CC theory for open shell nuclei

Titus Morris

Progress in Ab-Initio@TRIUMF

March 3rd, 2017

Collaborators

- Michigan State University
  - Scott Bogner
  - Heiko Hergert
  - Nathan Parzuchowski
- TRIUMF
  - Jason Holt
  - Ragnar Stroberg
- Oak Ridge
  - Gaute Hagen
  - Thomas Papenbrock
  - Gustav Jansen
  - ZhongHao Sun

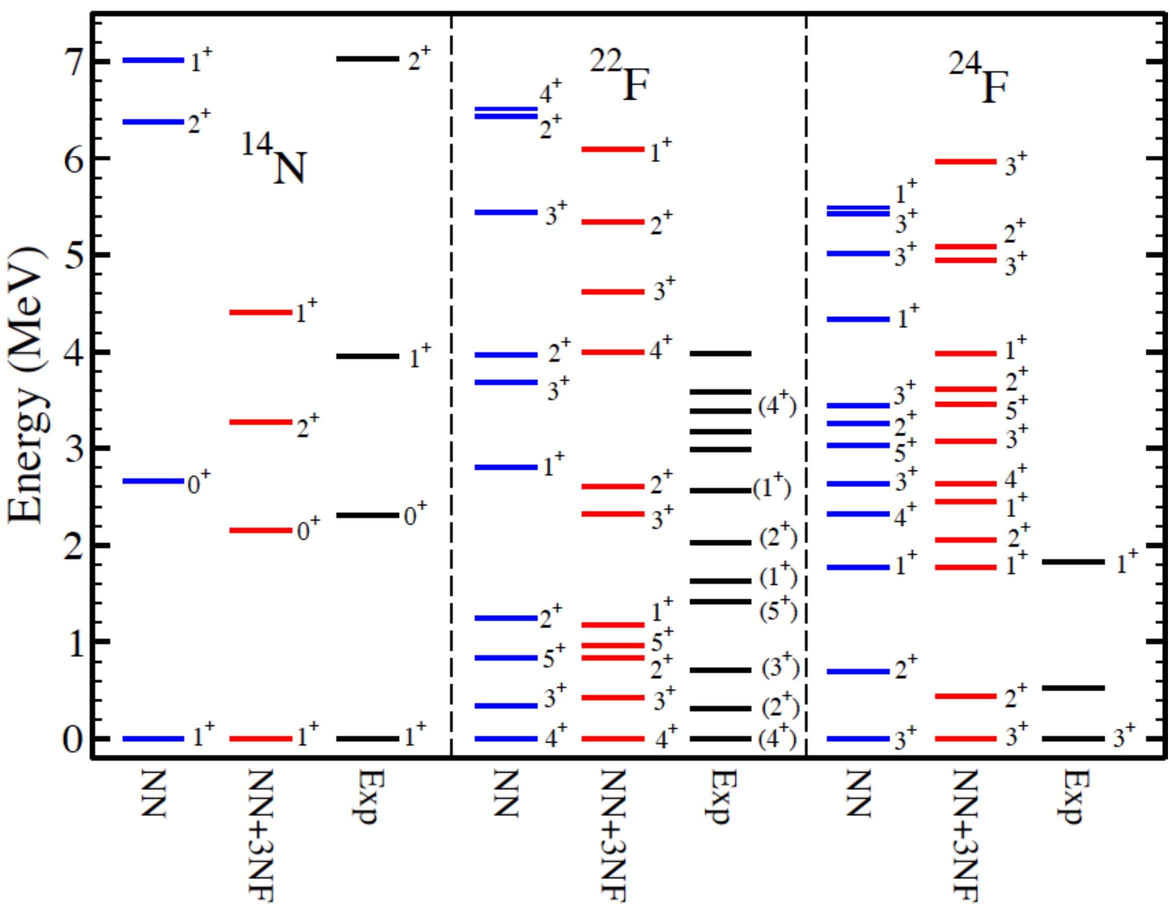
Outlook

- Improving current CC results (EOM)
  - How/why hybridizing CC-EOM further
  - Results and Future
- Shell Model derived interactions
  - Framework
  - Preliminary results

Coupled cluster calculations of odd-odd nuclei

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

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



- Compute spectra of daughter nuclei as beta decays of mother nuclei
- Level densities in daughter nuclei increase slightly with 3NF
- Predict several states in neutron rich Fluorine

CC-EOM

- Hybrid plus CI type
  - $\{\bar{H} R_\nu\}_c |\Phi_0\rangle = \omega_\nu R_\nu |\Phi_0\rangle$ (and L_ν)

Nucleus	Typical R_ν	Iterative Cost	Neglected $\tilde{R}_\nu$	Iterative Cost
A-2	1p3h	o^4u^2	2p4h	o^3u^4
A-1	1p2h	o^3u^2	2p3h	o^3u^4
A	2p2h	o^2u^4	3p3h	o^3u^5
A+1	2p1h	ou^4	3p2h	o^2u^5
A+2	3p1h	ou^5	4p2h	o^2u^6

  - Can we verify $\tilde{\boldsymbol{R}}_{\boldsymbol{\nu}}$ is small, account for its effect on ω_ν, o_ν, for each of these types?

CC-EOM

- Hybrid plus CI type
  - $\{\overline{H}R_\nu\}_c|\Phi_0\rangle = \omega_\nu R_\nu|\Phi_0\rangle$ (and L_ν)

Nucleus	Typical R_ν	Iterative Cost	Neglected $\widetilde{R}_\nu$	Iterative Cost
A-2	1p3h	o^4u^2	2p4h	o^3u^4
A-1	1p2h	o^3u^2	2p3h	o^3u^4
A	2p2h	o^2u^4	3p3h	o^3u^5
A+1	2p1h	ou^4	3p2h	o^2u^5
A+2	3p1h	ou^5	4p2h	o^2u^6

Doesn't this already exist for 3p3h?

  - Can we ve… …nt for its effect on ω_ν, o_ν, for each of these types?

EOM-ΛCCSD(T)

- Invoke energy functional

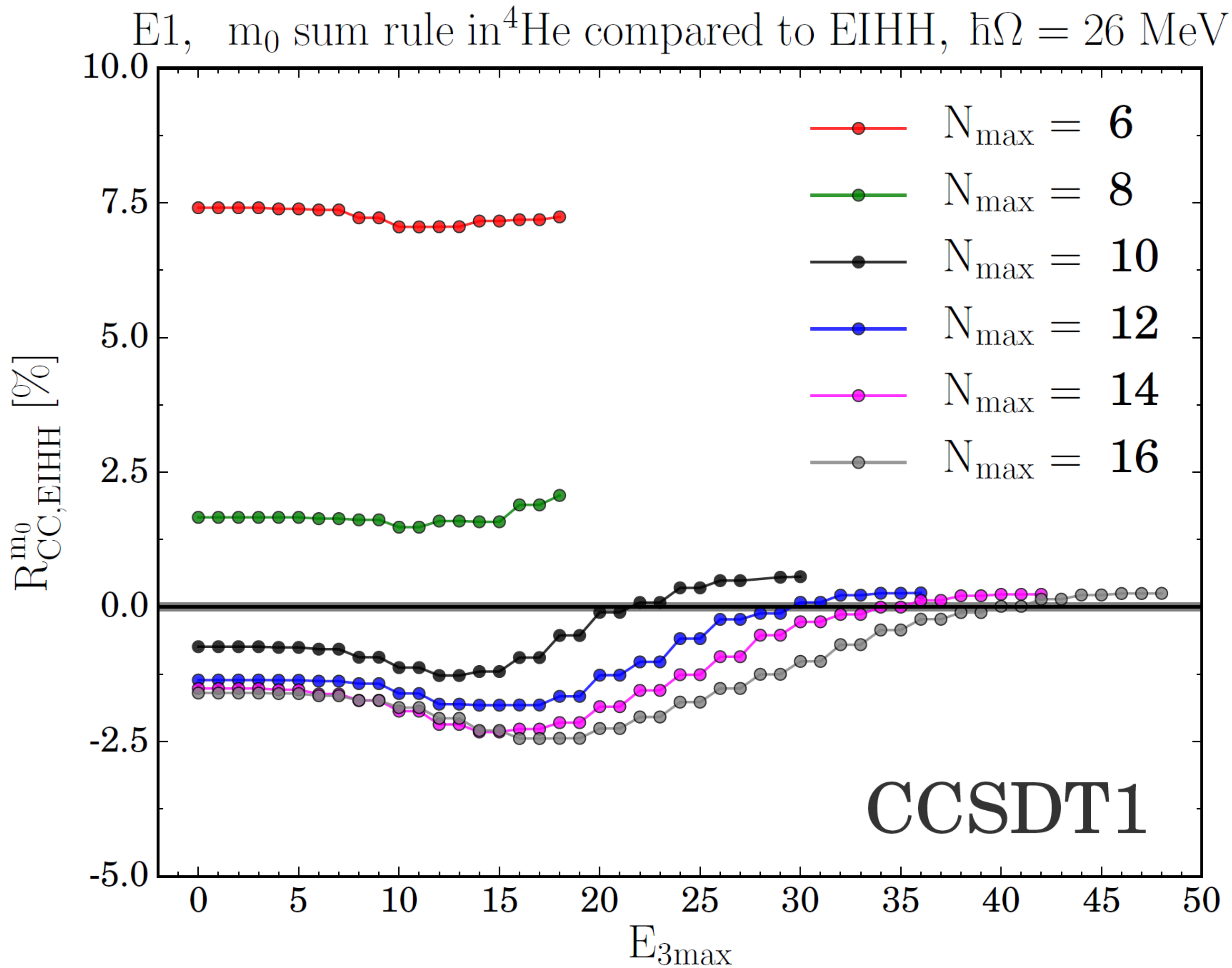
$$\langle\Phi_0|L_\nu\{\bar{H}R_\nu\}_c|\Phi_0\rangle = \omega_\nu\langle\Phi_0|L_\nu R_\nu|\Phi_0\rangle = \omega_\nu$$

