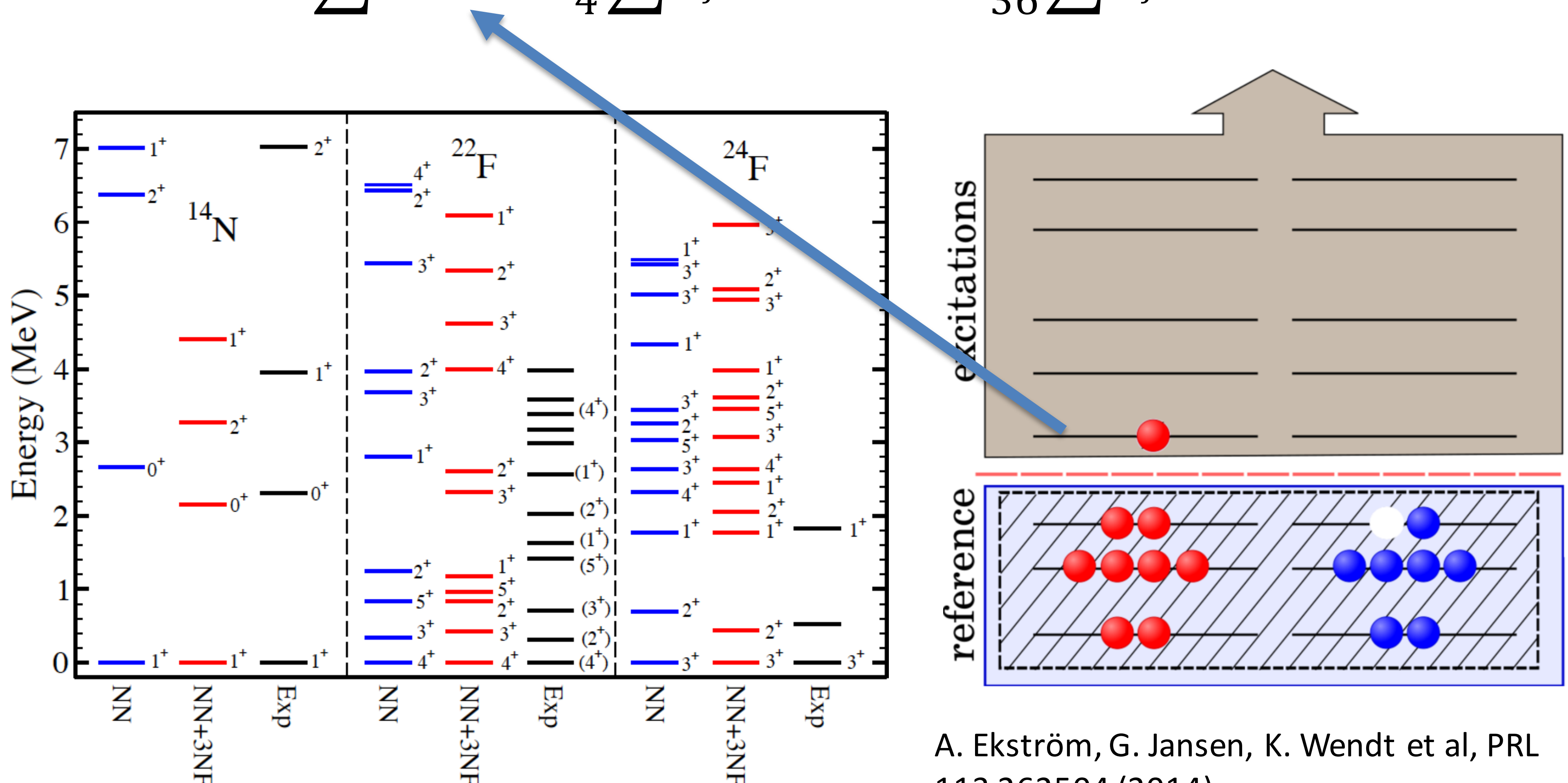

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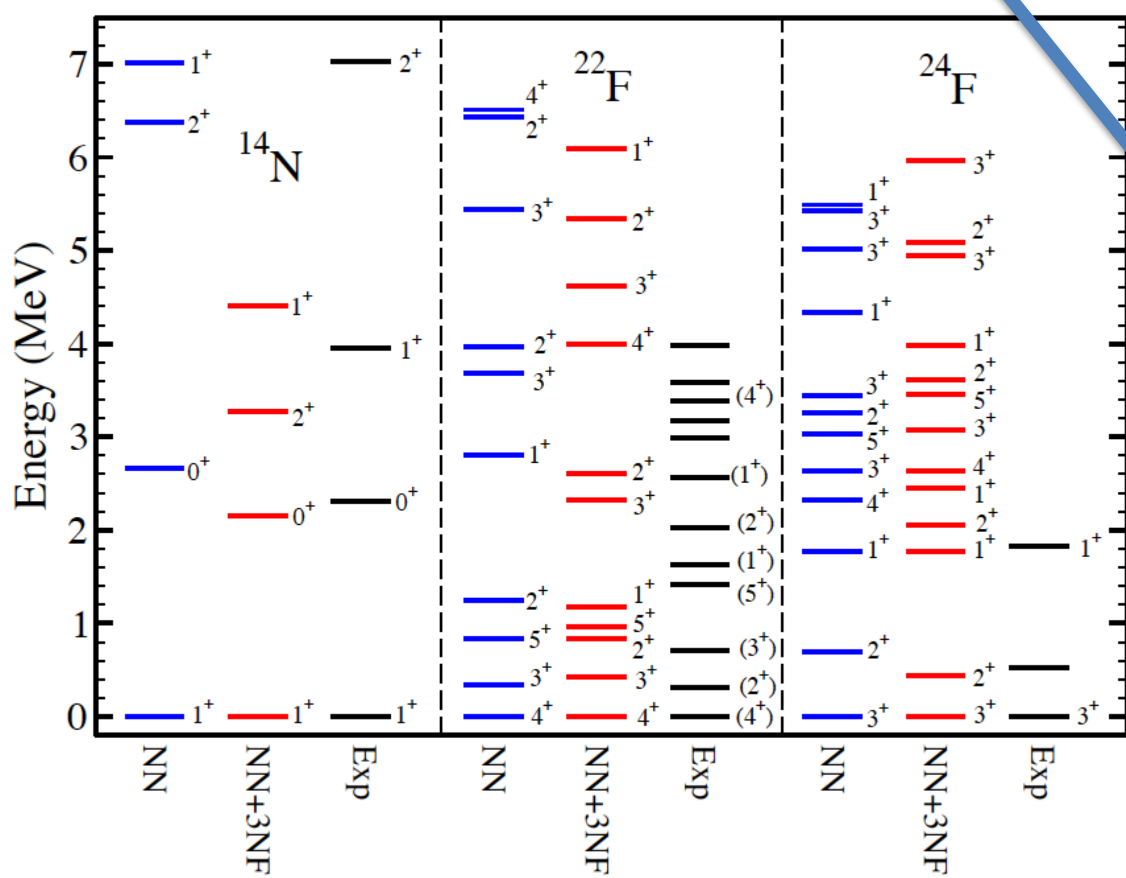

