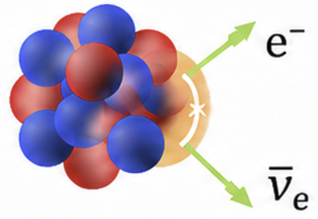


Ab initio many-body approaches

Ab initio many-body developments for weak processes: from 0νββ NMEs to precision beta decay

Bingcheng He (何秉承)

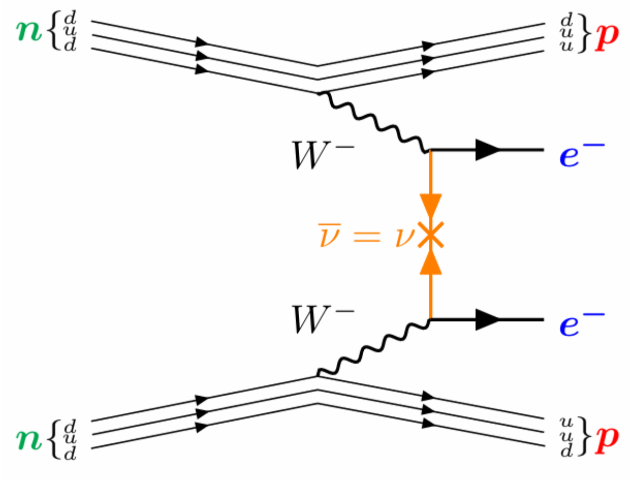
Department of Physics and Astronomy
University of Tennessee, Knoxville

INT Workshop: Recommended Values for Neutrinoless Double-Beta Decay Nuclear Matrix Elements
Seattle, July 2, 2026

NDB Collaboration
Advancing Theory for Nuclear Double-Beta Decay

THE UNIVERSITY OF TENNESSEE KNOXVILLE

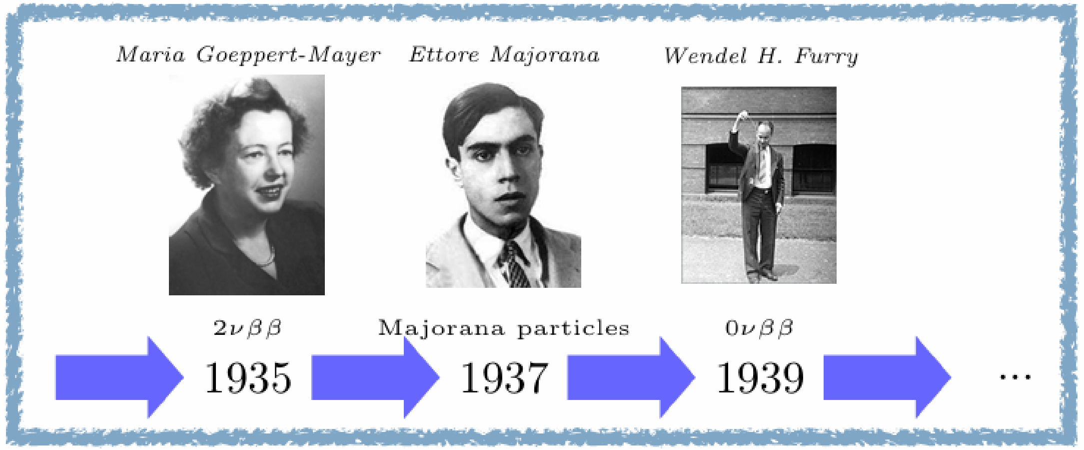
- ***11 institutions***
- ***Compute NMEs***
- ***Quantify uncertainties***



Attendees at the first in-person @NDB meeting, at the University of Notre Dame.

Advancing the 0νββ Through Ab Initio Calculations?

Neutrinoless double beta decay (0νββ)



$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu}\left|M^{0\nu}\right|^2\langle m_{\beta\beta}\rangle^2$$

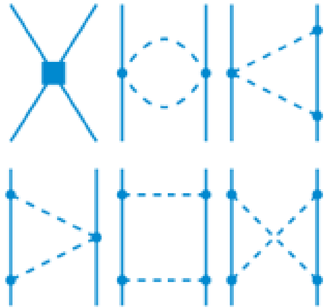
NME: must be calculated

- Lepton-number violation
- Majorana character of neutrino
- Matter/antimatter asymmetry
- Absolute neutrino mass scale

Ab initio nuclear structure theory

Chiral Effective Field Theory

New physics



$$H|\psi\rangle = E|\psi\rangle$$

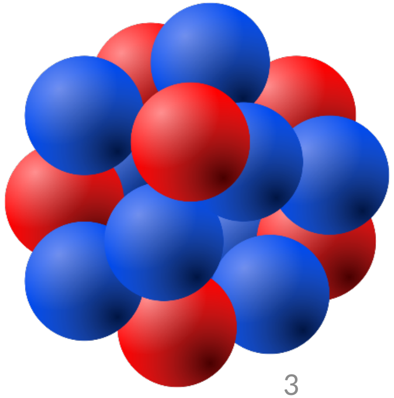
No free parameters

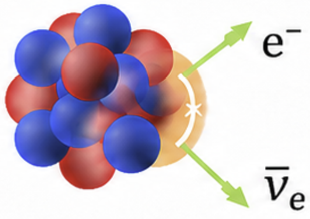
Many-body theory

VS-IMSRG and Coupled-cluster

Uncertainty quantification

$$M^{0\nu\beta\beta} = \langle\Psi_f|O_{eff}|\Psi_i\rangle$$





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Outline:

- Status of Coupled-cluster development

  Gaute Hagen, Thomas Papenbrock

- Preliminary results from VS-IMSRG(3f2)

- Application to superallowed beta decay

Start from chiral EFT Hamiltonian, solve correlations

Many-body Schrödinger equation

$$H|\Psi_\alpha\rangle = E_\alpha|\Psi_\alpha\rangle$$

$$\hat{H} = \hat{H}^{[1]} + \hat{H}^{[2]} + \hat{H}^{[3]}$$

Hartree–Fock (Spherical)

Normal-ordered two-body approximation(NO2B)

$$\hat{H}_\mathrm{N} = \hat{H}_\mathrm{N}^{[1]} + \hat{H}_\mathrm{N}^{[2]} + \hat{H}_\mathrm{N}^{[3]}$$

Solve correlations with ab initio many-body methods:

Coupled-cluster

VS-IMSRG

TABLE I. The recommended value for the total NME of $0\nu\beta\beta$ decay in ^{76}Ge, together with the uncertainties from different sources.

$M^{0\nu}$	ϵ_{LEC}	$\epsilon_{\chi\mathrm{EFT}}$	ϵ_{MBT}	ϵ_{OP}	ϵ_{EM}
$2.60^{+1.28}_{-1.36}$	0.75	0.3	0.88	0.47	< 0.06

Belley et al., Phys. Rev. Lett. 132, 182502 (2024)

Coupled-cluster theory

correlated state: $|\Psi\rangle = e^T|\phi\rangle$

Reference state :HF

cluster operator: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots + \hat{T}_A$ Only excitations

similarity-transformed Hamiltonian:

non-Hermitian $\bar{H} = e^{-T} H e^T$ $E_{CC}| = \langle\phi|\bar{H}|\phi\rangle$

Baker–Campbell–Hausdorff

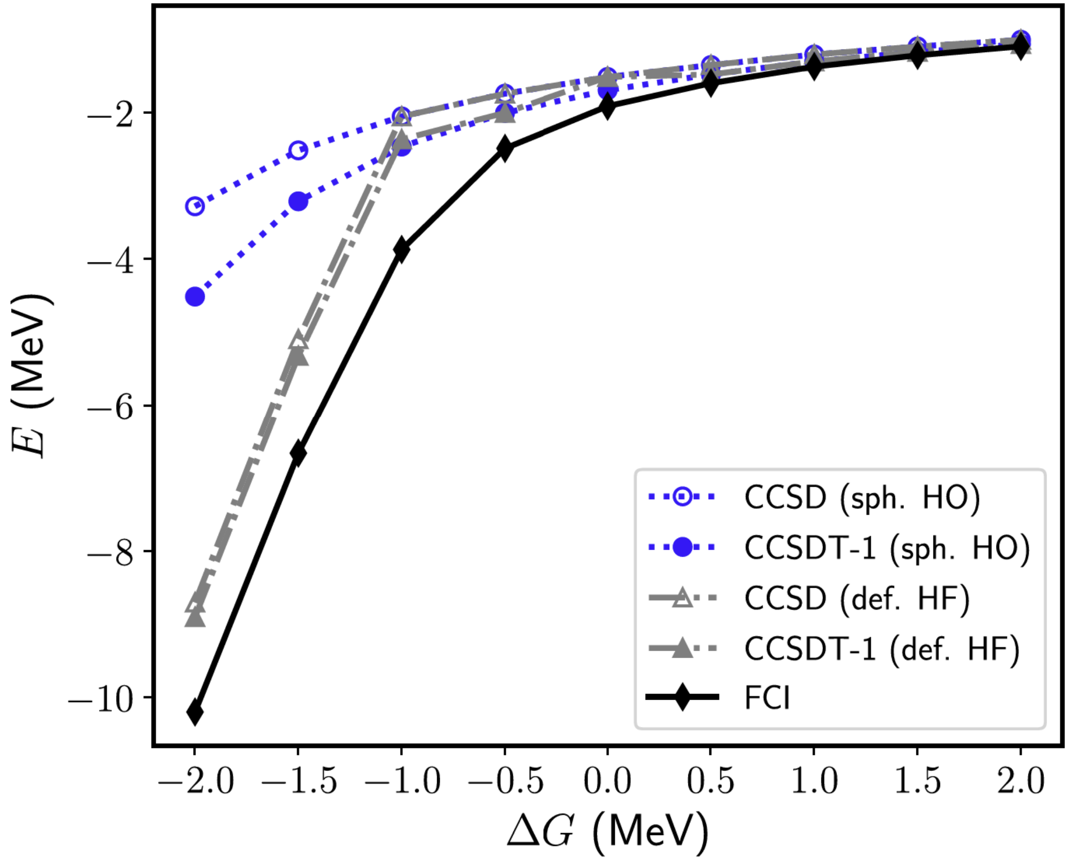
$$\langle O\rangle = \frac{\langle\Psi_L|O|\Psi_R\rangle}{\langle\Psi_L|\Psi_R\rangle}$$

$$|\Psi_R\rangle = e^T|\Phi_0\rangle$$

$$\langle\Psi_L| = \langle\Phi_0|(1+\Lambda)e^{-T}$$

Convergence of coupled-cluster method

Ground-state energy of ^{56}Ni based on the GXPF1A interaction as a function of the shift G between the f7/2 orbital and the unoccupied orbitals.



Z. H. Sun, G. Hagen, and T. Papenbrock, Phys. Rev. C 108, 014307 (2023)

Exact CI:

$$|\Psi\rangle = \Omega|\Phi\rangle = (1 + \sum_{i=1}^{A} C_i)|\Phi\rangle$$

$$C_1 = T_1,$$

$$C_2 = T_2 + \frac{1}{2}T_1^2,$$

$$C_3 = T_3 + T_1T_2 + T_1^3/3!,$$

$$C_4 = T_4 + T_2^2/2 + T_1T_3 + T_1^2T_2/2 + T_1^4/4!,$$

… …

CCSD Exact for the two-body problem

CCSDT Exact for the three-body problem

Higher-rank clusters systematically approach exact CI

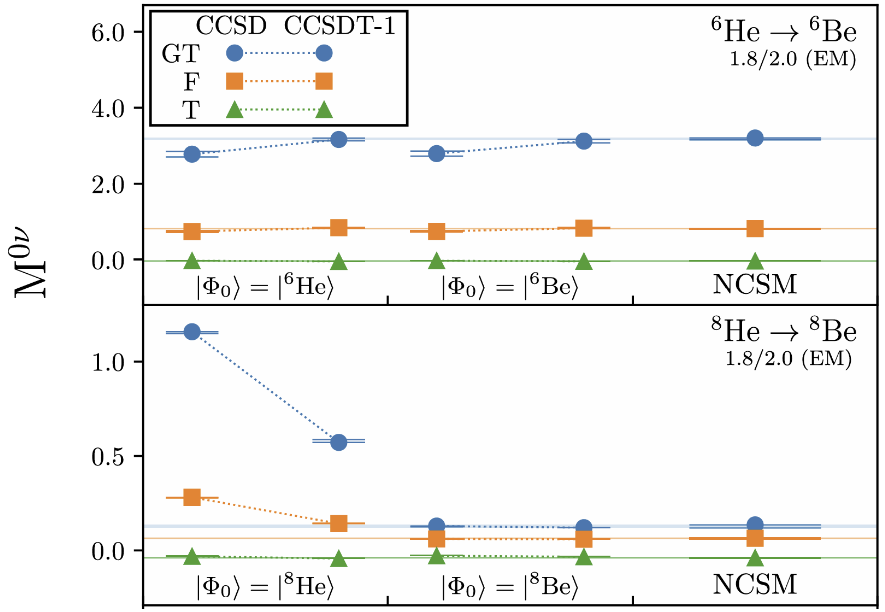
Coupled-cluster for the 0νββ NMEs

Basis:

