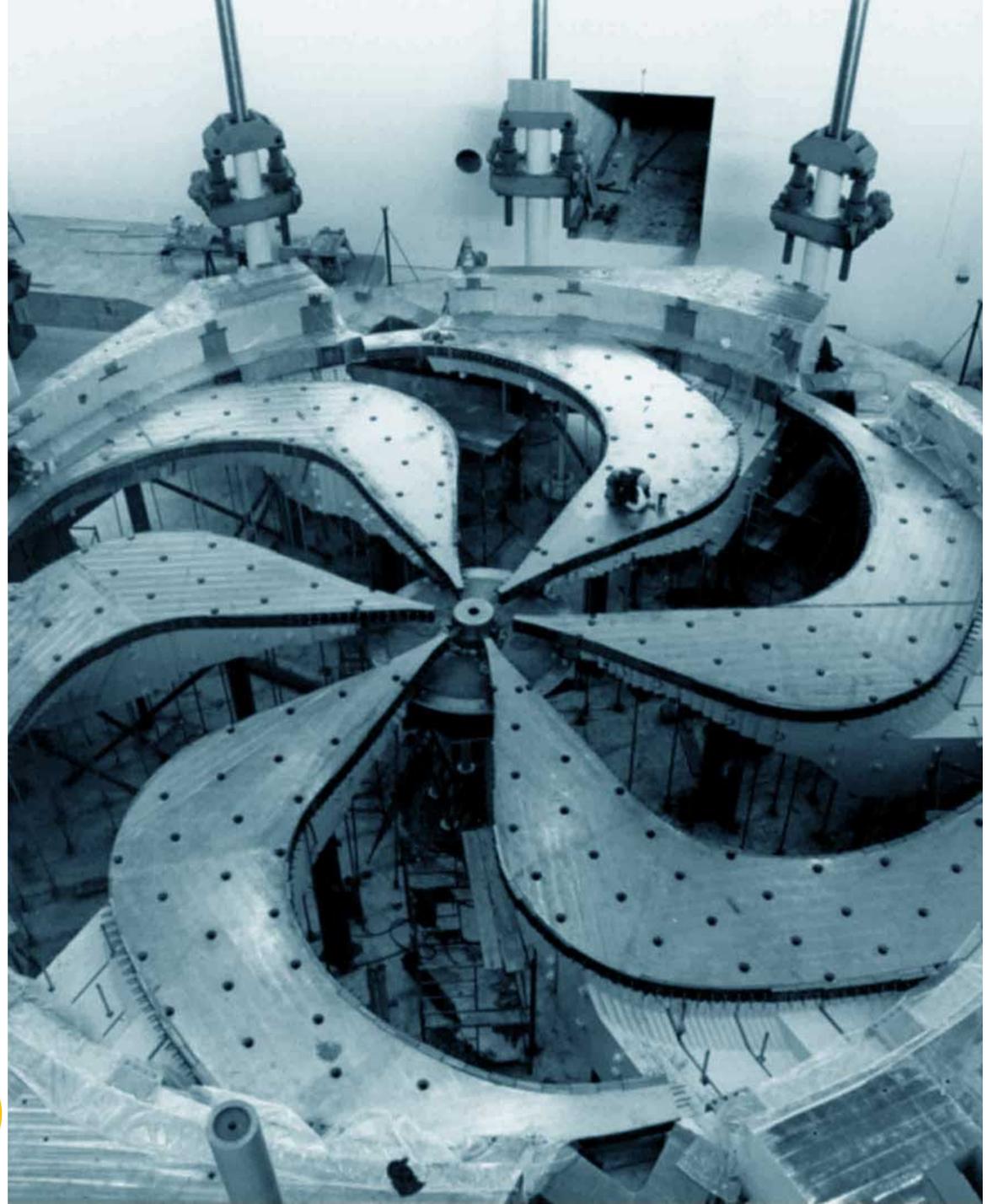


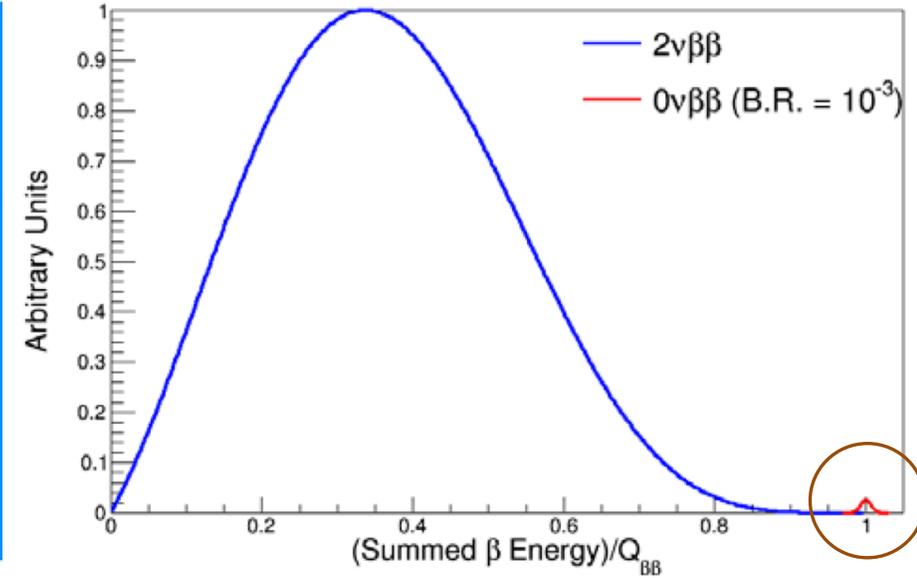
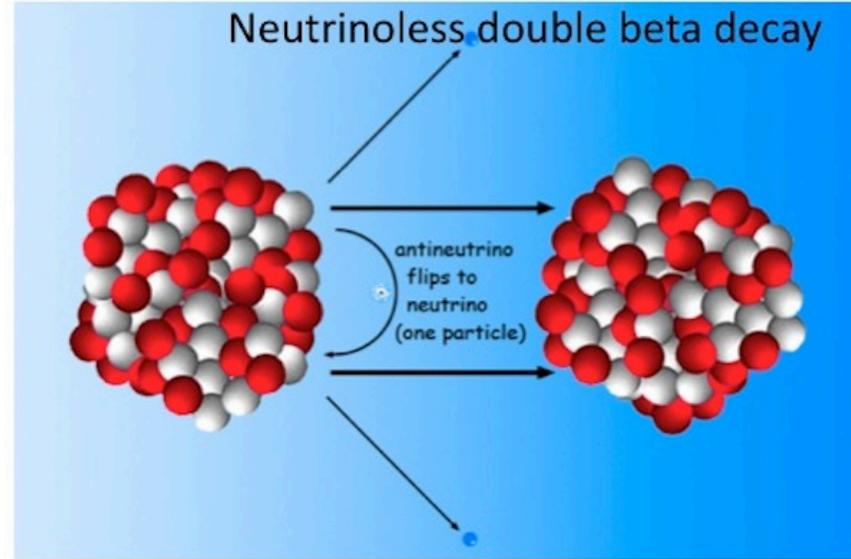
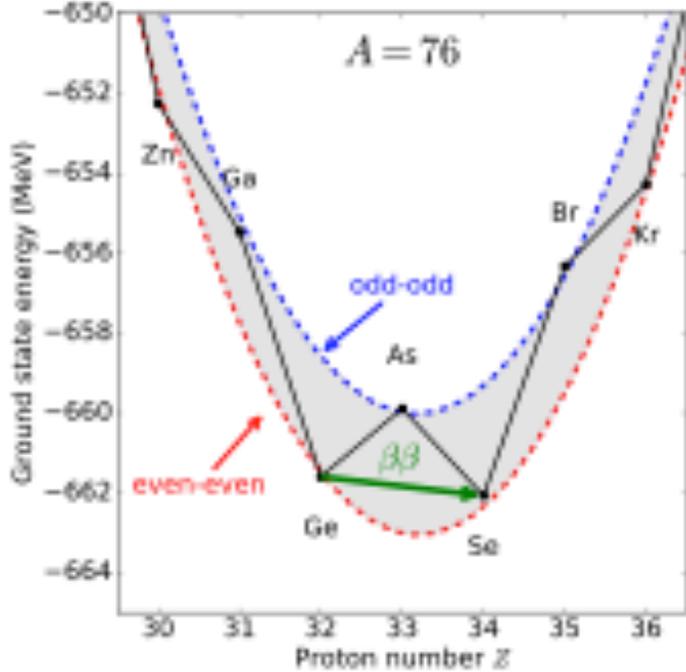
# Ab initio nuclear theory for beyond standard- model physics

Jason D. Holt  
Scientist, Theory Department  
Conference on Neutrino and Nuclear Physics  
February 26, 2020

work of S.R. Stroberg, T. Miyagi



Neutrino own antiparticle  $\longleftrightarrow$   $0\nu\beta\beta$  decay



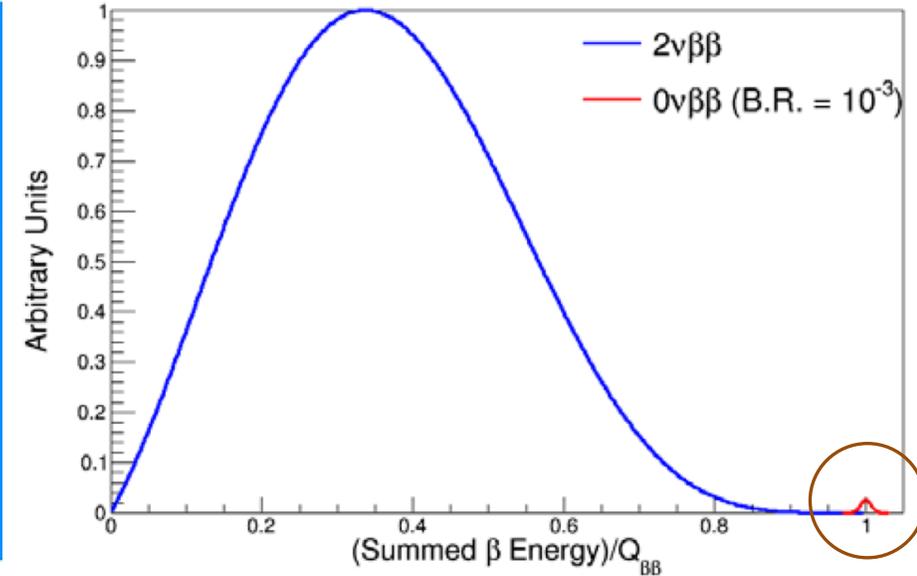
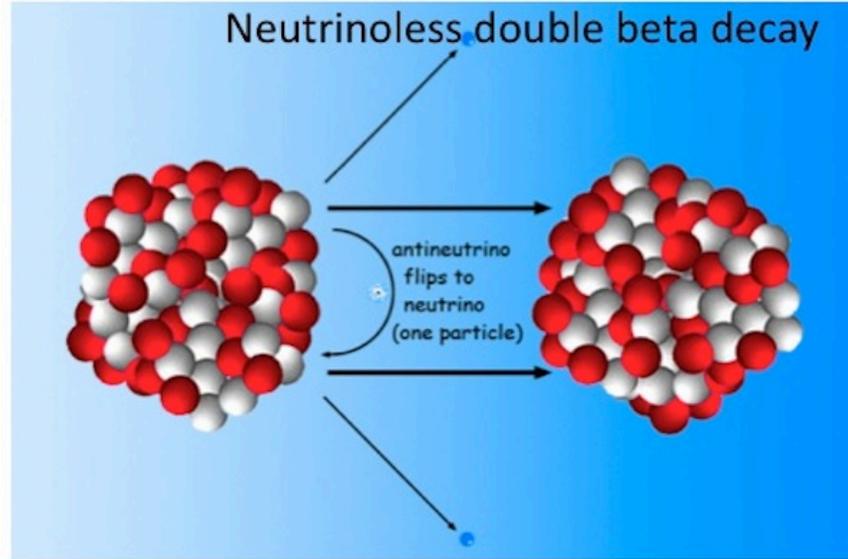
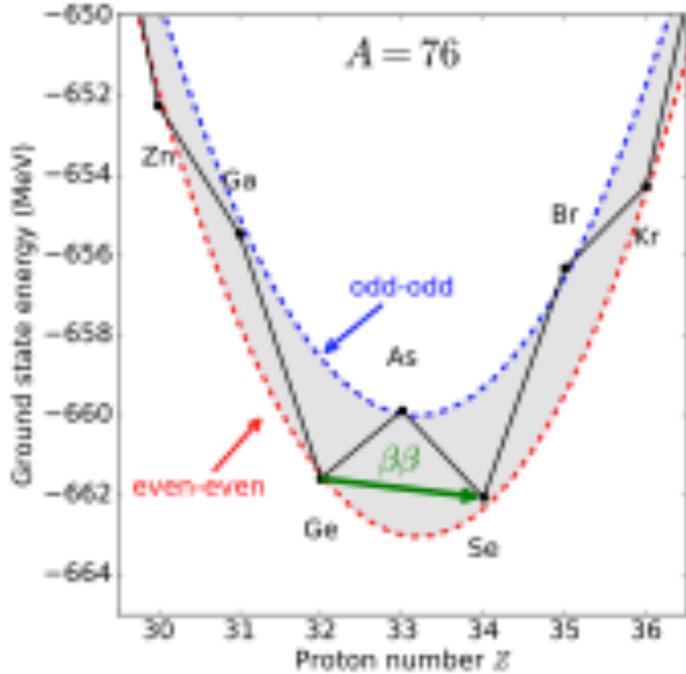
**Tremendous impact on BSM physics:**

**Lepton-number violating process**

Majorana character of neutrino

Absolute neutrino mass scale

Neutrino own antiparticle  $\longleftrightarrow 0\nu\beta\beta$  decay



**Tremendous impact on BSM physics:**

Lepton-number violating process

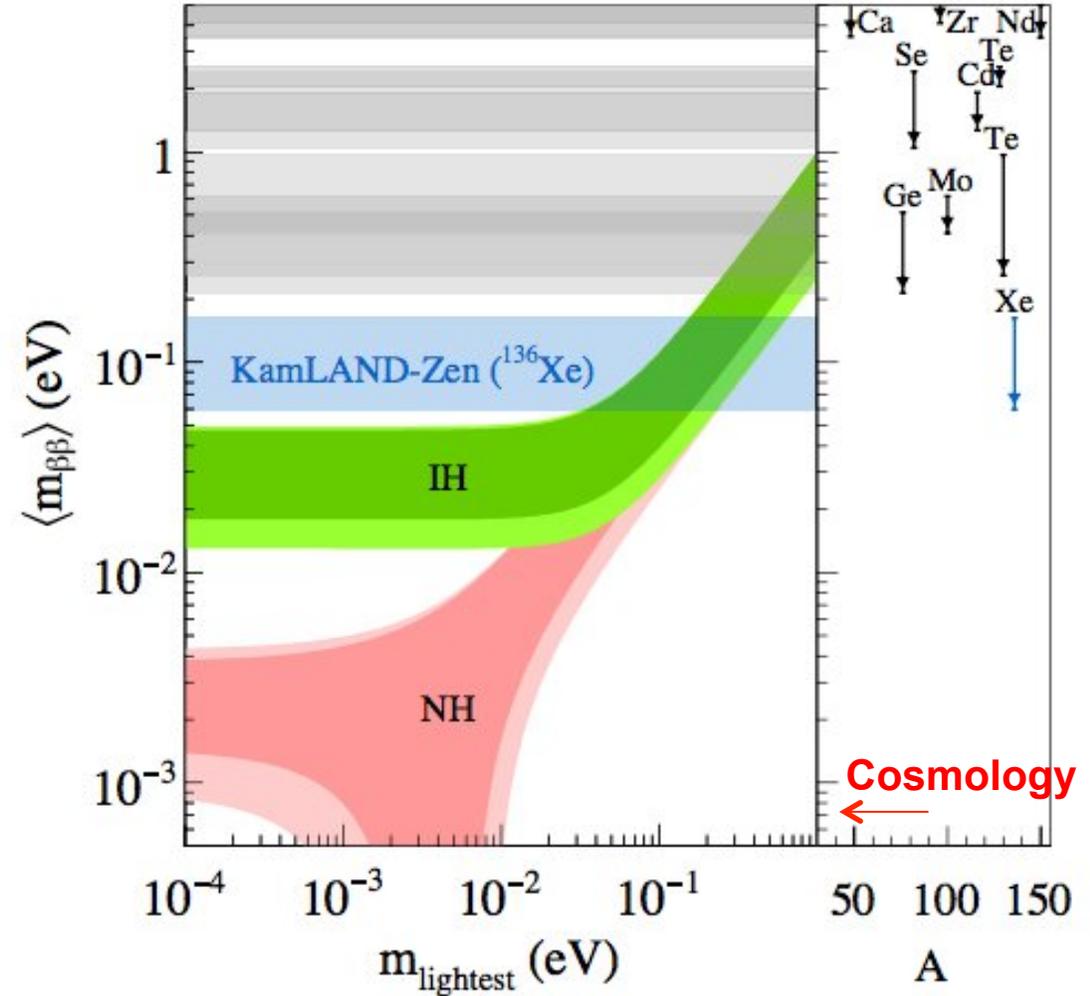
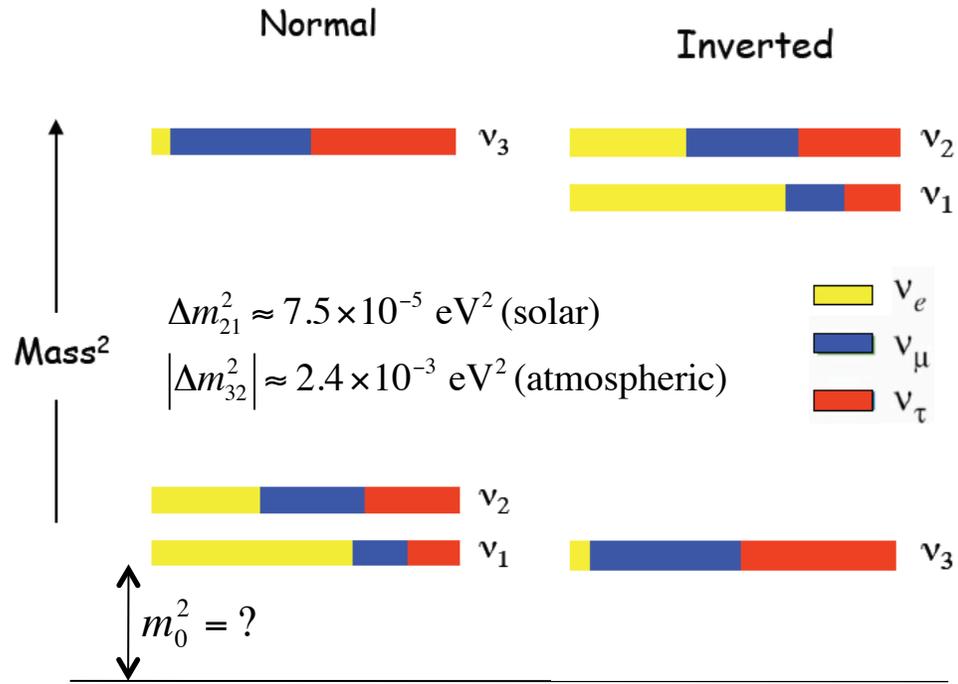
Majorana character of neutrino

**Absolute neutrino mass scale**

$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu} \boxed{M^{0\nu}}^2 \langle m_{\beta\beta} \rangle^2 \langle m_{\beta\beta} \rangle = \left| \sum_{i=1}^3 U_{ei} m_i \right|$$