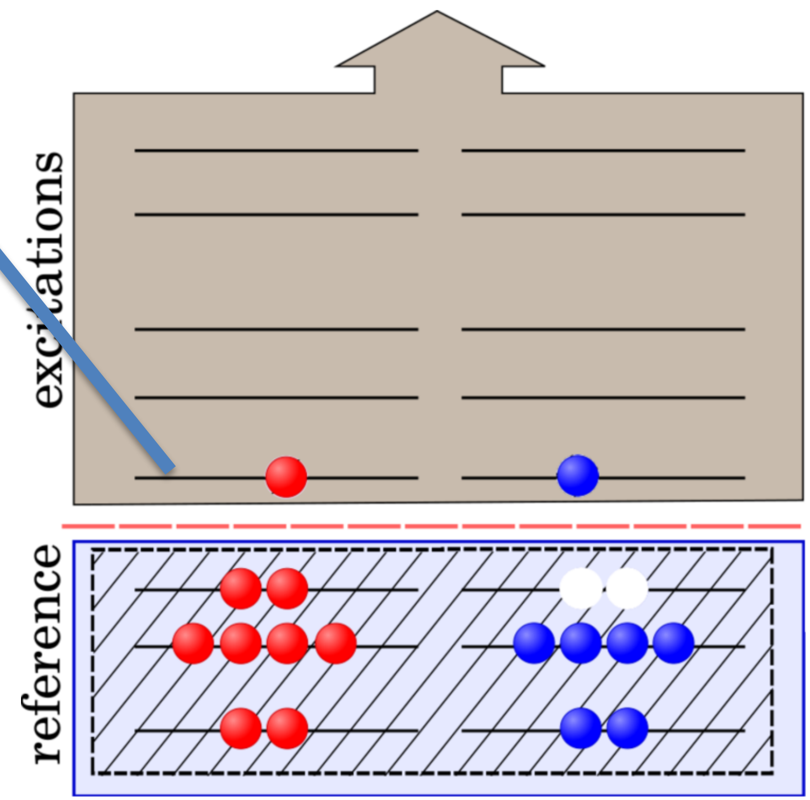

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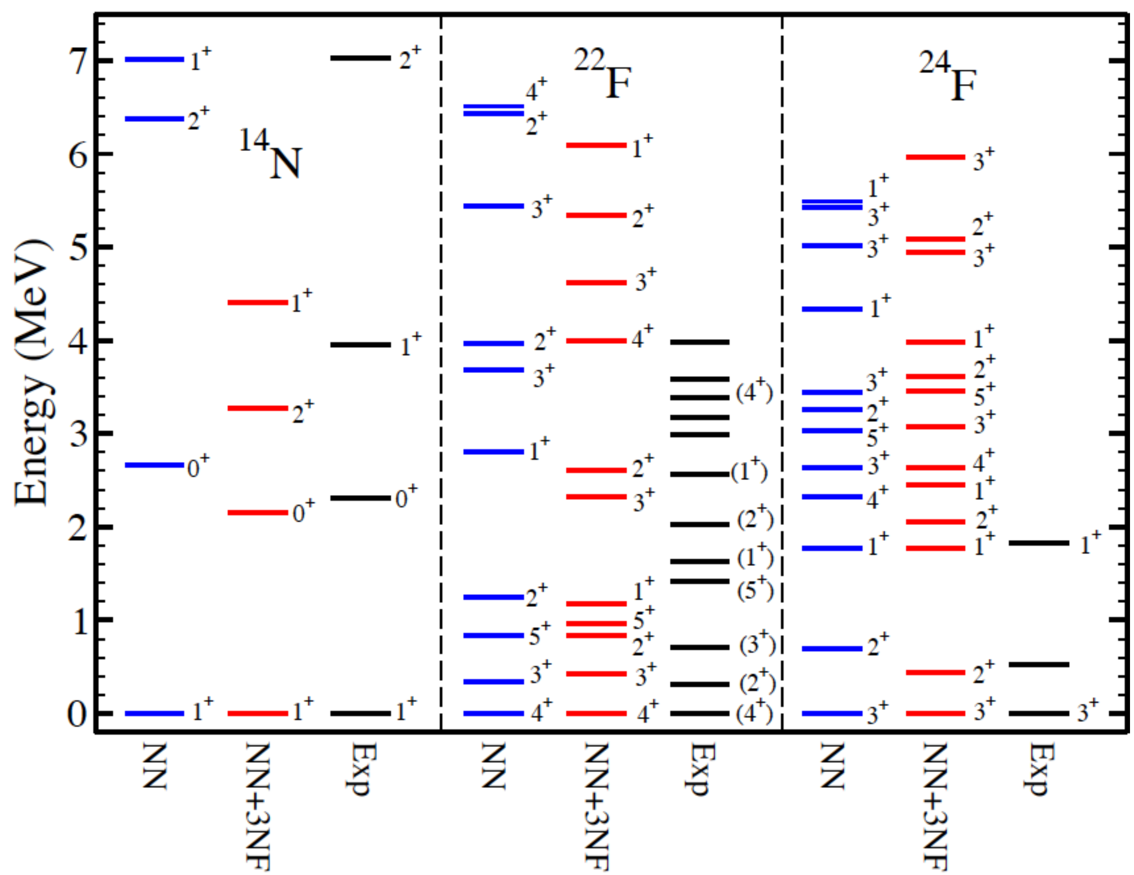

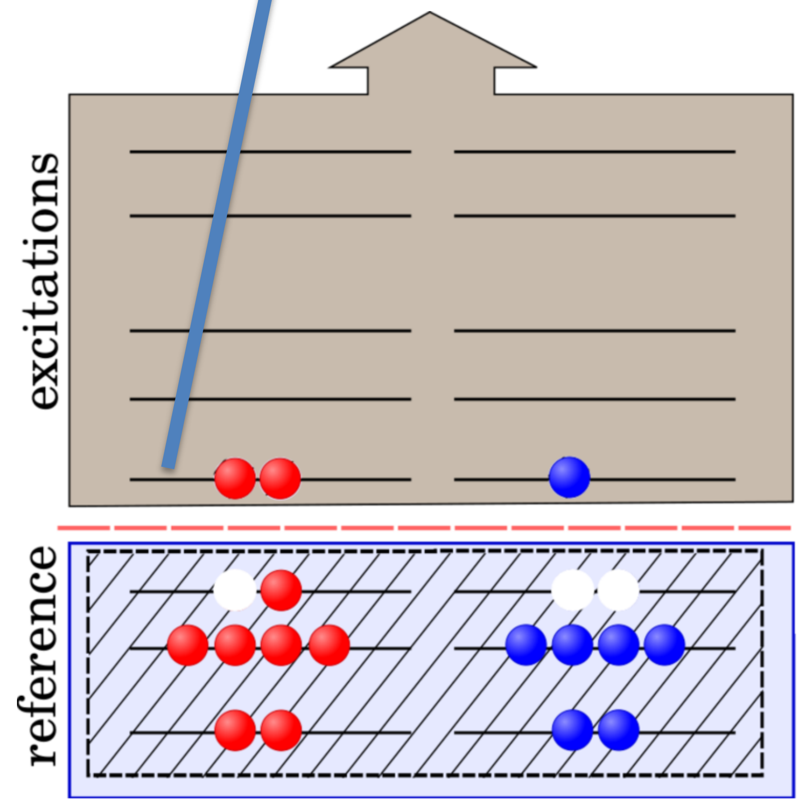

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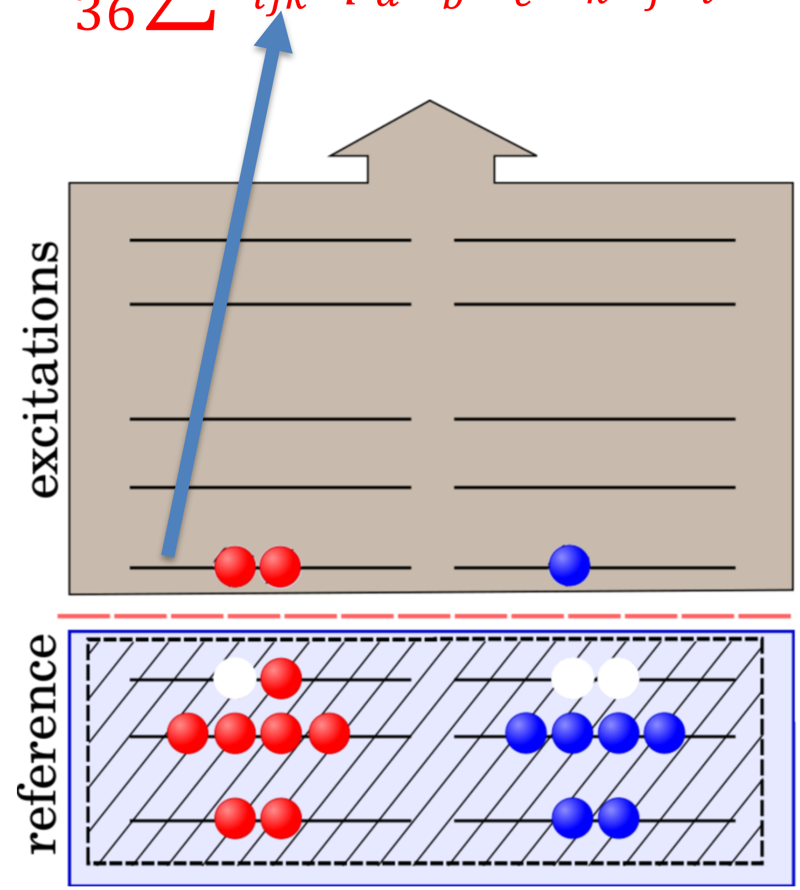
Introduce an energy cut on allowed three-particle three-hole excitations:

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

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

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



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

Charge exchange EOM-CCSDT-1

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

Charge exchange EOM-CCSDT-1

P-space

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

Q-space

Charge exchange EOM-CCSDT-1

P-space

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

Q-space

- Bloch-Horowitz is exact; iterative solution poss.

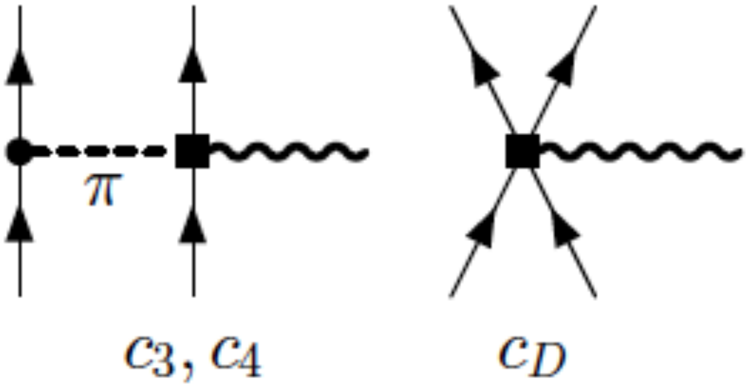
$$\overline{H}_{PP}R_P + \overline{H}_{PQ}(\omega - \overline{H}_{QQ})^{-1}\overline{H}_{QP}R_P = \omega R_P$$