- Expand ω_ν into its CCSD, and leading order (HF) MBPT expression

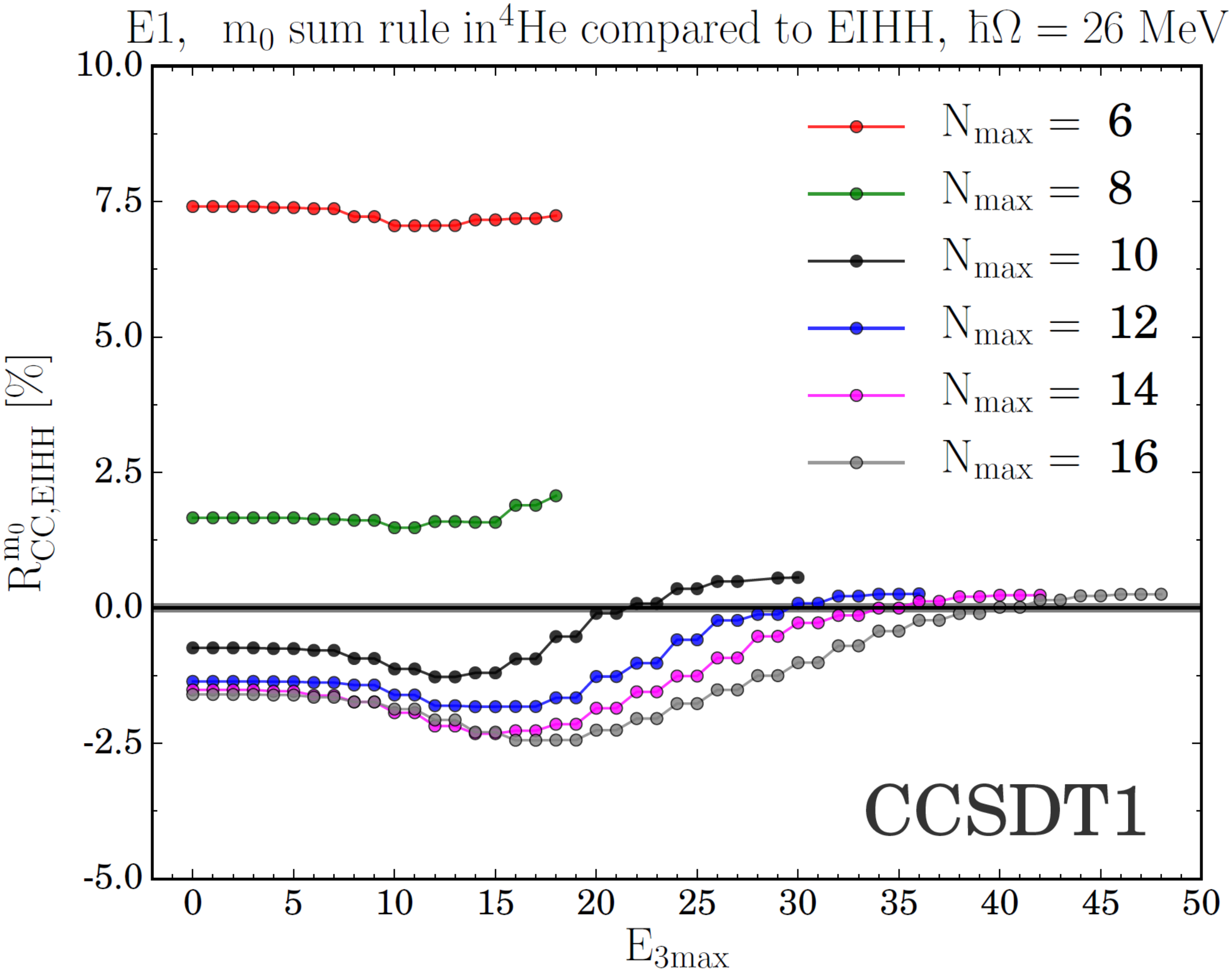
$$\Delta\omega_\nu^{[4]} \subset \langle\Phi_0|L_{CCSD}V\ \mathrm{M}\ \{VR_{CCSD}\}_c|\Phi_0\rangle \quad M = \frac{|\Phi_{ijk}^{abc}\rangle\langle\Phi_{ijk}^{abc}|}{\epsilon_i+\epsilon_j+\epsilon_k-\epsilon_a-\epsilon_b-\epsilon_c}$$

- Uses only knowledge of HF
- Is not suitable for other observables
- Exceedingly difficult to derive for A$\pm$1,2

Observables?



Observables?



Generalizing EOM-CC PT

- Partition $\bar{H}$ into P,Q spaces
  - Feasible R_ν, L_ν calculation lives in P, (Zeroth order)
  - $\bar{H}^{[1]} = \bar{H} - P\bar{H}\mathrm{P} - \Delta^q |\Phi_q\rangle\langle \Phi_q|$ $\quad \Delta^q = \langle \Phi_q|\bar{H}|\Phi_q\rangle$

- Expand $\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu}}$, $\widetilde{\boldsymbol{L}}_{\boldsymbol{\nu}}$ around CCSD

$$\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]} = \frac{\langle \Phi_q|\{\bar{H}^{[1]}R_\nu^{[0]}\}_c|\Phi_0\rangle}{\omega_\nu^{[0]} - \Delta^q} \qquad \widetilde{\boldsymbol{L}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]} = \frac{\langle \Phi_q|L_\nu^{[0]}\bar{H}^{[1]}|\Phi_0\rangle}{\omega_\nu^{[0]} - \Delta^q}$$

$$\Delta o_\nu^{[2]} = \langle\Phi_0|\widetilde{\boldsymbol{L}}_{\boldsymbol{\nu}}^{[\mathbf{1}]}\{\bar{O}^{[1]}R_\nu^{[0]}\}_c|\Phi_0\rangle + \langle\Phi_0|L_\nu\{\bar{O}^{[1]}\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu}}^{[\mathbf{1}]}\}_c|\Phi_0\rangle - \widetilde{\boldsymbol{L}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]}(\Delta o_\nu^{[0]} - \langle \Phi_q|\bar{O}|\Phi_q\rangle)\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]}$$

- $\omega_\nu^{[0]} - \Delta^q$ not based on HF
- Correction appropriate for $\bar{O}$
- General for A$\pm$1,2

$<\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]}\ \widetilde{\boldsymbol{L}}_{\boldsymbol{\nu},\boldsymbol{q}}^{[\mathbf{1}]}>$ measures whether $\widetilde{\boldsymbol{R}}_{\boldsymbol{\nu}}$, $\widetilde{\boldsymbol{L}}_{\boldsymbol{\nu}}$ are perturbative

EOM-CR-CCSD(T)

- Implemented and benchmarked 3p2h $\widetilde{R}_{\nu,q}^{[1]}$, $\widetilde{L}_{\nu,q}^{[1]}$
  - Phys. Rev. Lett. **101**, 052501 (UTK remote access down)

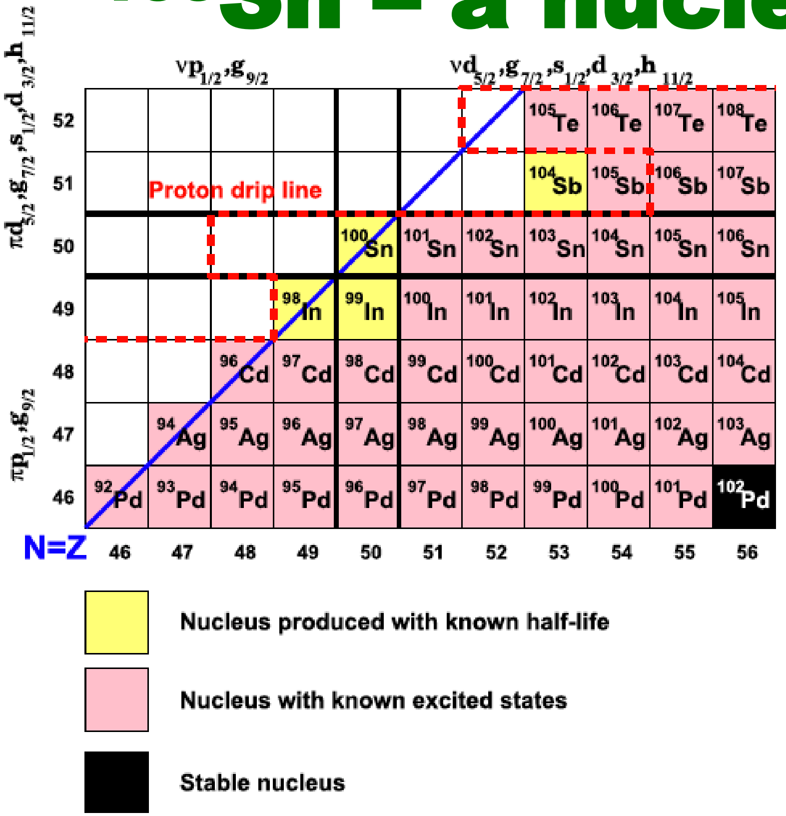
TABLE I. Binding energies (in MeV) of ^{55}Ni and ^{57}Ni relative to the corresponding reference energies $\langle\Phi_0^{(A)}(j)|H|\Phi_0^{(A)}(j)\rangle$, $A = 55$ and 57, respectively, as functions of the shell gap shift ΔG (in MeV). $S_0^{(A)}(j)$ is defined as $|\langle\Phi_0^{(A)}(j)|\Psi_{0,A}^{\text{full-CI}}(j)\rangle|$.

ΔG	−2	−1	0	1	2
^{55}Ni					
EOMCC(2h-1p)	−3.649	−2.459	−1.884	−1.542	−1.313
EOMCC(3h-2p)	−3.844	−2.567	−1.951	−1.587	−1.344
CI(2p-2h)	−2.505	−2.013	−1.672	−1.427	−1.244
CI(3p-3h)	−3.295	−2.449	−1.922	−1.580	−1.344
CI(4p-4h)	−4.457	−2.967	−2.150	−1.693	−1.406
CI(6p-6h)	−6.397	−3.519	−2.262	−1.723	−1.417
Full CI	−9.091	−3.920	−2.279	−1.725	−1.417
$S_0^{(55)}(\frac{7}{2})$	0.0362	0.4023	0.8015	0.8919	0.9287
^{57}Ni					
EOMCC(2p-1h)	−3.868	−2.671	−2.080	−1.721	−1.476
EOMCC(3p-2h)	−4.295	−2.871	−2.186	−1.783	−1.516
CI(2p-2h)	−2.692	−2.192	−1.840	−1.584	−1.389
CI(3p-3h)	−3.622	−2.717	−2.146	−1.772	−1.513
CI(4p-4h)	−4.697	−3.217	−2.370	−1.884	−1.575
CI(6p-6h)	−6.534	−3.768	−2.493	−1.918	−1.588
Full CI	−9.391	−4.151	−2.511	−1.921	−1.588
$S_0^{(57)}(\frac{3}{2})$	0.0335	0.4062	0.7802	0.8774	0.9182

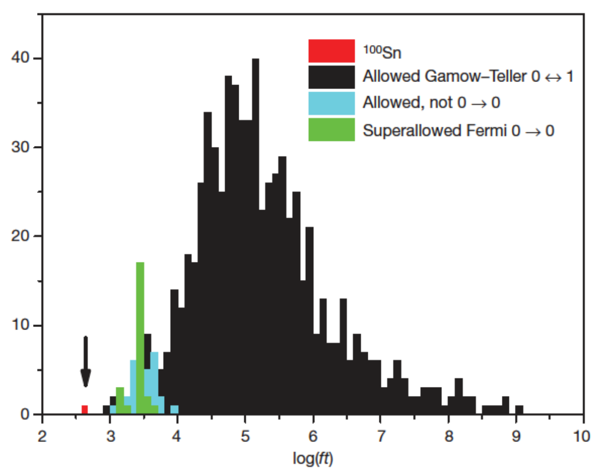
TABLE II. Excitation energies (in MeV) of the low-lying states of ^{57}Ni as functions of the shell gap shift ΔG (in MeV). $S_0^{(A)}(j)$ is defined as $|\langle\Phi_0^{(A)}(j)|\Psi_{0,A}^{\text{full-CI}}(j)\rangle|$.