HF: Spherical, Axial

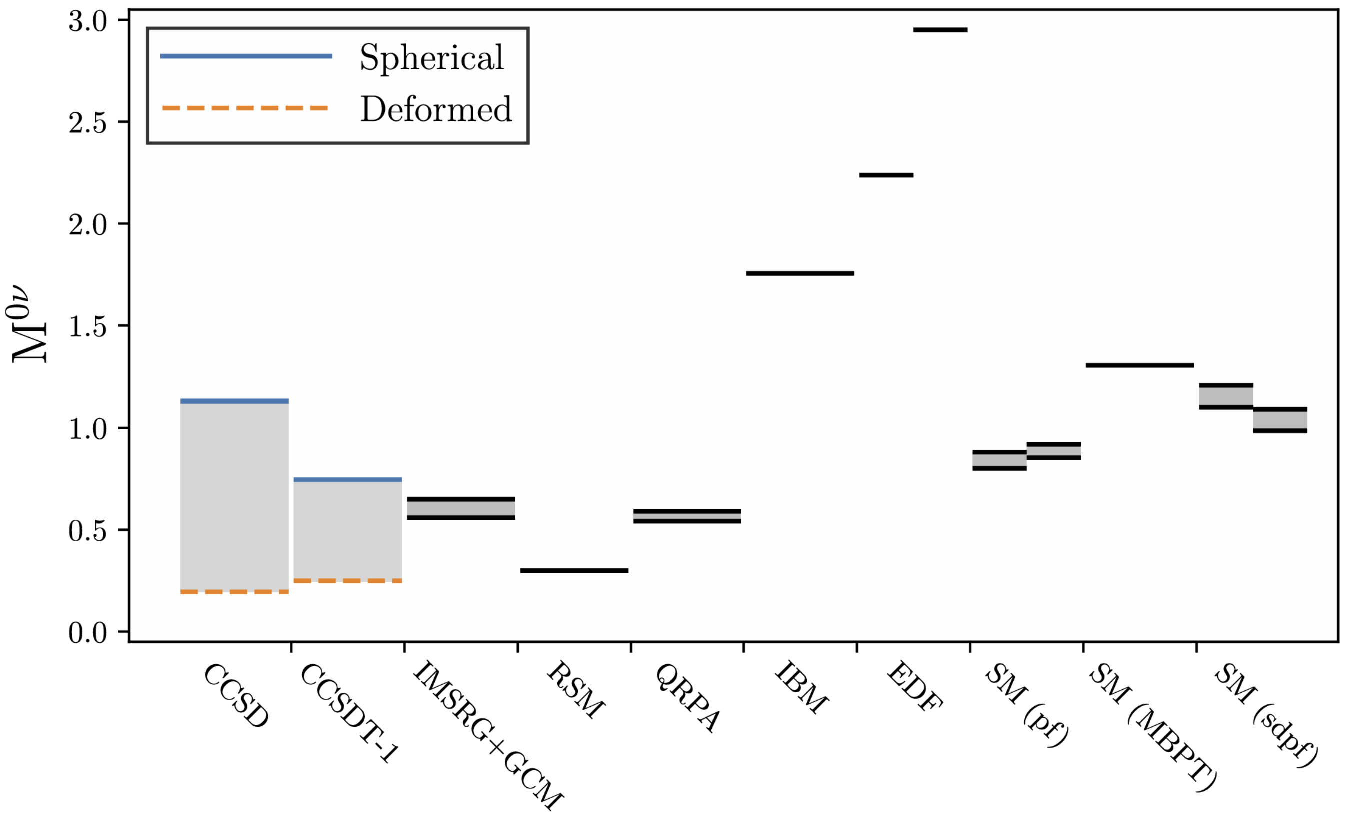
CCSD(T): Spherical, Axial

Reference dependence



Novario et al., PRL 126, 182502 (2021)

Comparison of the NME for the 0νββ decay of ^{48}Ca

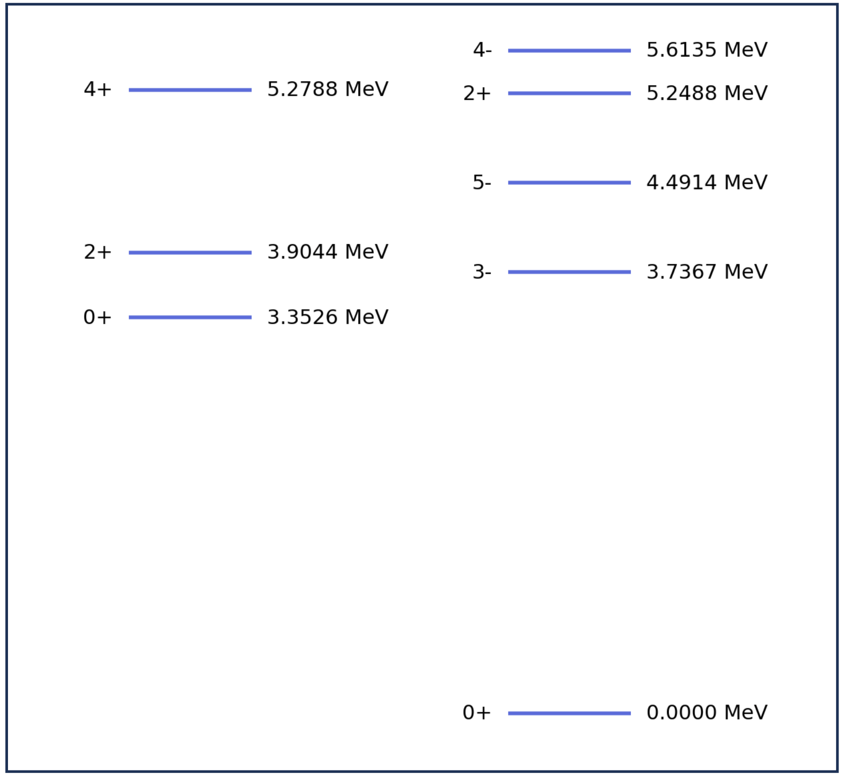


Developing:

HF/CCSD(T): Triaxiality, J-projection

Preliminary results from triaxial CC for ^{40}Ca

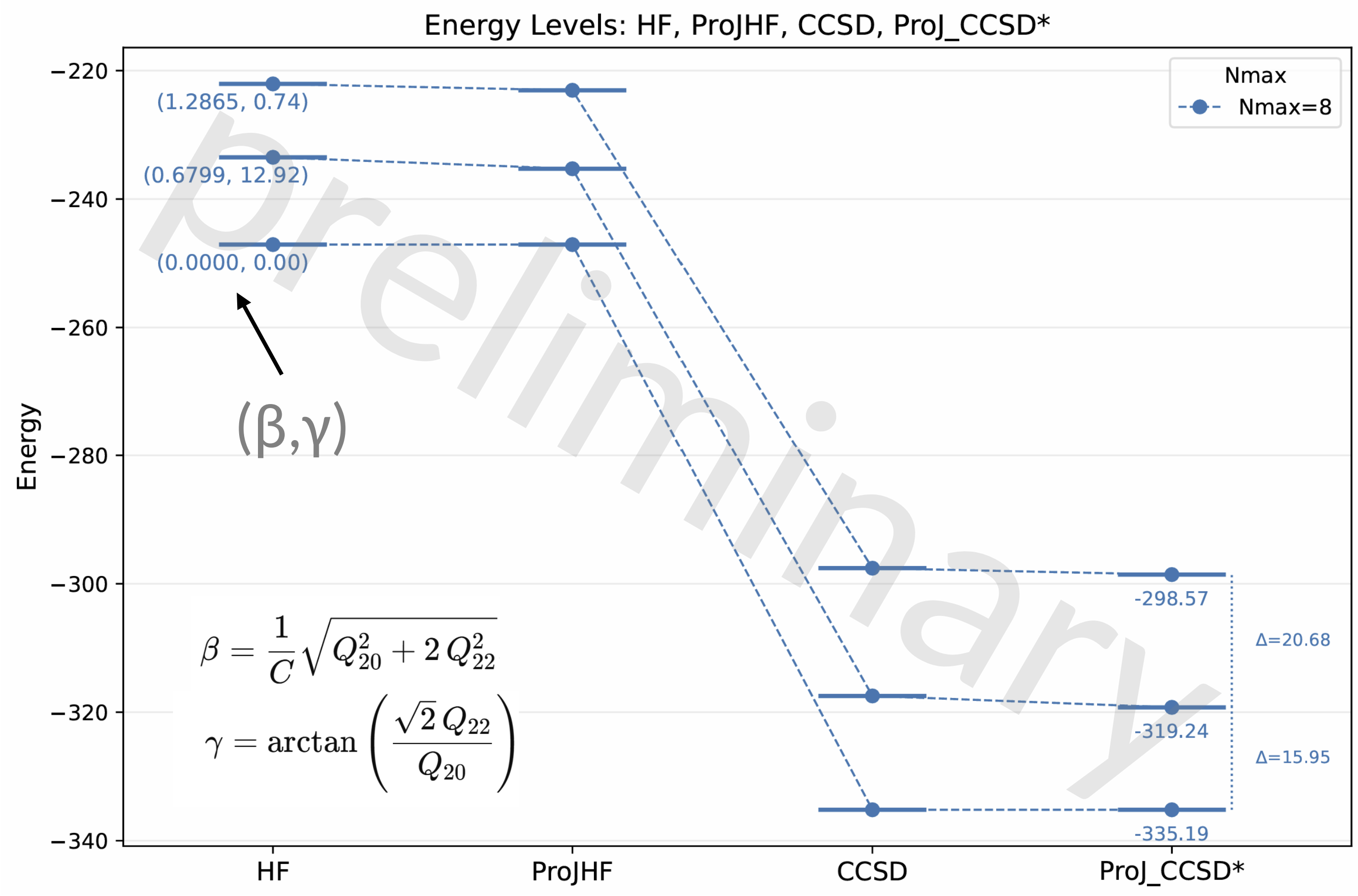
Exp.



$$H = H_0 - \lambda_{q20} \cdot Q_{20} - \lambda_{q22} \cdot Q_{22}$$

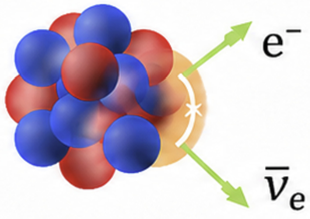
$$< H_0 >< Q_{20} >< Q_{22} >$$

Projected triaxial HF and triaxial CC



EM 1.8/2.0 with e_{max}=8

Toward NMEs with triaxial reference states

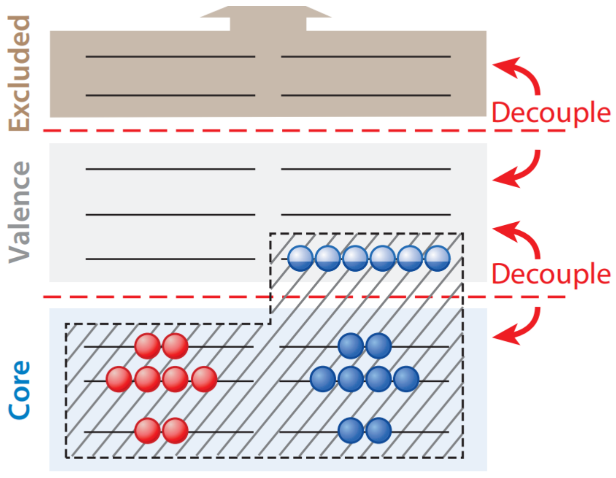


Outline:

- Status of Coupled-cluster development
- Preliminary results from VS-IMSRG(3f2)

  Alex Todd, Antoine Belley, J. D. Holt, S. R. Stroberg
- Application to superallowed beta decay

VS-IMSRG: Valence Space In-medium similarity renormalization group



flow parameter

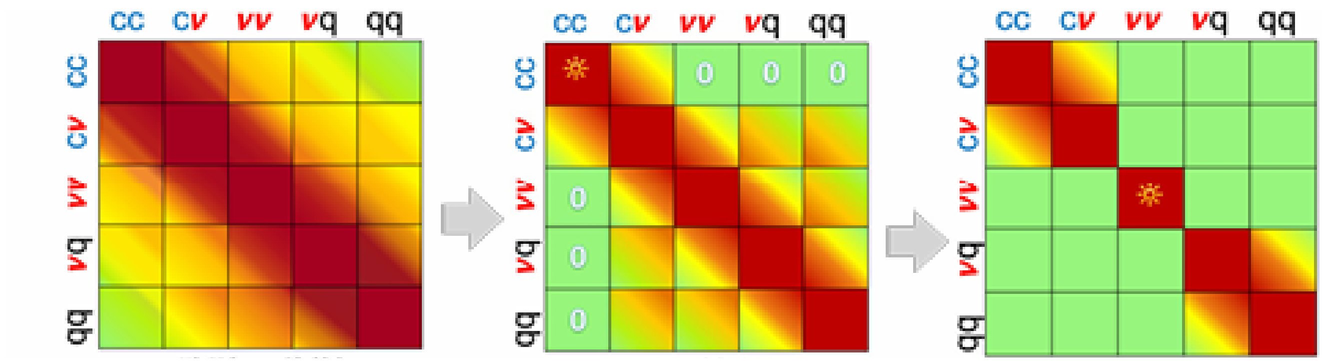
$$\frac{\mathrm{d}H(s)}{\mathrm{d}s} = [\eta(s), H(s)]$$

flow equation

$$H(s) = U(s)\ H\ U^{\dagger}(s)$$

Baker–Campbell–Hausdorff

$\langle \phi_i | H | \phi_j \rangle$



Initial Hamiltonian → Evolving Hamiltonian → Decoupled Hamiltonian

IMSRG(2) Two-body truncation (≈ $O(N^6)$ cost)