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

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

Normal ordered one- and two-body current

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



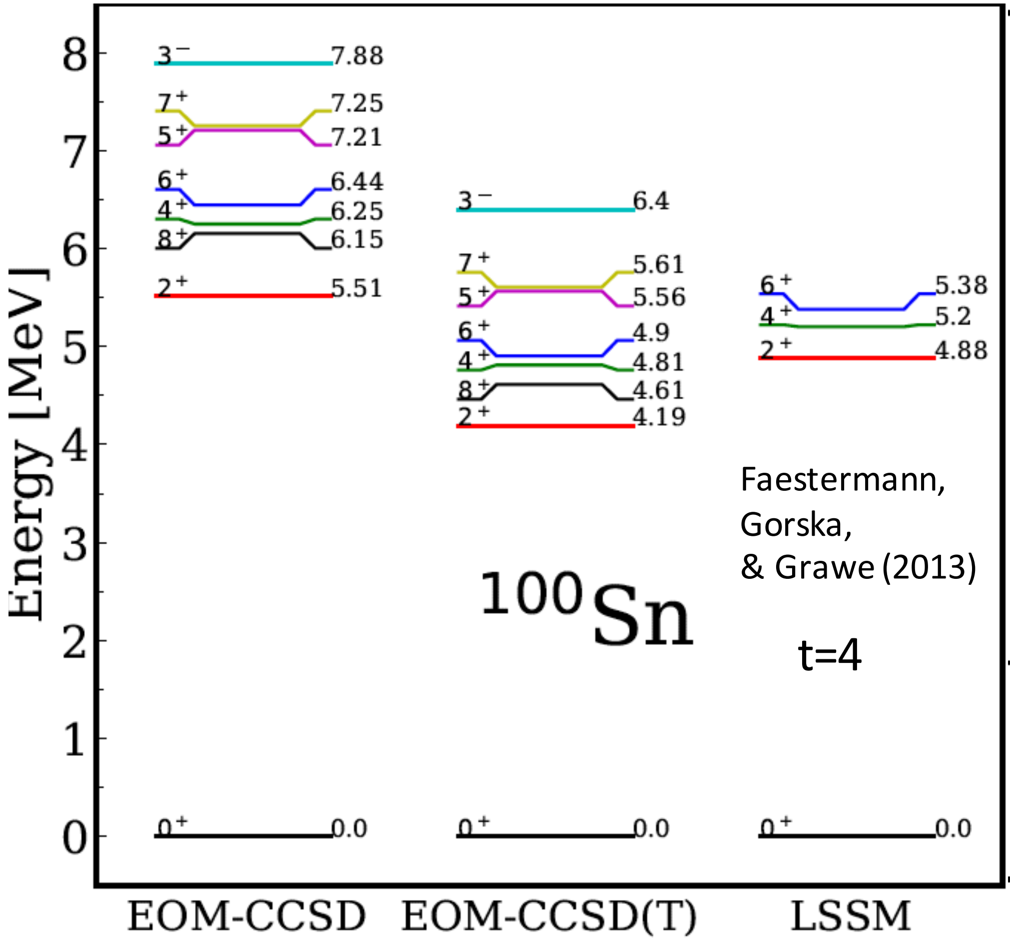
Normal ordered operator:

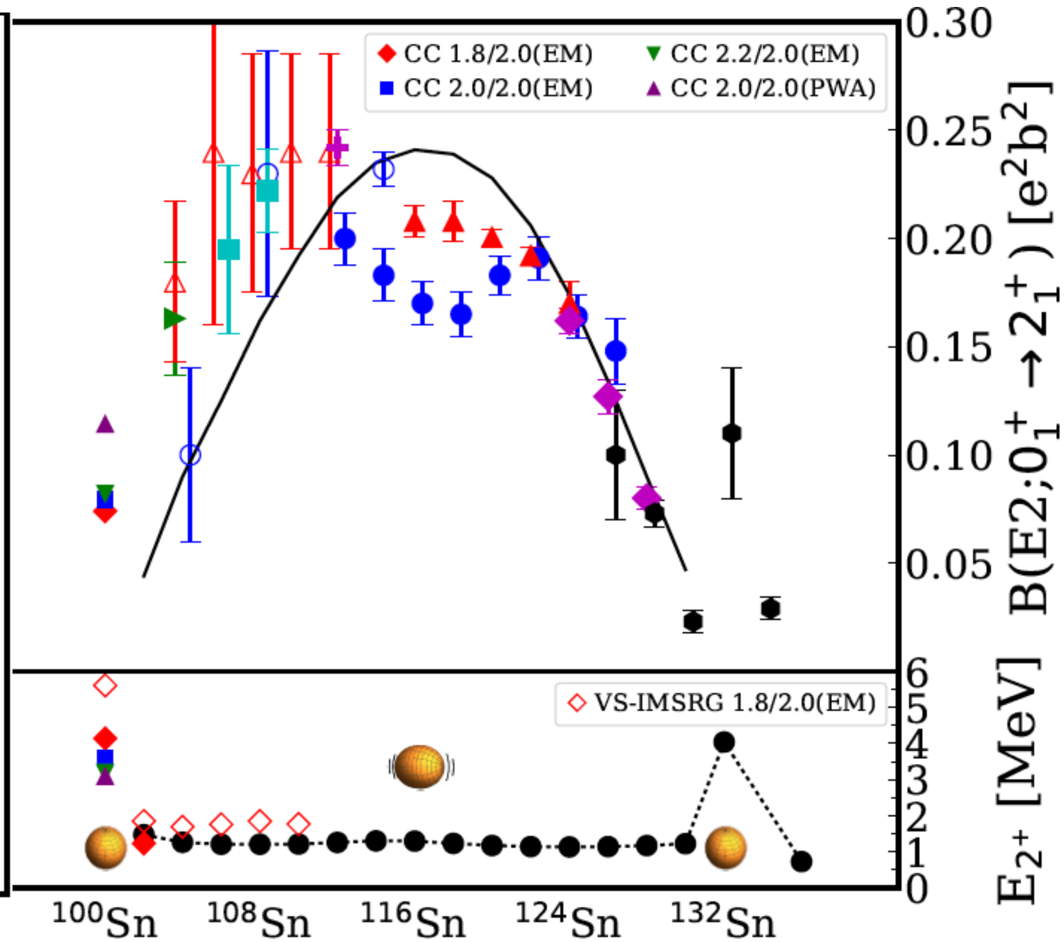
$$\hat{O}_{\mathrm{GT}} = O^1_N + O^2_N$$

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

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)

Structure of the ligthest tin isotopes





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

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

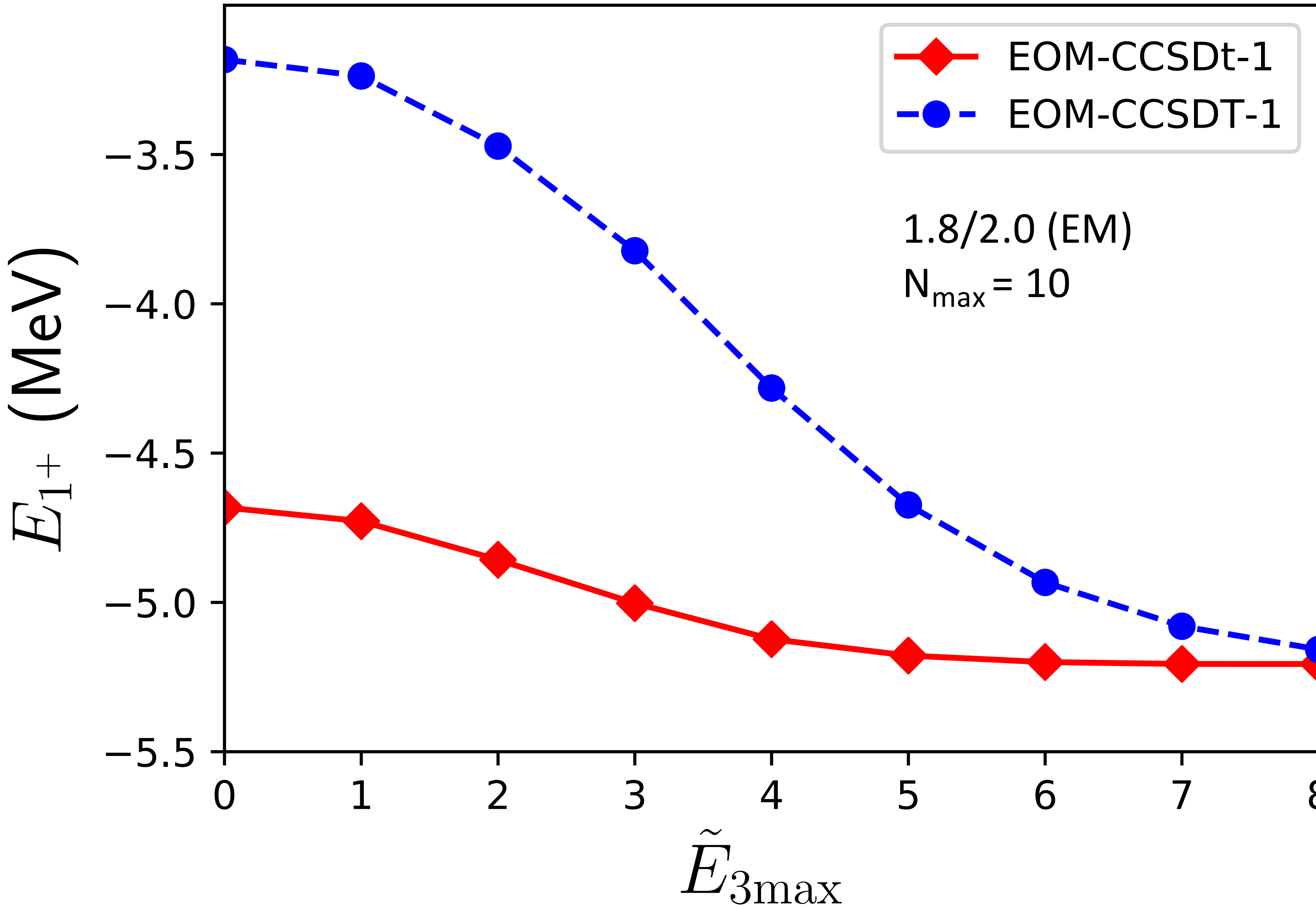
$$Q \equiv \tilde{e}_p + \tilde{e}_q + \tilde{e}_r \leq \tilde{E}_{3\mathrm{max}}$$

$$Q' \equiv \tilde{e}_p + \tilde{e}_q + \tilde{e}_r > \tilde{E}_{3\mathrm{max}}$$

Perturbative energy correction accounting for excluded 3p3h states in Q':