ΔG	−2	−1	0	1	2
$(5/2)^-$					
EOMCC(2p-1h)	0.658	0.819	0.895	0.937	0.961
EOMCC(3p-2h)	0.625	0.771	0.856	0.908	0.939
CI(2p-2h)	0.812	0.856	0.897	0.927	0.948
CI(3p-3h)	0.781	0.827	0.878	0.917	0.944
CI(4p-4h)	0.692	0.776	0.852	0.904	0.937
CI(6p-6h)	0.360	0.658	0.832	0.900	0.936
Full CI	−0.118	0.402	0.825	0.900	0.936
$S_0^{(57)}(\frac{5}{2})$	0.0193	0.2640	0.7443	0.8596	0.9077
$(1/2)^-$					
EOMCC(2p-1h)	1.259	1.494	1.639	1.739	1.813
EOMCC(3p-2h)	0.669	1.071	1.366	1.562	1.694
CI(2p-2h)	1.279	1.451	1.592	1.699	1.781
CI(3p-3h)	1.009	1.218	1.426	1.588	1.706
CI(4p-4h)	0.763	1.021	1.312	1.530	1.676
CI(6p-6h)	0.395	0.739	1.211	1.499	1.665
Full CI	0.050	0.434	1.184	1.496	1.665
$S_0^{(57)}(\frac{1}{2})$	0.0293	0.2561	0.6577	0.8049	0.8701

^{100}Sn – a nucleus of superlatives



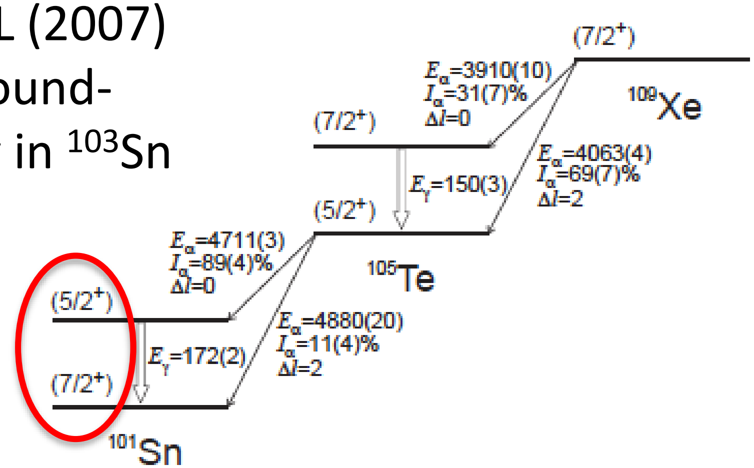
- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline
- At the endpoint of the rapid proton capture process (Sn-Sb-Te cycle)
- Unresolved controversy regarding s.p. structure of ^{101}Sn



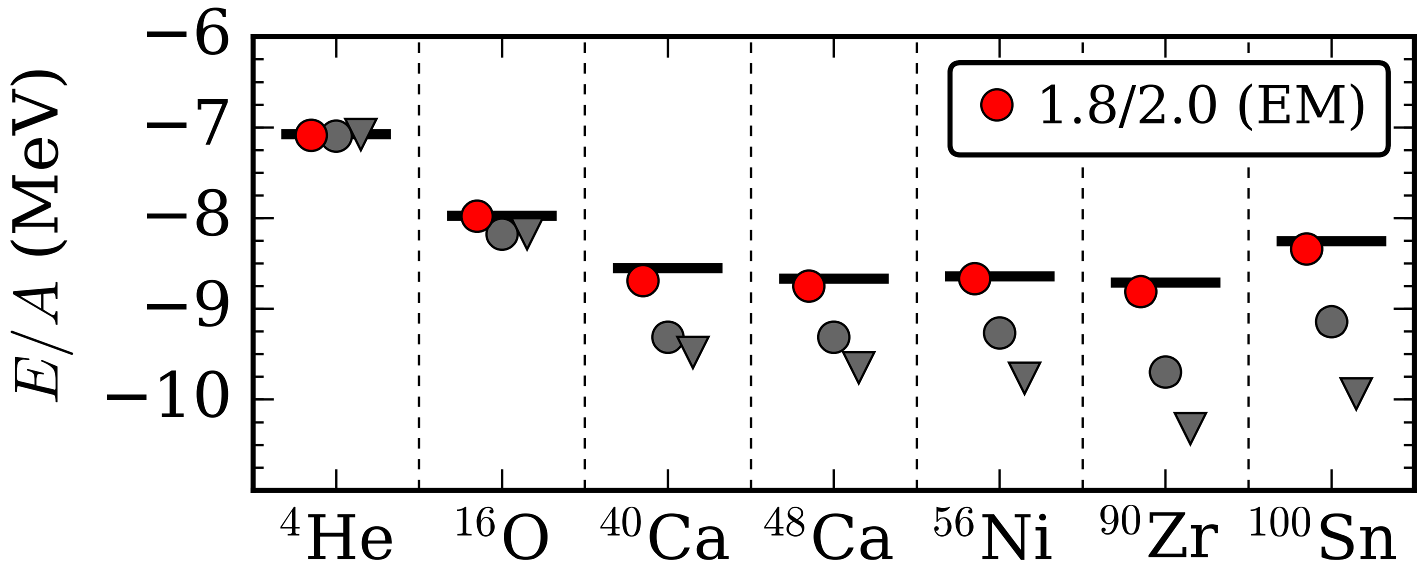
Hinke et al, Nature (2012)

Sewernyiak et al PRL (2007) predicted a 5/2+ ground-state as presumably in ^{103}Sn

Darby et al, PRL (2010)