**NME not observable: must be calculated**

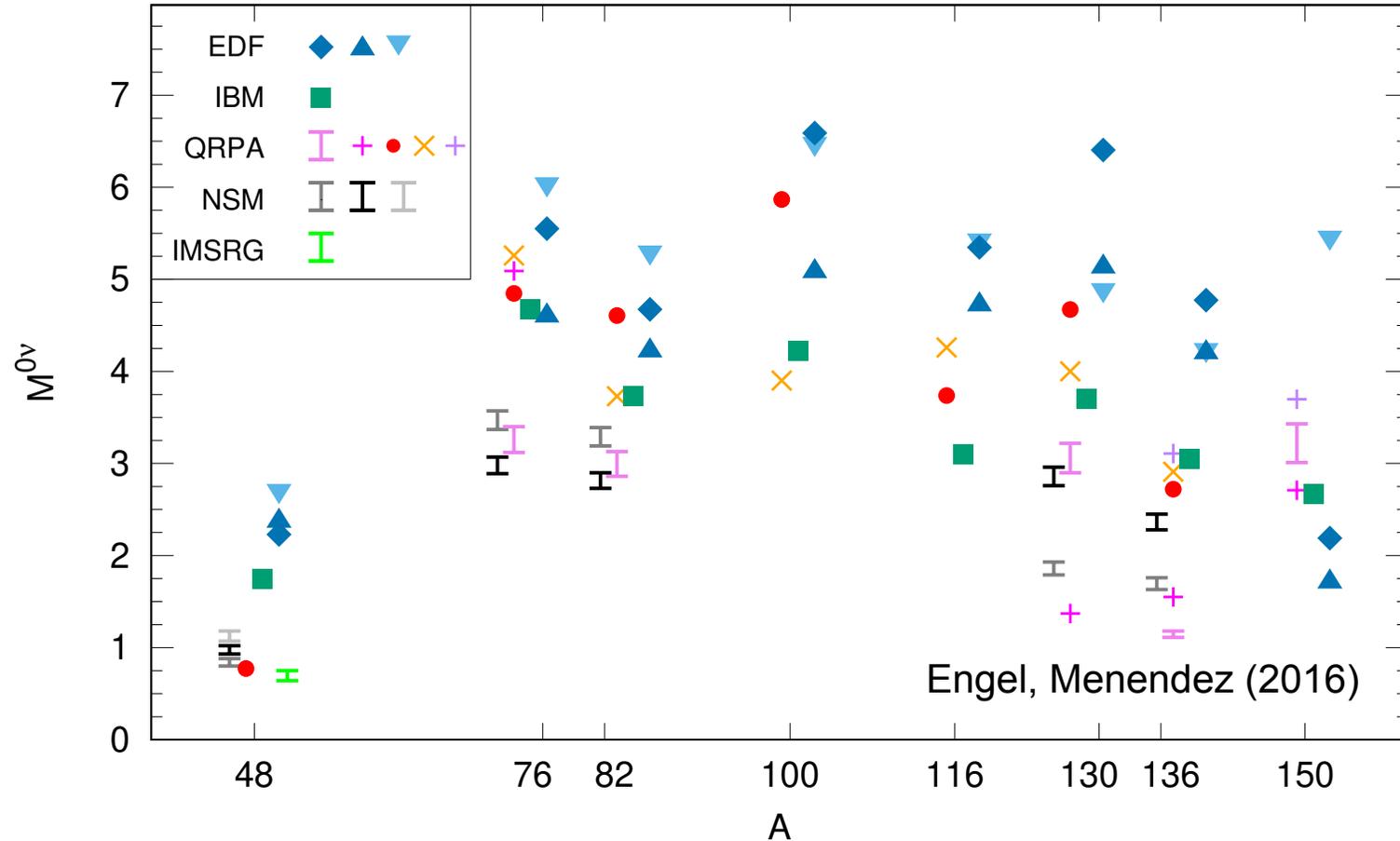
## Progress in large-scale searches pushing towards IH



$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu} \left(M^{0\nu}\right)^2 \langle m_{\beta\beta} \rangle^2 \quad \langle m_{\beta\beta} \rangle = \left| \sum_{i=1}^3 U_{ei} m_i \right|$$

Uncertainty from **Nuclear Matrix Element**; bands do not represent rigorous uncertainties

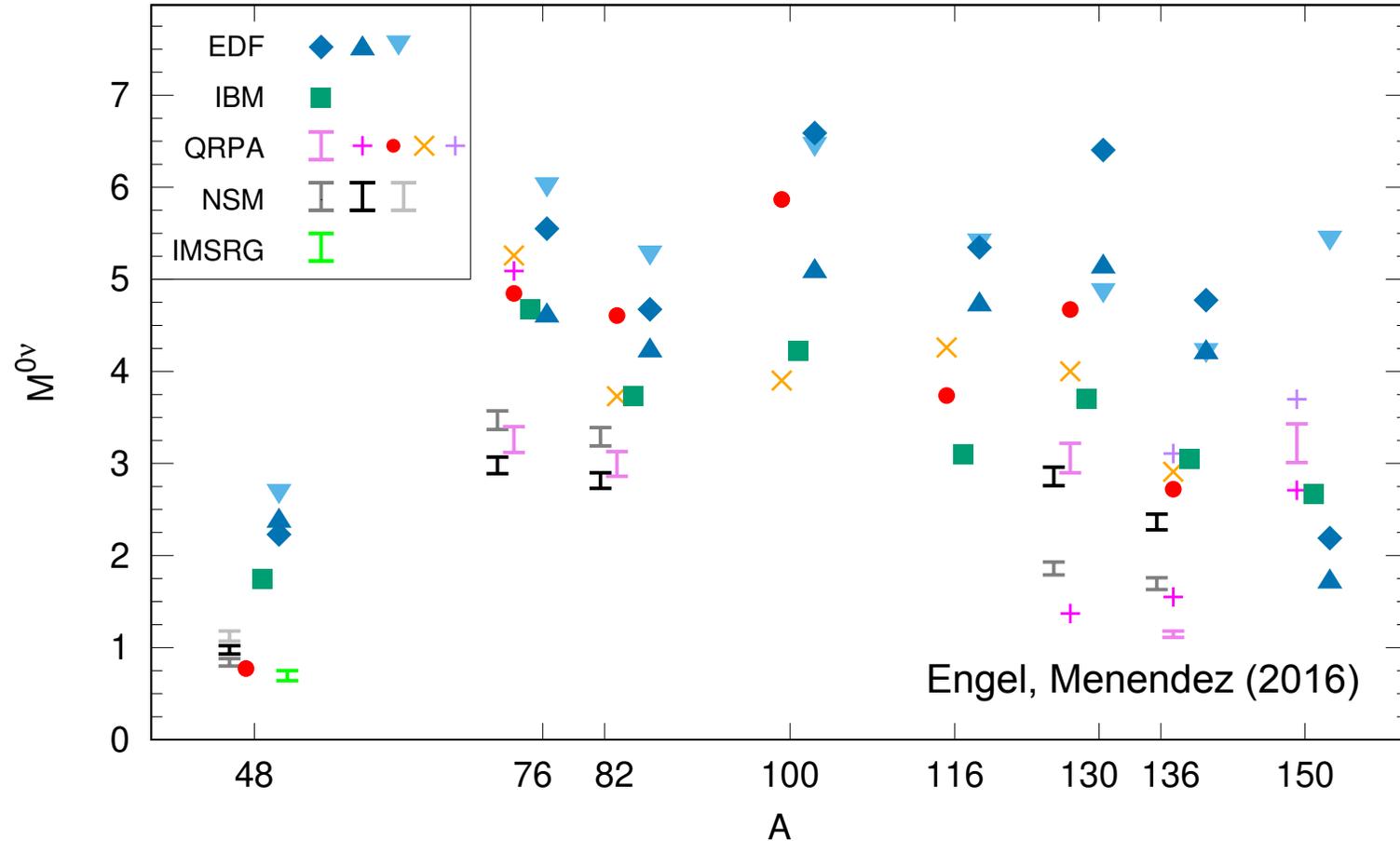
All calculations to date from **extrapolated** phenomenological models; large spread in results



**All models missing essential physics**

**Impossible to assign rigorous uncertainties**

All calculations to date from **extrapolated** phenomenological models; large spread in results

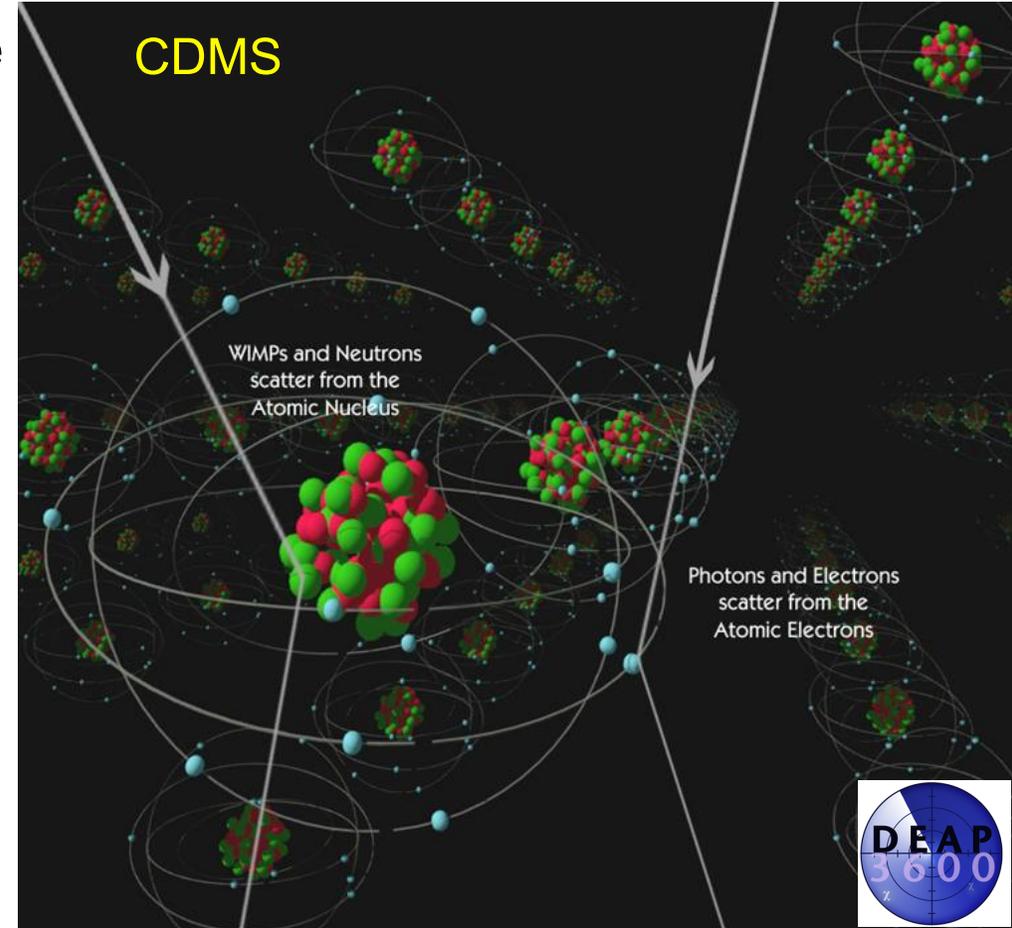
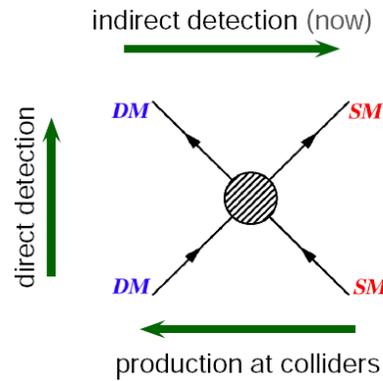
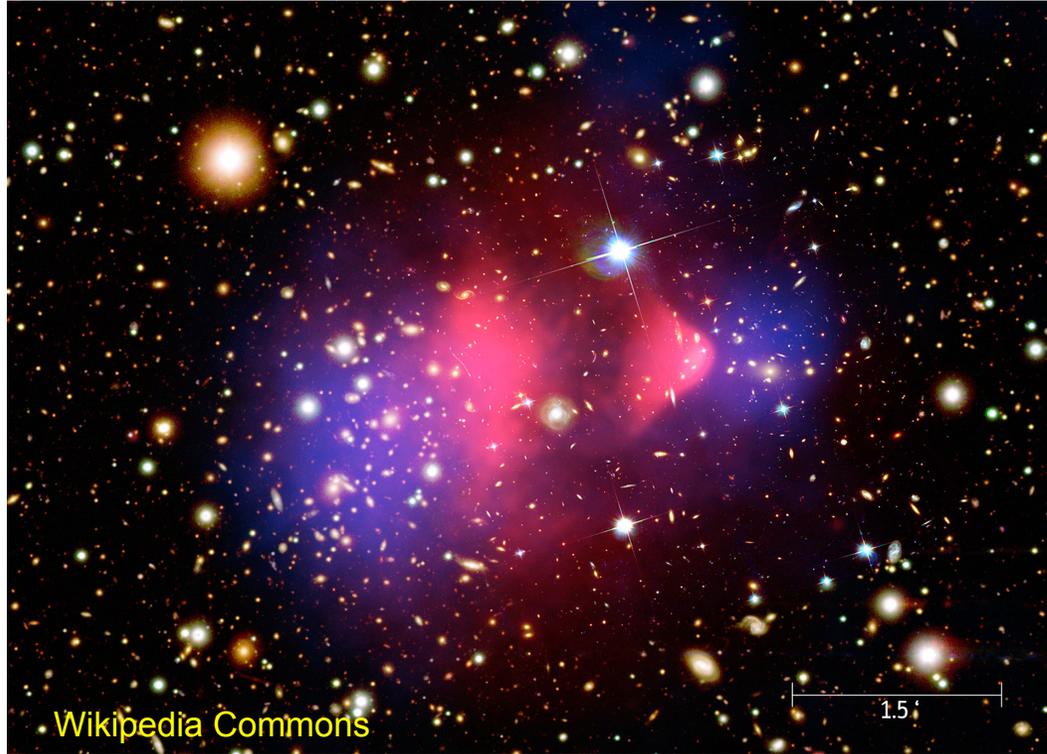


All models missing essential physics

Impossible to assign rigorous uncertainties

Explore new approaches to nuclear theory

Large-scale direct-detection searches underway worldwide



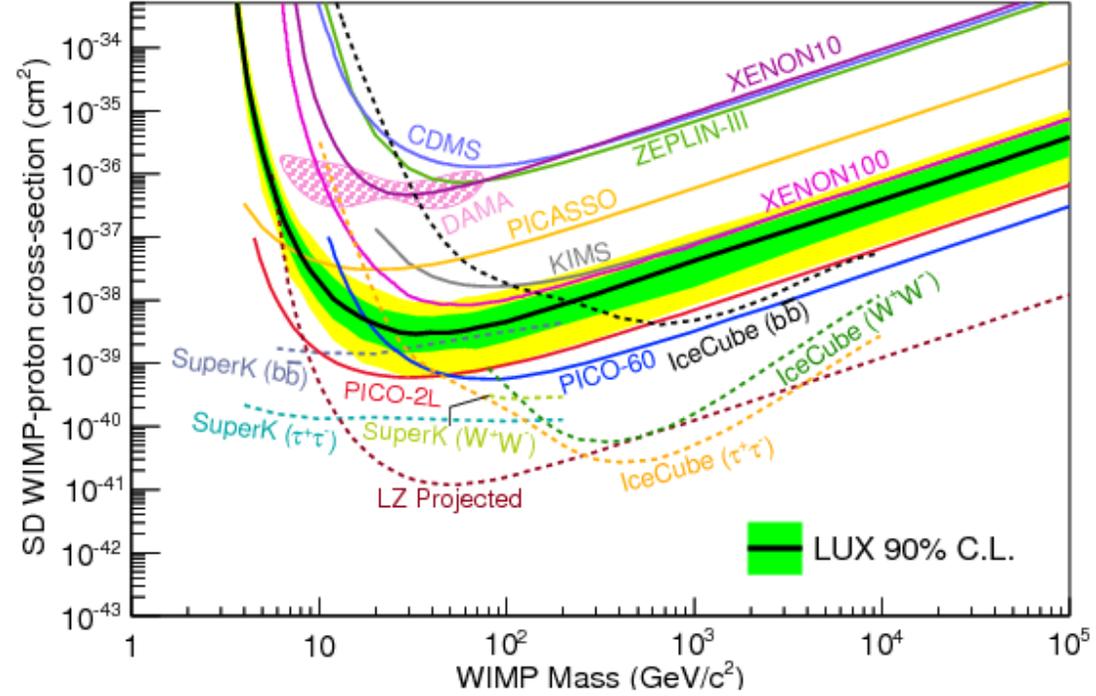
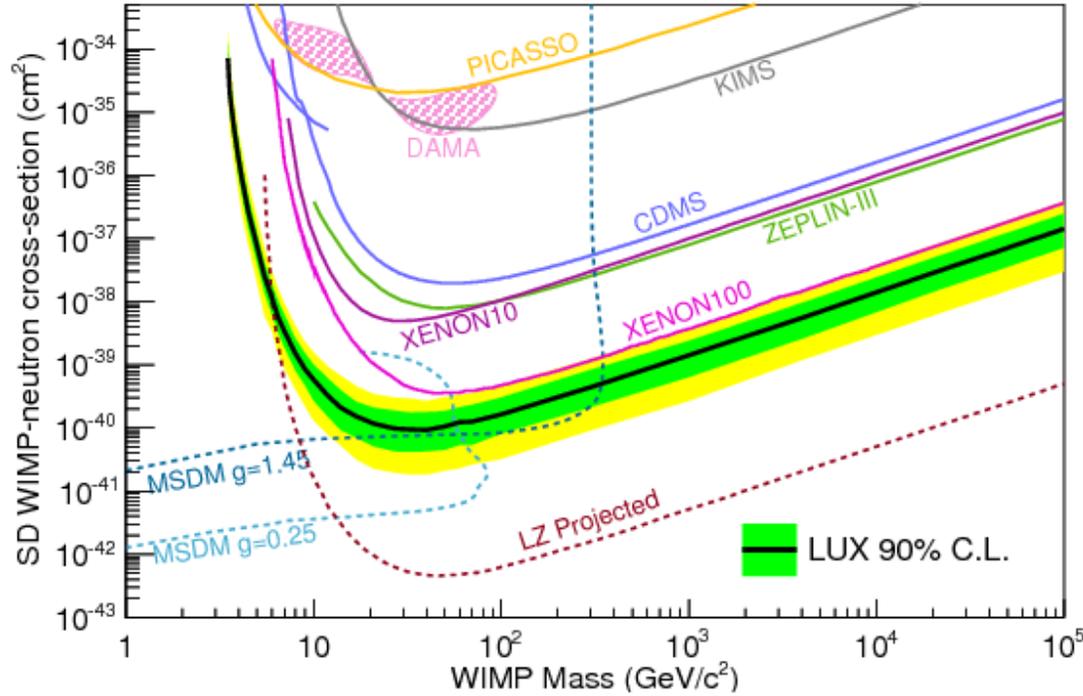
Observation of nuclear recoil

Direct detection:  $X \text{ SM} \rightarrow X \text{ SM}$

Leading candidates: neutralinos, ...?