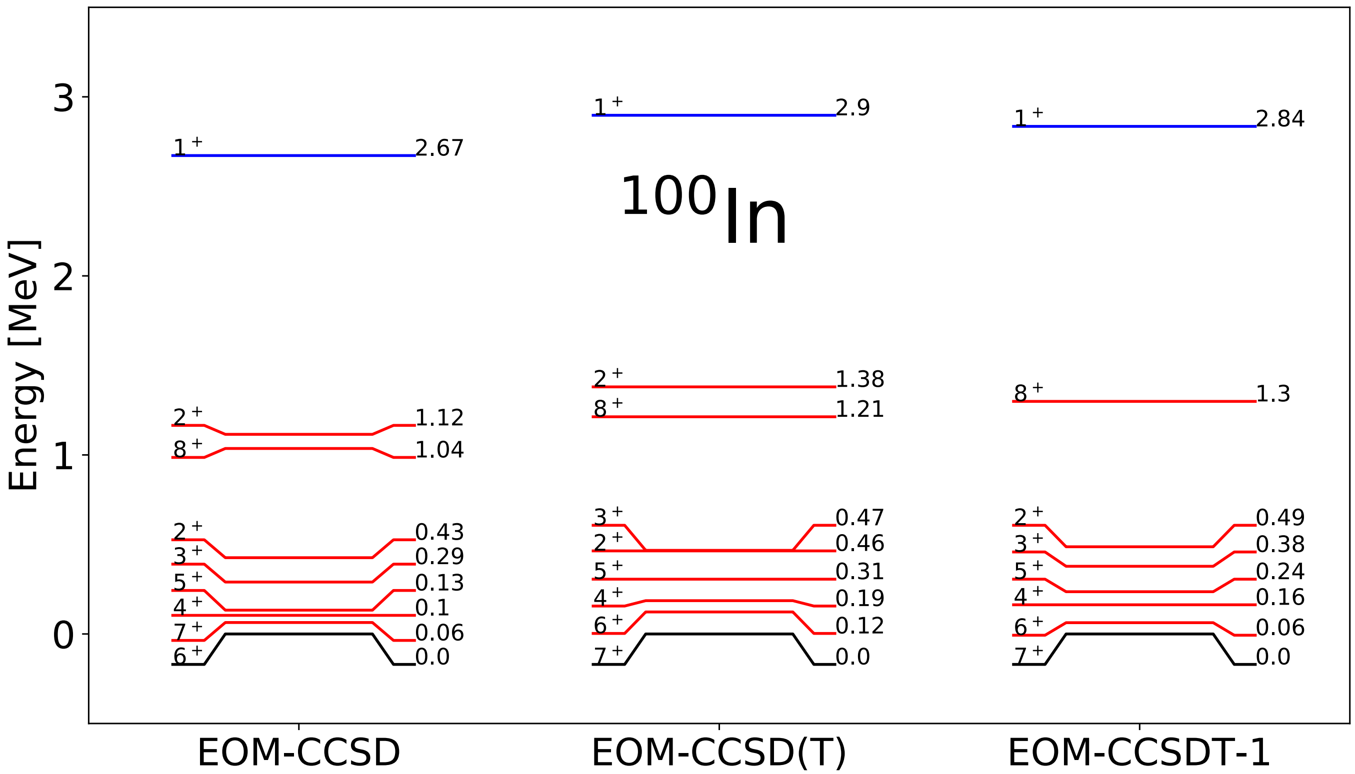
$$\Delta\omega_\mu = \langle \Phi_0 | L_\mu \overline{H}_{PQ'} (\omega_\mu - \overline{H}_{Q'Q'})^{-1} \overline{H}_{Q'P} R_\mu | \Phi_0 \rangle$$

Convergence of excited states in ^{100}In

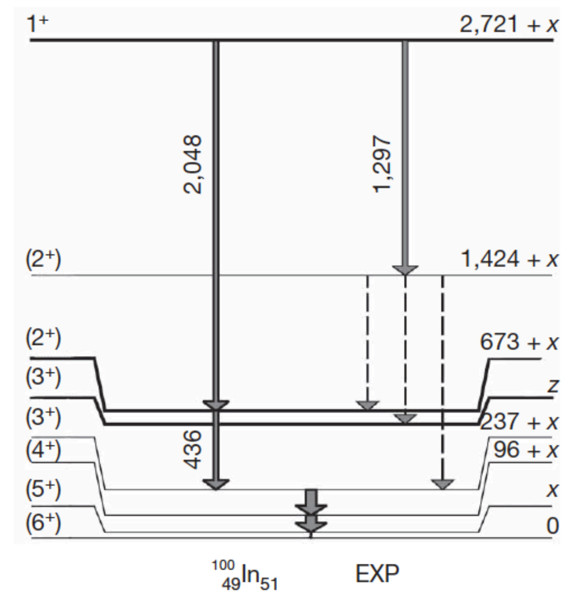


^{100}In from charge exchange coupled-cluster equation-of-motion method

1.8/2.0 (EM)



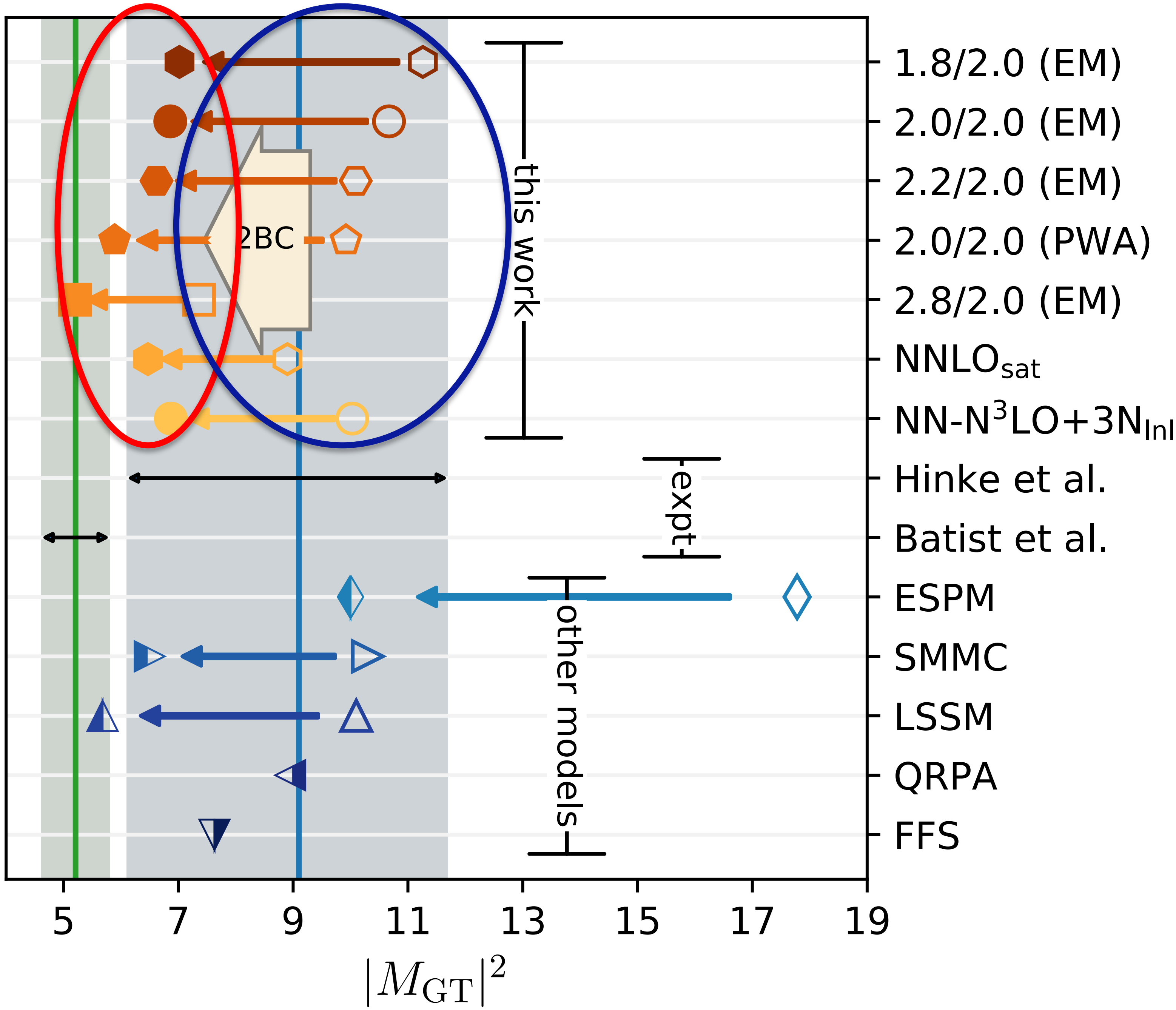
Hinke et al, Nature (2012)