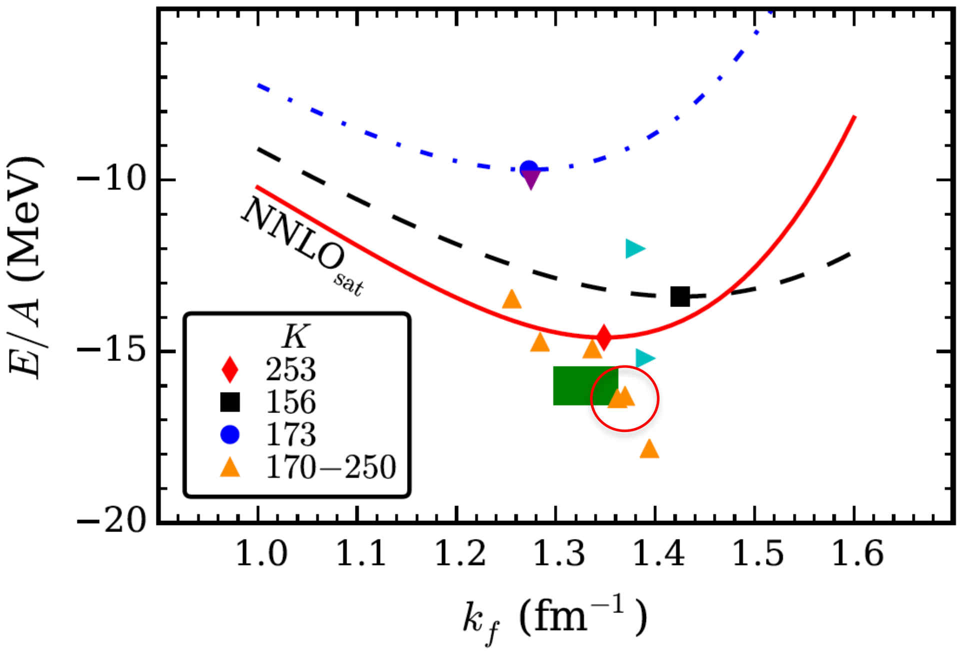


Accurate BEs from light → heavy → infinite matter from a chiral interaction

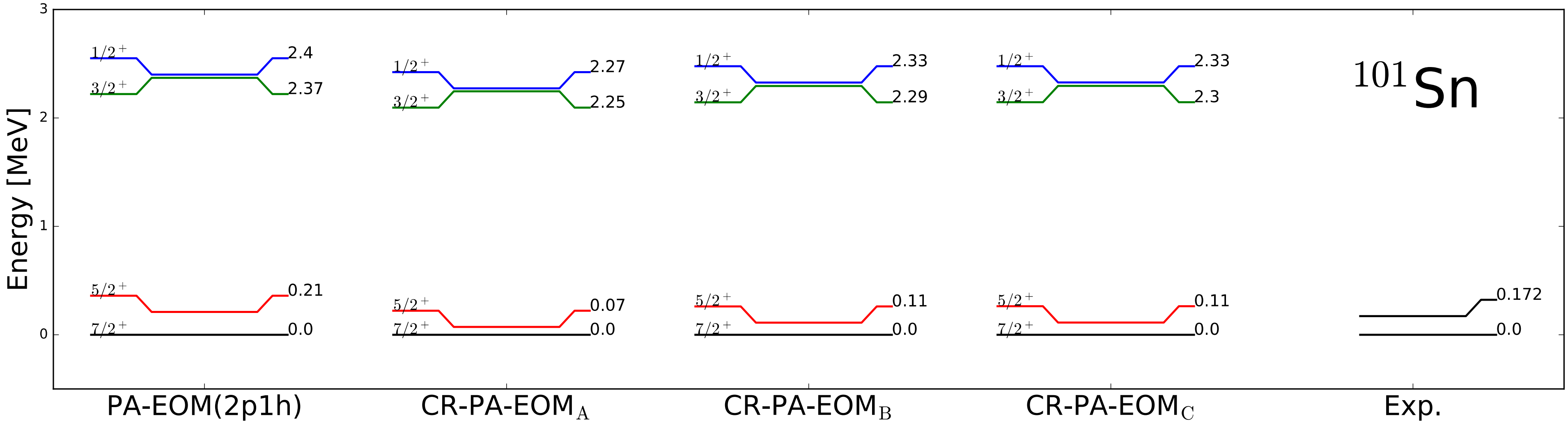


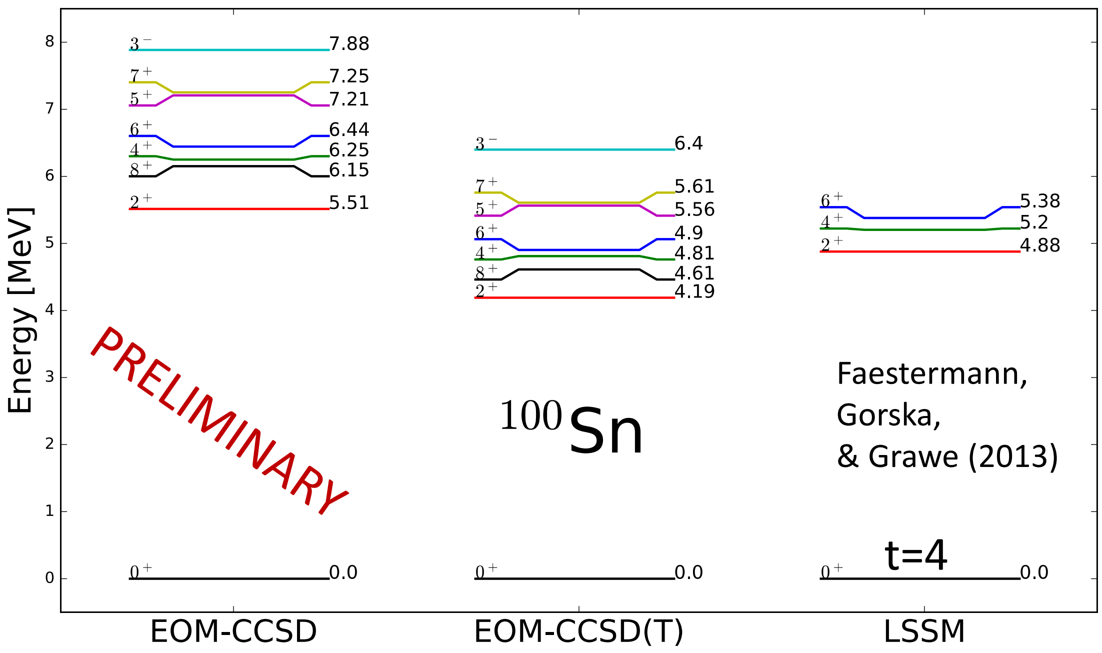
1.8/2.0 (EM) from K. Hebeler *et al* PRC (2011)
The other chiral NN + 3NFs are from Binder et al, PLB (2014)

- Accurate binding energies up to mass 100 from a chiral NN + 3NF
- Fit to nucleon-nucleon scattering and BEs and radii of A=3,4 nuclei
- Reproduces saturation point in nuclear matter within uncertainties
- Deficiencies: Radii are less accurate



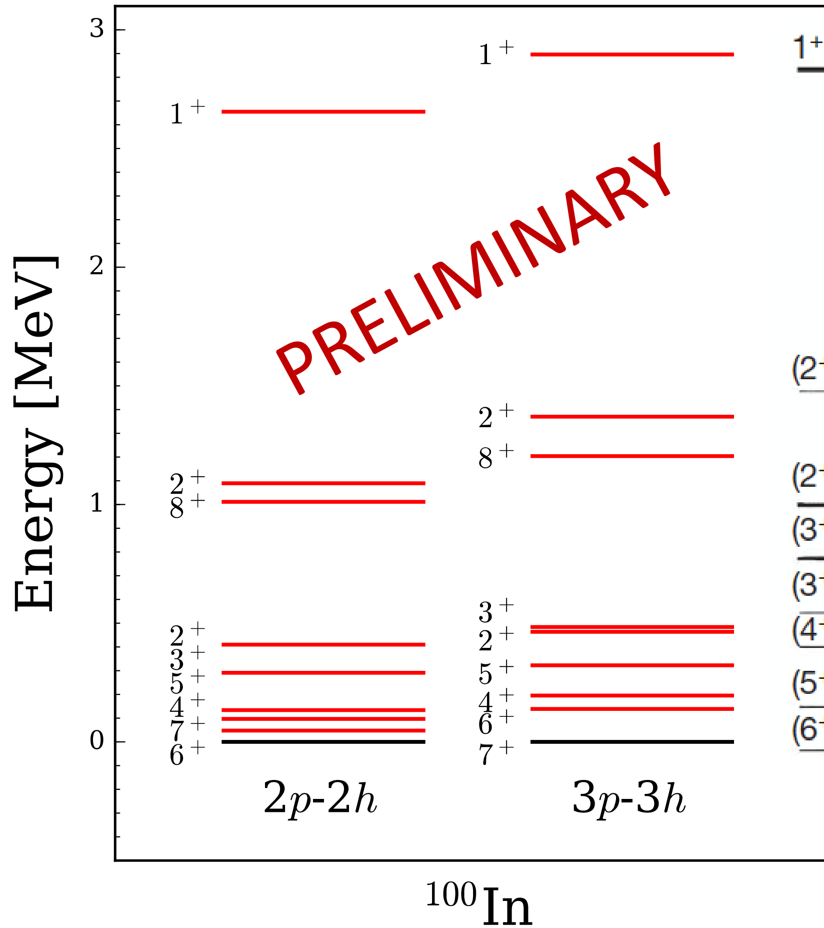
Structure of the ligthest tin isotopes

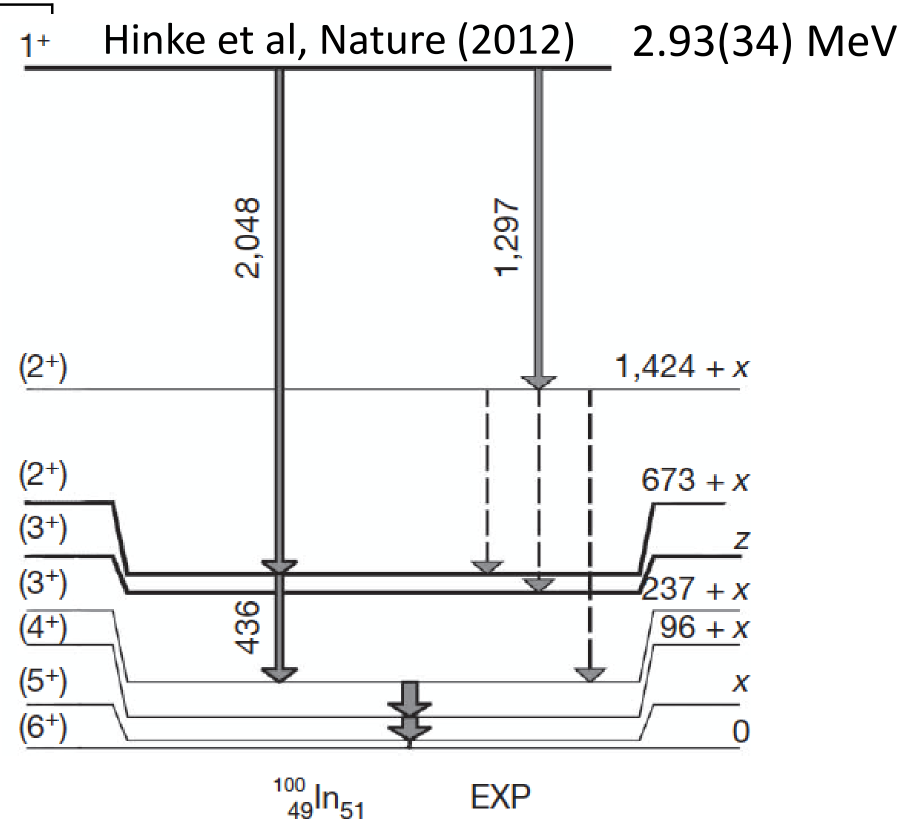




- High 2^+ energy in ^{100}Sn
- Predict $7/2^+$ ground-state in ^{101}Sn
- Experimental splitting between $7/2^+$ and $5/2^+$ reproduced
- Ground-state spins of $^{101-121}$Sn will be measured at CERN (CRIS collaboration)

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





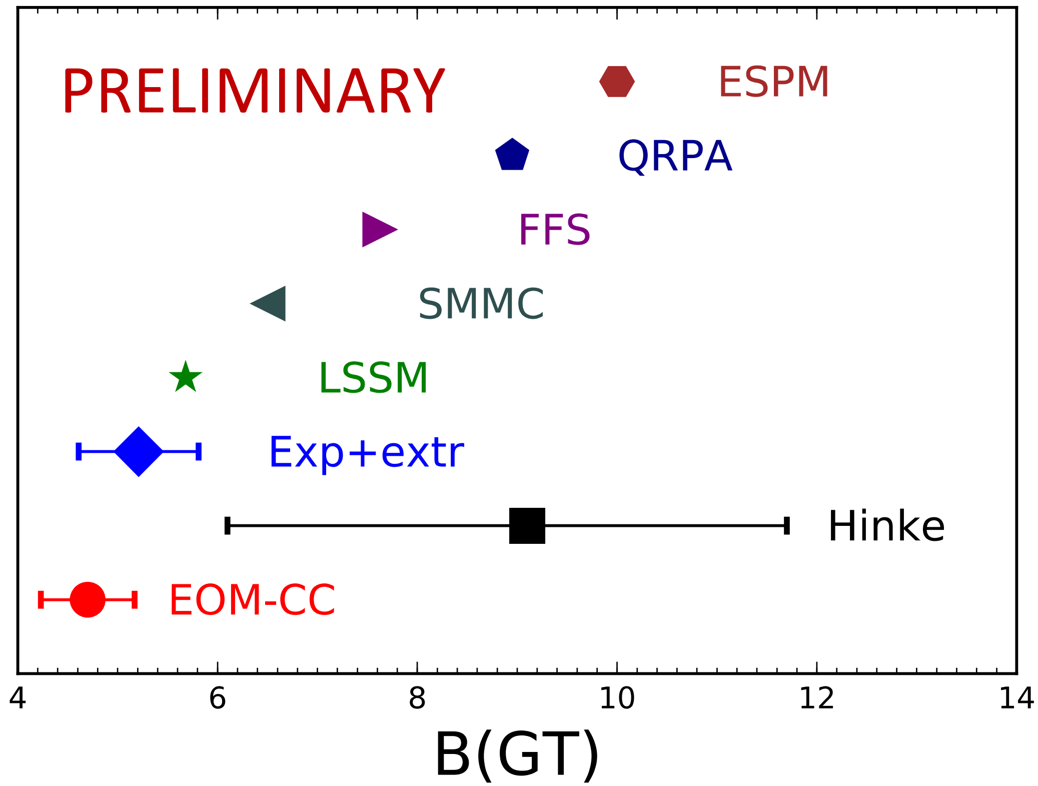
New method: 3p-3h charge-exchange EOM

$$\overline{H}_N R_\mu |\Phi_0\rangle = E_\mu R_\mu |\Phi_0\rangle$$

- Reproduce known 1^+ state at 2.93(34) MeV
- Predict a 7^+ ground-state for ^{100}In
- Ground-state spin of ^{100}In can be measured by CRIS collab. at CERN

Superallowed Gamow-Teller transition

- Prediction for the Gamow-Teller transition consistent with data
- Towards understanding the quenching of g_A
- Important implications for computations of $0\nu\beta\beta$ decay



Hinke et al, Nature (2012)

Model	Ref	unquenched	quenched
ESPM	[30]	17.78	10.00
MCSM	[8]	10.3	6.5
QRPA	[9]	8.95	
FFS	[9]	7.63	
extrapol.	[10]	9.8	5.2
SM+corr.	[7]	14.2	
LSSM	this work	~ 13.90	~ 7.82
LSSM (only 1_1^+)	this work	10.10	5.68