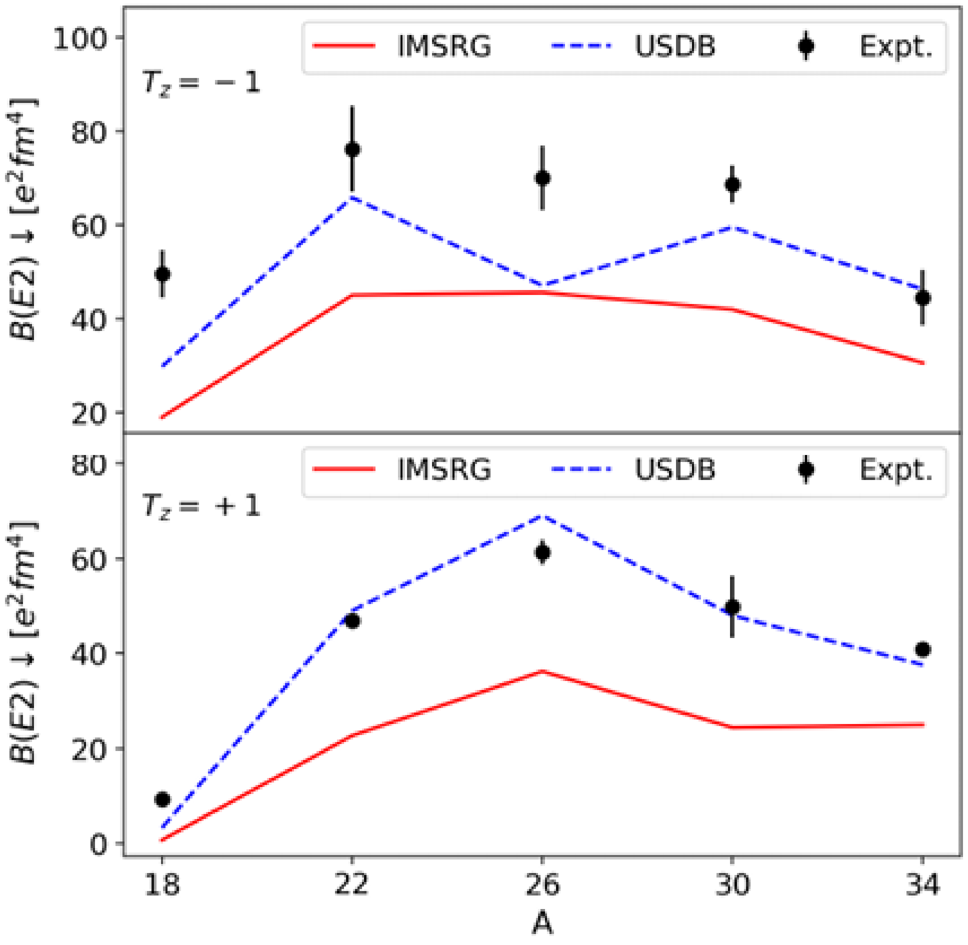
IMSRG(3n7) Complexity scale (≈ $O(N^7)$ cost)

IMSRG(3) Three-body truncation (≈ $O(N^9)$ cost)

IMSRG(2A) A-body truncation Exact solution

Problem: IMSRG(2) **underestimates** B(E2)

B(E2)↓values for(top) Tz=−1 and (bottom) Tz=+1 nuclei.



Stroberg et al. (2022), Phys. Rev. C 105, 034333

E2 transitions provide sensitive probes of nuclear deformation and collective motion.

Possible reason:

- Interaction
- E2 operator
- Many-body truncation: IMSRG(2)

Motivates introducing full IMSRG(3) treatment

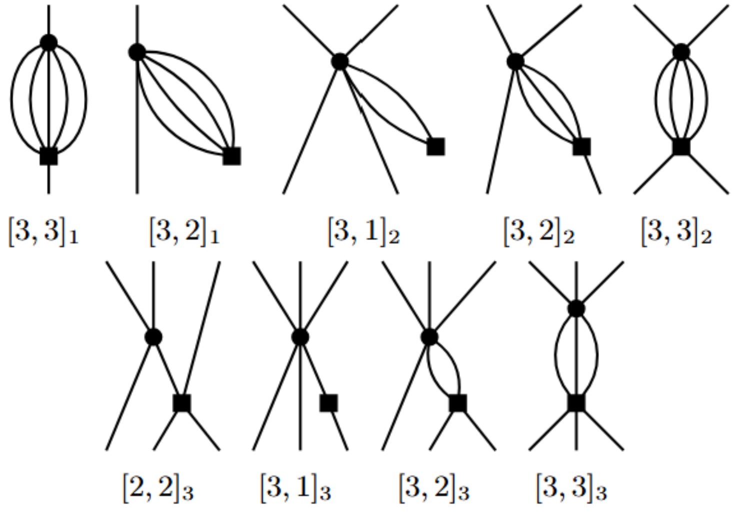
Full IMSRG(3) treatment of Hamiltonians and Observables

Effective Hamiltonian (scalar)

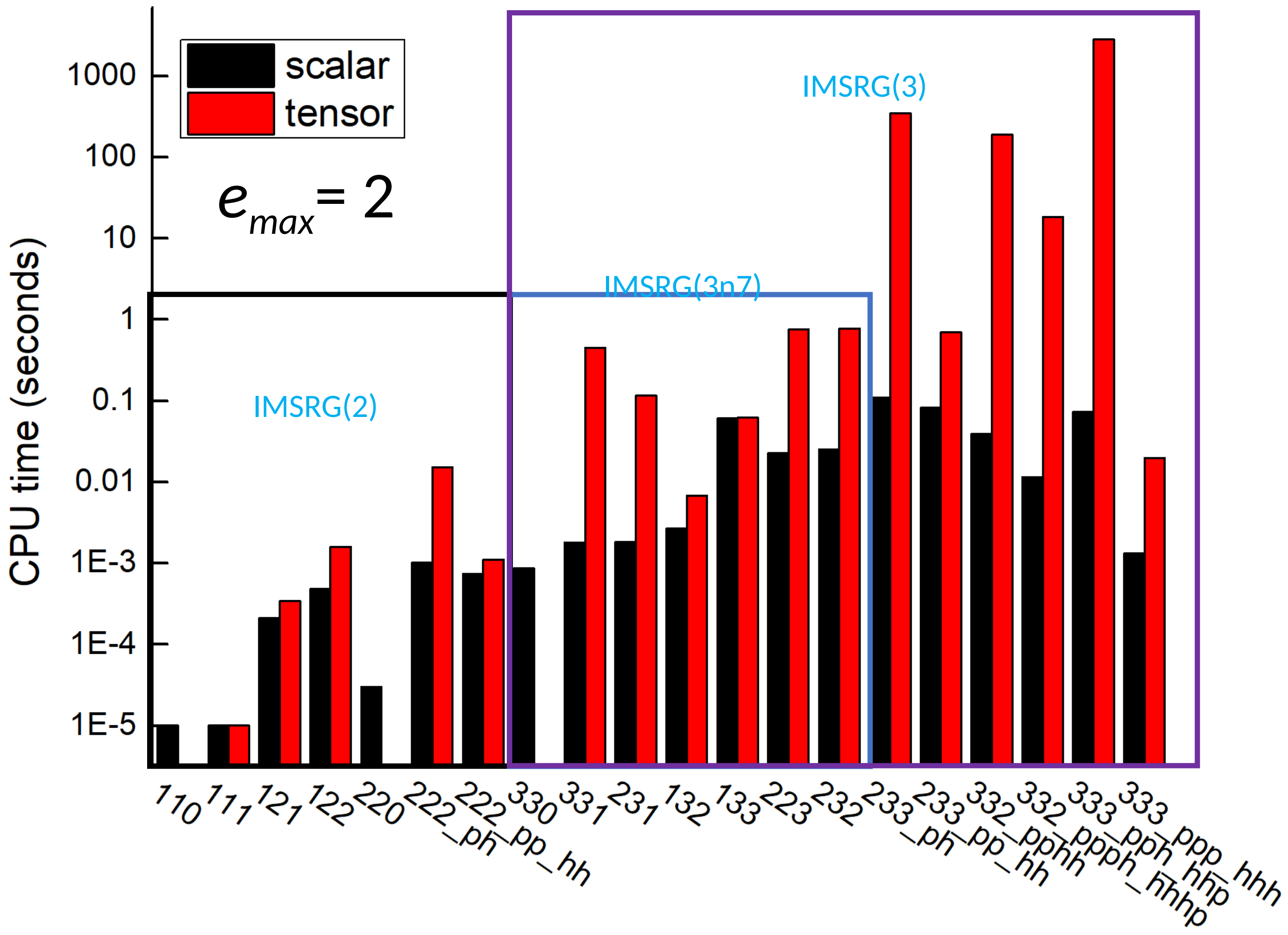
$$\mathcal{H}_{eff} = e^{\Omega}\mathcal{H}e^{-\Omega}$$

Effective operators (tensor)

$$\mathcal{O}_{eff} = e^{\Omega}\mathcal{O}e^{-\Omega}$$ (E2, M1, etc.)