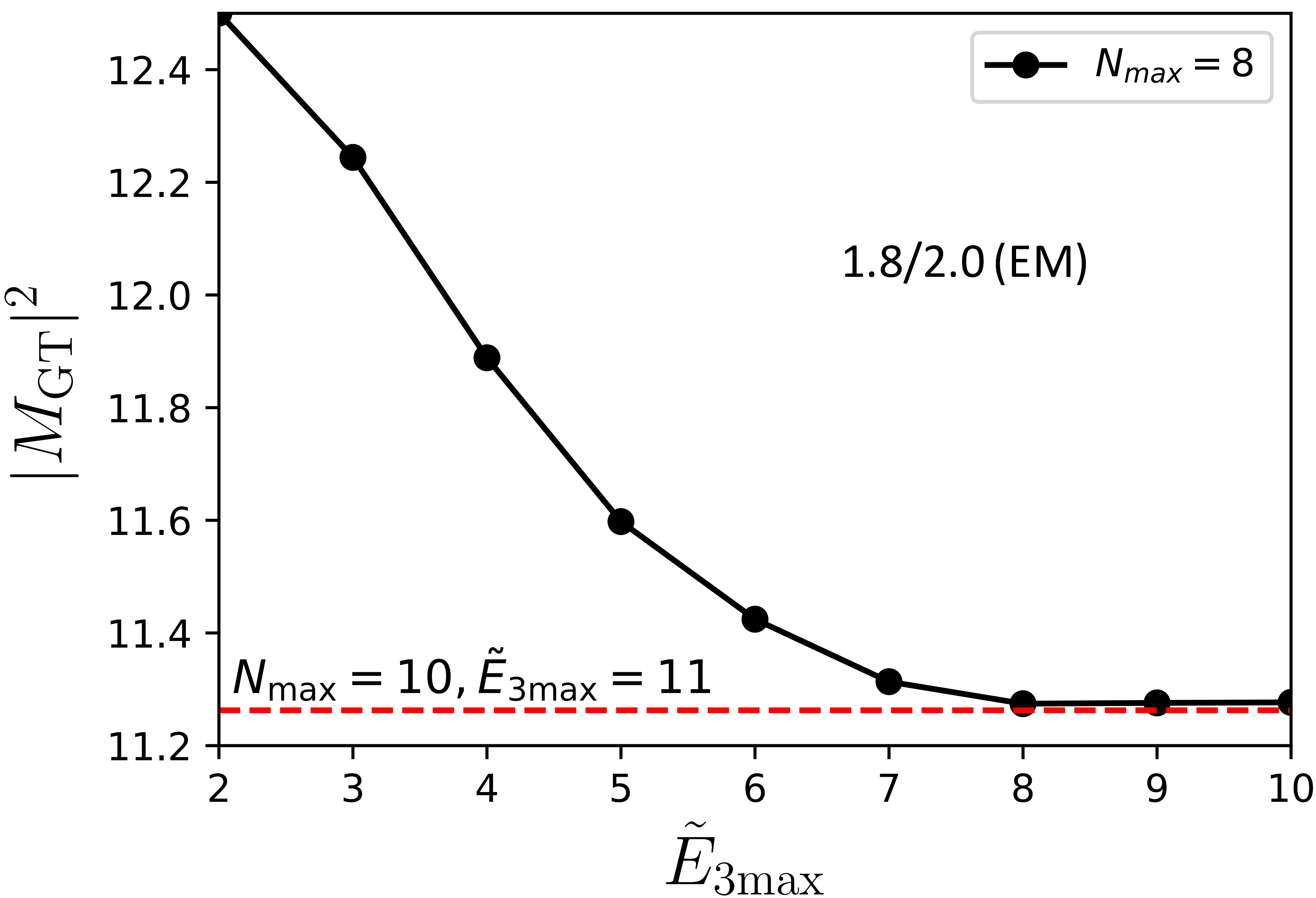
Charge-exchange EOM-CC with perturbative corrections accounting for excluded 3p3h states:

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

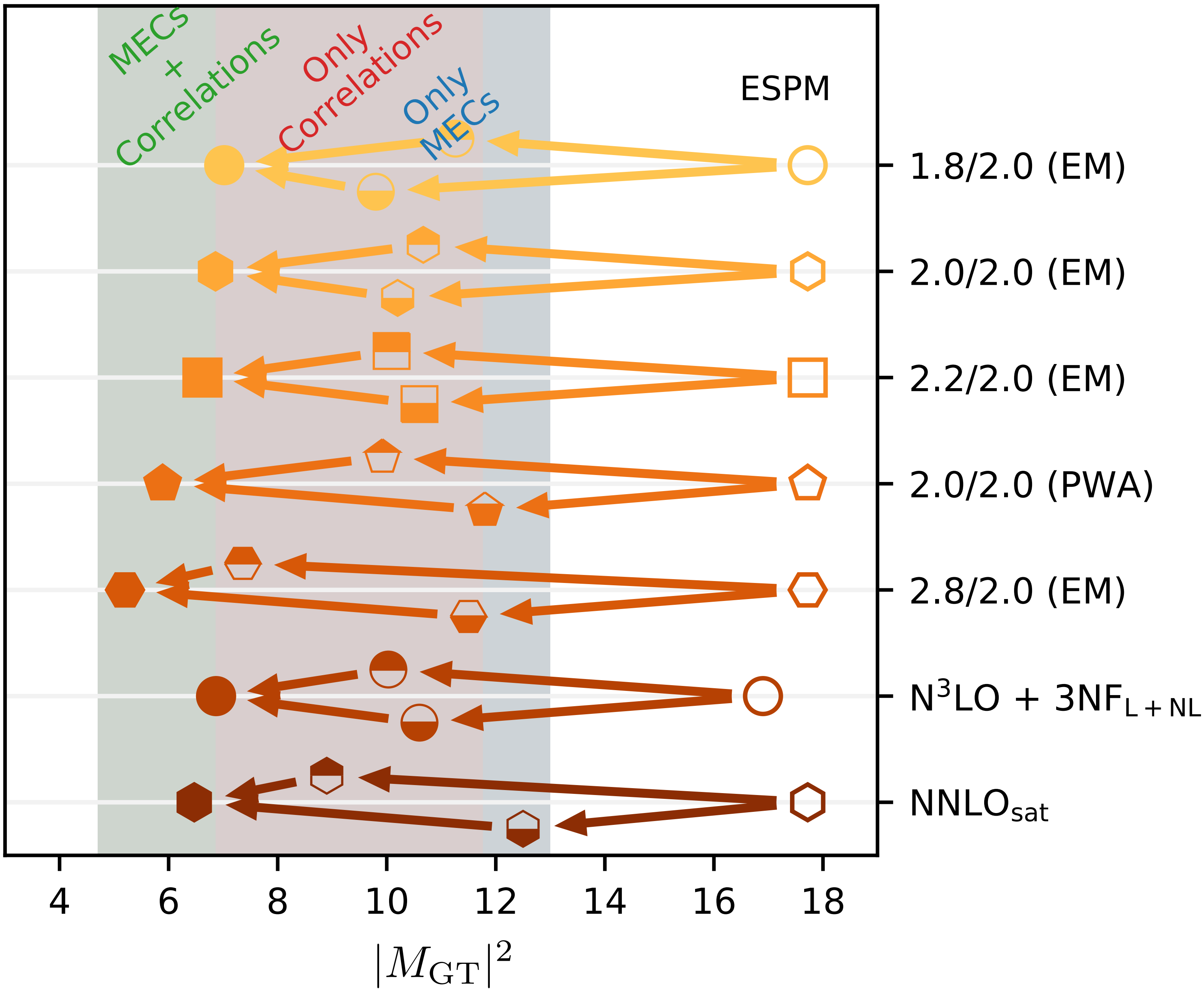
Super allowed Gamow-Teller decay of ^{100}Sn



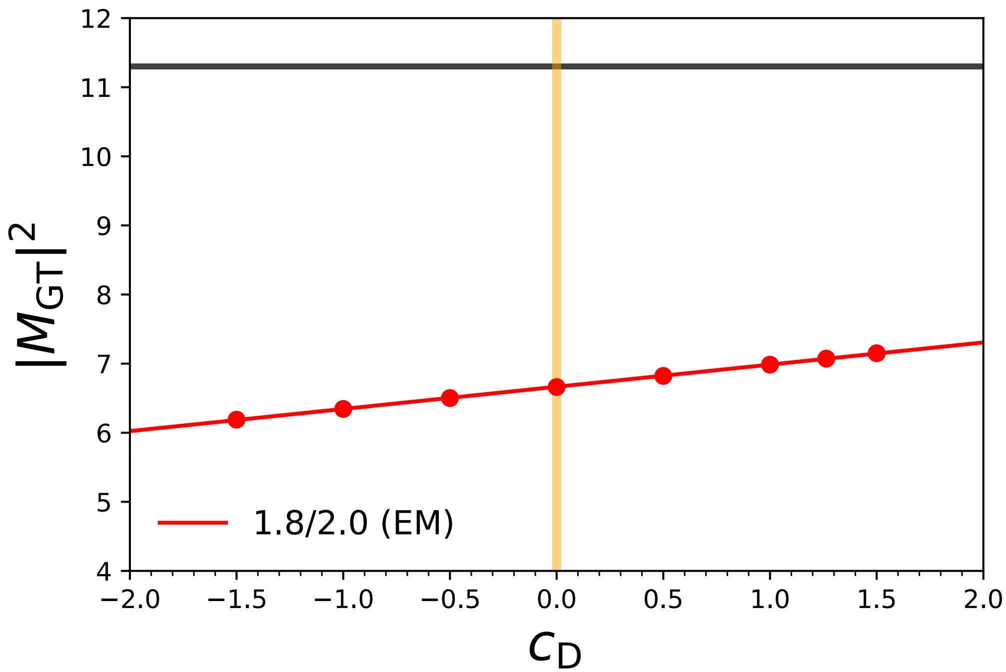
Convergence of GT transition in ^{100}Sn