- Coupled-cluster computations predict a B(GT) of **4.7(5)**
- B(GT) is currently targeted by upcoming precision measurements

Neutrinoless ββ-decay of ^{48}Ca

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

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

$$M^{0\nu}_{GT} + \left(\frac{g_V}{g_A}\right)^2 M^{0\nu}_F + M^{0\nu}_T$$

The ground-state of ^{48}Ca is computed in the CCSD approximation:

$$\overline{H}_N|\Phi_0\rangle = E_0|\Phi_0\rangle,\ \ \overline{H}_N = e^{-T}H_N e^T,\ \ T = T_1 + T_2$$

The CC energy functional is expressed in term of left/right ground-states

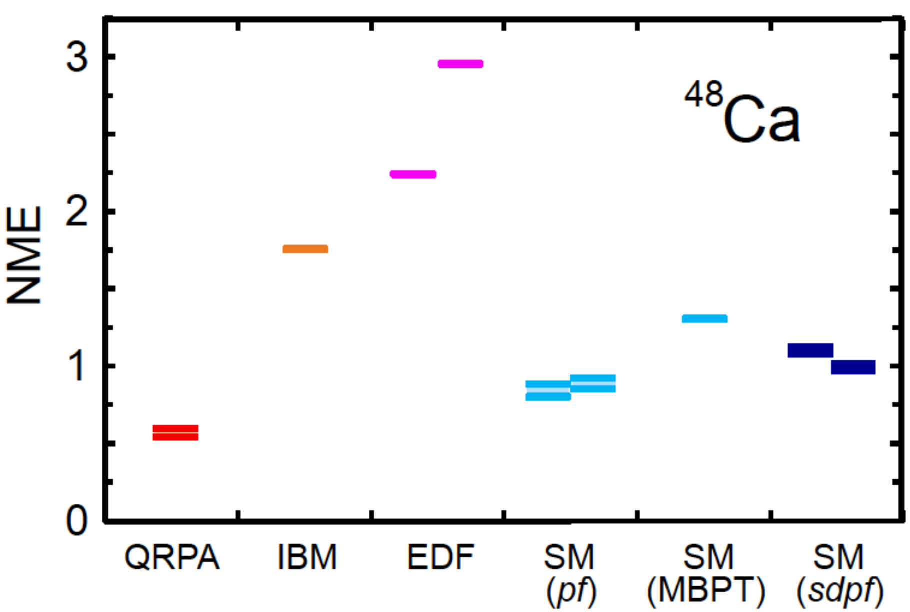
$$\langle\Phi_0|(1+\Lambda)\overline{H}_N|\Phi_0\rangle = E_0,\ \ \langle\Phi_0|(1+\Lambda)|\Phi_0\rangle = 1.$$

$$\Lambda = \sum_{ia}\lambda^i_a a_a a^\dagger_i + \frac{1}{2}\sum_{ijab}\lambda^{ij}_{ab} a_b a_a a^\dagger_i a^\dagger_j$$

Neutrinoless ββ-decay of ^{48}Ca

NME for 0νββ			
Method	GT	Fermi	Tensor
CCSD	0.97	0.31	-0.12
CCSDT-1(10)	0.44	0.09	-0.11
CCSDT-1(12)	0.50	0.11	-0.11
CCSDT-1(14)	0.45	0.10	-0.11

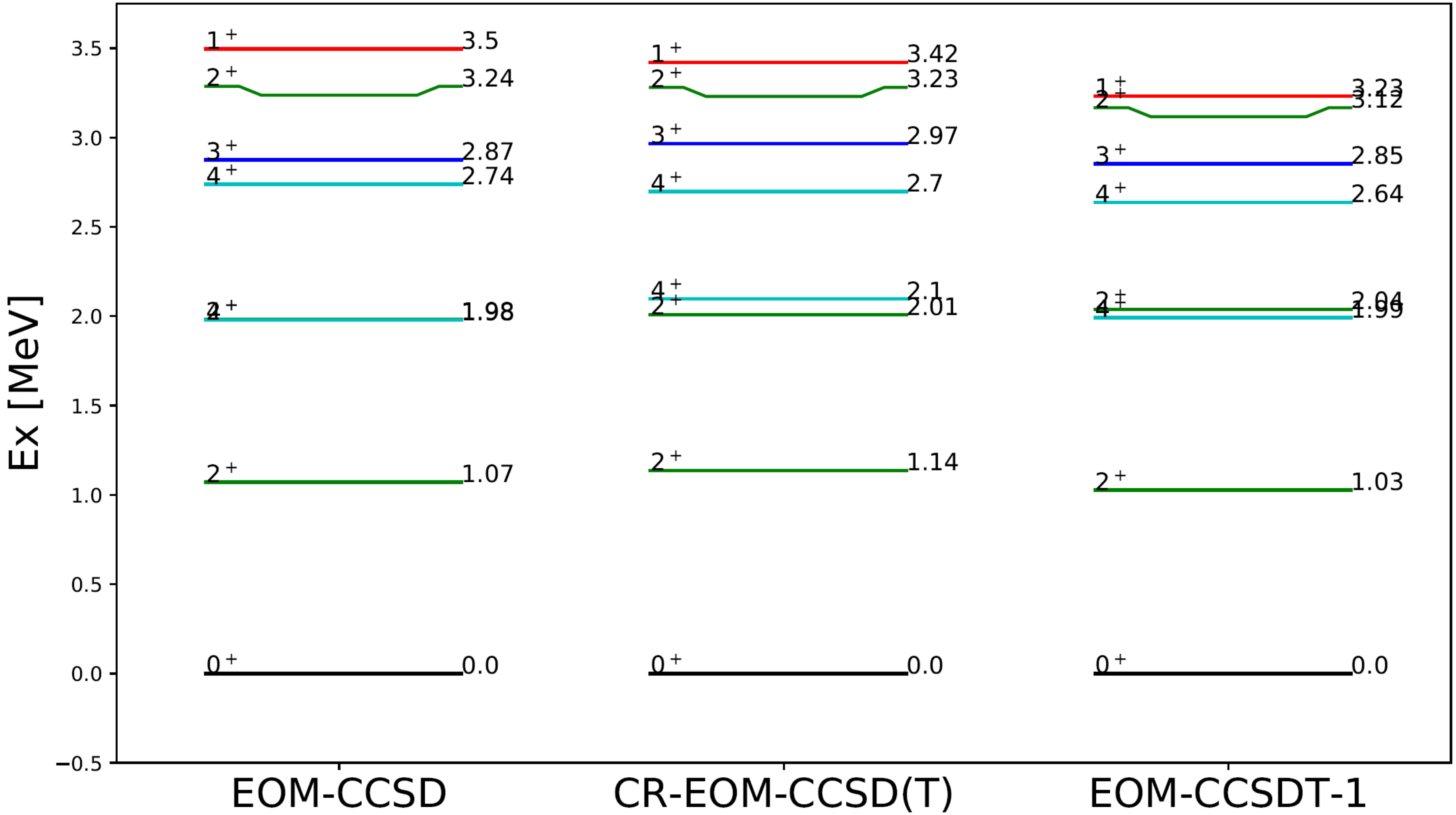
PRELIMINARY



- NME computed with the chiral NN + 3N interaction 1.8/2.0 (EM) [K. Hebeler *et al* PRC (2011)]
- Model-space N_{max} =10, hw = 22MeV.
- Not converged with respect to model-space or truncation in 3p3h amplitudes
- Preliminary CC results agree with QRPA

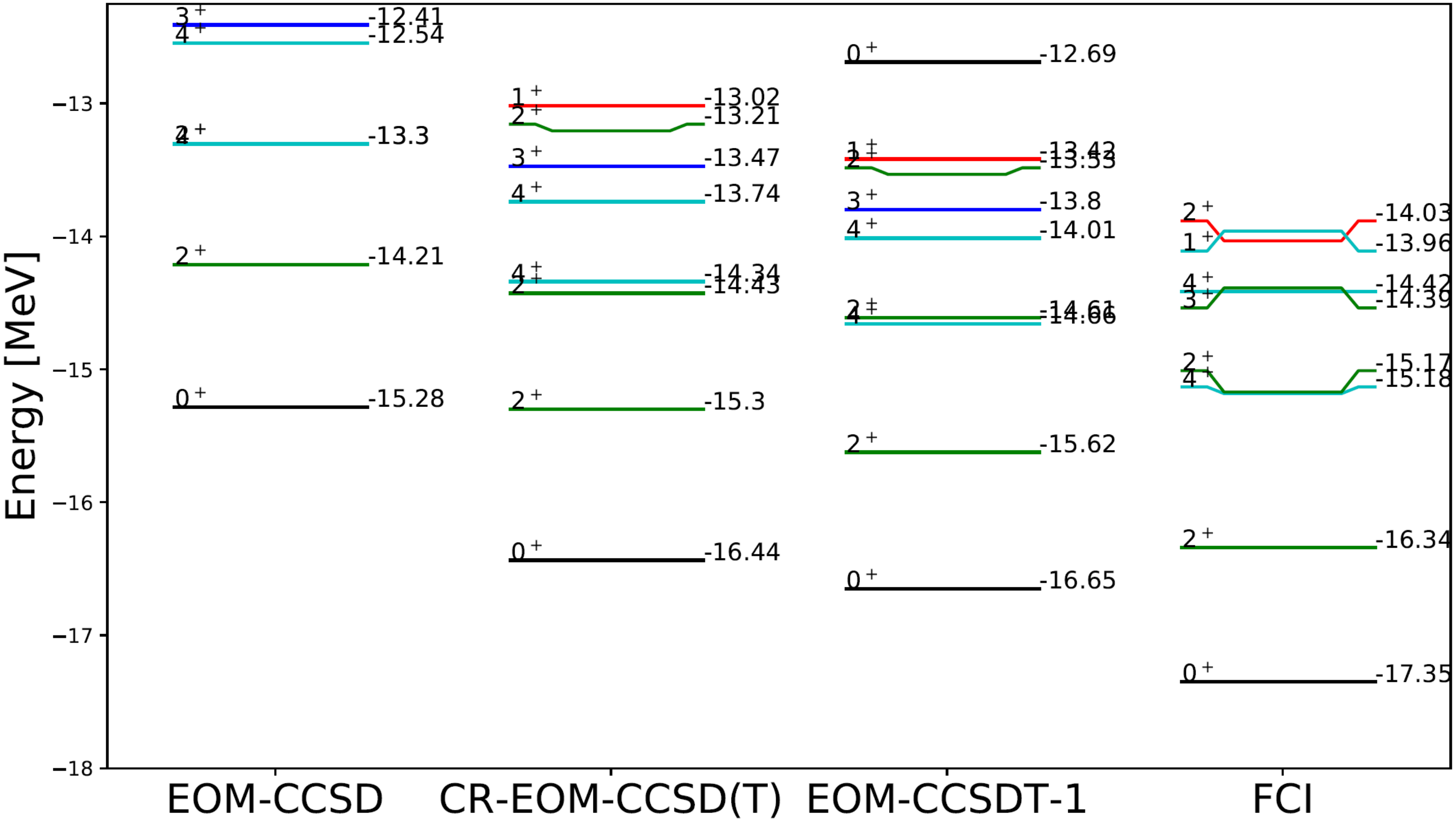
Ti48 CR-EOM-CCSD(T)

$$R_\nu = \frac{1}{4}\sum r_{ij}^{ab}\, p_a^\dagger p_b^\dagger n_j n_i \qquad + \frac{1}{3!^2}\sum r_{ijk}^{abc}\, p_a^\dagger p_b^\dagger N_c^\dagger N_k n_j n_i$$