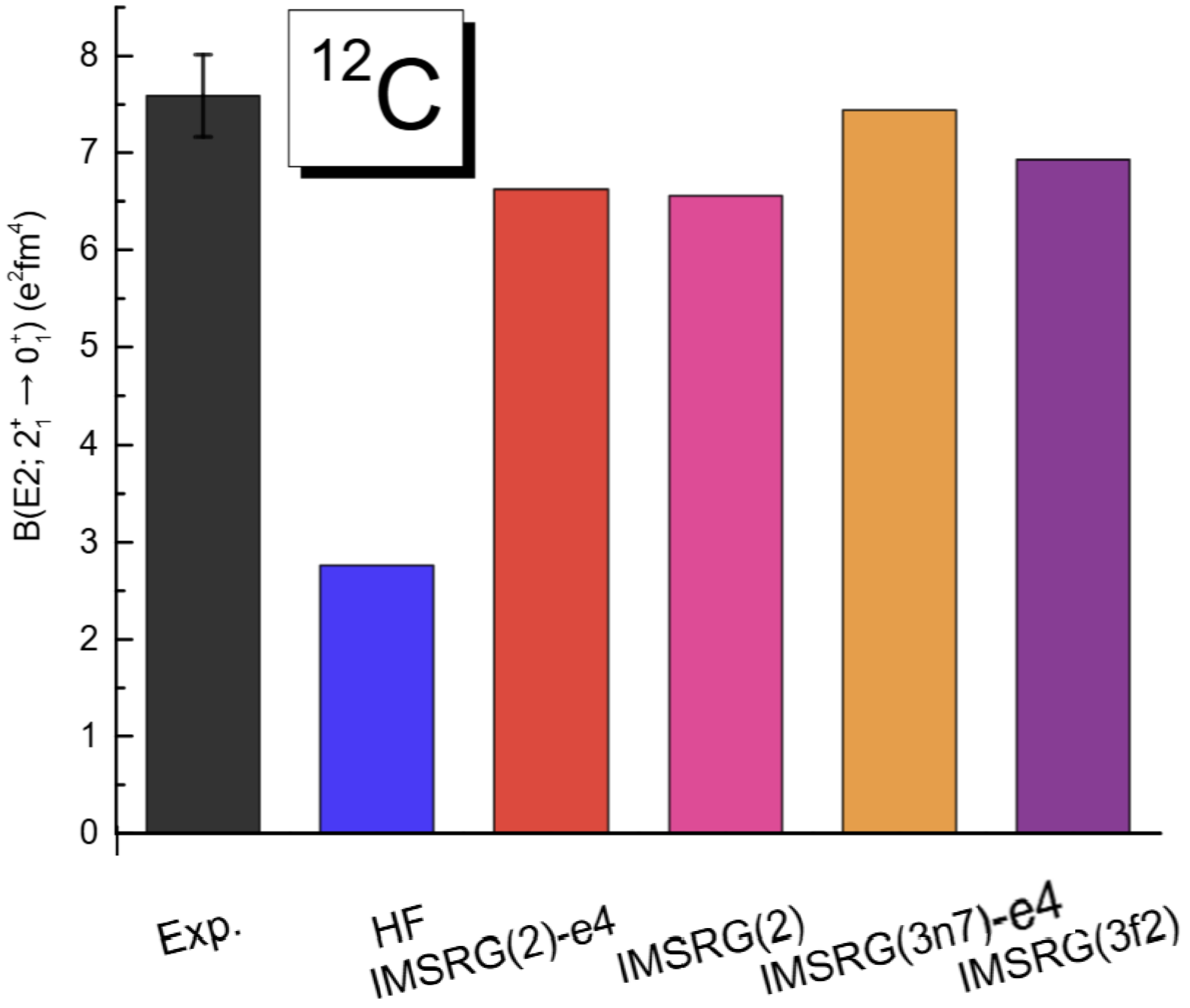


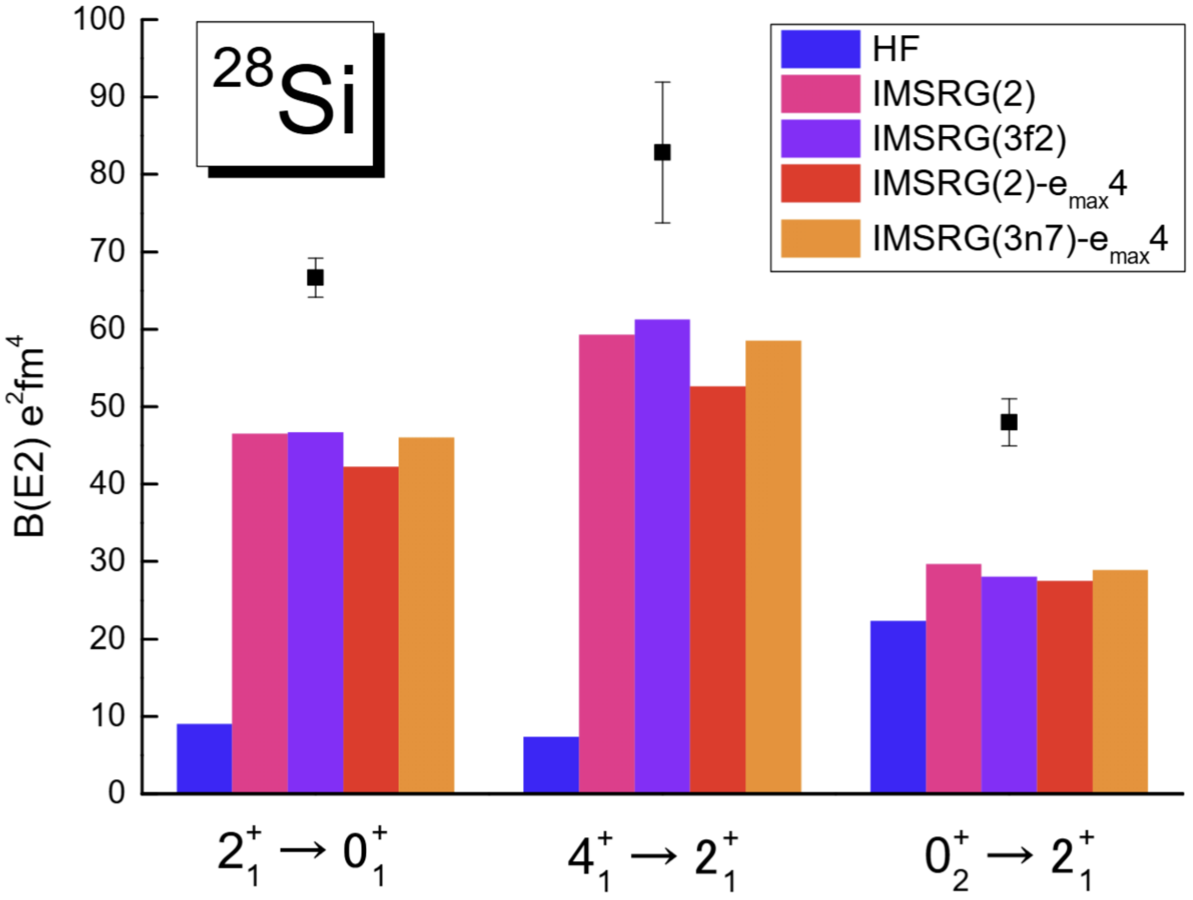
CPU time for one commutator [O, Ω]



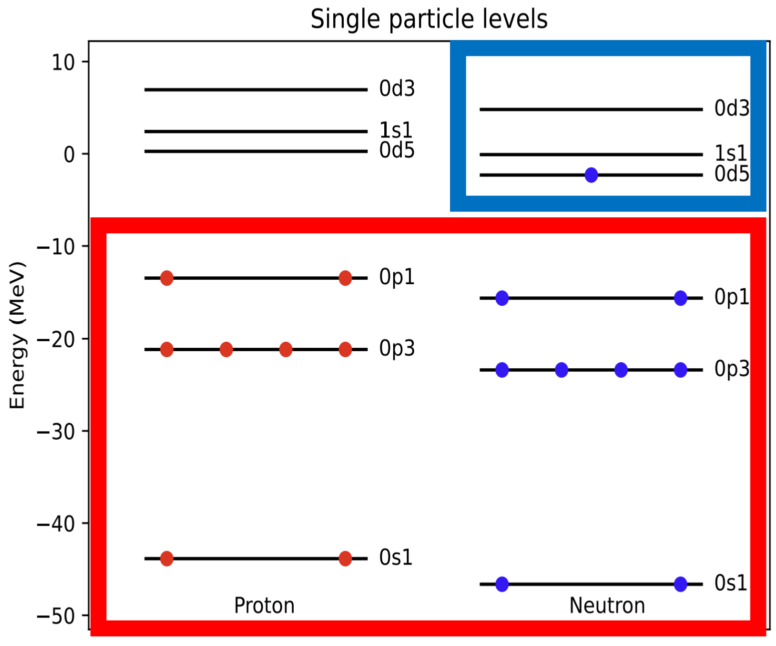
B. He and S. R. Stroberg, *Induced Three-Body Effects on E2 Observables with IMSRG(3)*, in preparation.

Transitions in ^{12}C and ^{28}Si





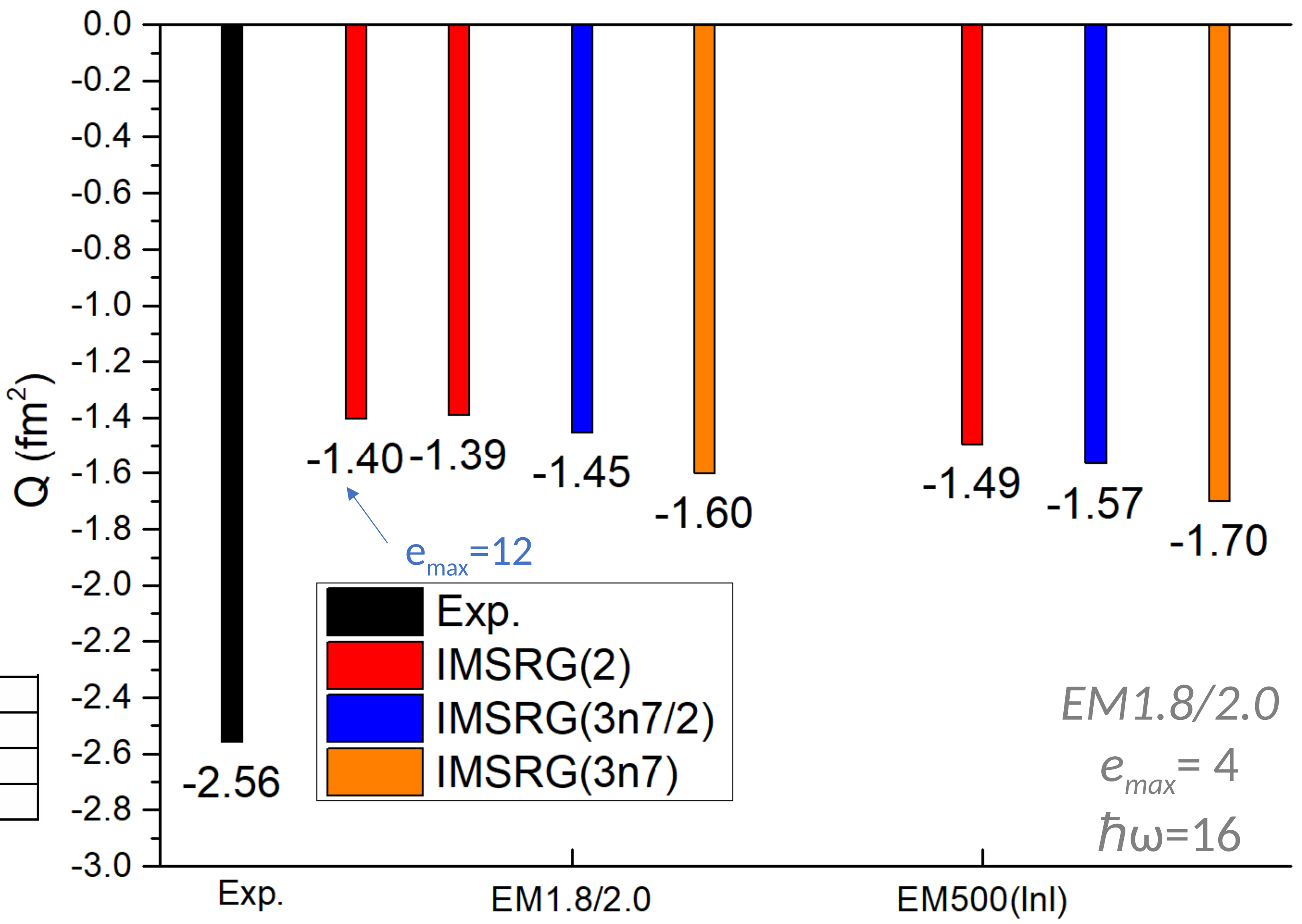
Quadrupole Moment of ^{17}O: Sensitivity to Induced 3-Body operator



Ground state energy (MeV)

Exp.	-131.750
IMSRG(2)_emax12	-130.777
IMSRG(2)	-121.359
IMSRG(3n7)	-121.453

EM1.8/2.0



Quadrupole observables remain puzzling in VS-IMSRG

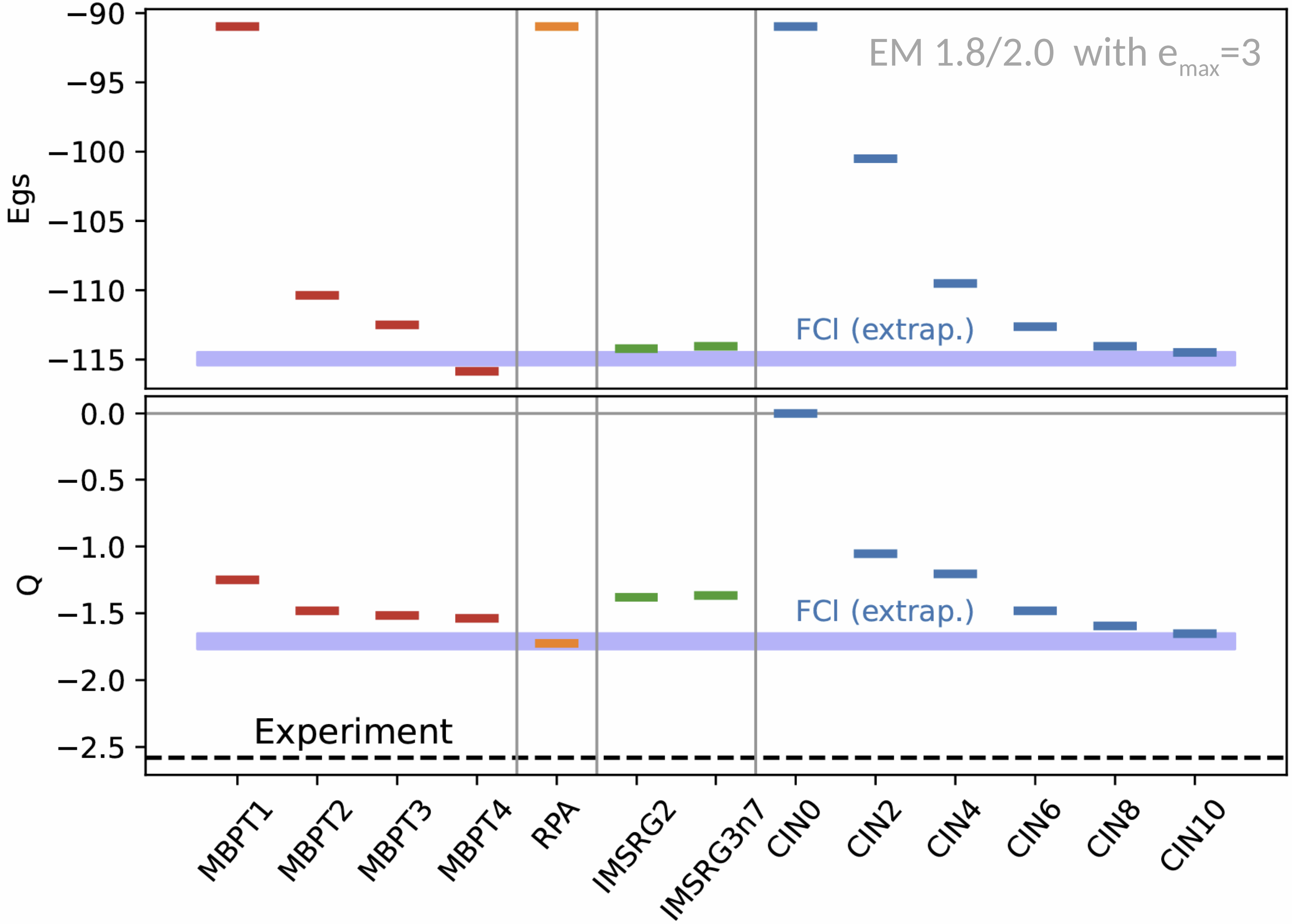


Figure courtesy of Ragnar Stroberg and Zhonghao Sun

Improving VS-IMSRG: IMSRG(3f2)

IMSRG(2) Two-body truncation
(≈ O(N^6) cost)

IMSRG(3f2)