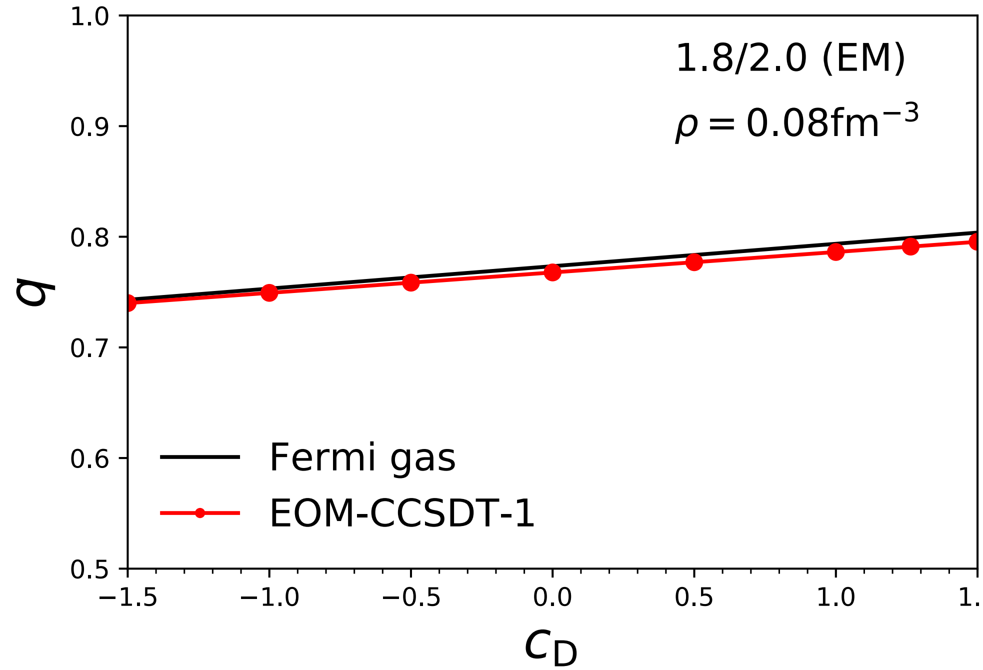


Role of 2BC and correlations in ^{100}Sn



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



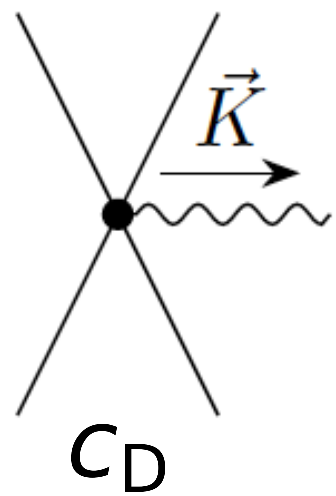


J. Menéndez, D. Gazit, A. Schwenk

PRL 107, 062501 (2011)

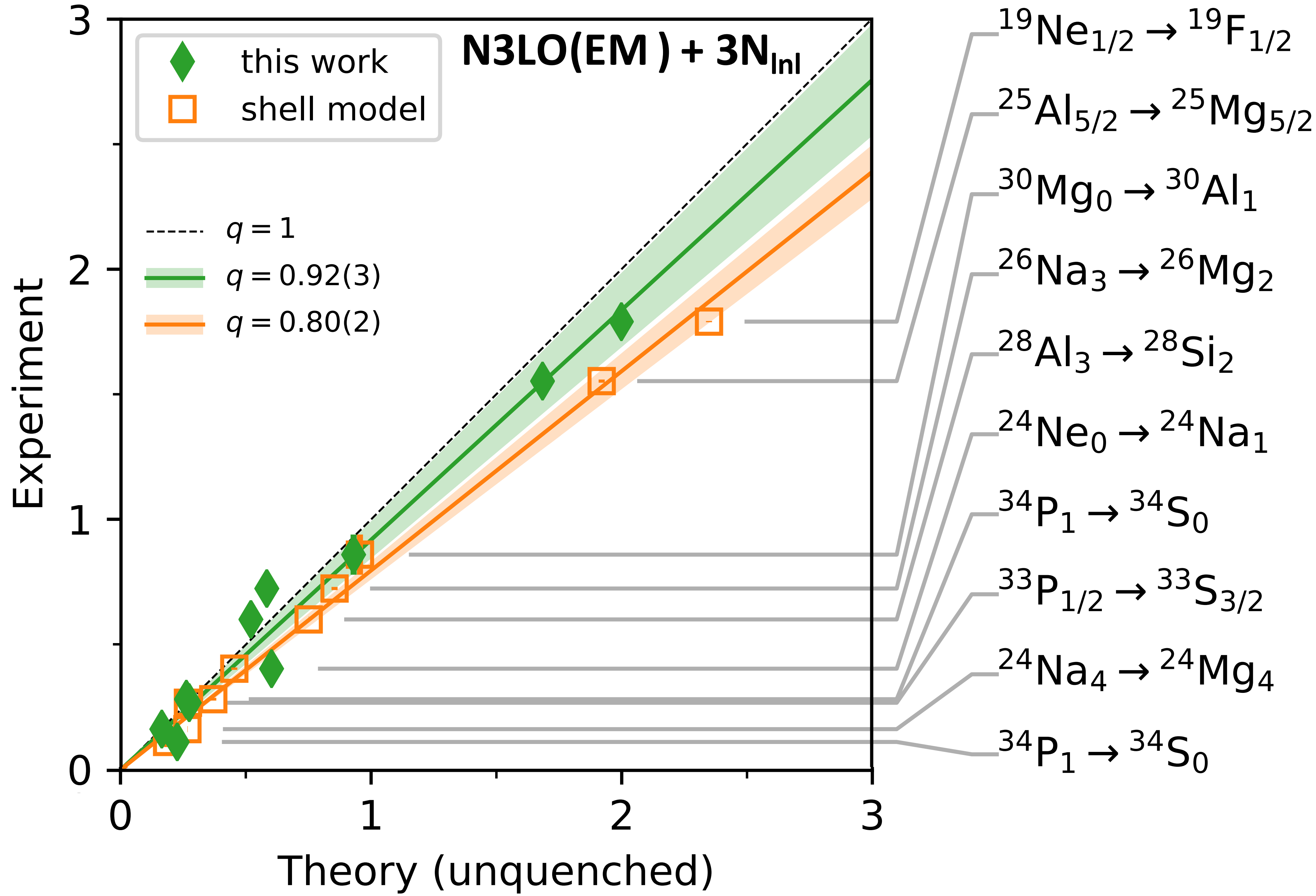
One-body normal ordering of 2BC in free Fermi gas