Couple to scalar and axial-vector currents in atomic nuclei

Exclusion plots for WIMP-nucleon total cross section require nuclear structure



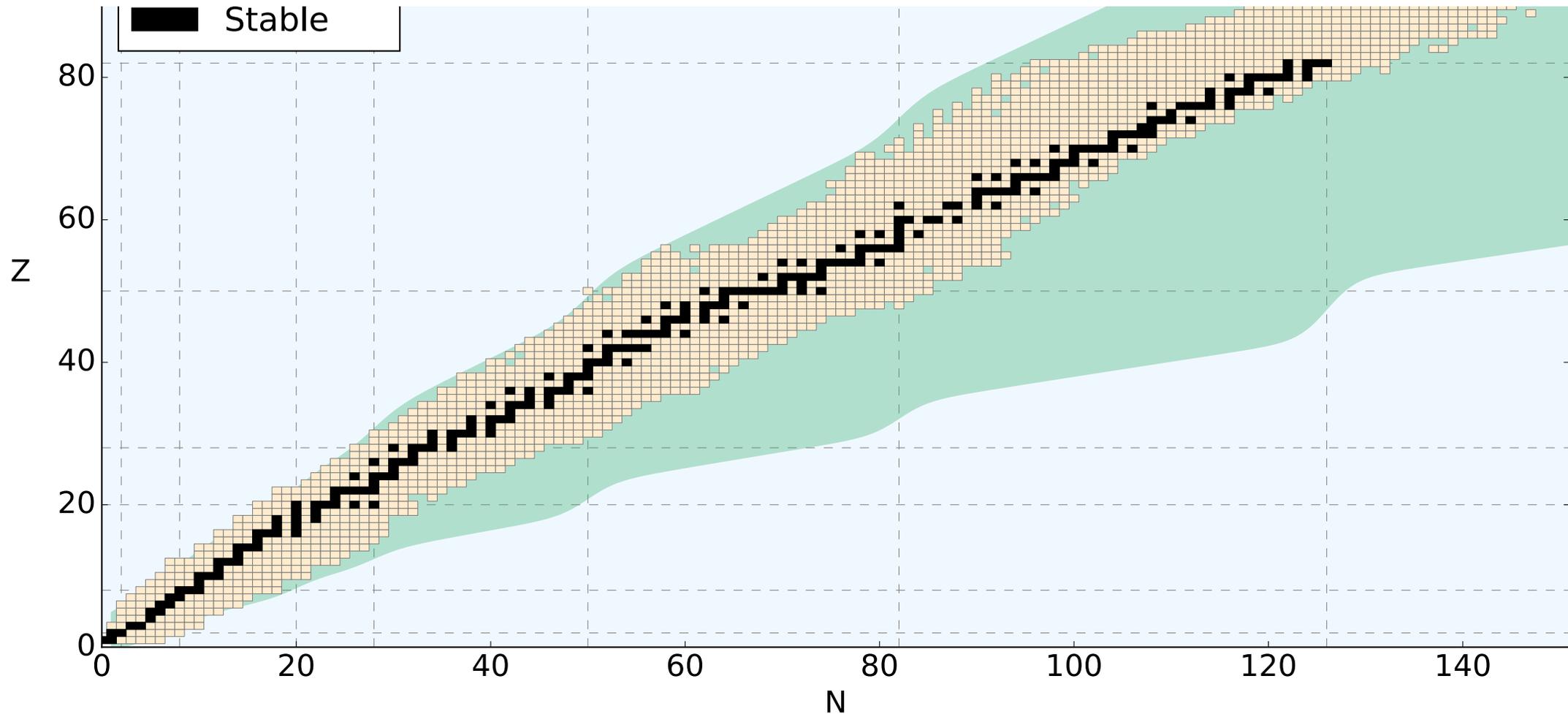
Differential cross section: compare results from different target nuclei

$$\frac{d\sigma}{dp^2} = \frac{8G_F^2}{(2J_i + 1)v^2} S_A(p)$$

**Structure functions** required from nuclear theory

Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

$$H\psi_n = E_n\psi_n$$

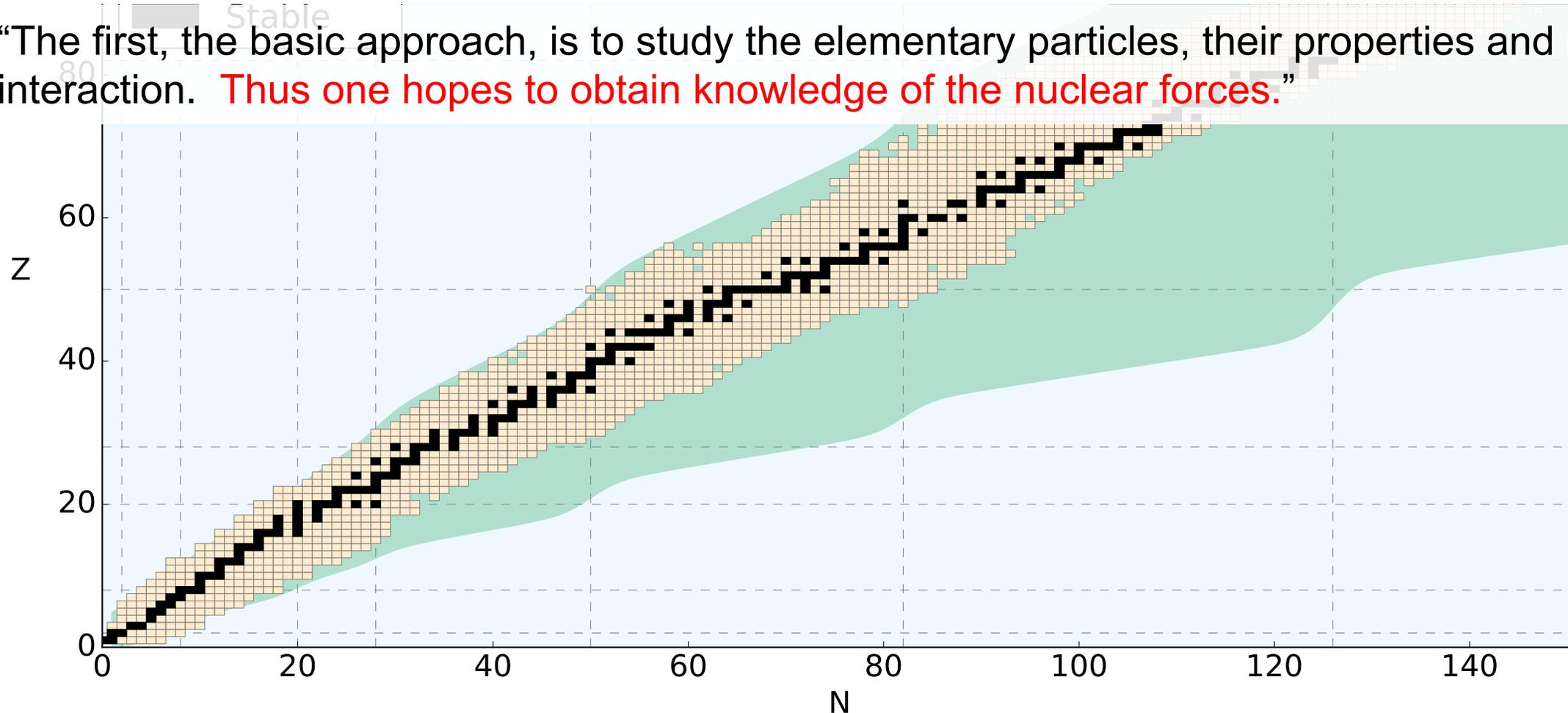


Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

- Nuclear forces (low-energy QCD)
- Electroweak physics

$$\boxed{H}\psi_n = E_n\psi_n$$

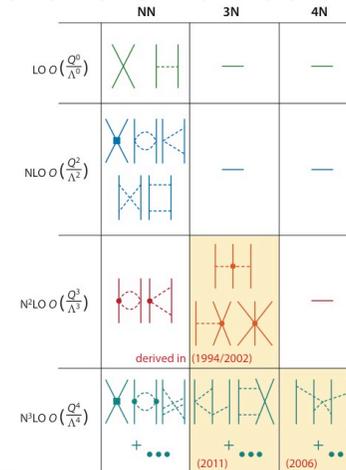
“The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces.”



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- Nuclear forces (low-energy QCD)
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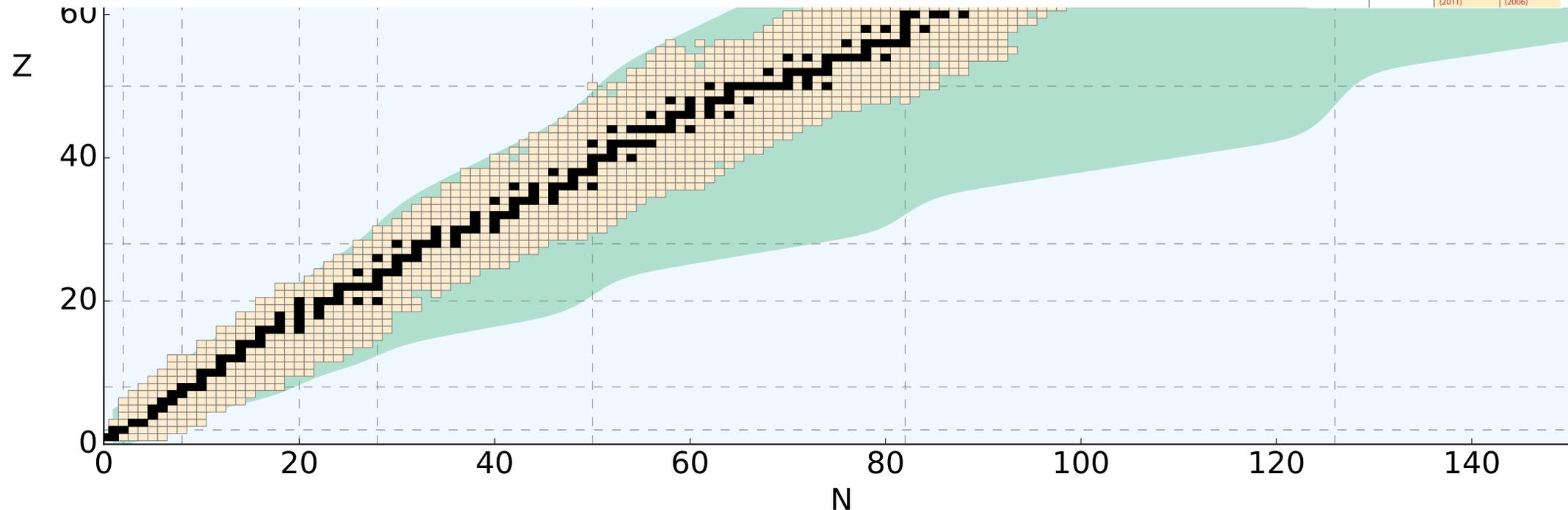
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**Chiral effective field theory:** systematic expansion of nuclear interactions

Consistent 3N forces, electroweak currents

Quantifiable uncertainties possible

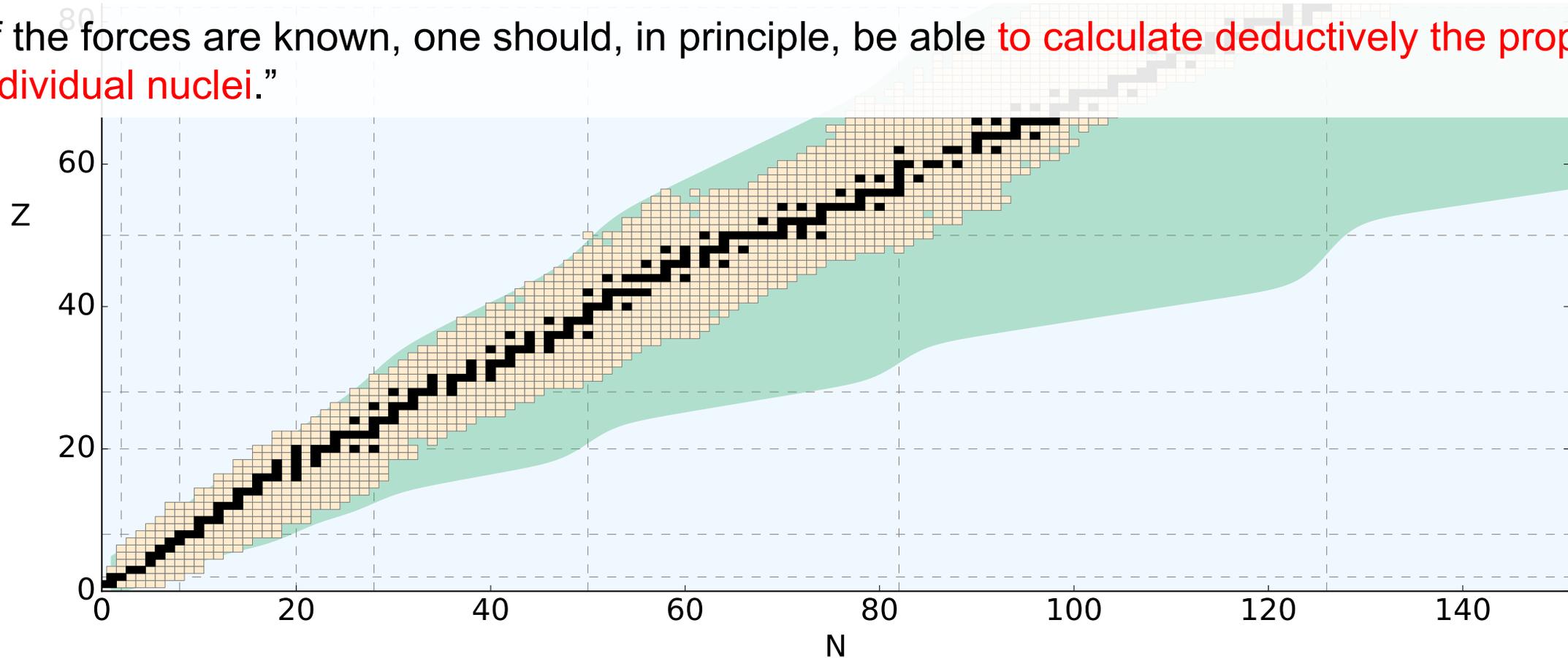


Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

- Nuclear forces (low-energy QCD)
- Electroweak physics
- **Nuclear many-body problem**

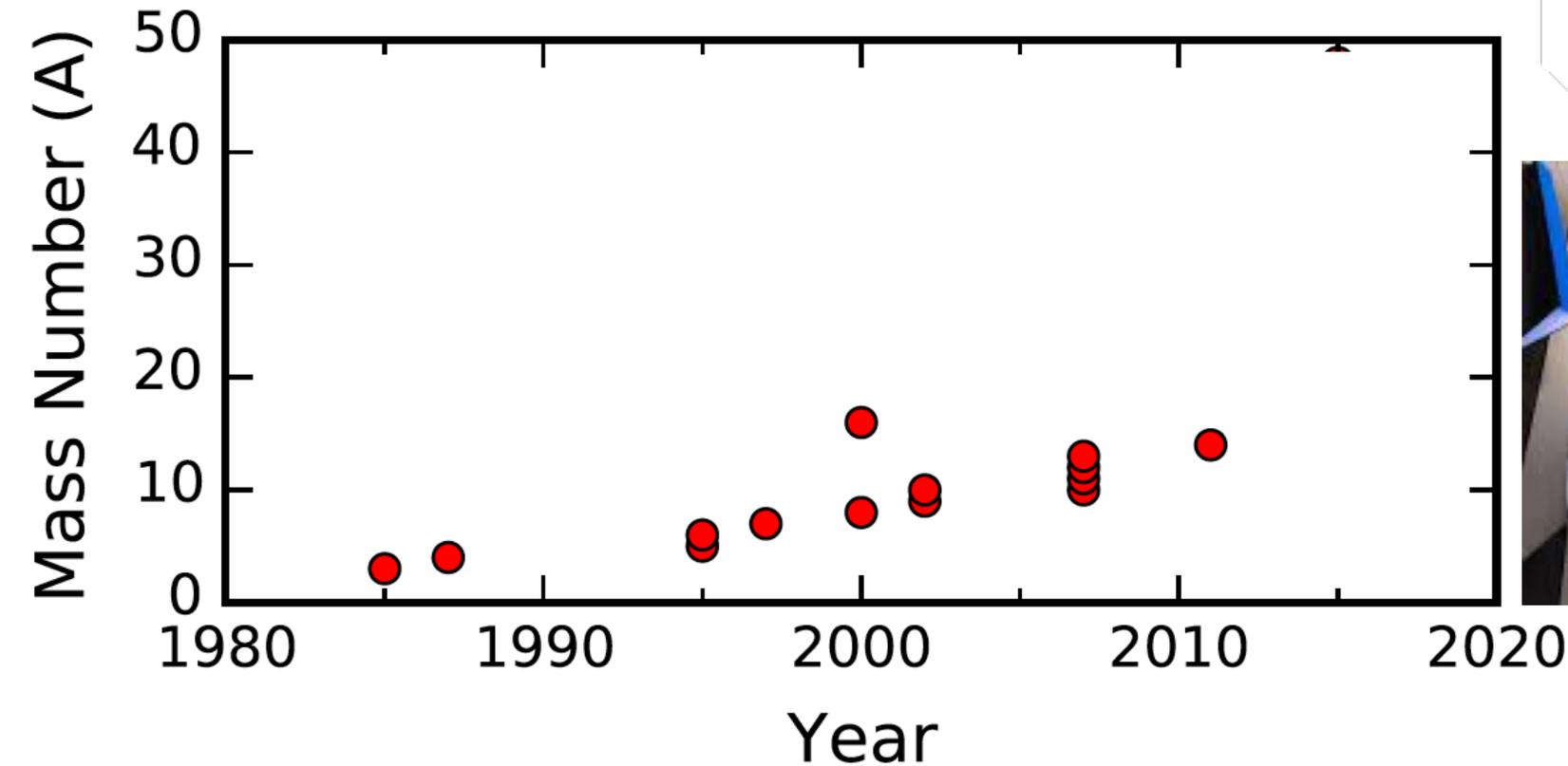
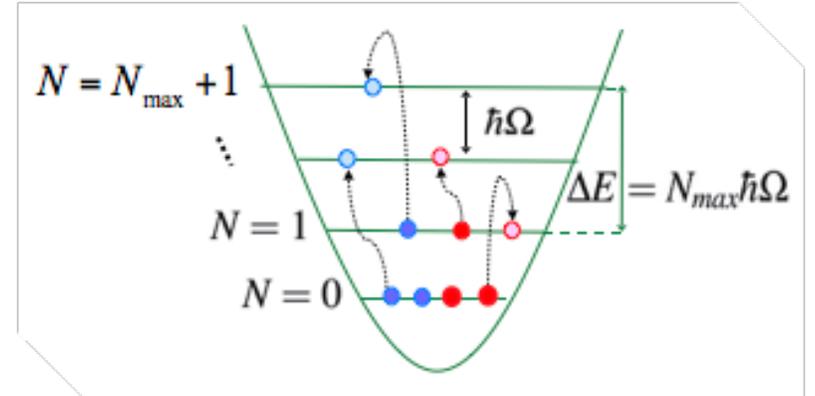
$$H\psi_n = E_n\psi_n$$

“If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei.”