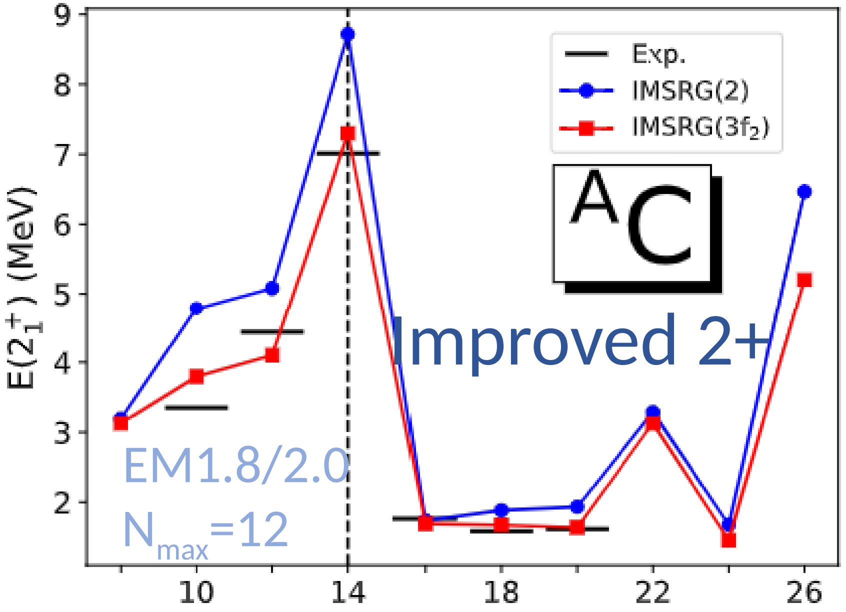
Factorized double commutators

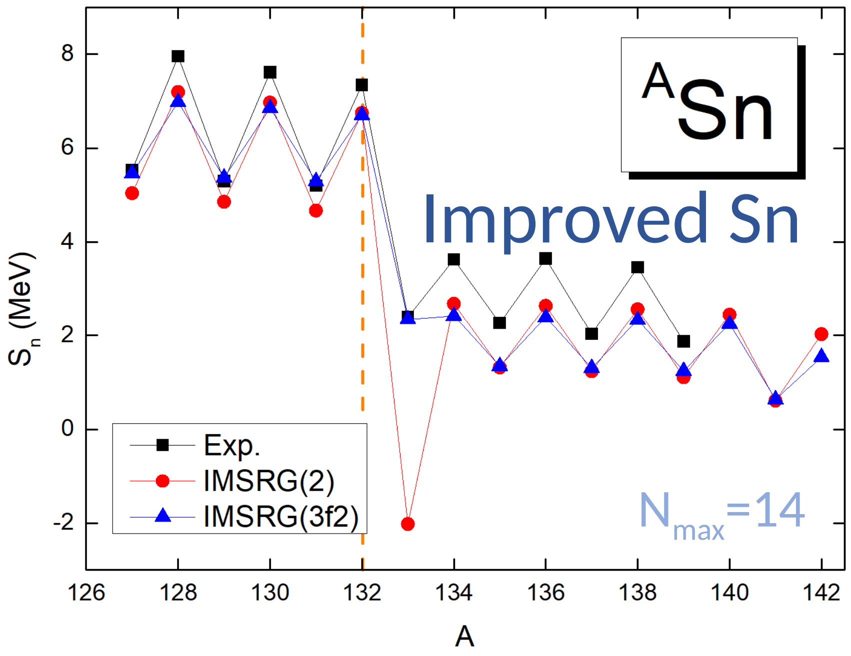
IMSRG(3n7)

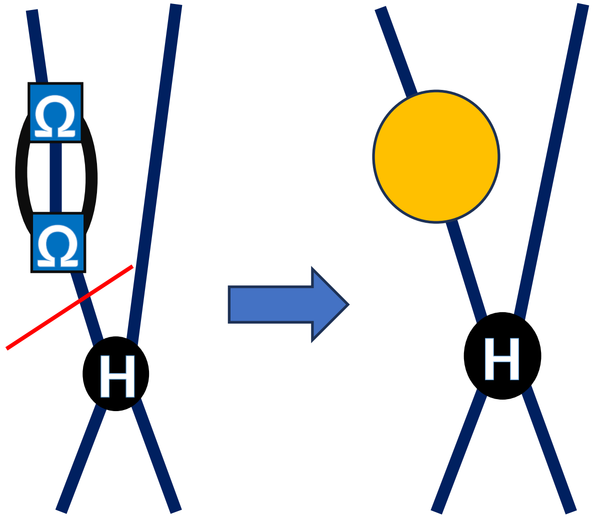
Complexity scale
(≈ O(N^7) cost)

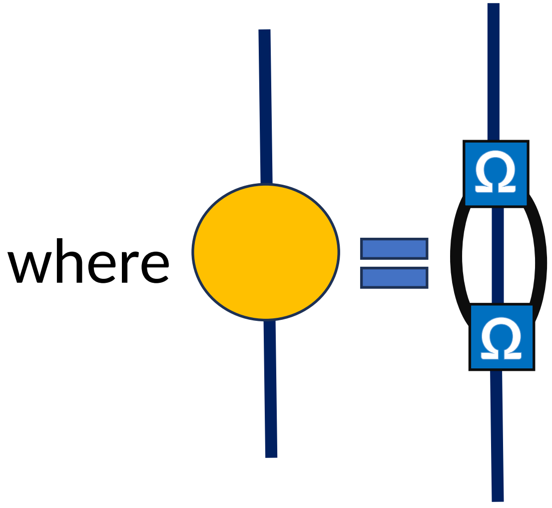
IMSRG(3) Three-body truncation
(≈ O(N^9) cost)

IMSRG(2A) A-body truncation
Exact solution





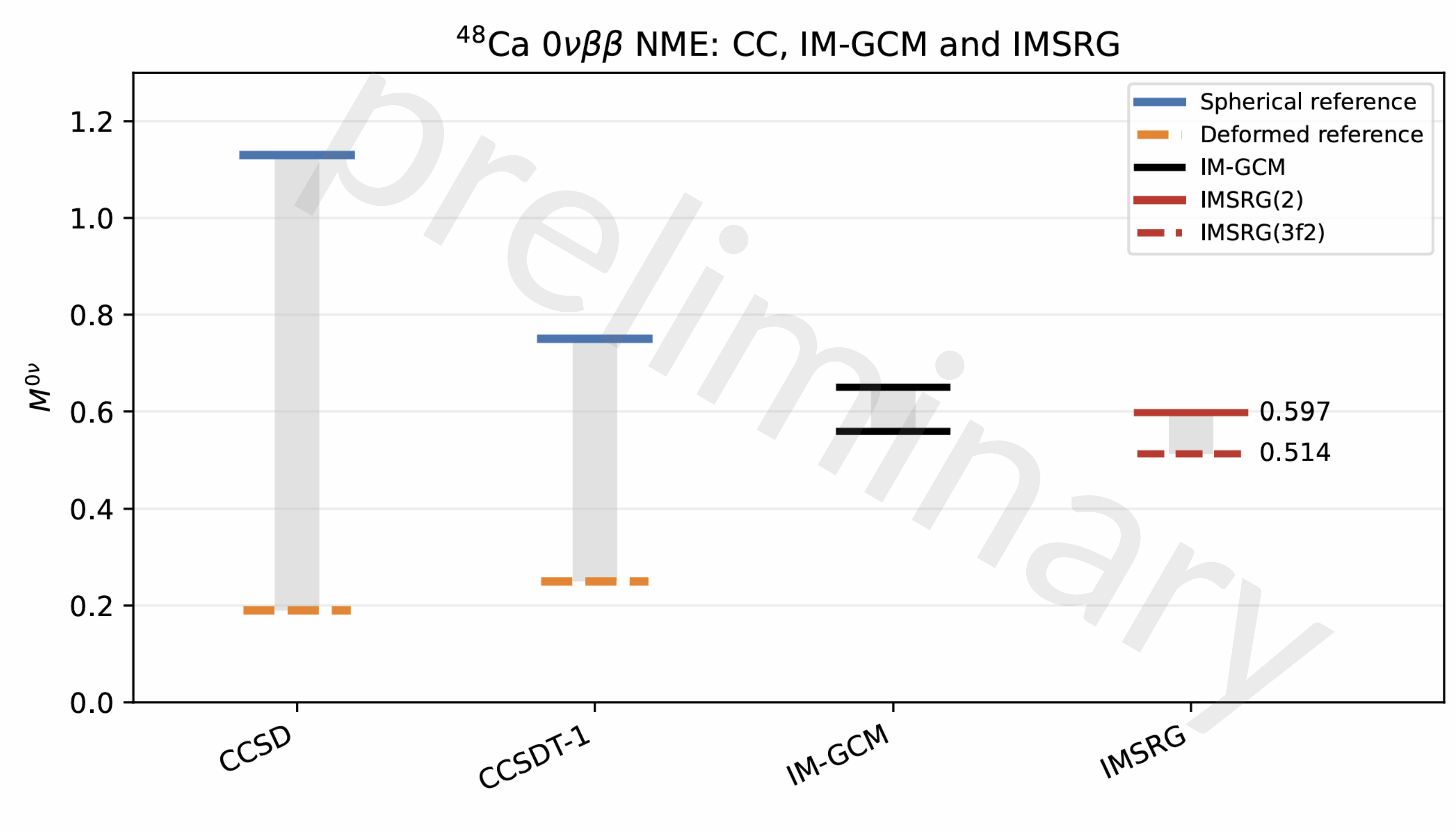


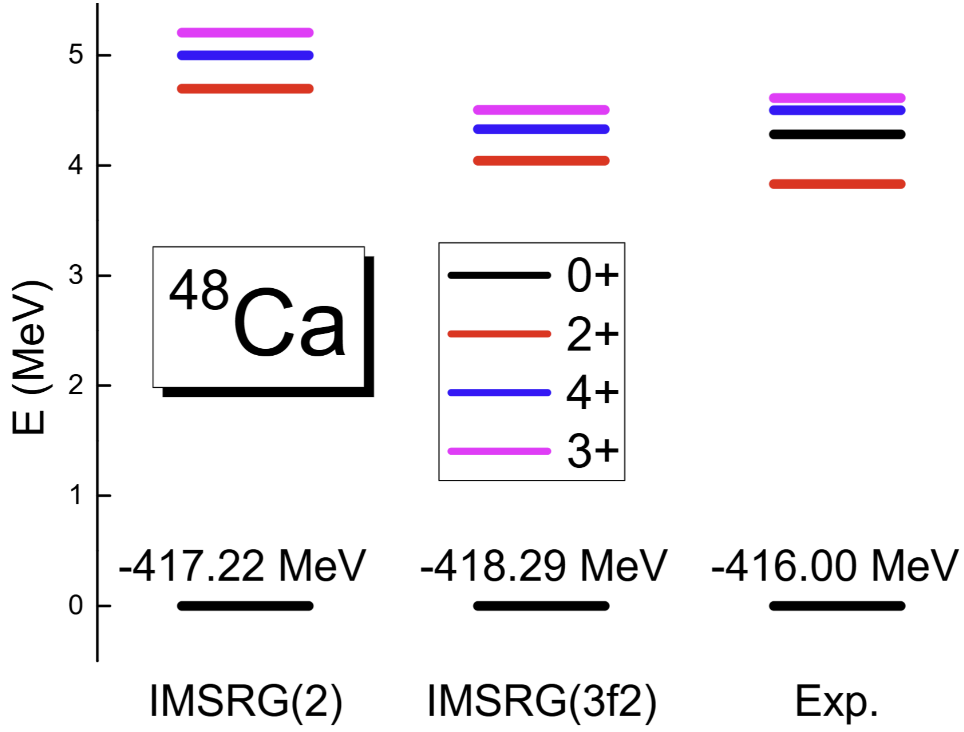


Intermediate 1b

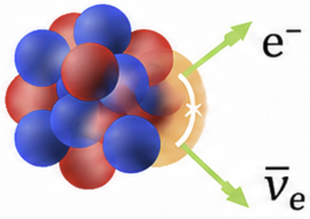
B. C. He and S. R. Stroberg, PRC,110,044317 (2024)

Preliminary results of ^{48}Ca from VS-IMSRG(3f2)





EM 1.8/2.0 with e_{max}=12



Outline:

- Status of Coupled-cluster development
- Preliminary results from VS-IMSRG(3f2)
- Application to superallowed beta decay

BCH, Mikhail Gorchtein , Matthias Heinz, Ben Ohayon , Lucas Platter, Chien-Yeah Seng
arXiv:2605.13985

Help on testing of CKM unitarity

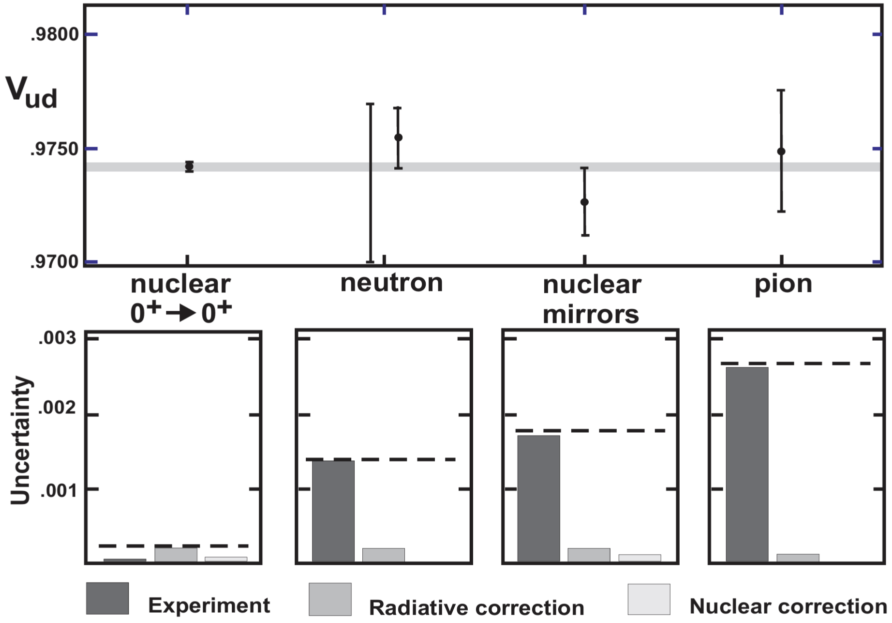
In SM, CKM matrix is unitary, describing the strength of flavor-changing weak interaction