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

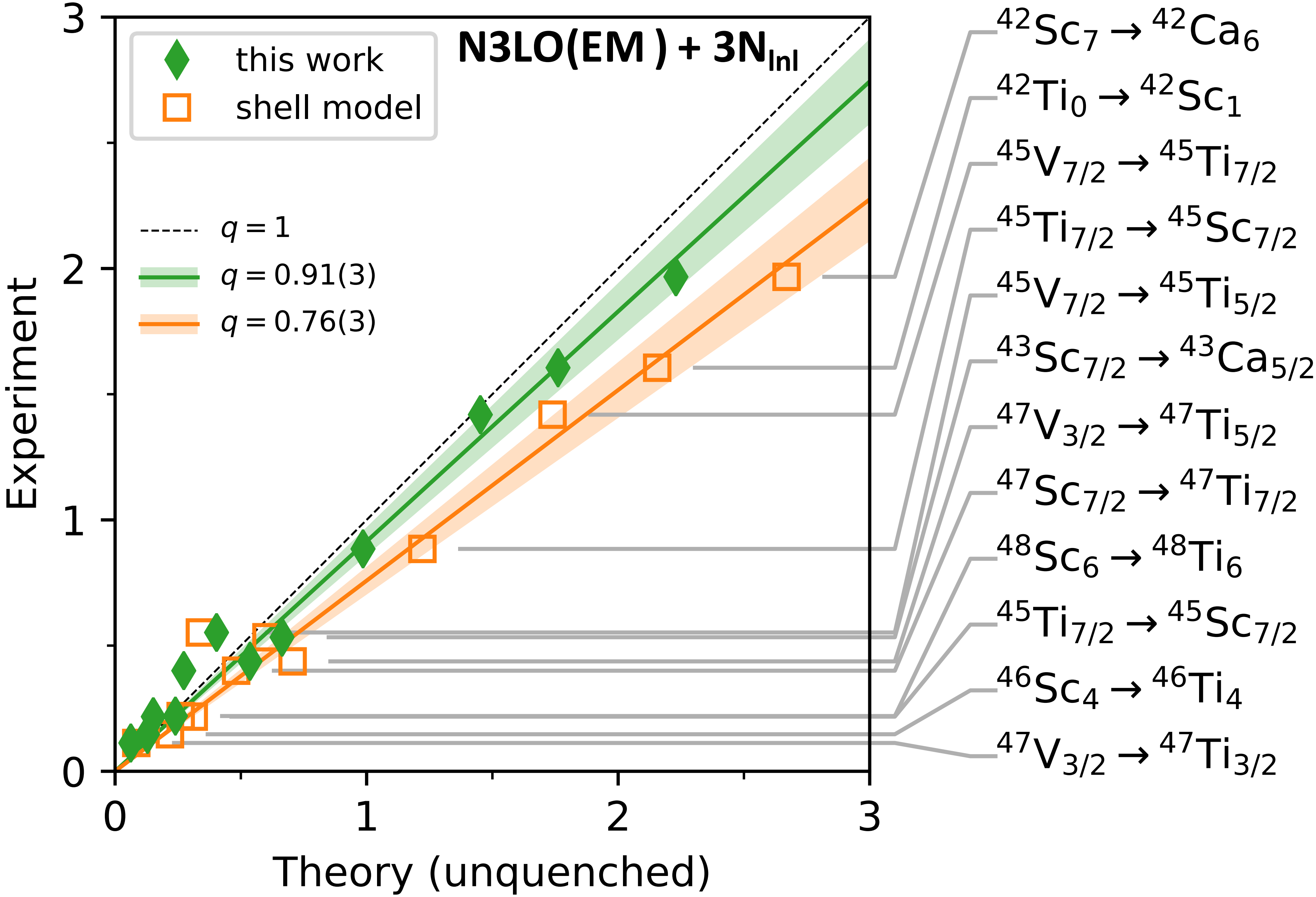


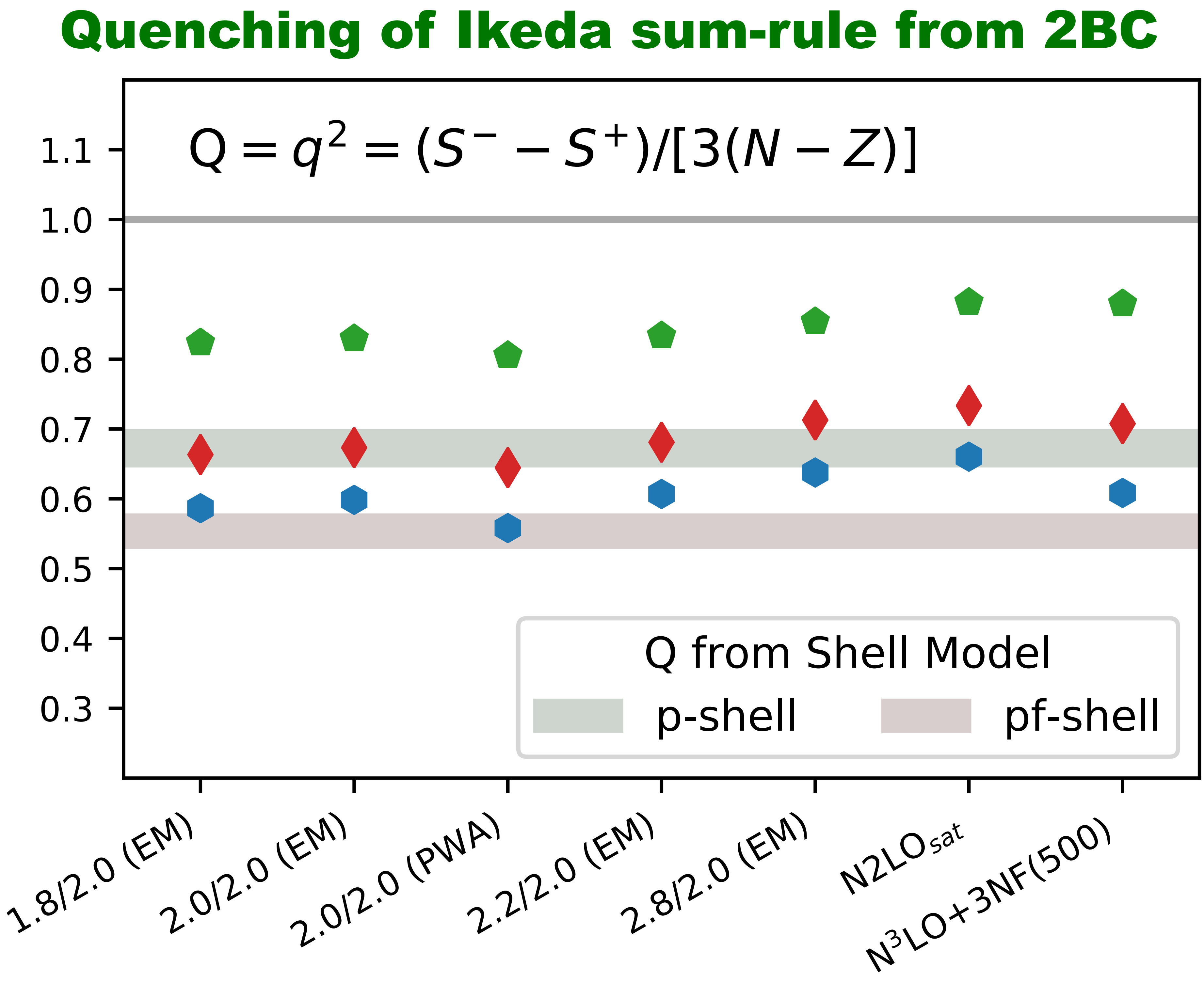
Short-ranged contact term of 2BC (heavy meson exchange)

The role of 2BC in the sd-shell



The role of 2BC in the pf-shell





Quenching of Ikeda sum-rule from 2BC
$Q = q^2 = (S^- - S^+)/[3(N - Z)]$
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
Q from Shell Model
p-shell
pf-shell
1.8/2.0 (EM)
2.0/2.0 (EM)
2.0/2.0 (PWA)
2.2/2.0 (EM)
2.8/2.0 (EM)
N2LO$_{sat}$
N^{3}LO+3NF(500)

Inclusive electron scattering and the Coulomb sum rule

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

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

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

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

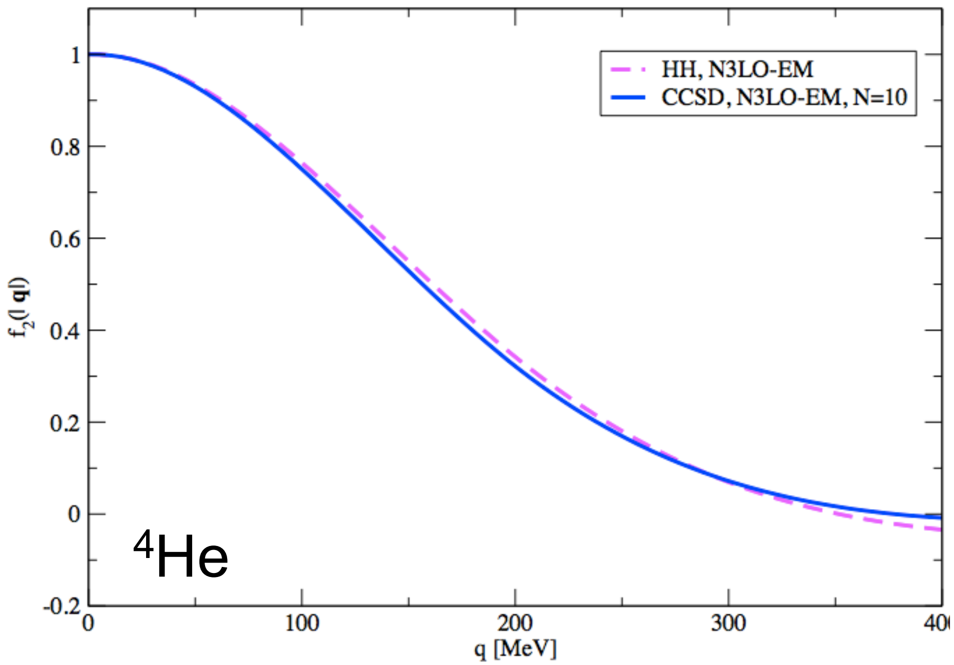
We approached the problem as we do for the calculation of the total strength of the dipole response function in PRL **111**, 122502 (2013).

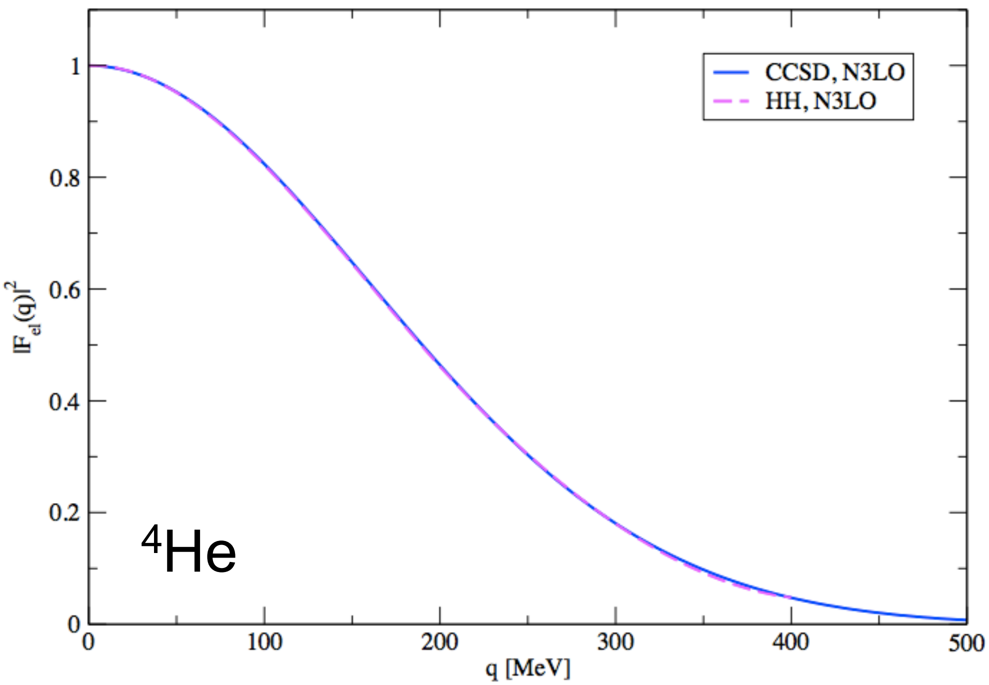
Coulomb sum rule

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

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

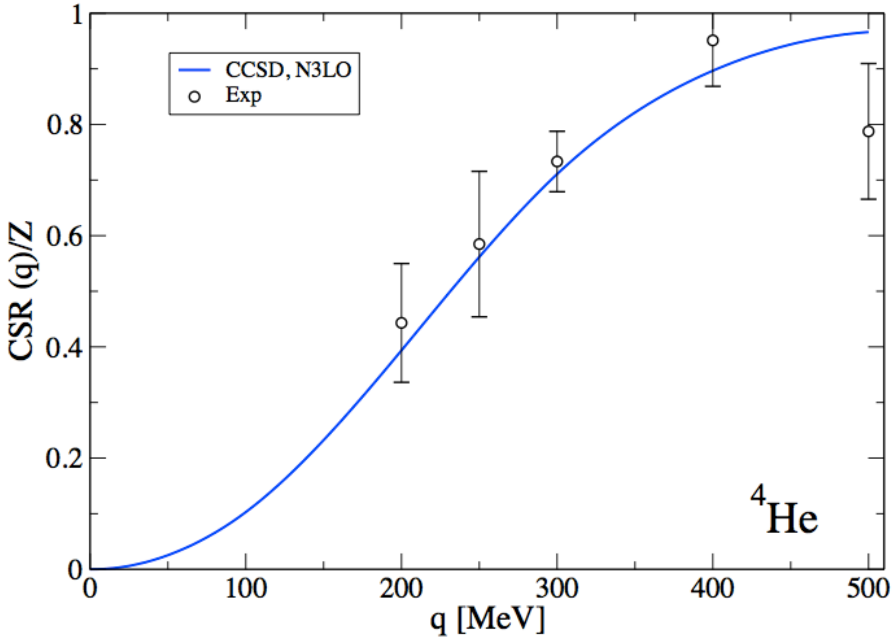
$$\langle 0|\sum_{i \neq j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)}|0\rangle = Z(Z-1) f_2(|\mathbf{q}|)$$