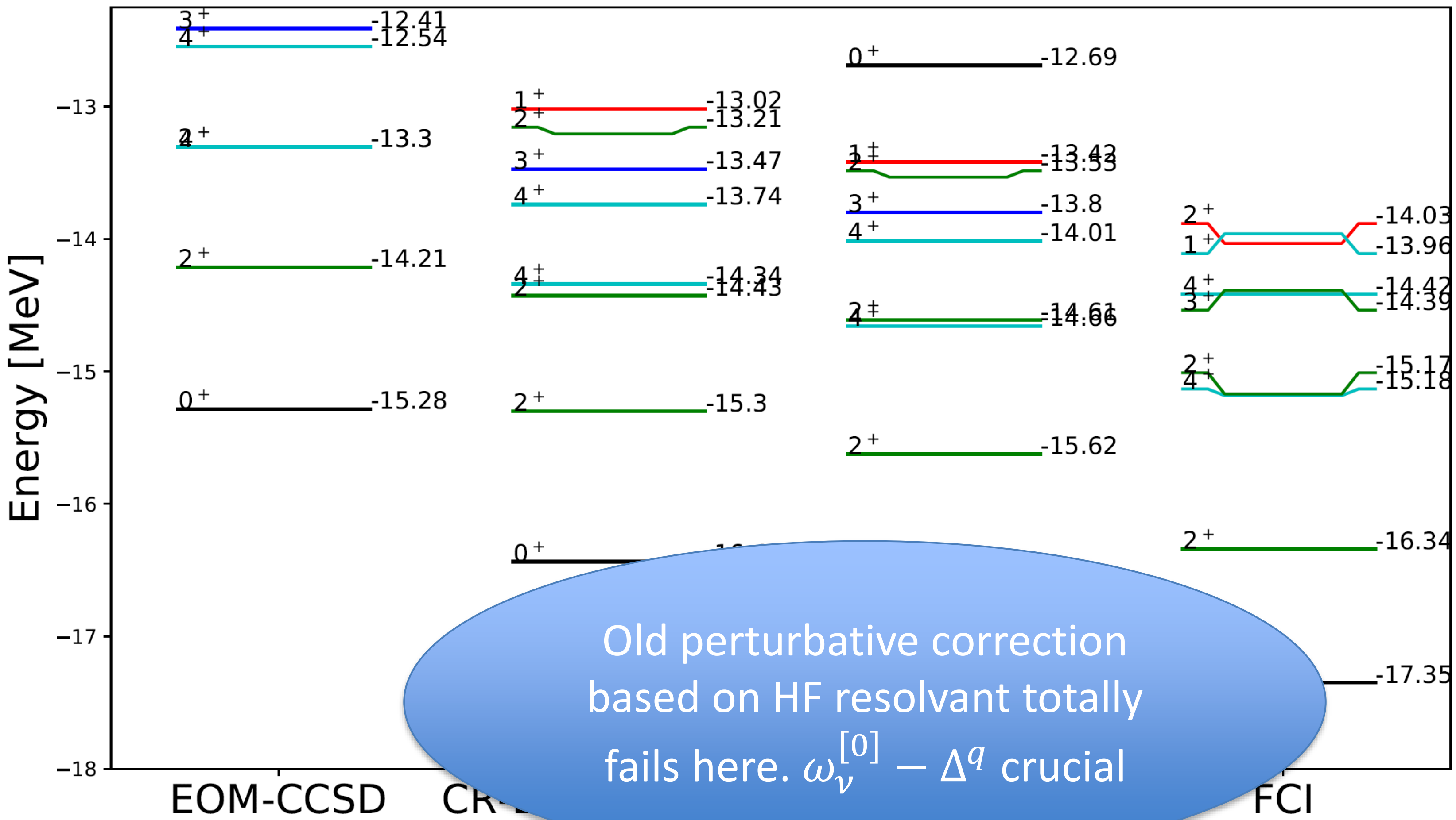
Ti48 CR-EOM-CCSD(T)

$$R_\nu = \frac{1}{4}\sum r_{ij}^{ab}\, p_a^\dagger p_b^\dagger n_j n_i \qquad + \frac{1}{3!^2}\sum r_{ijk}^{abc}\, p_a^\dagger p_b^\dagger N_c^\dagger N_k n_j n_i$$



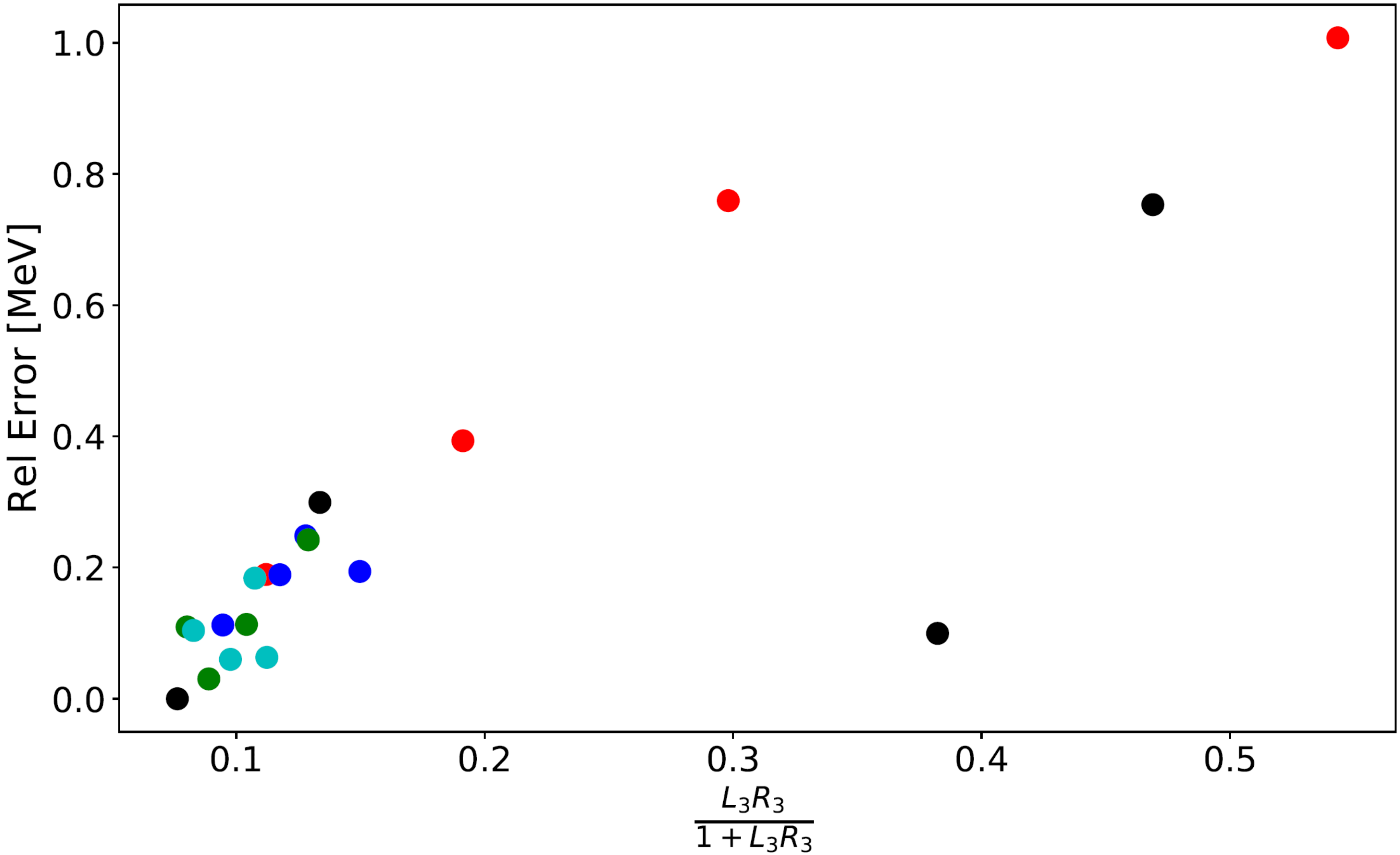
Ti48 CR-EOM-CCSD(T)

$$R_\nu = \frac{1}{4}\sum r_{ij}^{ab}\, p_a^\dagger p_b^\dagger n_j n_i \qquad + \frac{1}{3!^2}\sum r_{ijk}^{abc}\, p_a^\dagger p_b^\dagger N_c^\dagger N_k n_j n_i$$