Cabibbo Kobayashi Maskawa

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

$$\underset{\sim 0.95}{|V_{ud}|^2} + \underset{\sim 0.05}{|V_{us}|^2} + \underset{\sim 10^{-5}}{|V_{ub}|^2} = 0.9985(6)_{V_{ud}}(4)_{V_{us}}$$

sub-permille level



J.C. Hardy and I.S. Towner, arXiv:1807.01146v1

$$\mathcal{F}t \equiv ft(1 + \delta'_{\rm R})(1 + \delta_{\rm NS} - \delta_{\rm C})$$

statistical rate function

$$= \frac{K}{2G_F^2 V_{ud}^2 (1 + \Delta_R^v)}$$

How to determine the statistical rate function *f*

$$f = m_e^{-5} \int_{m_e}^{E_0} pE(E_0 - E)^2 F(E) C(E) Q(E) R(E) r(E)\, dE$$

Fermi function — $(E_0-E)^2$ … $F(E)$; shape factor — $C(E)$; atomic screening — $Q(E)$; kinematic recoil — $R(E)$; atomic overlap — $r(E)$

Nuclear-size and shape dependence enters through $F(E)$ and $C(E)$:

- The Fermi function *F(E)* solving the Dirac equation $\rho_{\text{ch}}(r)$
- The shape factor *C(E)*, computed from a charged weak density $\rho_{\text{cw}}(r)$

Model-Independent Determination of Nuclear Weak Form Factors

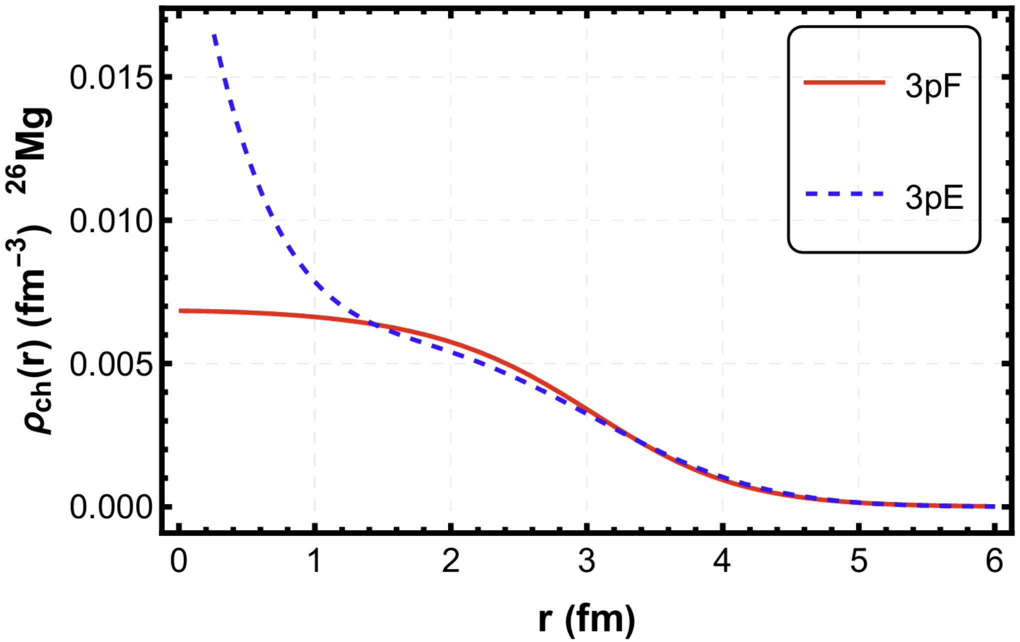
$$\rho_{\text{cw}} = \rho_{\text{ch}}^{1} + Z_0(\rho_{\text{ch}}^{0} - \rho_{\text{ch}}^{1}) = \rho_{\text{ch}}^{1} + (Z_{-1}/2)(\rho_{\text{ch}}^{-1} - \rho_{\text{ch}}^{1})$$

$$2Z_0\rho_{\text{ch}}^{0} = Z_1\rho_{\text{ch}}^{1} + Z_{-1}\rho_{\text{ch}}^{-1}$$

Chien-Yeah Seng, PRL, 130, 152501 (2023)

The statistical rate function *f* depends on nuclear size.

Nuclear charge density for 26Mg in two different models with the first three moments fixed:
$\langle r^2\rangle = 9.1809\text{fm}^2$, $\langle r^4\rangle = 125.521\text{fm}^4$, $\langle r^6\rangle = 2204.11\ \text{fm}^6$



The three-parameter Fermi (**3pF**) model:

$$\rho_{3\text{pF}}(r; c, a, w) = \rho_0 \frac{1 + wr^2/c^2}{1 + \exp[(r-c)/a]}$$

Three-parameter exponential (**3pE**) model:

$$\rho_{3\text{pE}}(r; R_1, R_2, R_3) = C_1\, \rho_{1\text{pE}}(r; R_1) + C_2\, G_2(r) + C_3\, G_3(r)$$

$$G_i(r) \equiv \frac{\exp\left[-\frac{(r-R_i)^2}{\gamma^2}\right] + \exp\left[-\frac{(r+R_i)^2}{\gamma^2}\right]}{2\pi^{3/2}\gamma\left(2R_i^2 + \gamma^2\right)}$$

$$\rho_{1\text{pE}}(r; R) = \frac{3\sqrt{3}}{\pi R^3} \exp\left(-\frac{2\sqrt{3}\, r}{R}\right)$$

Fix $\langle r^2\rangle$,$\langle r^4\rangle$ and $\langle r^6\rangle$ → *f* model independent

f values:

$$^{10}\text{C} \to {}^{10}\text{B}^* \ :\ 2.30160\ (3\text{pF})\ \text{vs.}\ 2.30161\ (3\text{pE})$$

$$^{26\text{m}}\text{Al} \to {}^{26}\text{Mg} \ :\ 478.027\ (3\text{pF})\ \text{vs.}\ 478.034\ (3\text{pE})$$

≤ 0.001%

The precision goal for Vud is **0.01%**..

Computing r moments from ab initio methods

It's hard for VS-IMSRG to evaluate r^4 and r^6 directly:

$$\mathcal{H}_{eff} = e^{\Omega}\mathcal{H}e^{-\Omega} \qquad \mathcal{O}_{eff} = e^{\Omega}\mathcal{O}e^{-\Omega}$$

Extracting charge moments from low-q form factors:

$$F_{\text{ch}}(q^2) = e\sum_{i=1}^{A}\left\{G_E^i(q^2)\left(1 - \frac{q^2}{8m^2}\right)j_0(qr_i) - \frac{q^2}{2m^2}\left[G_M^i(q^2) - \frac{1}{2}G_E^i(q^2)\right](\ell_i\cdot\sigma_i)\frac{j_1(qr_i)}{qr_i}\right\}$$

$$\left\langle r^2\right\rangle_{\text{ch}} = -6\left.\frac{d\widetilde{F}_{\text{ch}}}{dx}\right|_{x=0},$$

$$\left\langle r^4\right\rangle_{\text{ch}} = 60\left.\frac{d^2\widetilde{F}_{\text{ch}}}{dx^2}\right|_{x=0},$$

$$\left\langle r^6\right\rangle_{\text{ch}} = -840\left.\frac{d^3\widetilde{F}_{\text{ch}}}{dx^3}\right|_{x=0}.$$

$$\widetilde{F}_{\text{ch}}(q) \equiv \frac{F_{\text{ch}}(q)}{F_{\text{ch}}(0)}$$

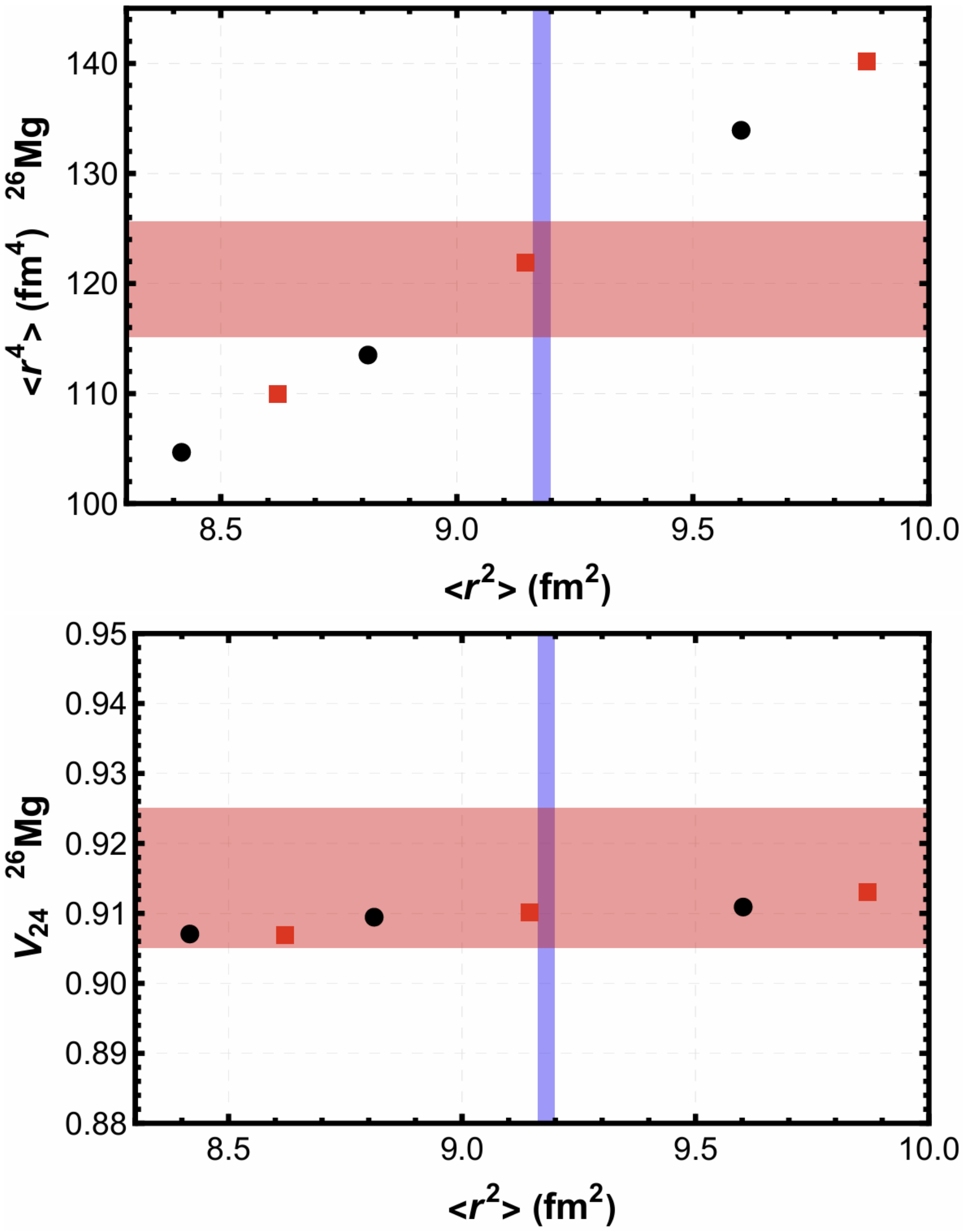
center-of-mass contamination

$$F_{\text{ch}}^{\text{int}}(q^2) = e^{q^2 b_{\text{cm}}^2/4}F_{\text{ch}}(q^2)_{2})$$

Mesh grid size:

- IMSRG(2) q goes up to 1 GeV
- IMSRG(3f2) q < 200 MeV

R moments and V factors



Many-body methods:

- IMSRG(2)
- IMSRG(3f2)

Nuclear interactions:

- 1.8/2.0 (EM)
- 1.8/2.0 (EM7.5)
- ΔN2LO$_{GO}$(394)

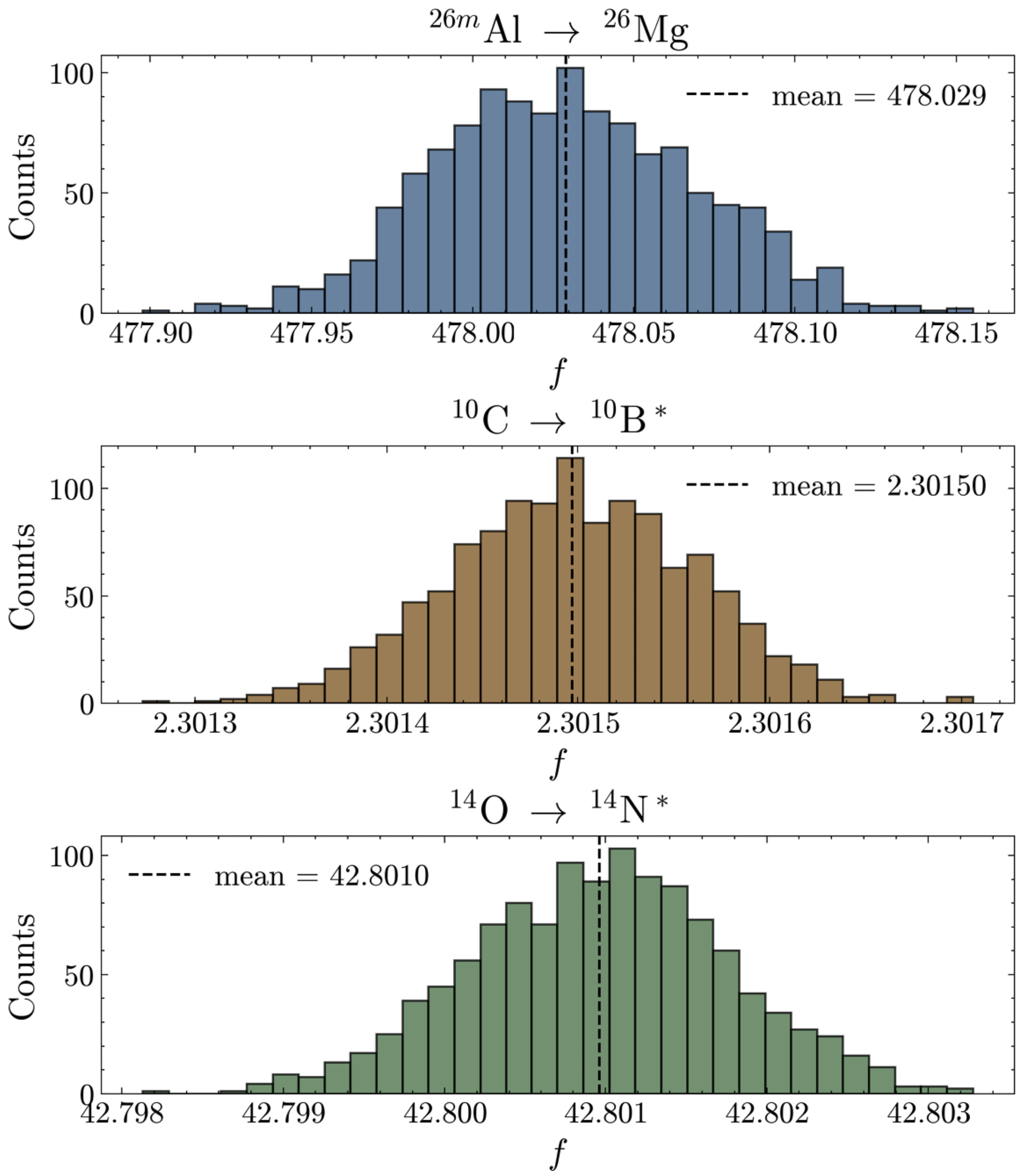
Dimensionless moment ratios:

$$V_{2\,2n} \equiv \langle r^2 \rangle^{1/2} / \langle r^{2n} \rangle^{1/2n}$$

Moment ratios are more robust than absolute moments:

$$\langle r^2 \rangle_{\text{exp}} + V_{24}^{\text{th}} + V_{26}^{\text{th}} \Rightarrow \langle r^4 \rangle, \langle r^6 \rangle$$