Moore's law: **exponential** growth in computing power

Methods for light nuclei (QMC, **NCSM**) scale **exponentially** with mass

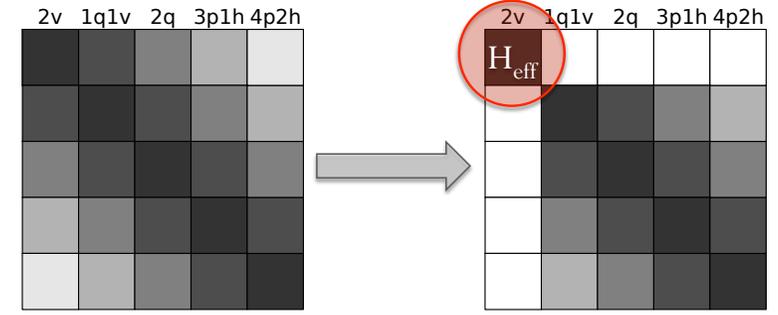


Moore's law: **exponential** growth in computing power

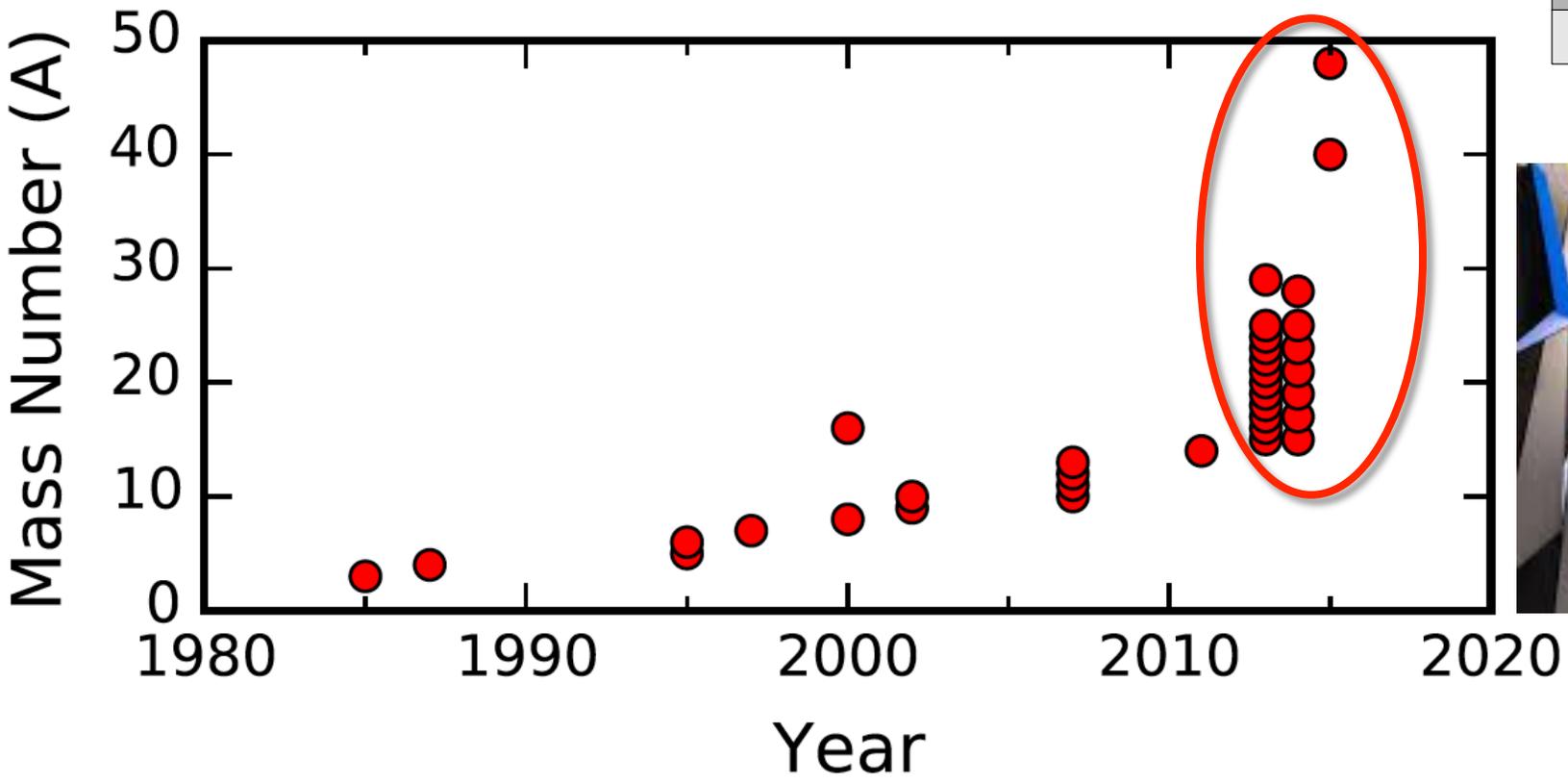
Methods for light nuclei (QMC, NCSM) scale exponentially with mass

Polynomial scaling methods developed (**CC**, **IMSRG**, SCGF)

**Explosion in limits of ab initio theory** 



$$H(s=0) \rightarrow H(\infty)$$



Moore's law: exponential growth in computing power

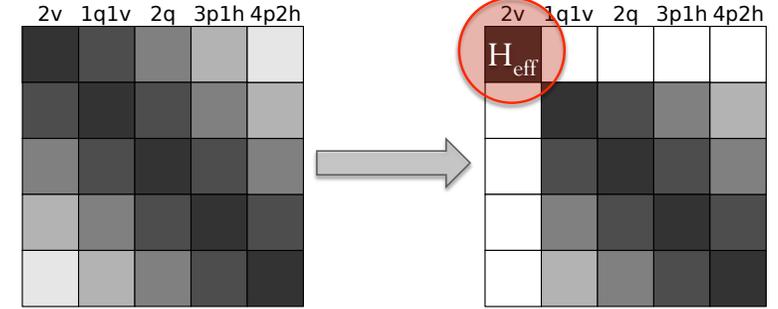
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Polynomial scaling methods developed (CC, IMSRG,...)

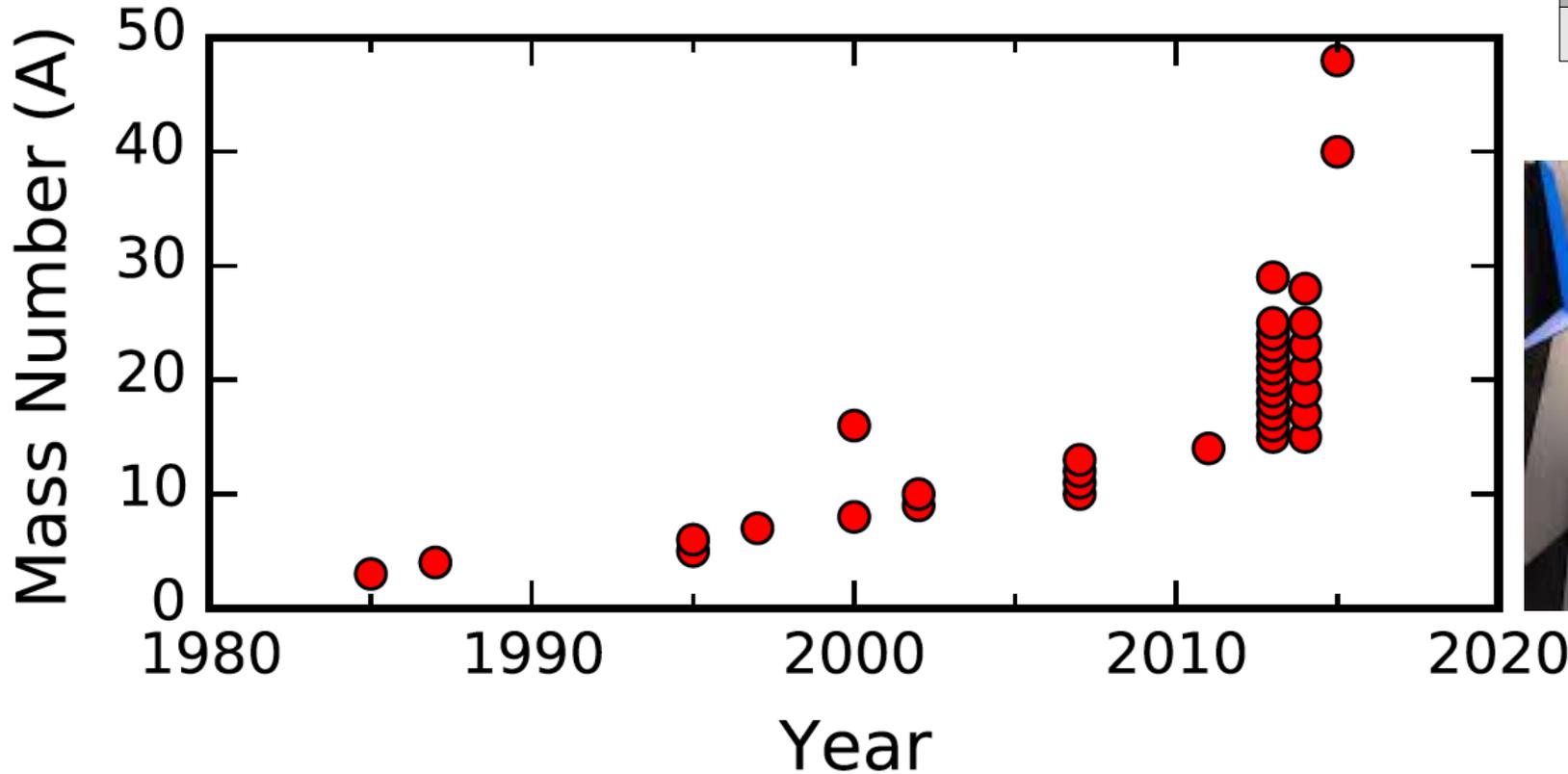
**Explosion in limits of ab initio theory**



**2020:  $A > 132$**



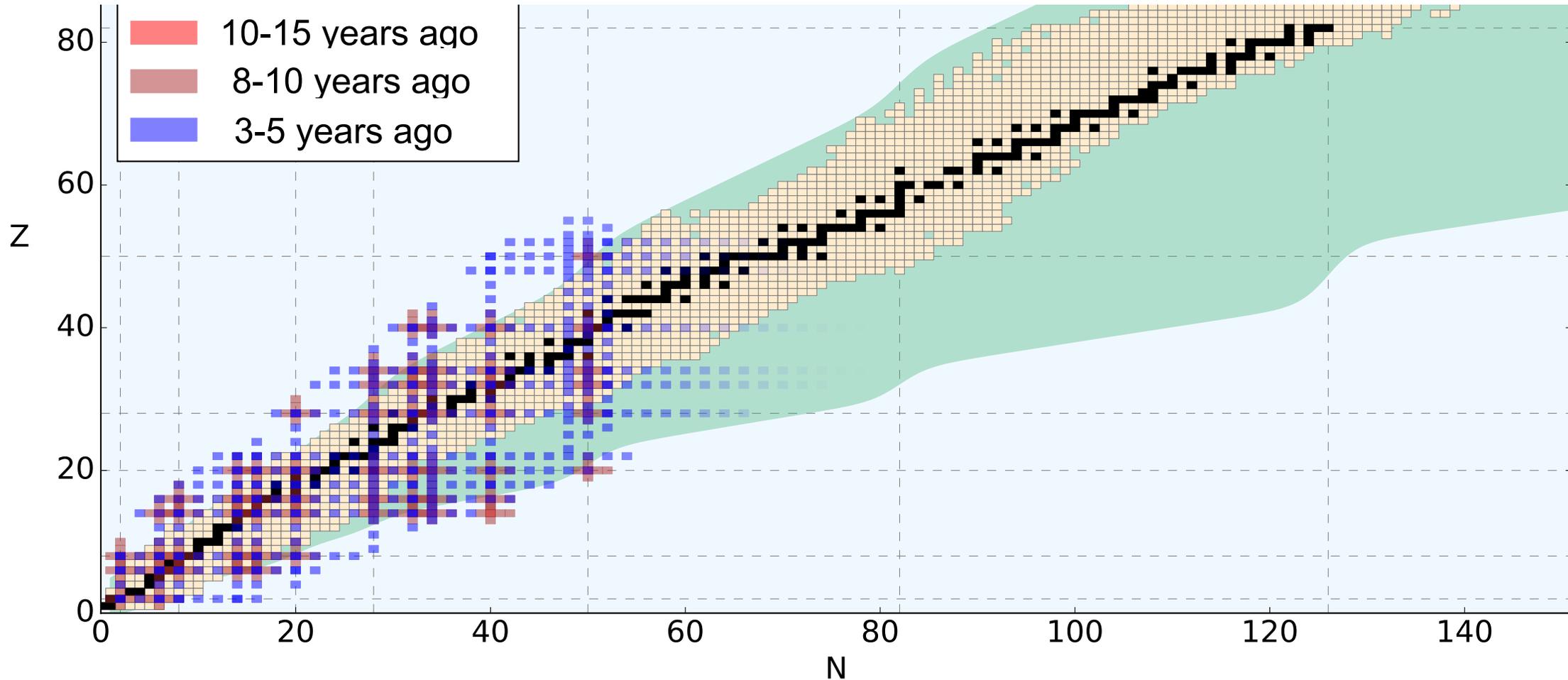
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- Nuclear forces, electroweak physics
- **Nuclear many-body problem**

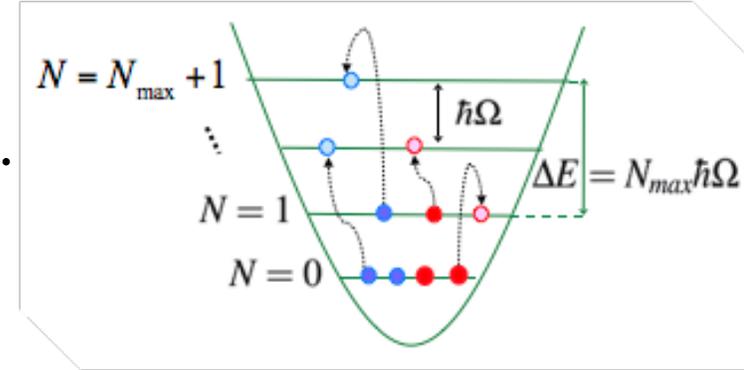
$$H\psi_n = E_n\psi_n$$



Explicitly construct unitary transformation from sequence of rotations

$$U = e^{\Omega} = e^{\eta_n} \dots e^{\eta_1} \quad \eta = \frac{1}{2} \arctan \left( \frac{2H_{\text{od}}}{\Delta} \right) - \text{h.c.}$$

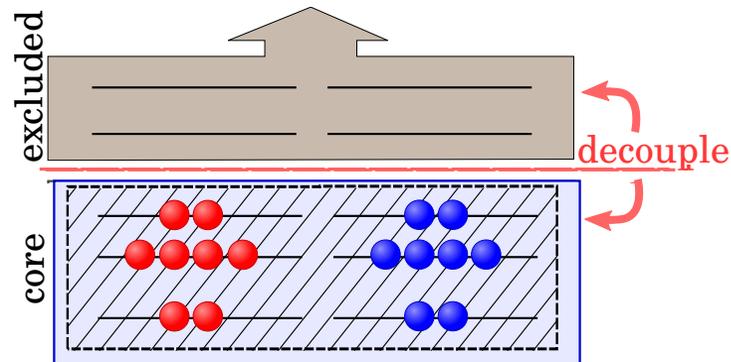
$$\tilde{H} = e^{\Omega} H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2} [\Omega, [\Omega, H]] + \dots$$



**All operators truncated at two-body level IMSRG(2)**  
**IMSRG(3) in progress (S.R. Stroberg)**

Tsukiyama, Bogner, Schwenk, PRC 2012  
 Morris, Parzuchowski, Bogner, PRC 2015

## Step 1: Decouple core



Can we achieve accuracy  
of large-space methods?

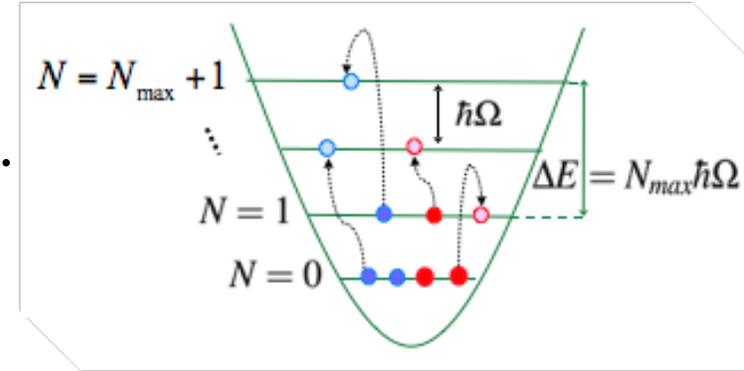
$$\langle \tilde{\Psi}_n | P \tilde{H} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

$$|\Phi_0\rangle = |^{16}\text{O}\rangle$$

Explicitly construct unitary transformation from sequence of rotations

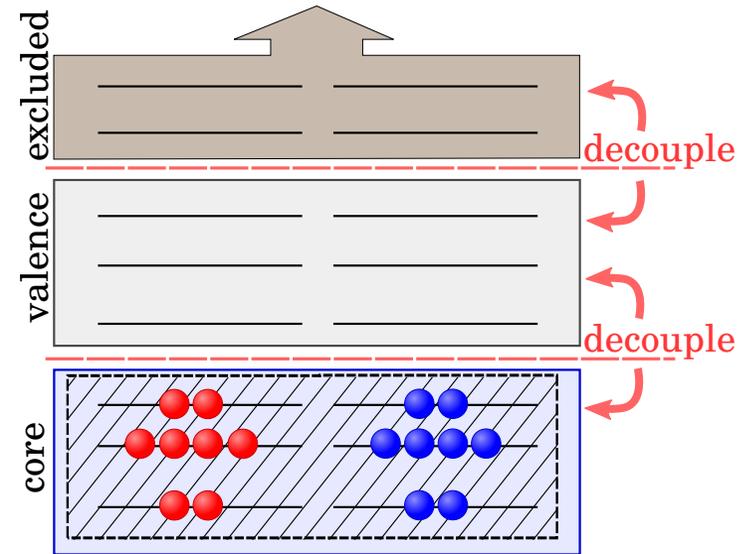
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**Step 1: Decouple core**  
**Step 2: Decouple valence space H**

Can we achieve accuracy  
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$$\langle \tilde{\Psi}_n | P \tilde{H} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

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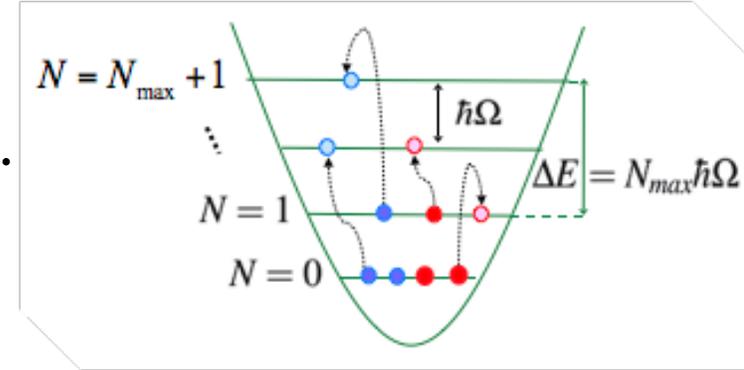
$\langle P   H   P \rangle$	$\langle P   H   Q \rangle \rightarrow 0$
$\langle Q   H   P \rangle \rightarrow 0$	$\langle Q   H   Q \rangle$

Explicitly construct unitary transformation from sequence of rotations

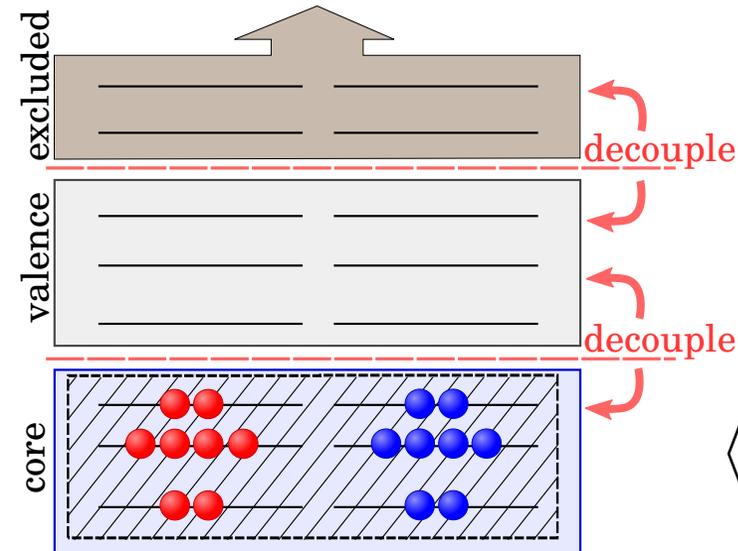
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$$\tilde{H} = e^\Omega H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2} [\Omega, [\Omega, H]] + \dots$$

$$\tilde{\mathcal{O}} = e^\Omega \mathcal{O} e^{-\Omega} = \mathcal{O} + [\Omega, \mathcal{O}] + \frac{1}{2} [\Omega, [\Omega, \mathcal{O}]] + \dots$$



Tsukiyama, Bogner, Schwenk, PRC 2012  
Morris, Parzuchowski, Bogner, PRC 2015



- Step 1: Decouple core**
- Step 2: Decouple valence space H**
- Step 3: Transform additional operators**

$$\langle \tilde{\Psi}_n | P \tilde{H} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