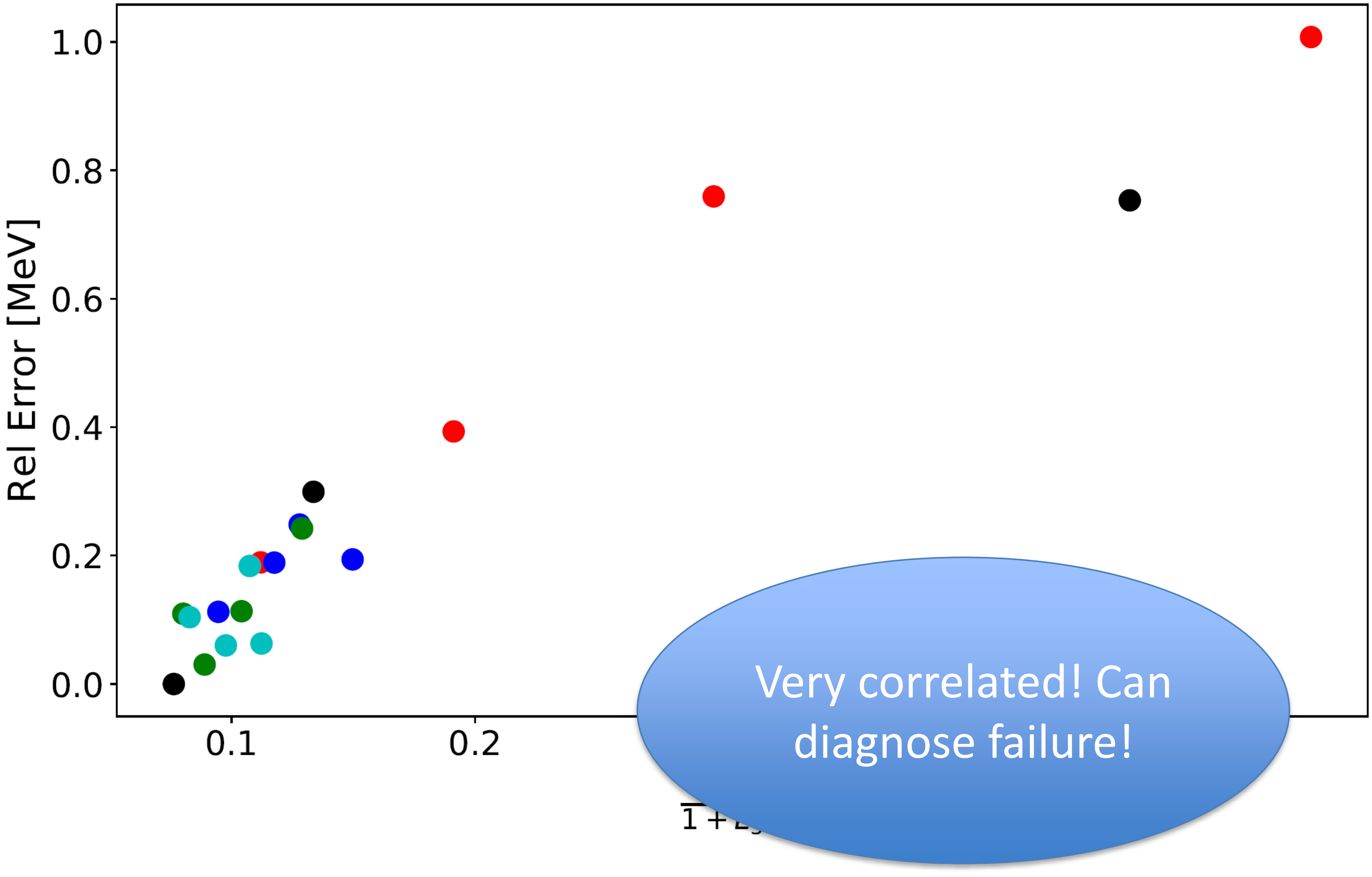


Old perturbative correction based on HF resolvant totally fails here. $\omega_\nu^{[0]} - \Delta^q$ crucial

Ti48 CR-EOM-CCSD(T)

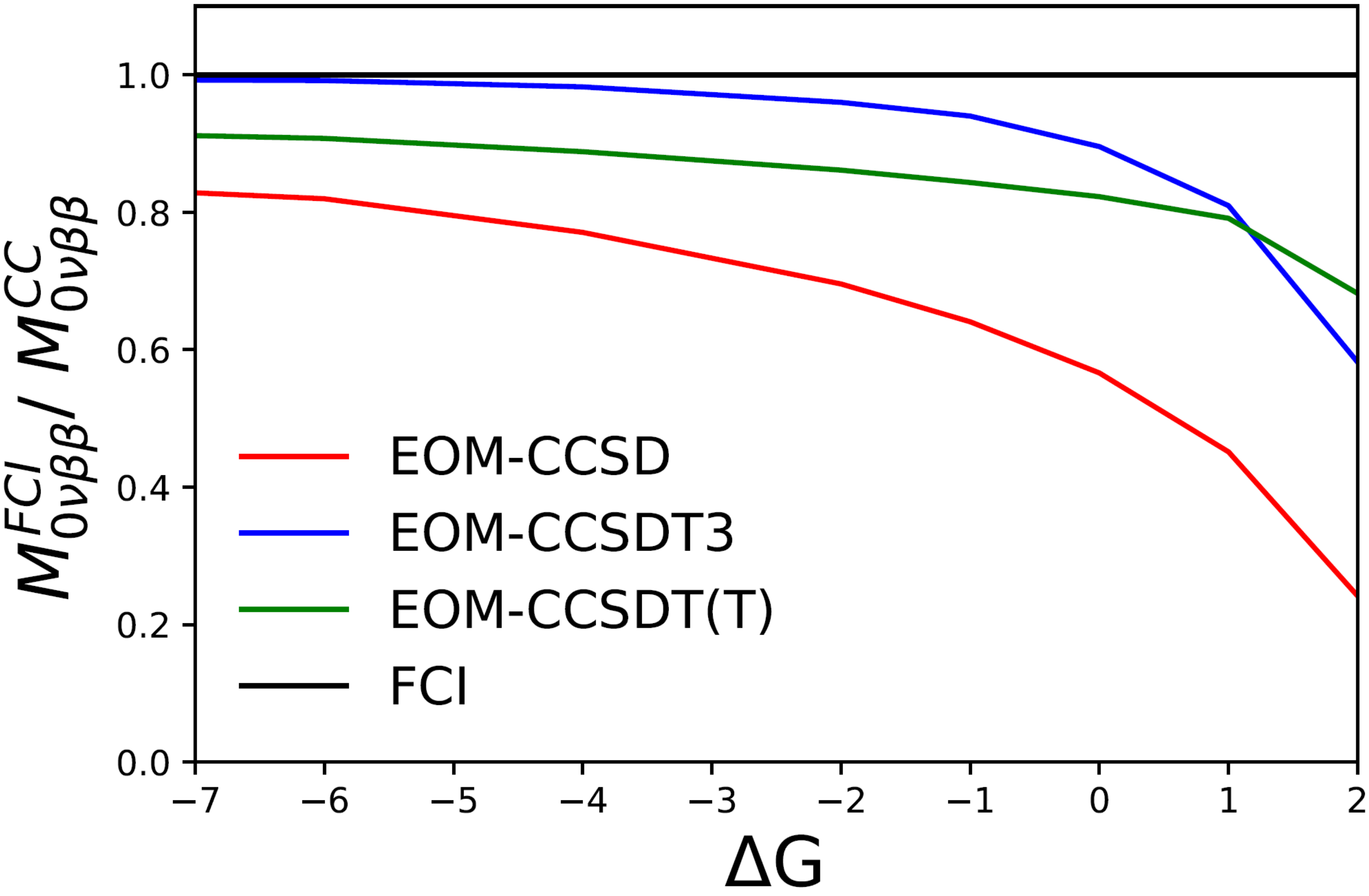


Ti48 CR-EOM-CCSD(T)



EOM-CR-CCSD(T)

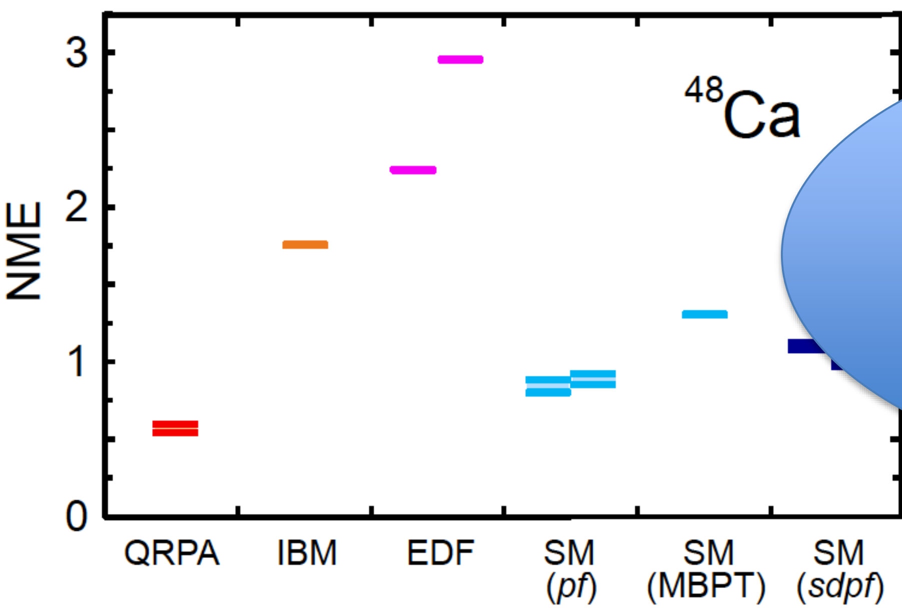
- Implemented and benchmarked 3p2h $\tilde{\boldsymbol{R}}_{\nu,q}^{[1]}$, $\tilde{\boldsymbol{L}}_{\nu,q}^{[1]}$
  - Phys. Rev. Lett. **101**, 052501 (UTK remote access down)



Neutrinoless ββ-decay of ^{48}Ca

NME for 0νββ			
Method	GT	Fermi	Tensor
CCSD	0.97	0.31	-0.12
CCSDT-1(10)	0.44	0.09	-0.11
CCSDT-1(12)	0.50	0.11	-0.11
CCSDT-1(14)	0.45	0.10	-0.11

PRELIMINARY



- NME ... with the chiral NN + ... [K... ...y. ...el-
- Preliminary CC results agree with QRPA

CCSDT-1(e3max) "Pspace" solution. Effect of energy and $\beta\beta$ from Q 3p3h confs should be doable!

Coupled Cluster Shell Model

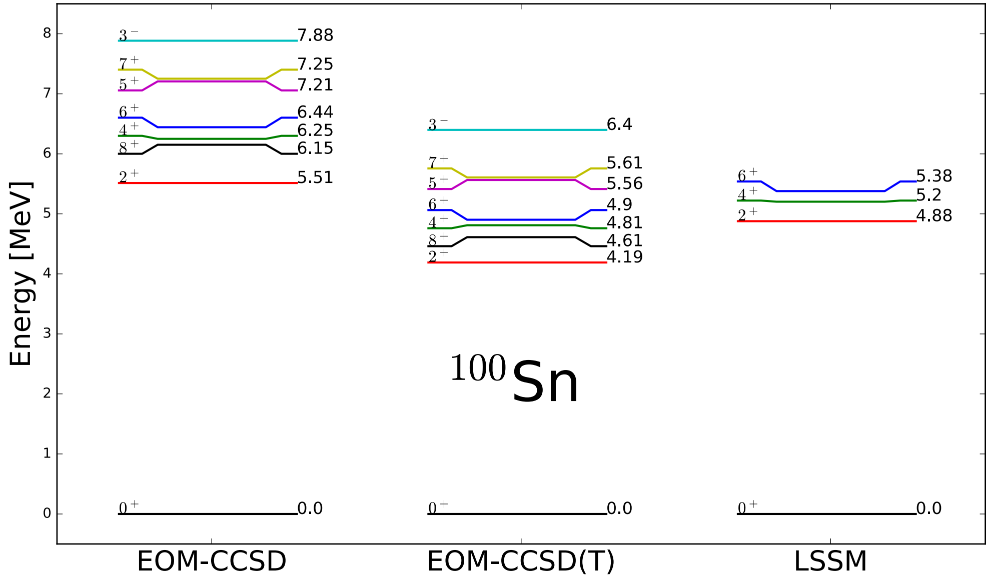
ZhongHao Sun
University of Tenn.
Oak Ridge Natl. Lab