Determining the statistical rate function *f*



Method 1:

$$r_{\rm ch}^{(k)} \sim \text{experimental radius uncertainty}$$

Method 2:

$$r_{\rm ch}^{(k)} \sim \text{experimental radius uncertainty}$$

$$V_{24}^{(k)}, V_{26}^{(k)} \sim \text{ab initio uncertainty.}$$

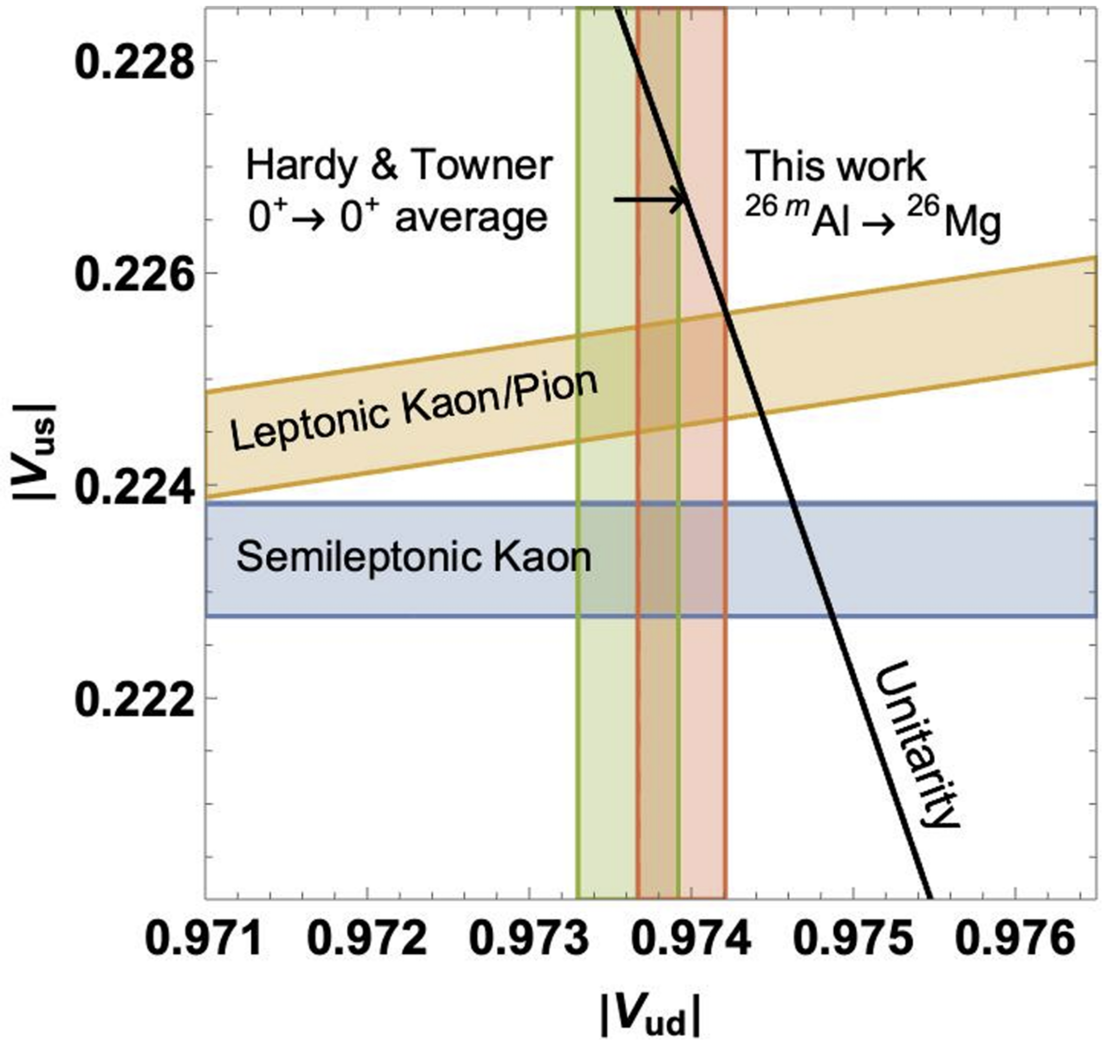
$$^{10}\mathrm{C} \rightarrow {}^{10}\mathrm{B}^* \;:\; f = 2.30150(71)_{Q_{\rm EC}}(43)_{\rm scr}(6)_{\rm den}$$

$$^{14}\mathrm{O} \rightarrow {}^{14}\mathrm{N}^* \;:\; f = 42.8010(77)_{Q_{\rm EC}}(63)_{\rm scr}(8)_{\rm den}$$

$$^{26\rm m}\mathrm{Al} \rightarrow {}^{26}\mathrm{Mg} \;:\; f = 478.029(101)_{Q_{\rm EC}}(82)_{\rm scr}(40)_{\rm den}$$

“den” is the charge density uncertainty, dominated by the charge radii. The V-factor contribution is O(**0.001%**) or smaller

Reduced nuclear-size uncertainty in V_{ud} for ^{26}Al



Using Ft = 3070.16(1.68) from 26mAl decay.

The green vertical band

|Vud| = 0.97373(31)

The red vertical band represents our new result

|Vud| = 0.97394(27)

$$|V_{ud}|^2 = \frac{2984.431(3)\,\mathrm{s}}{\mathcal{F}t(1+\Delta_R^V)}$$

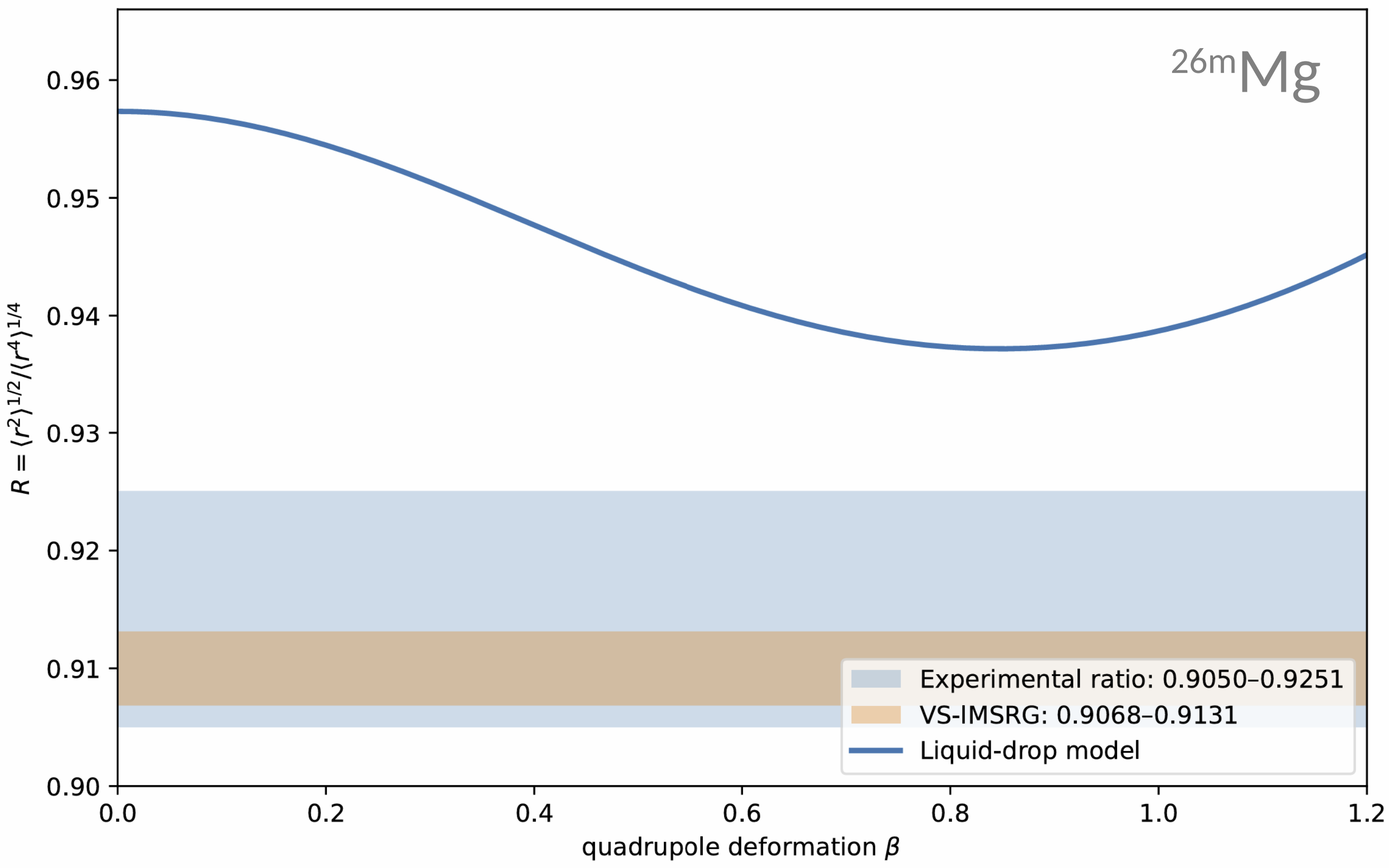
$$\mathcal{F}t \equiv ft(1+\delta'_{\mathrm{R}})(1+\delta_{\mathrm{NS}}-\delta_{\mathrm{C}})$$

$$\Delta_{\mathrm{CKM}} \equiv |V_{ud}|^2 + |V_{us}|^2 + |V_{ub}|^2 - 1$$

Thinking about the moment ratios

$$V_{2,2n}[\rho_{\rm ch}] = \frac{\left[4\pi \int_0^\infty dr\, r^4 \rho_{\rm ch}(r)\right]^{1/2}}{\left[4\pi \int_0^\infty dr\, r^{2n+2} \rho_{\rm ch}(r)\right]^{1/(2n)}}$$

Density is the only quantity we need



$$R(\theta,\phi) = R_0\left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi)\right]$$

$$\mathcal{R}(\beta) \equiv \frac{\langle r^2\rangle^{1/2}}{\langle r^4\rangle^{1/4}} = \frac{\left[\frac{3}{5}\left(1+\frac{5}{4\pi}\beta^2\right)\right]^{1/2}}{\left[\frac{3}{7}\left(1+\frac{7}{2\pi}\beta^2\right)\right]^{1/4}}$$

Ongoing project to understand the ratio in ab initio

Summary

- **Triaxial CCSD** framework is developing for 0νββ NMEs
- **VS-IMSRG(3f2)** enables practical inclusion of leading induced three-body effects in NME calculations
- Ab initio developments also benefit super-allowed β decay

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Finite size correction for Superallowed beta decay

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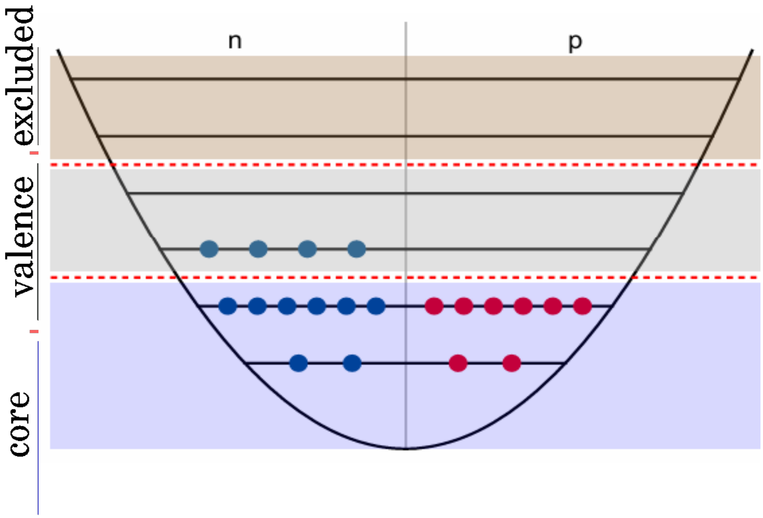
Thank you!