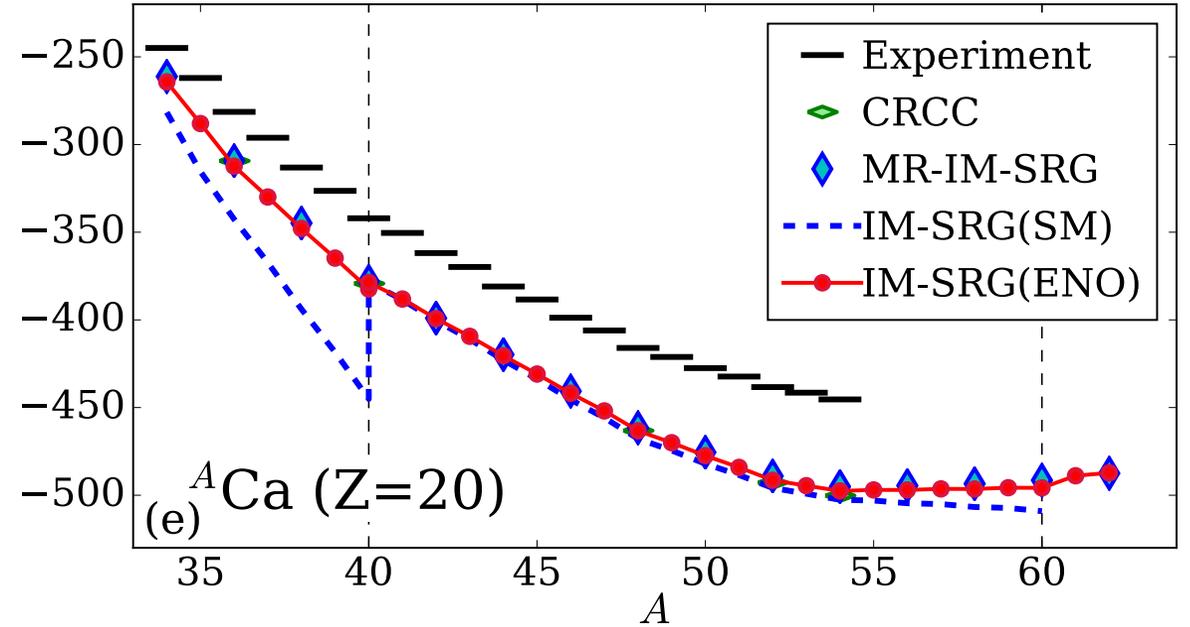
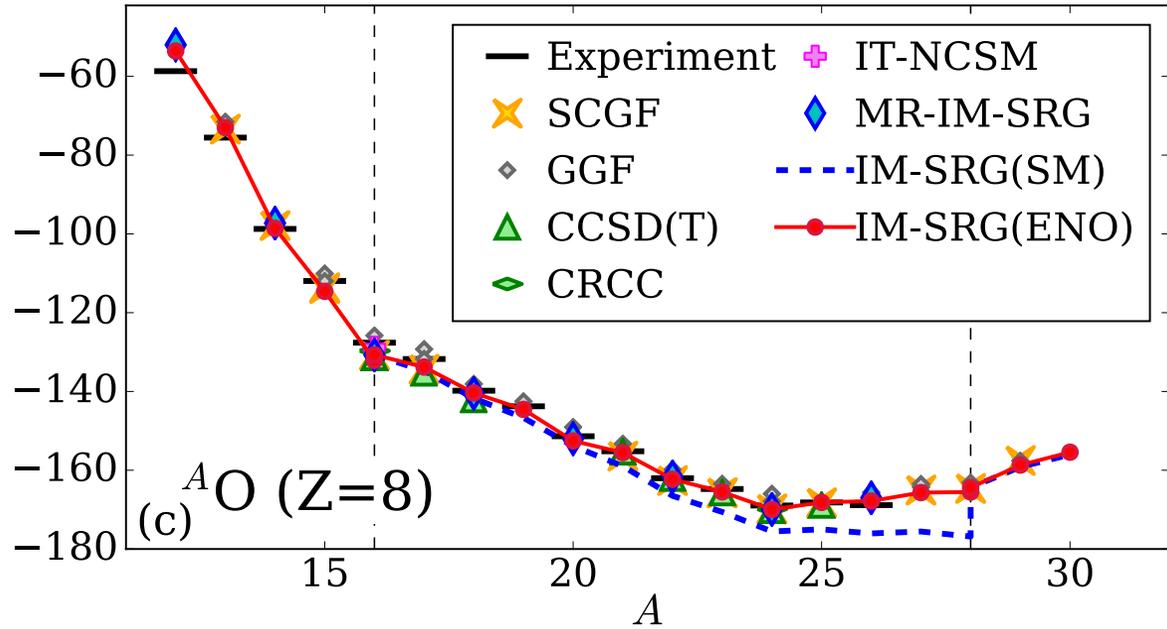
$$\langle \tilde{\Psi}_n | P \tilde{M}_{0\nu} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$

$\langle P   H   P \rangle$	$\langle P   H   Q \rangle \rightarrow 0$
$\langle Q   H   P \rangle \rightarrow 0$	$\langle Q   H   Q \rangle$

$$|\Phi_0\rangle = |^{16}\text{O}\rangle$$

**Careful benchmarking essential!**

**New approach accesses *\*all\** nuclei:** agrees to 1% with large-space methods



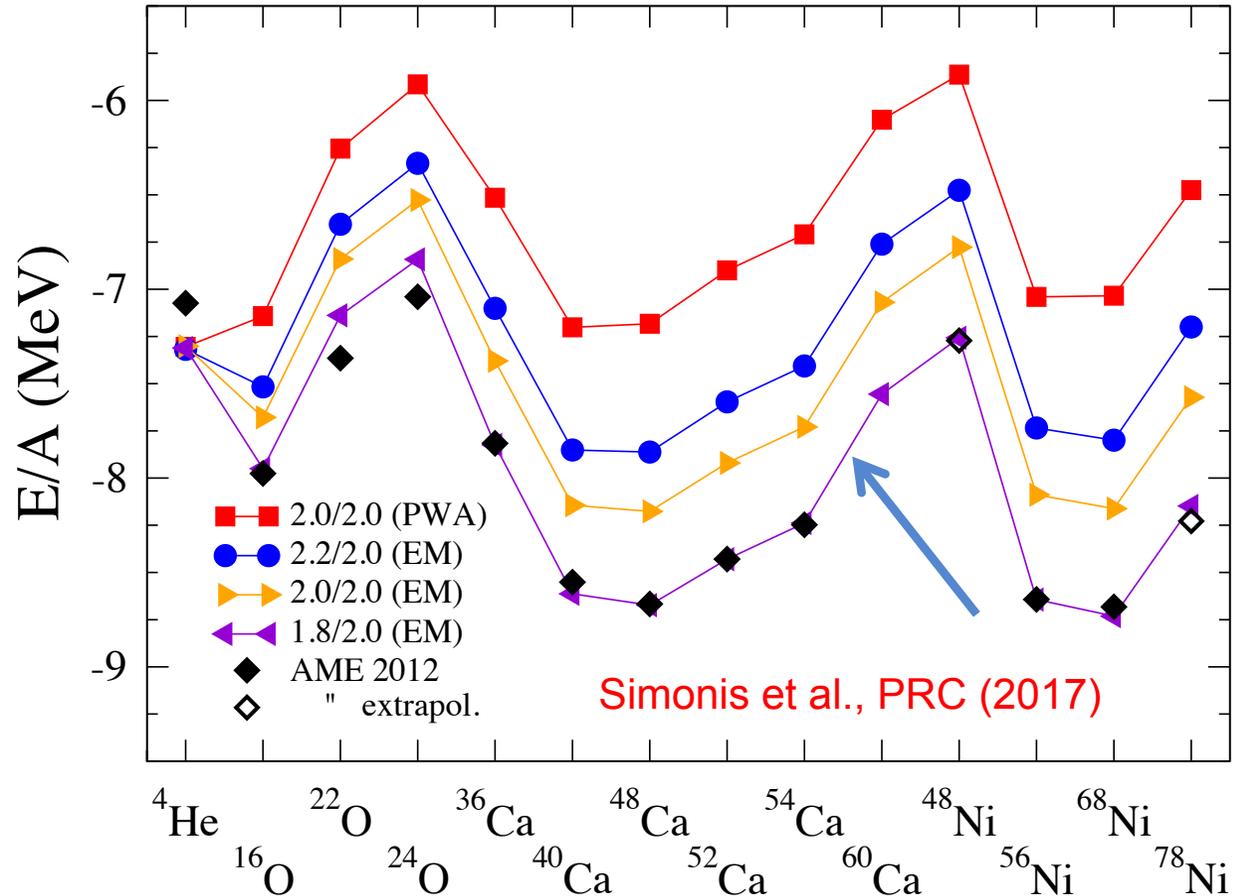
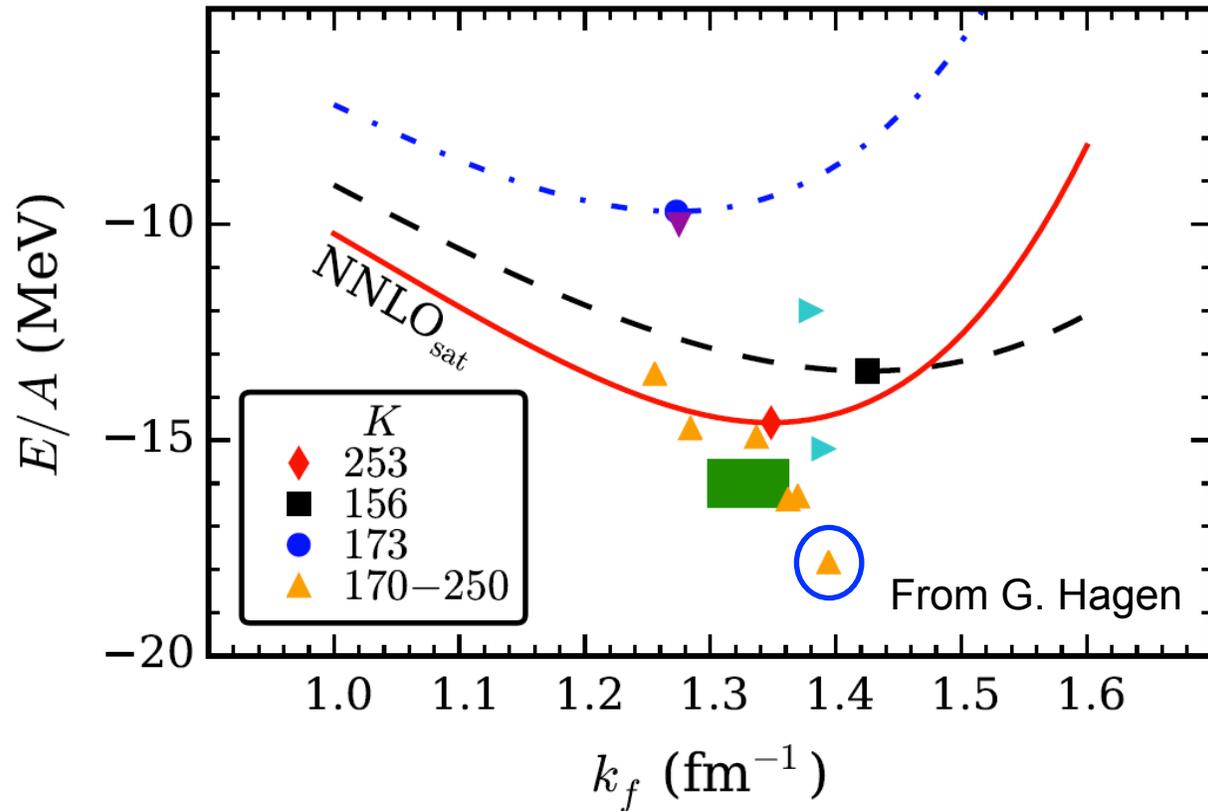
Stroberg et al., PRL (2017)

Agreement with *experiment* deteriorates for heavy chains (due to input Hamiltonian)

Significant gain in applicability with little/no sacrifice in accuracy; **Any operator can be calculated**

**Low computational cost:** ~1 node-day/nucleus

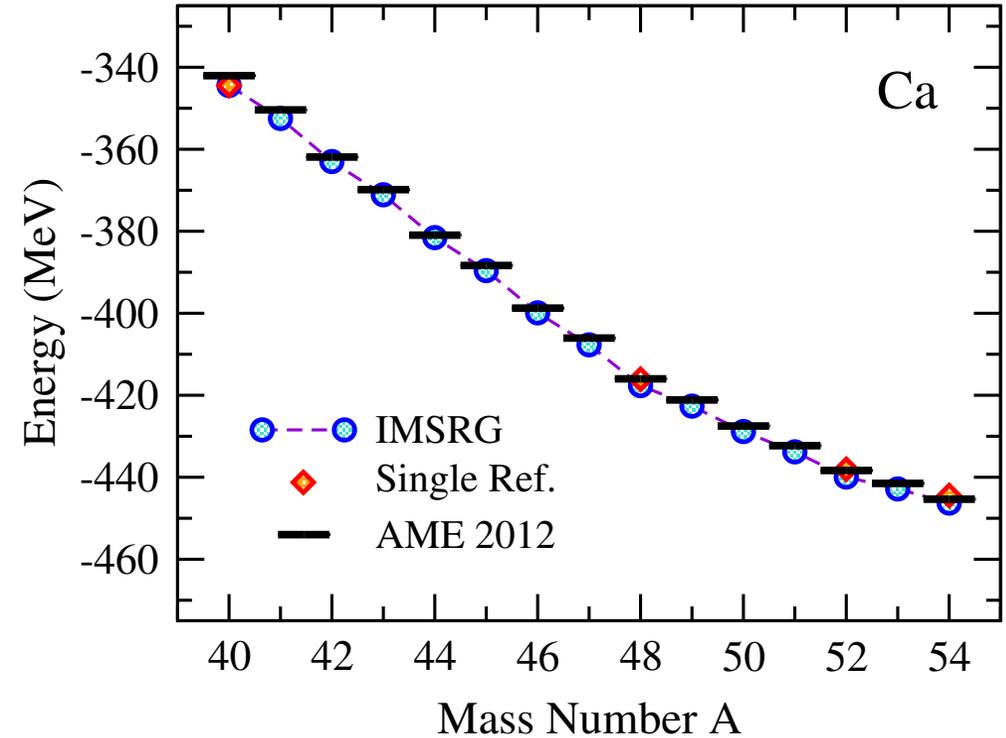
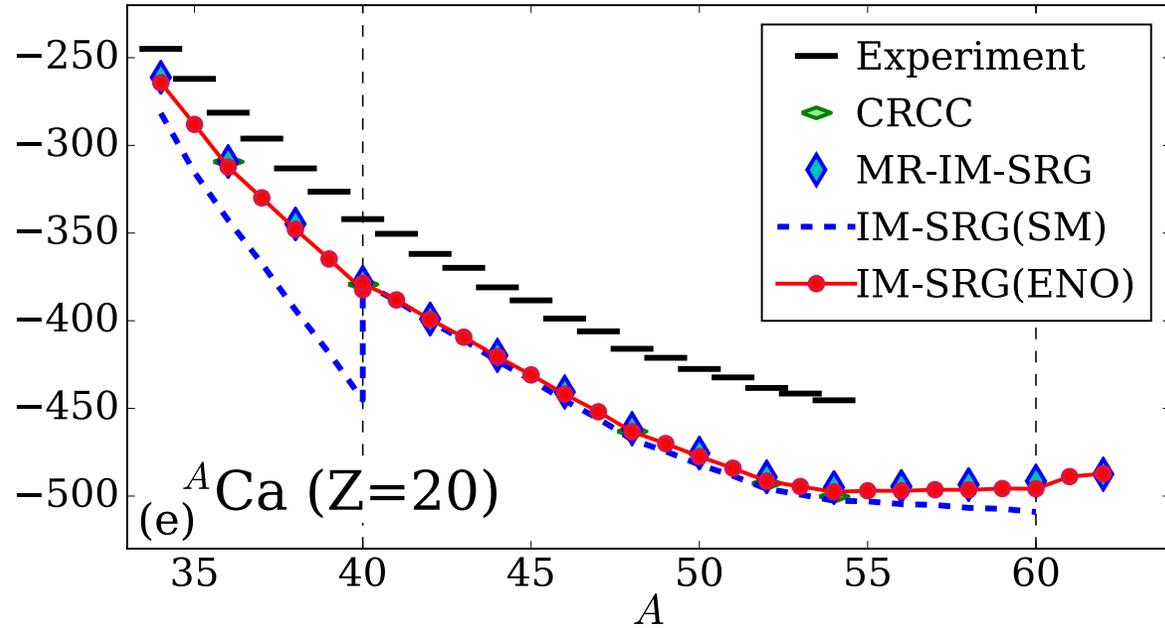
## NN+3N force with good reproduction of ground-state energies



**1.8/2.0 (EM) reproduces ground-state energies through  ${}^{78}\text{Ni}$**

Slight underbinding for neutron-rich oxygen

Dramatic improvement with respect to experimental data



Opens possibility for reliable ab initio predictions across the nuclear chart!