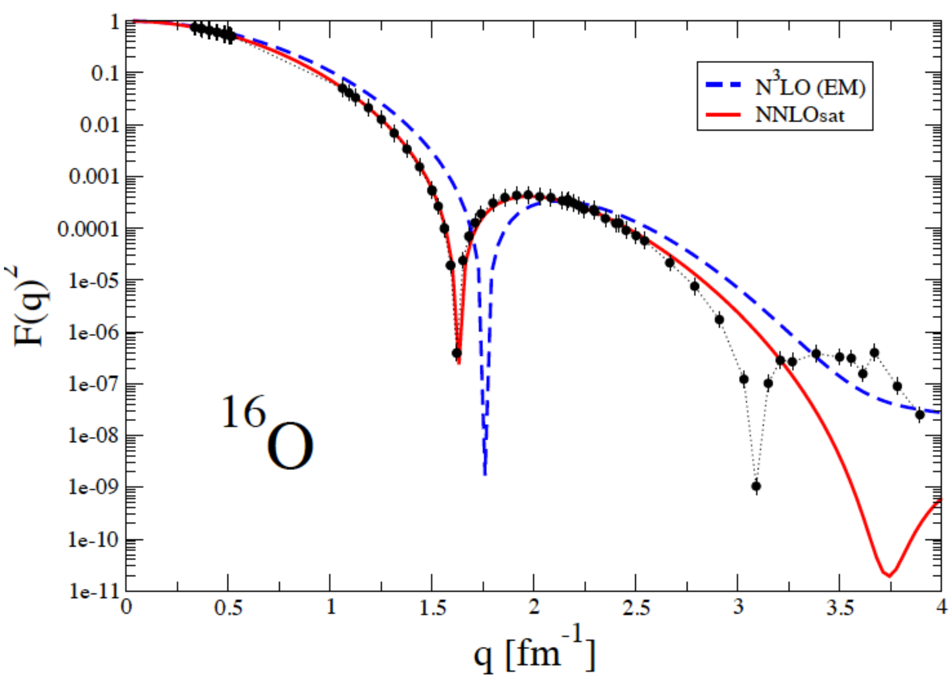


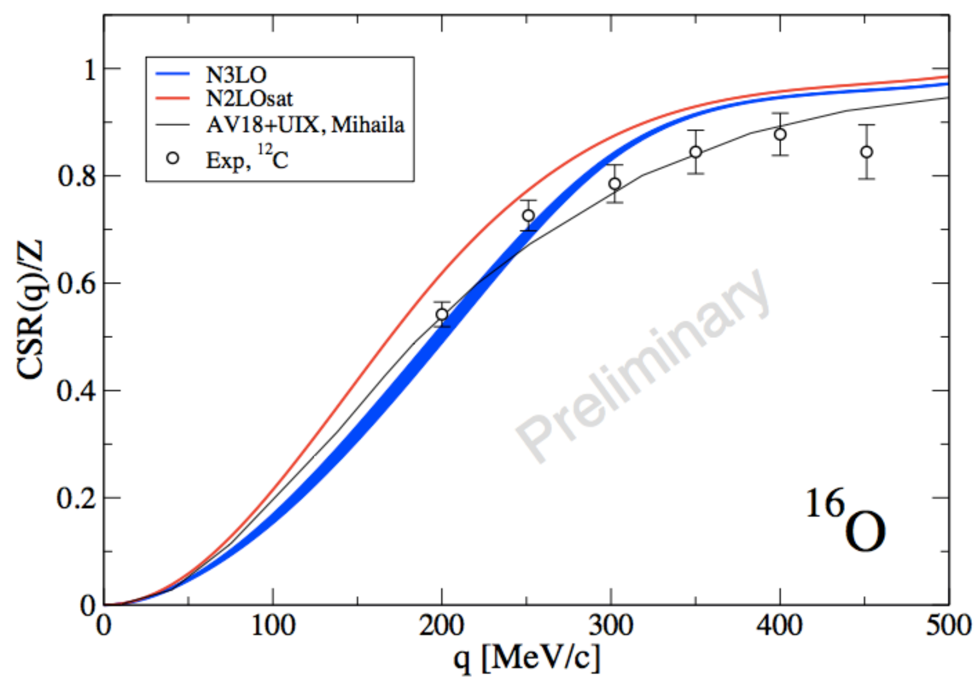
Very nice agreement!

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

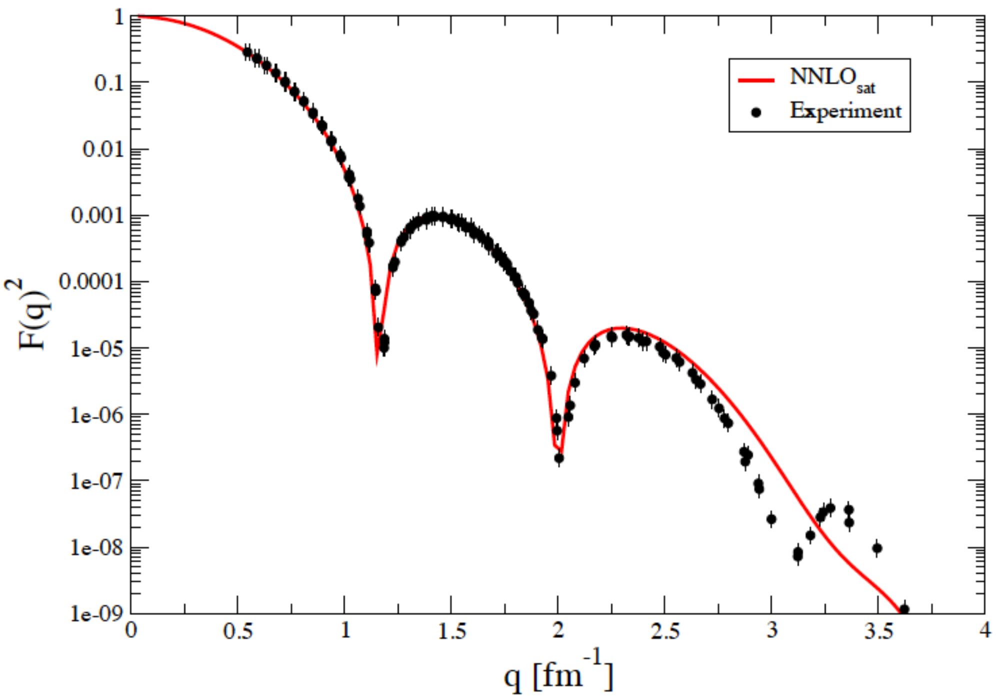


- Good agreement in ^{4}He
- CSR for 16O based on $NNLO_{sat}$ and N3LO(EM)
- Comparison to data in ^{12}C and to Mihaila and Heisenberg (PRL 2000)

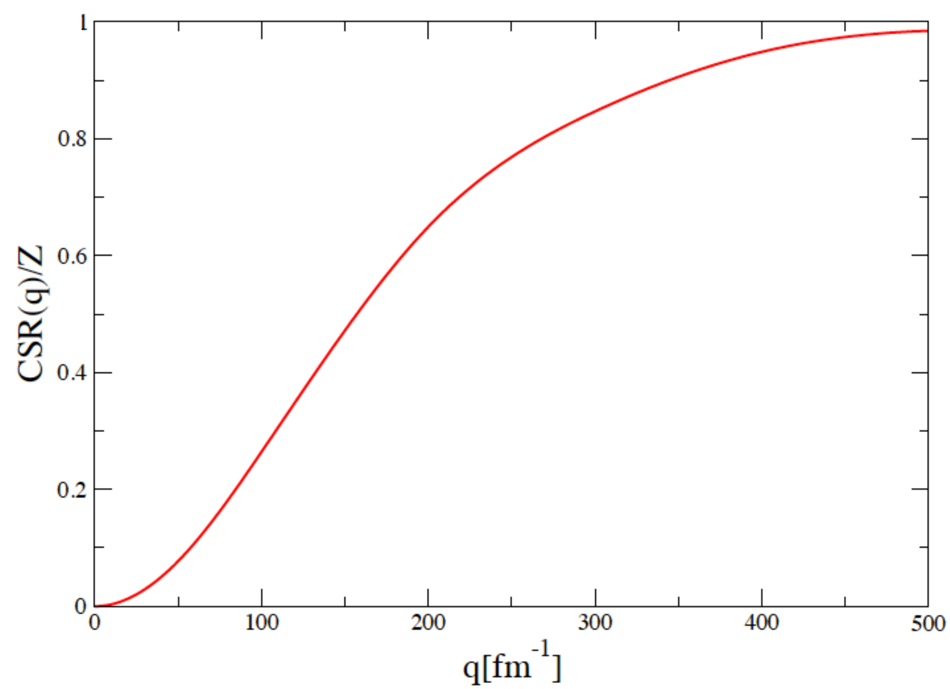




Comparison to data in ^{40}Ca



S. Bacca et al, in preparation.



Summary

- Forces and 2BCs from chiral EFT explain (to large extent) the quenching of GT strength in atomic nuclei
- Make predictions for the super allowed GT transition in ^{100}Sn
- Promising coupled-cluster results for total inelastic longitudinal response
- Next steps is to look at the inelastic longitudinal response function and neutrino response on ^{16}O and ^{40}Ar.

Collaborators

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