Many-body truncations in the IMSRG

$$H(s) = e^{\Omega(s)} H(0) e^{-\Omega(s)}$$ Baker–Campbell–Hausdorff

$$= H + [\Omega, H] + \frac{1}{2!}[\Omega, [\Omega, H]] + \ldots$$



$[\Omega, H]_{2b}$ IMSRG(2)

$[\Omega, H]_{3b}$ IMSRG(3)

… …

IMSRG(A)

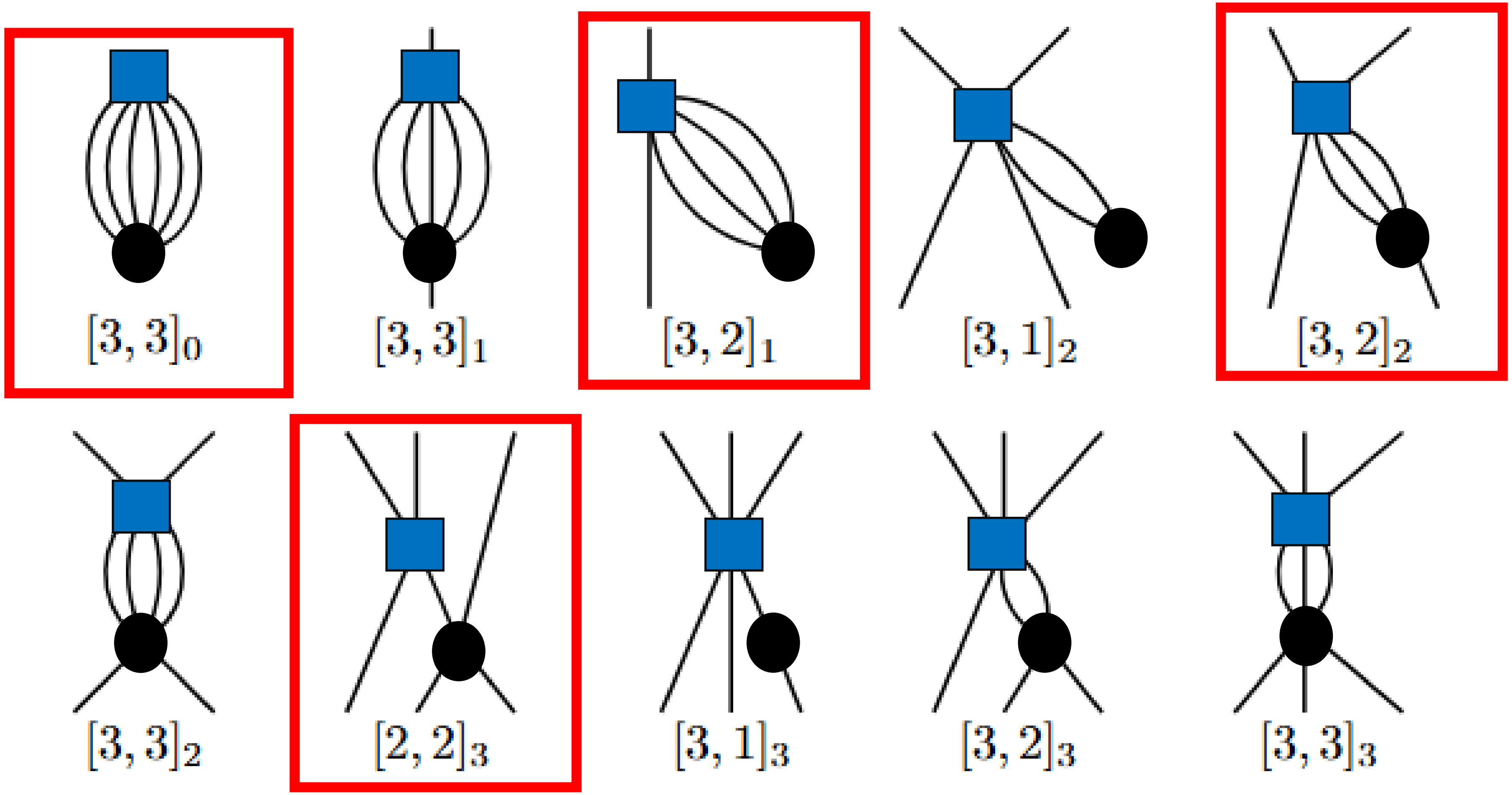
Step 1: Decouple core

Step 2: Decouple valence space

How to truncate IMSRG(3)

$e^{\Omega}\mathcal{H}e^{\Omega}$

$[\Omega, H]$

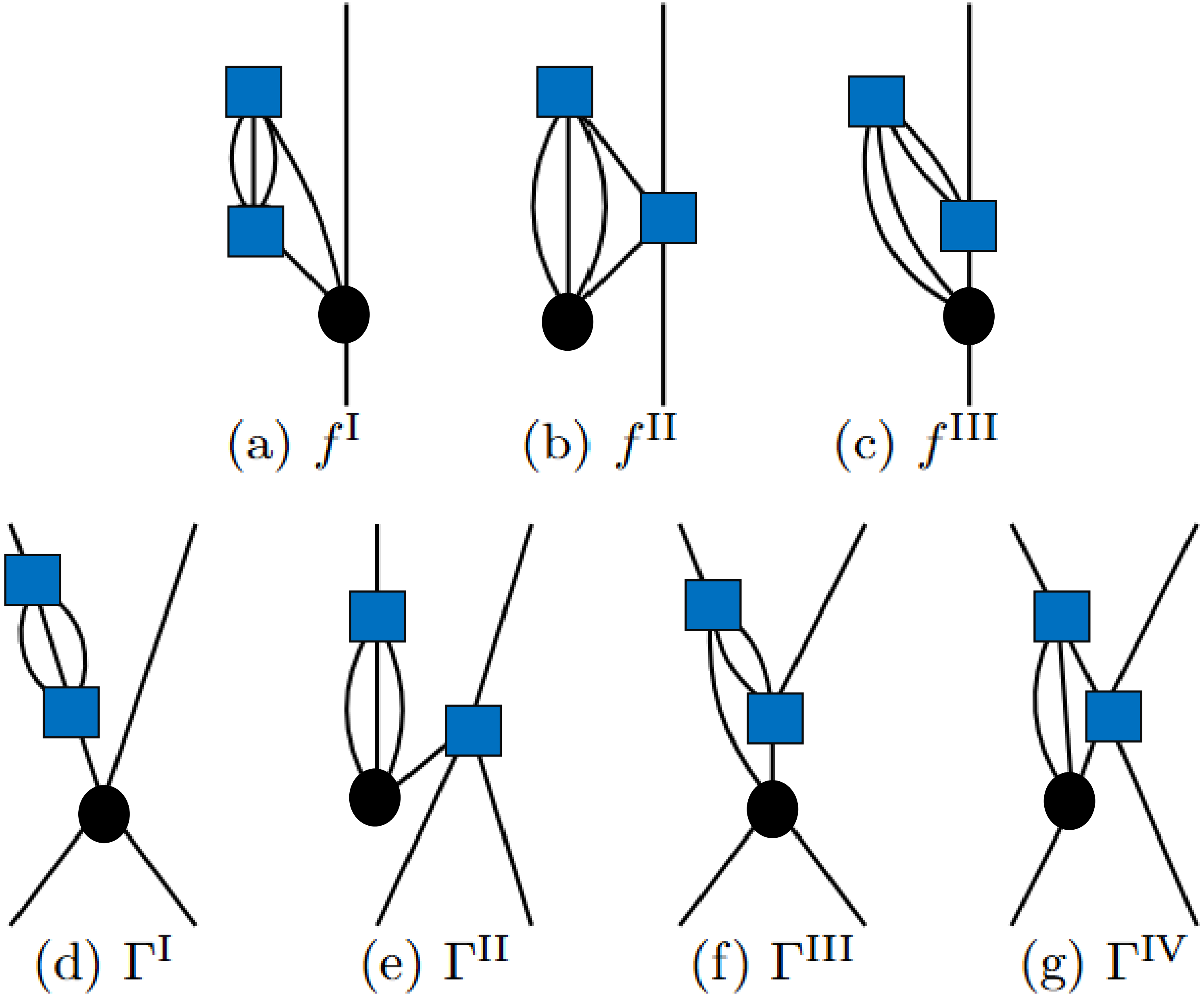


$$[\Omega, [\Omega, H]_{3b}]_{1b,2b}$$

Factorized double commutators

$$[\Omega, [\Omega, H]_{\color{red}{3b}}]_{1b}$$

$$[\Omega, [\Omega, H]_{\color{red}{3b}}]_{2b}$$



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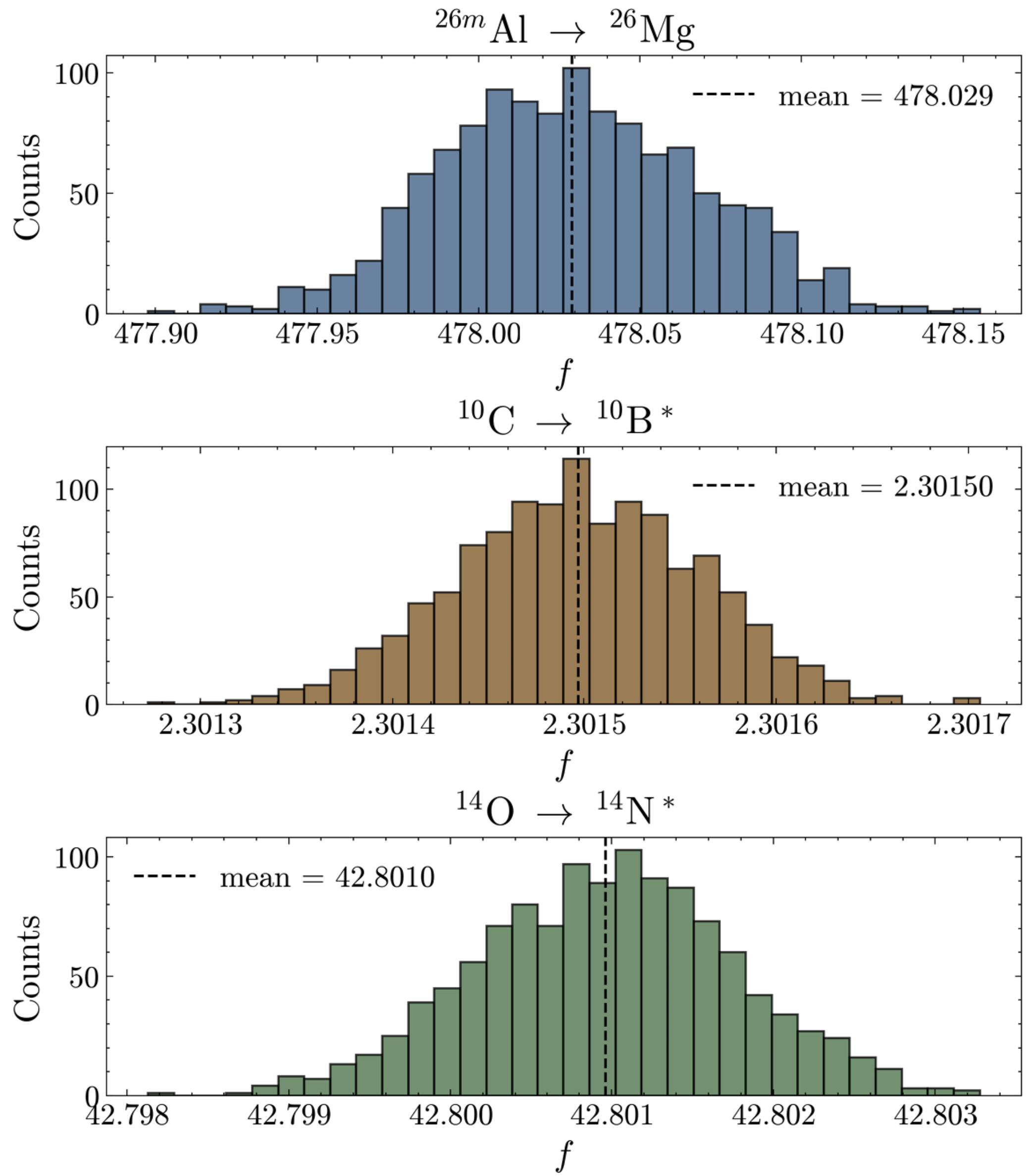
Determining the statistical rate function *f*



Method 1:
With V-factors fixed, we then vary the radii between the central and maximum values. This provides a straightforward assessment of uncertainty.

Method 2:
We randomly sample a large ensemble of charge densities by varying both radii and V-factors within their uncertainties, compute f for each sample, and take the standard deviation of the resulting distribution as the combined uncertainty from the radii and ab initio calculations.

$$^{10}\mathrm{C} \to {}^{10}\mathrm{B}^* \;:\; f = 2.30150(71)_{Q_{\mathrm{EC}}}(43)_{\mathrm{scr}}(6)_{\mathrm{den}}$$
$$^{14}\mathrm{O} \to {}^{14}\mathrm{N}^* \;:\; f = 42.8010(77)_{Q_{\mathrm{EC}}}(63)_{\mathrm{scr}}(8)_{\mathrm{den}}$$
$$^{26\mathrm{m}}\mathrm{Al} \to {}^{26}\mathrm{Mg} \;:\; f = 478.029(101)_{Q_{\mathrm{EC}}}(82)_{\mathrm{scr}}(40)_{\mathrm{den}}$$

“den” is the charge density uncertainty, dominated by the charge radii. The V-factor contribution is O(**0.001%**) or smaller