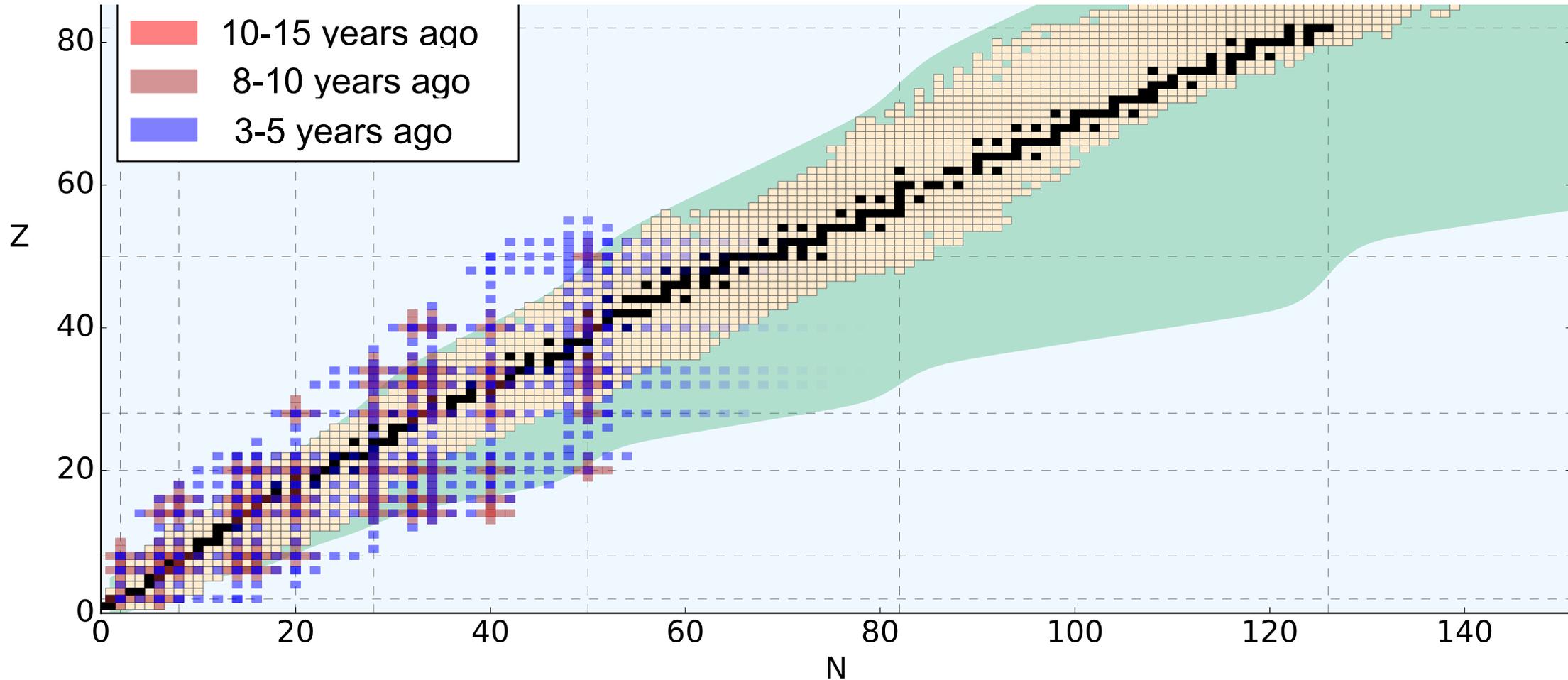
Accesses **all** properties of **all** nuclei:

- Ground states, excited states, charge radii, electroweak transitions...
- Test nuclear forces across wide range of nuclei

**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem

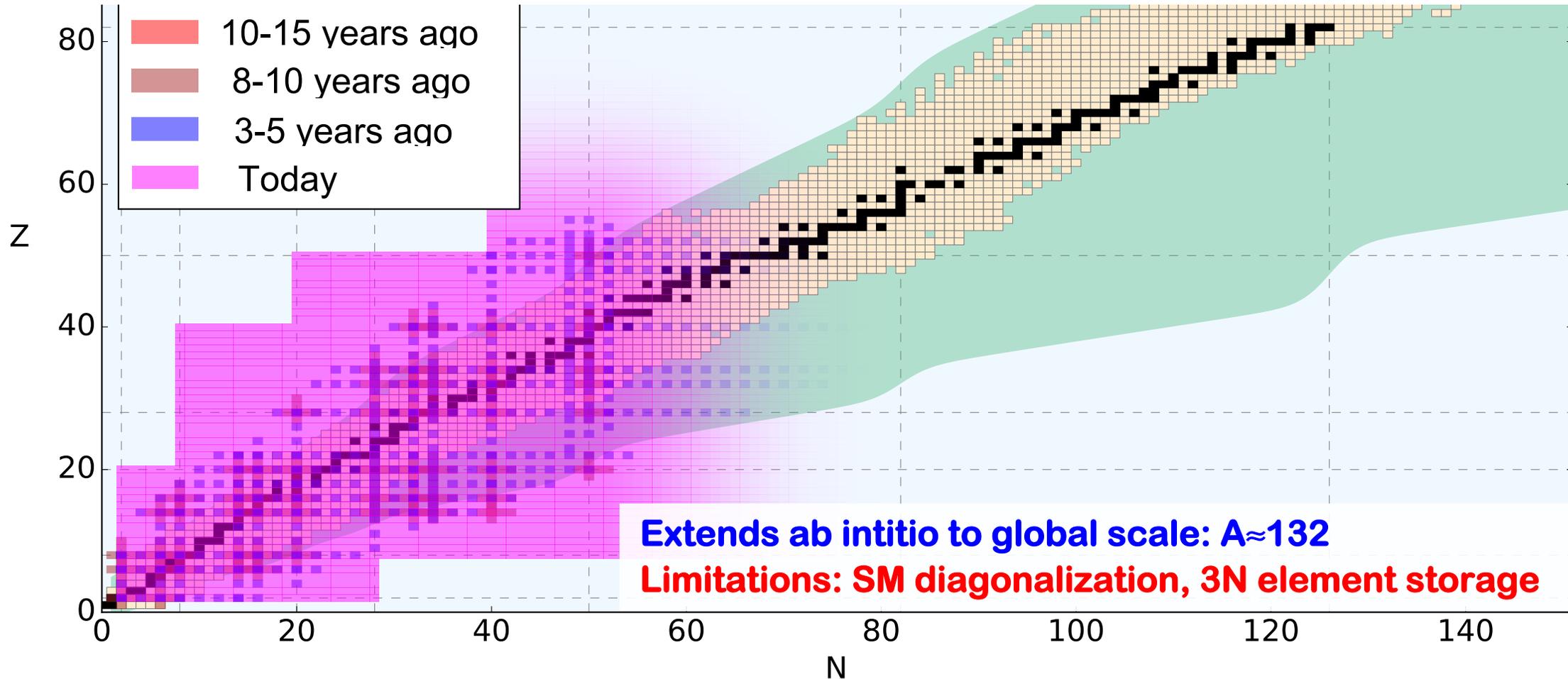
$$H\psi_n = E_n\psi_n$$



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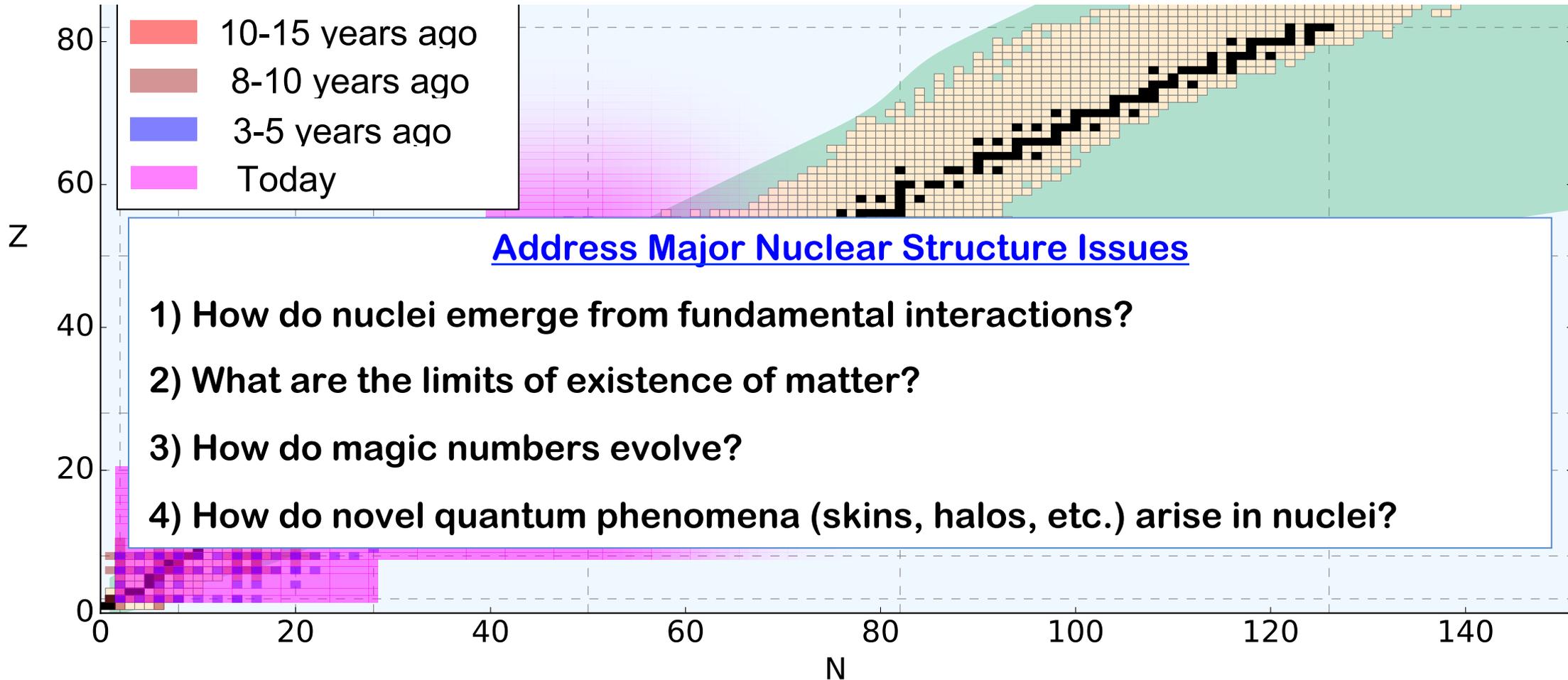
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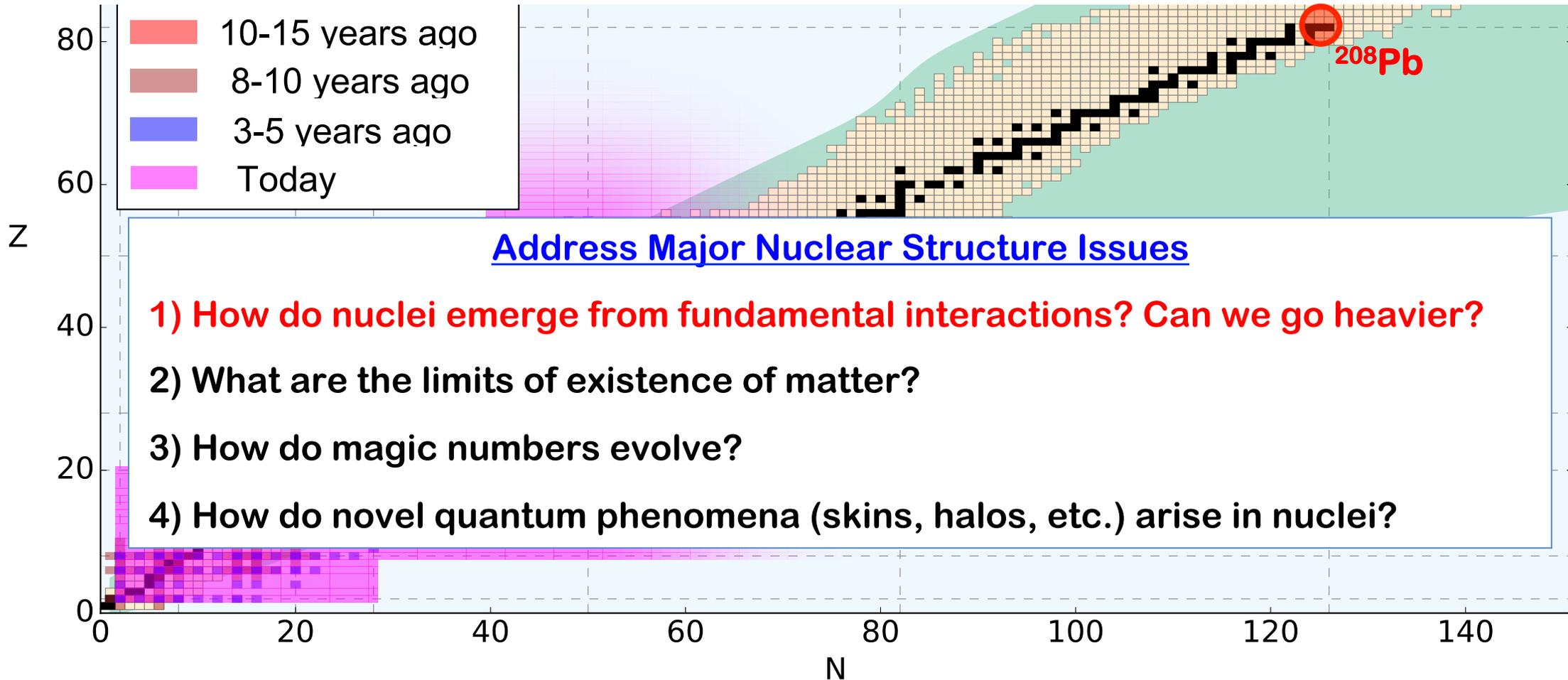
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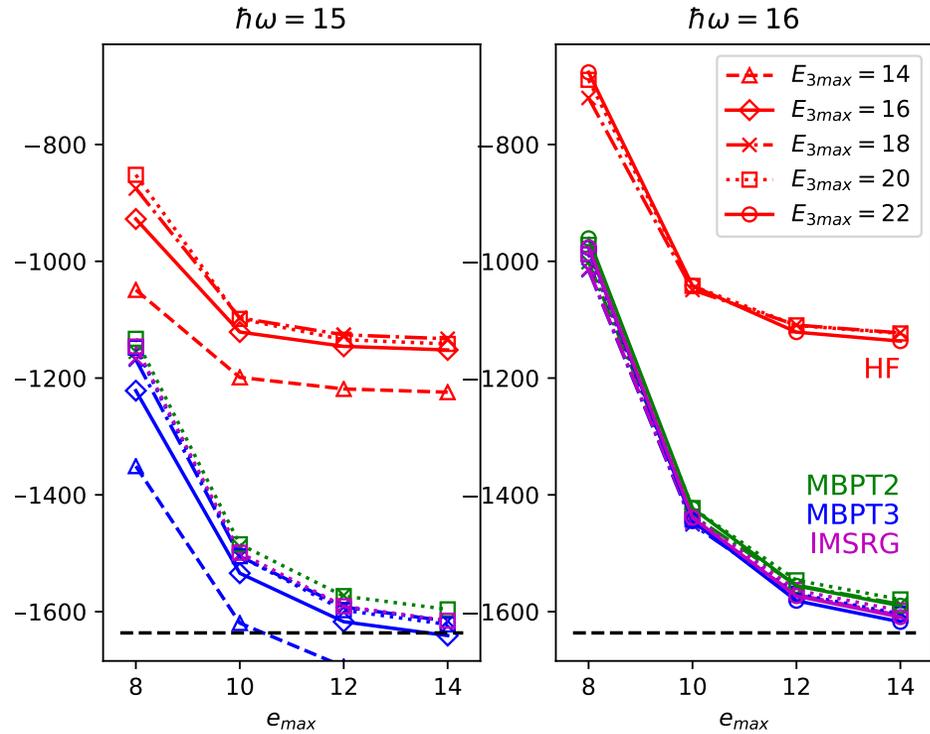
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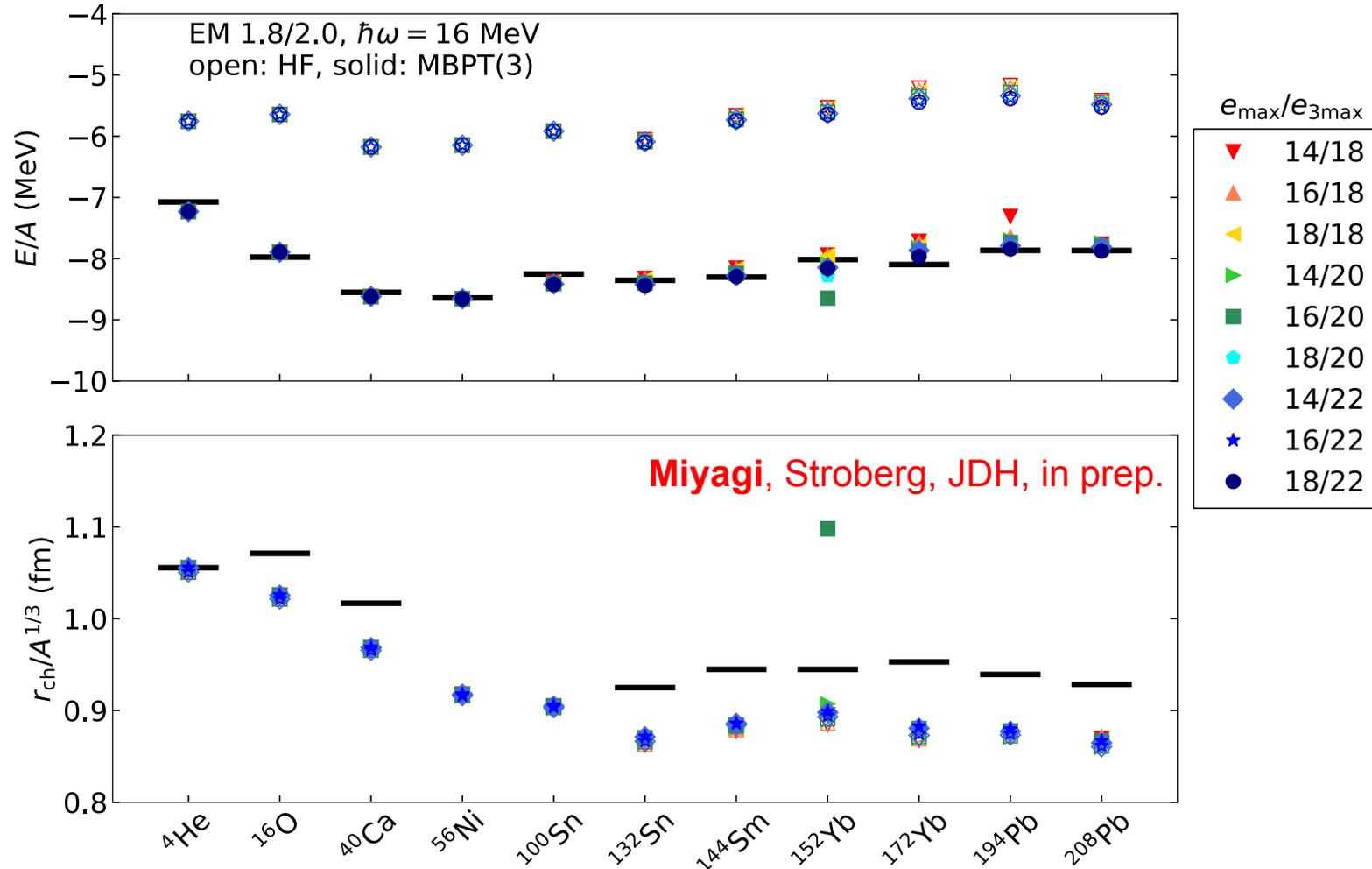


Improvements in storage of 3N matrix elements greatly expands reach of ab initio theory!



**\*Preliminary results\***

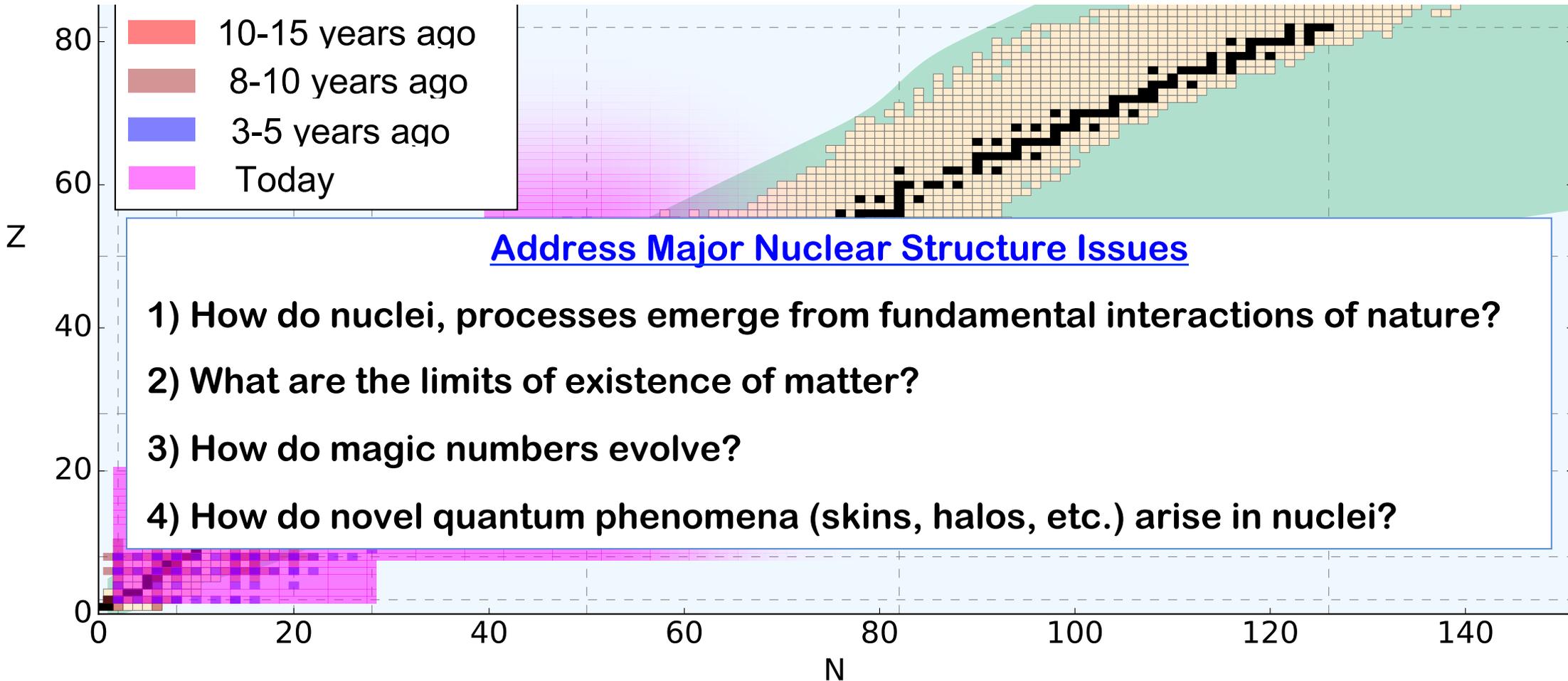
Promising for converged calculations in region of heavy Pb isotopes!