IMSRG and CC

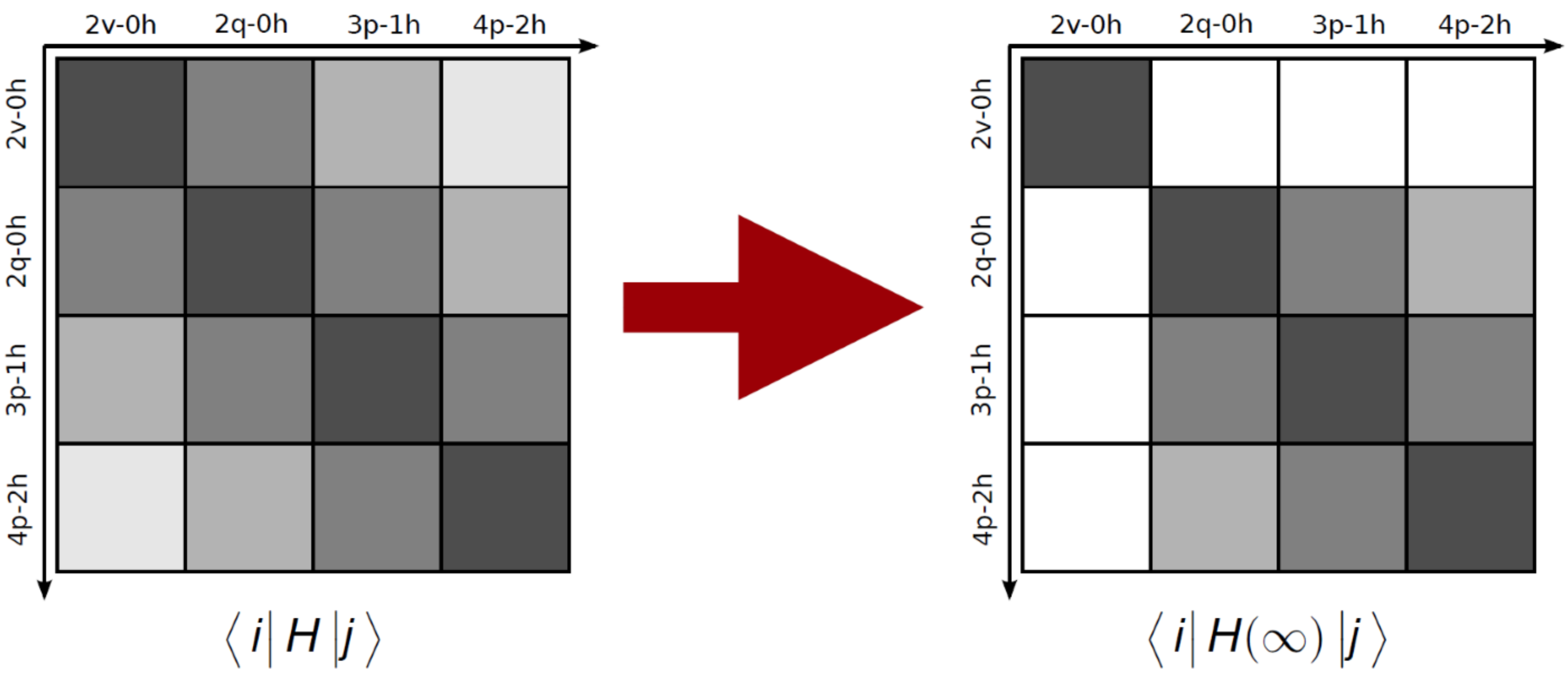
- Real difference is that CC does not attempt to conserve norm i.e. $\langle \Phi_0 | e^{-T^\dagger} e^{-T} | \Phi_0 \rangle \neq 1$
  - Leads to many fewer total diagrams/simple transformation
  - Must then appeal to left eigenstates

- Would the ease of analyzing diagrams make CC shell model a viable path?

- Answer why IMSRG sometimes produces EOM-CCSD quality results?



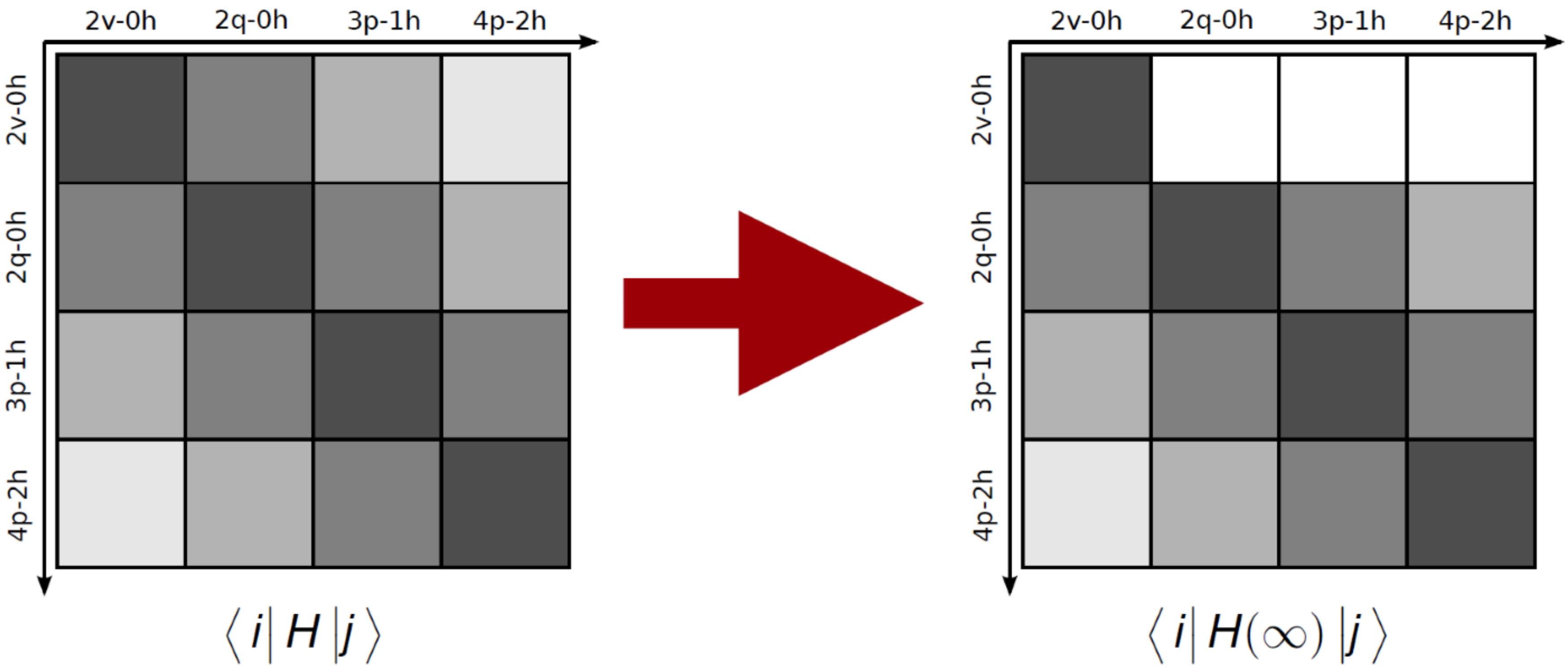
IMSRG Shell Model



change definition of off-diagonal Hamiltonian:

$$\left\{H^{od}\right\} = \{f_{h'}^{h}, f_{p'}^{p}, f_{h}^{p}, f_{v}^{q}, \Gamma_{hh'}^{pp'}, \Gamma_{hv}^{pp'}, \Gamma_{vv'}^{pq}\} \text{ \& H.c.}$$

CC Shell Model



change definition of off-diagonal Hamiltonian:

$$\left\{ H^{od} \right\} = \{ f^{h}_{h'}, f^{p}_{p'}, f^{p}_{h}, f^{q}_{v}, \Gamma^{pp'}_{hh'}, \Gamma^{pp'}_{hv}, \Gamma^{pq}_{vv'} \} \text{ \& H.c.}$$

CC Shell Model

- Decouple ground state first, obtaining $\overline{\boldsymbol{H}}_{\boldsymbol{CCSD}}$
  - Introduce a secondary transformation

$$\overline{\overline{\boldsymbol{H}}} = \mathbf{e}^{\boldsymbol{Z}}\overline{\boldsymbol{H}}_{\boldsymbol{CCSD}}\,\mathbf{e}^{-\boldsymbol{Z}} \qquad \dot{Z} = \eta(\overline{\overline{\boldsymbol{H}}})$$

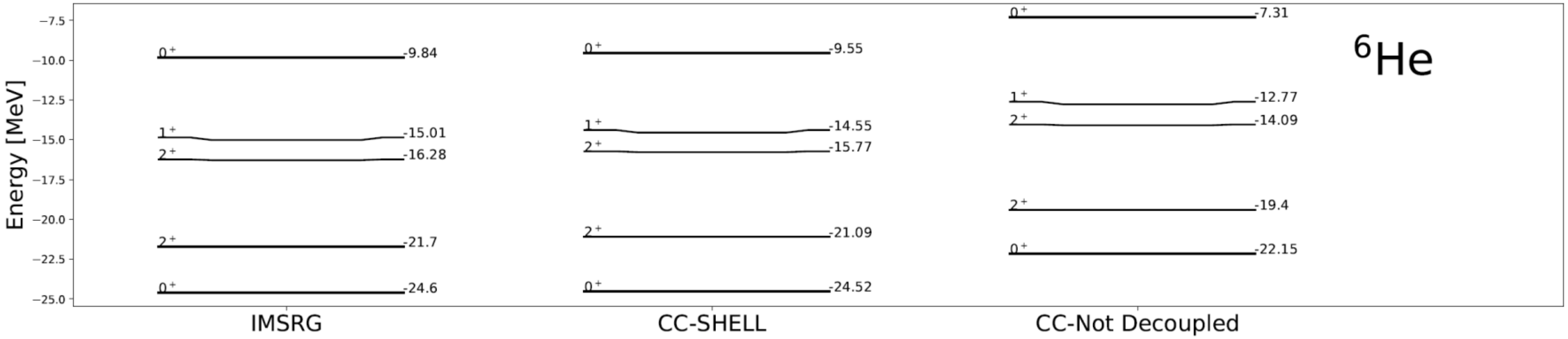
OR

$$\overline{\overline{\boldsymbol{H}}}_{\boldsymbol{k}} = \mathbf{e}^{\boldsymbol{Z}_{\boldsymbol{k}}}\overline{\boldsymbol{H}}_{\boldsymbol{CCSD}}\,\mathbf{e}^{-\boldsymbol{Z}_{\boldsymbol{k}}} \qquad Z_{k+1} = Z_k + \delta s\,\eta(\overline{\overline{\boldsymbol{H}}}_{\boldsymbol{k}})$$

  - Use same generators as IMSRG
  - Iterate until $\eta(\overline{\overline{\boldsymbol{H}}}_{\boldsymbol{k}})$ vanishes
  - Hermitize in order to feed to large scale SM

CC Shell Model

- Preliminary Results!
  - P-shell, emax=4, NN EM N3LO 2.0, M-Scheme



  - Still benchmarking, and investigating 3b-forces
  - Promising!

Thanks!

NUCLEI
Nuclear Computational Low-Energy Initiative

ICER