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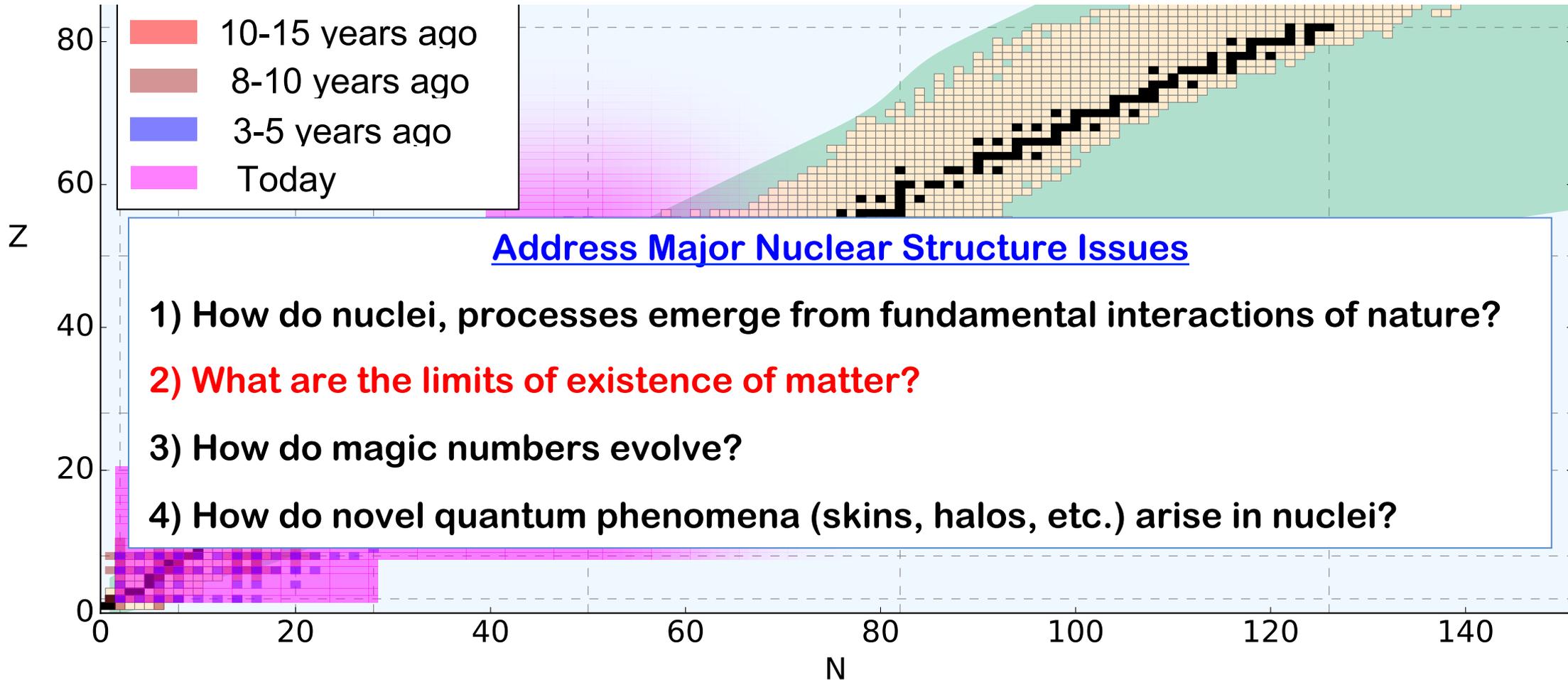
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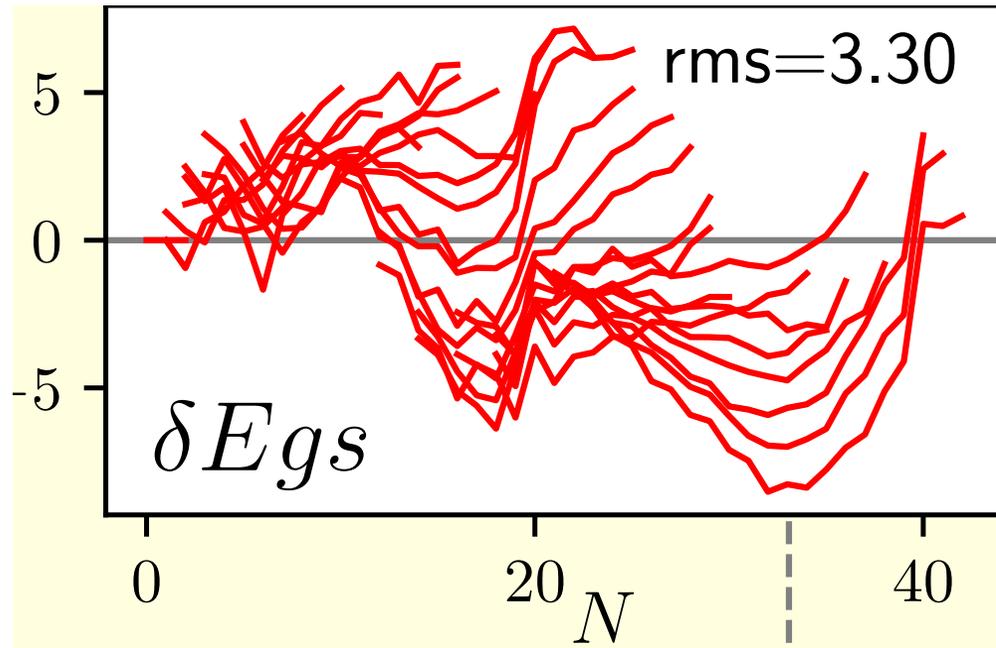
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$$H\psi_n = E_n\psi_n$$



Ab initio calculations of nearly 700 nuclei... how to analyze uncertainties?



$$\delta \mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$

B-W Mass formula: 3.1 MeV  $Z < 28$   
3.5 MeV  $Z < 20$

DFT: 0.6-2.0 MeV

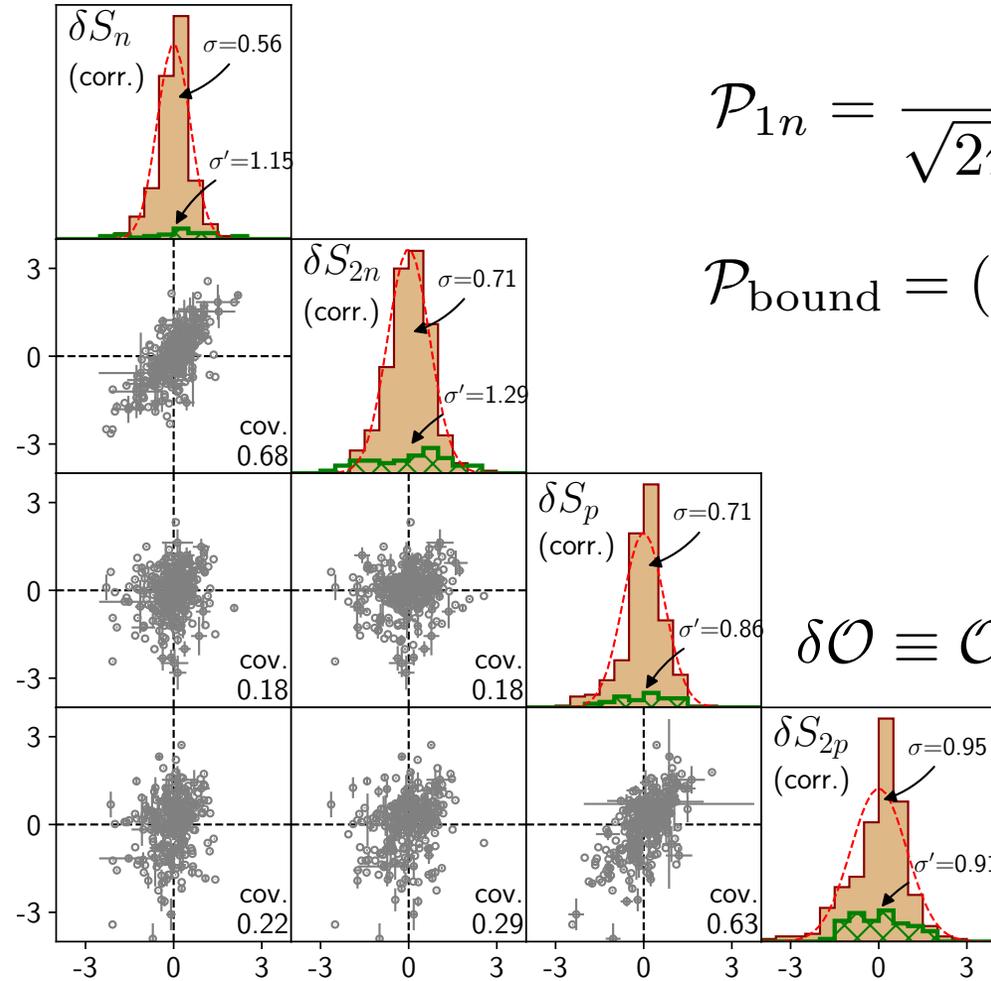
JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

rms deviation at level of BW Mass formula, approaching EDF models

Input Hamiltonians fit to  $A=2,3,4$  – not biased towards known data

What is deviation for separation energies? **Apply to nuclear driplines**

All corrected distributions approximately Gaussian centered at 0



$$\mathcal{P}_{1n} = \frac{1}{\sqrt{2\pi}\sigma_{1n}} \int_0^\infty \exp \left[ \frac{(x - S_n^{th.corr})^2}{2\sigma_{1n}^2} \right] dx$$

$$\mathcal{P}_{\text{bound}} = (\mathcal{P}_{1n}\mathcal{P}_{2n} + \xi_{1n,2n})(\mathcal{P}_{1p}\mathcal{P}_{2p} + \xi_{1p,2p})$$

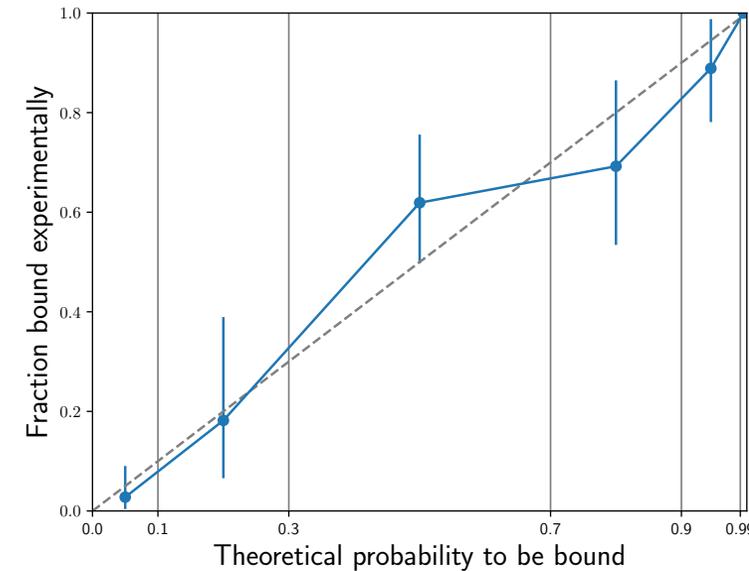
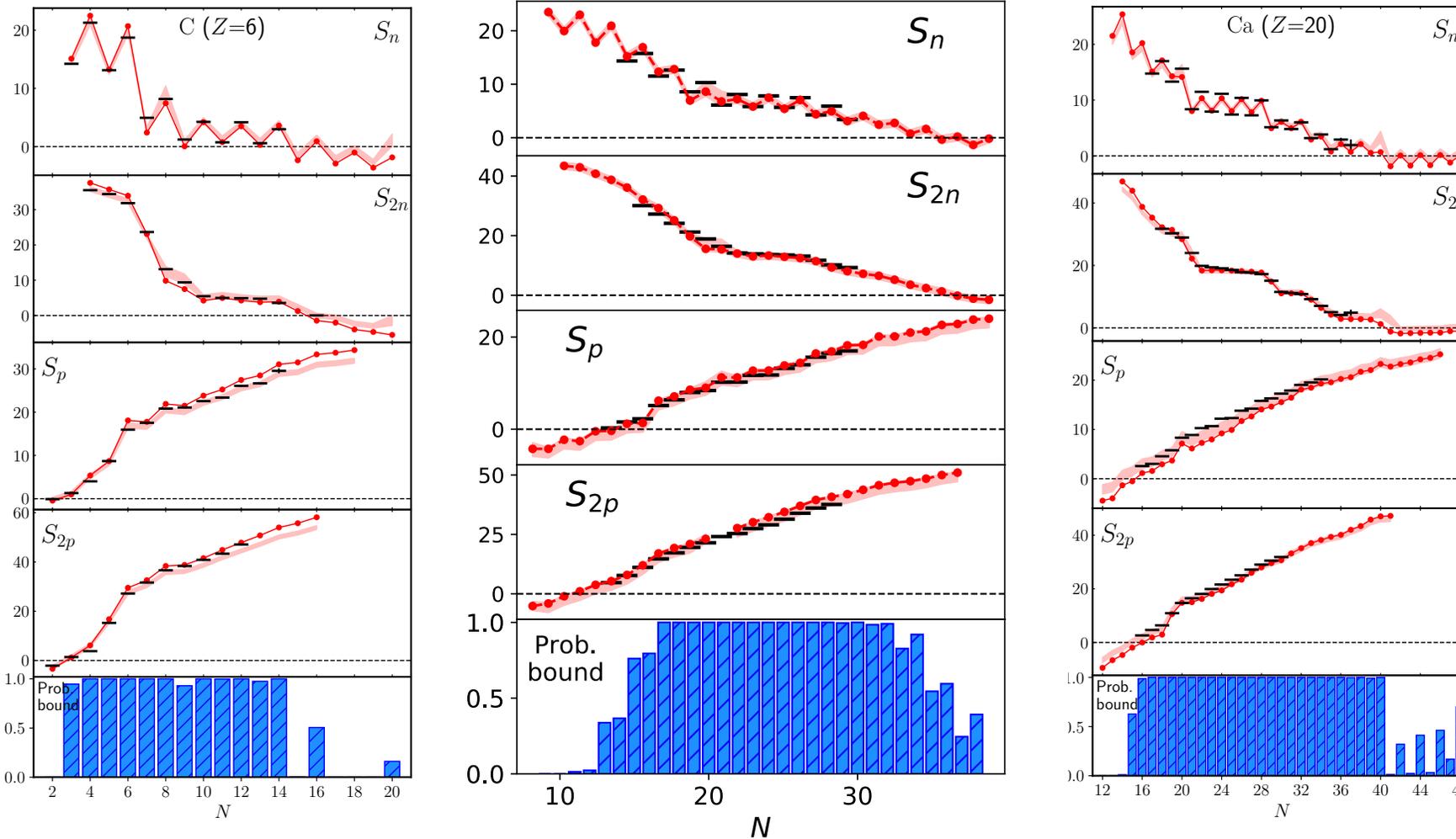
$$\delta\mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$

JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

Certain residuals correlated – must correct for this in probabilities

Assume unmeasured nuclei also follow this distribution

Determine rms deviation from experiment – extrapolate this uncertainty beyond data

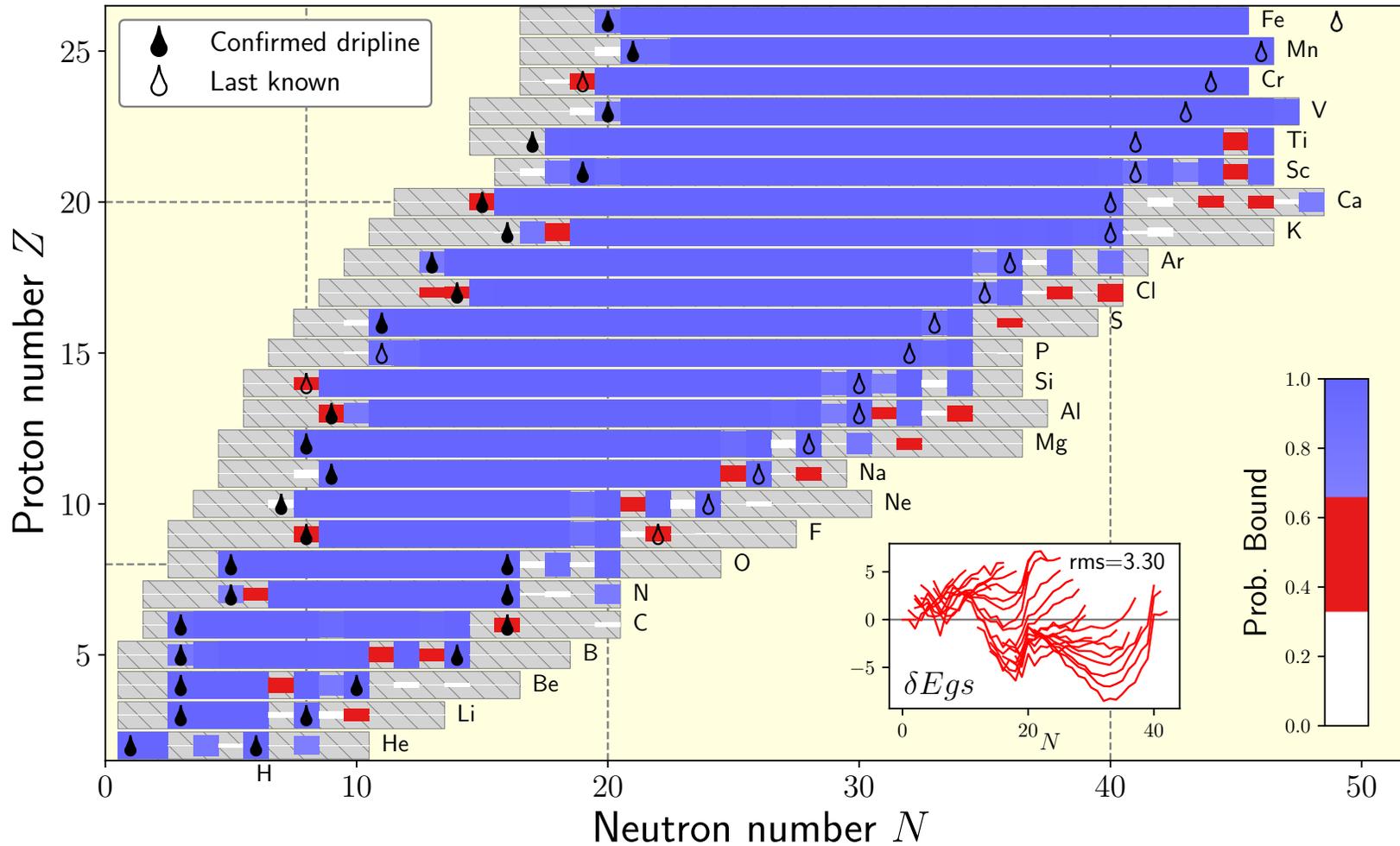


Determine range of likely separation energies reaching 0

Assign probability that a particular nucleus is bound

JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

## First predictions of proton and neutron driplines from first principles



$$\mathcal{P}_{1n} = \frac{1}{\sqrt{2\pi}\sigma_{1n}} \int_0^\infty \exp\left(-\frac{(x - S_n^{th.cor})^2}{2\sigma_{1n}^2}\right) dx$$

$$\mathcal{P}_{bound} = (\mathcal{P}_{1n}\mathcal{P}_{2n} + \xi_{1n,2n})(\mathcal{P}_{1p}\mathcal{P}_{2p} + \xi_{1p,2p})$$

JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

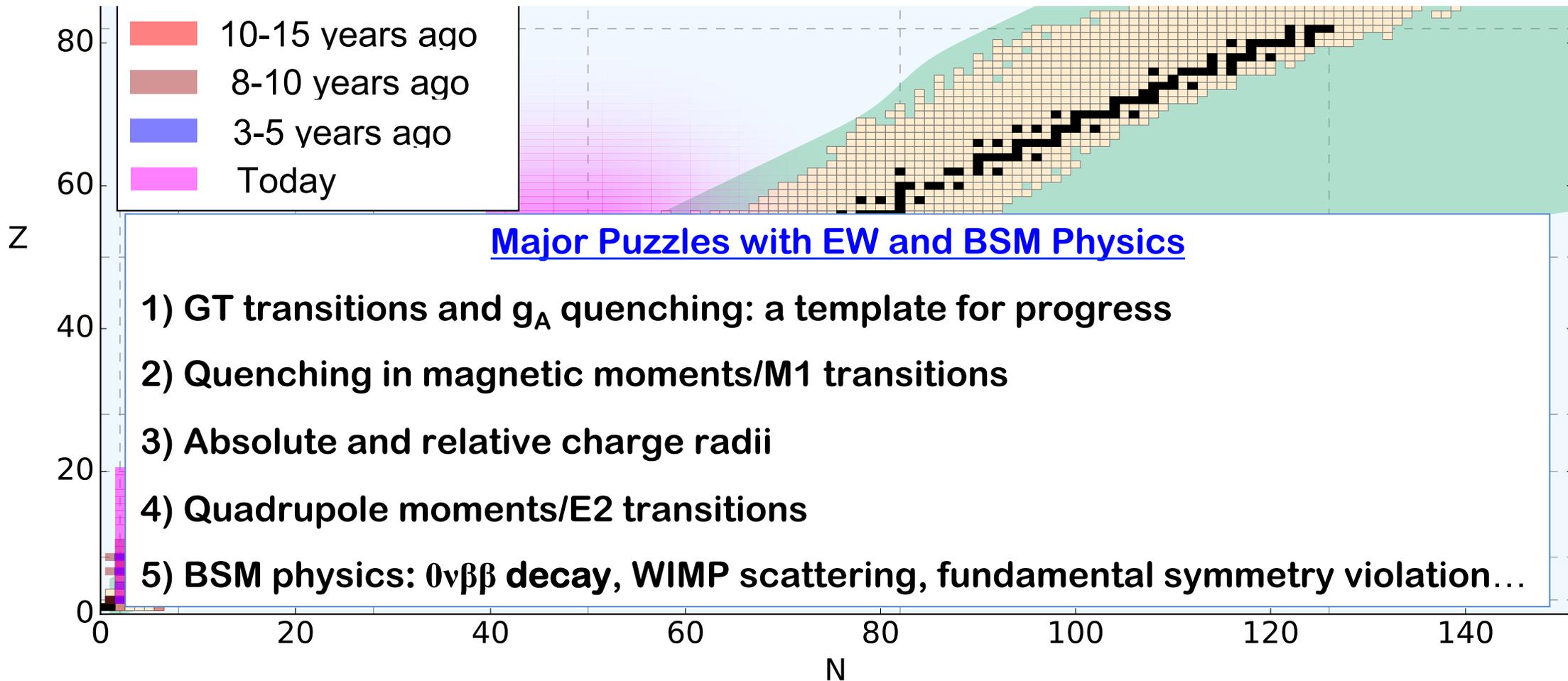
Known drip lines largely predicted within uncertainties (issues remain at shell closures)

Provide ab initio predictions for neutron-rich region

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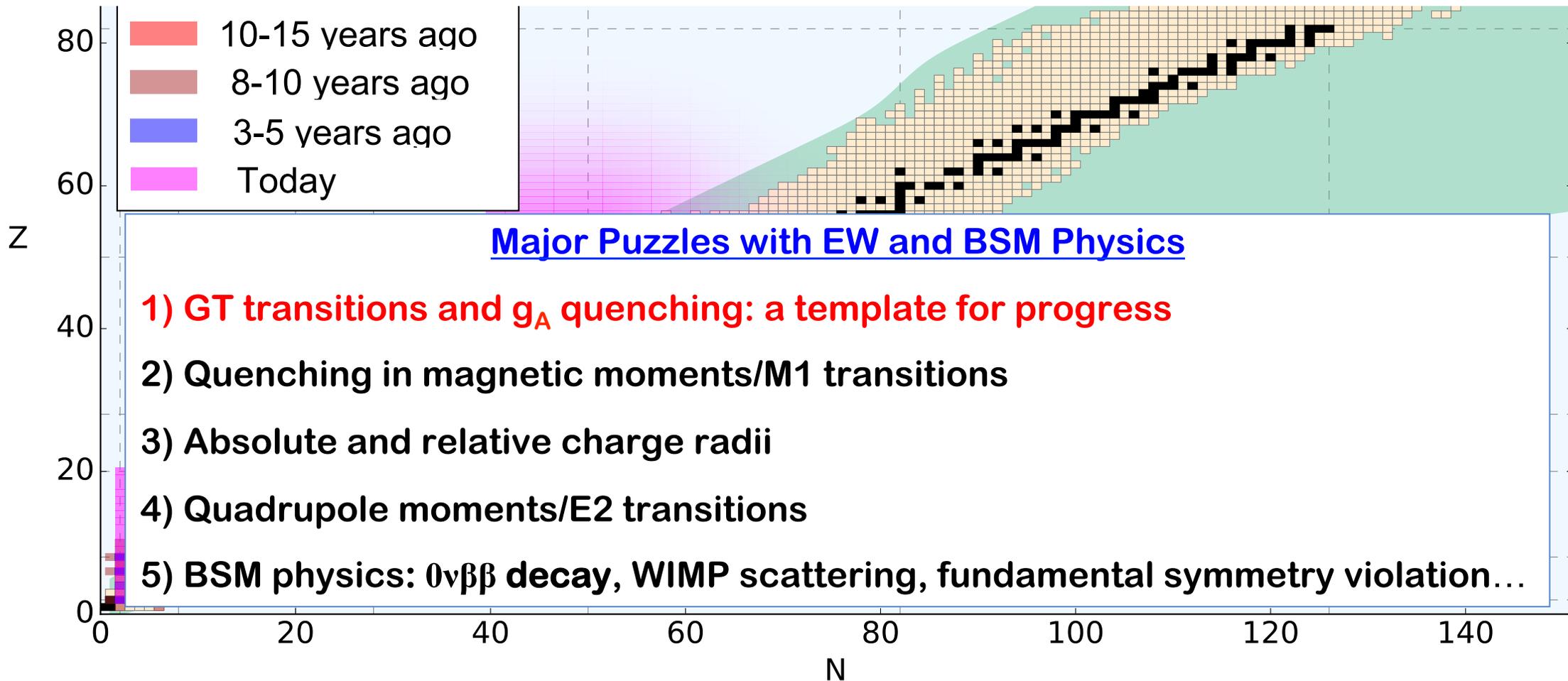
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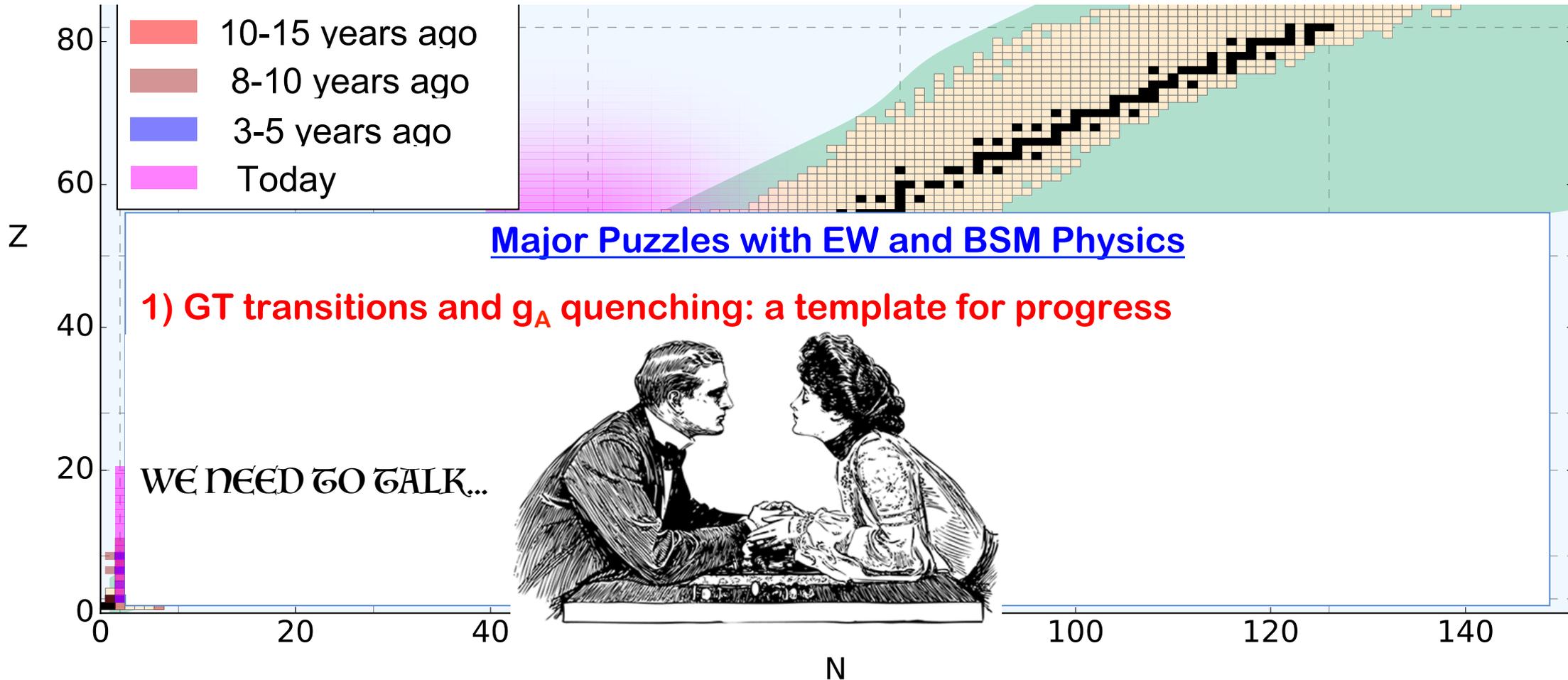
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**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem

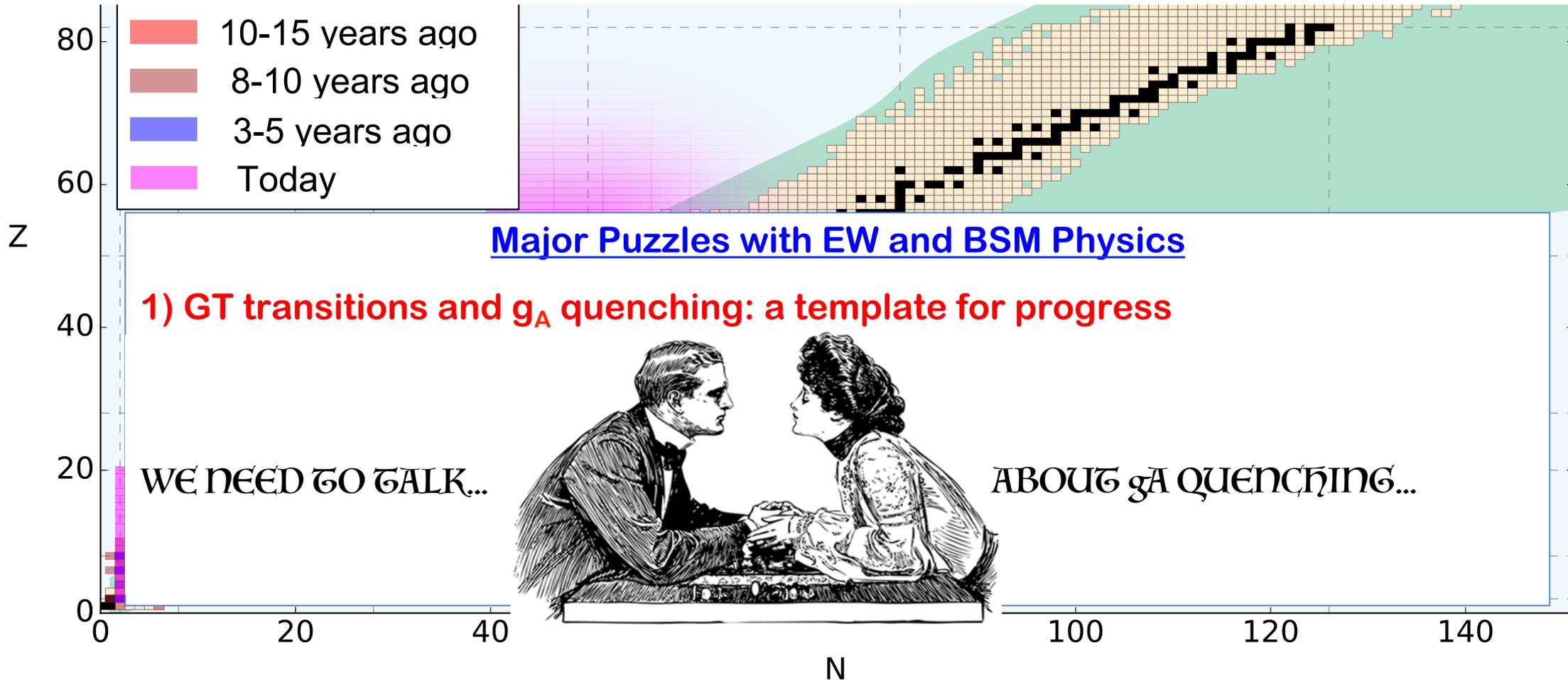
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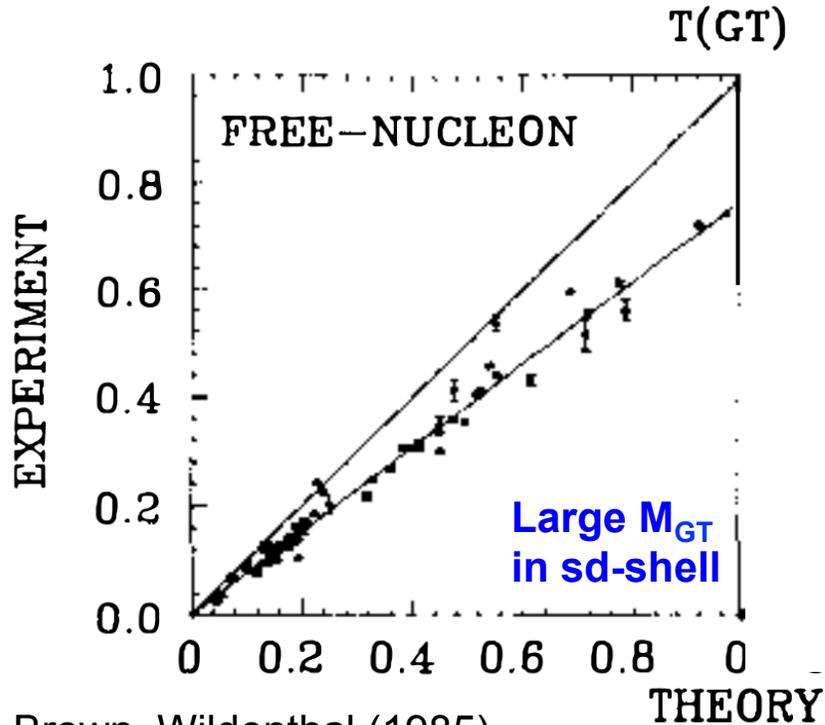
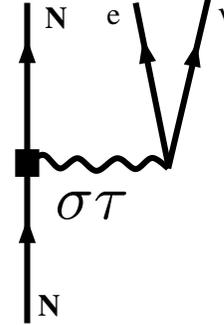
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“Long-standing problem”<sup>1</sup> in weak decays: **experimental values systematically smaller than theory**

$$M_{GT} = g_A \langle f | \mathcal{O}_{GT} | i \rangle \quad \mathcal{O}_{GT} = \mathcal{O}_{\sigma\tau}^{1b} + \mathcal{O}_{2BC}^{2b}$$



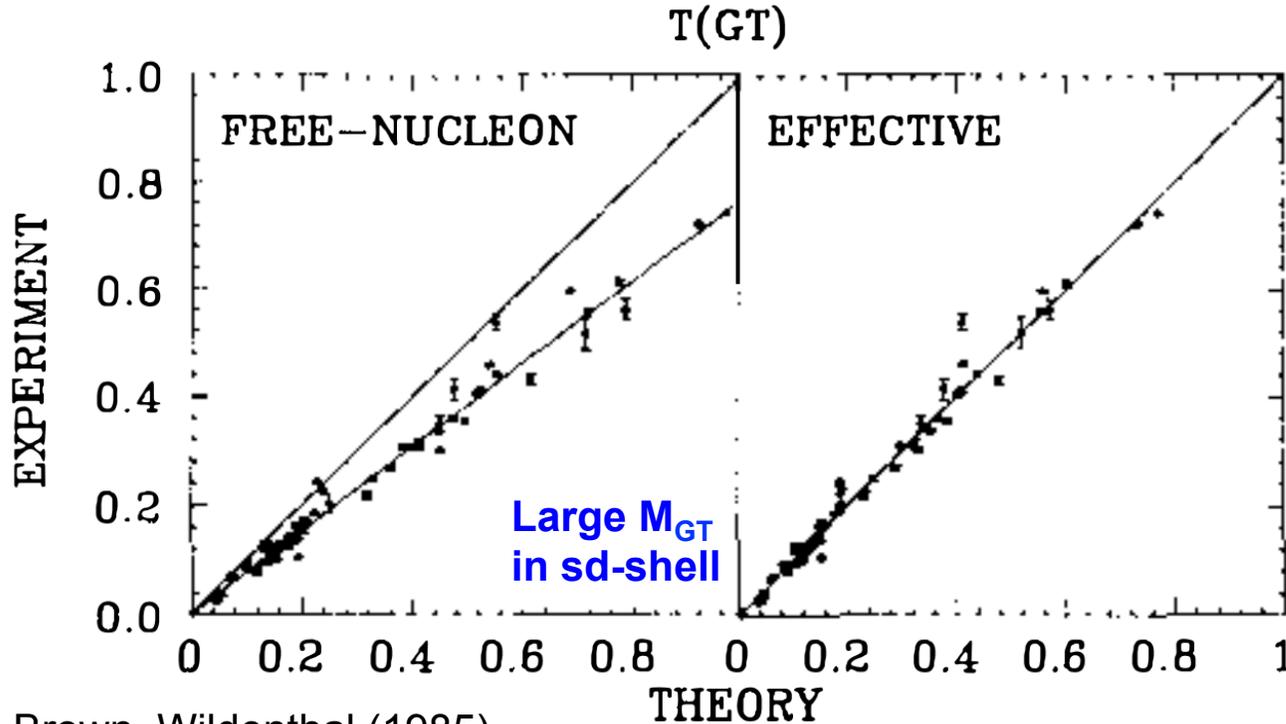
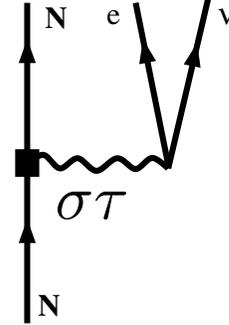
Brown, Wildenthal (1985)

<sup>1</sup> papers from the 1970's

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Using  $g_A^{\text{eff}} \approx 0.77 \times g_A^{\text{free}}$  agrees with data

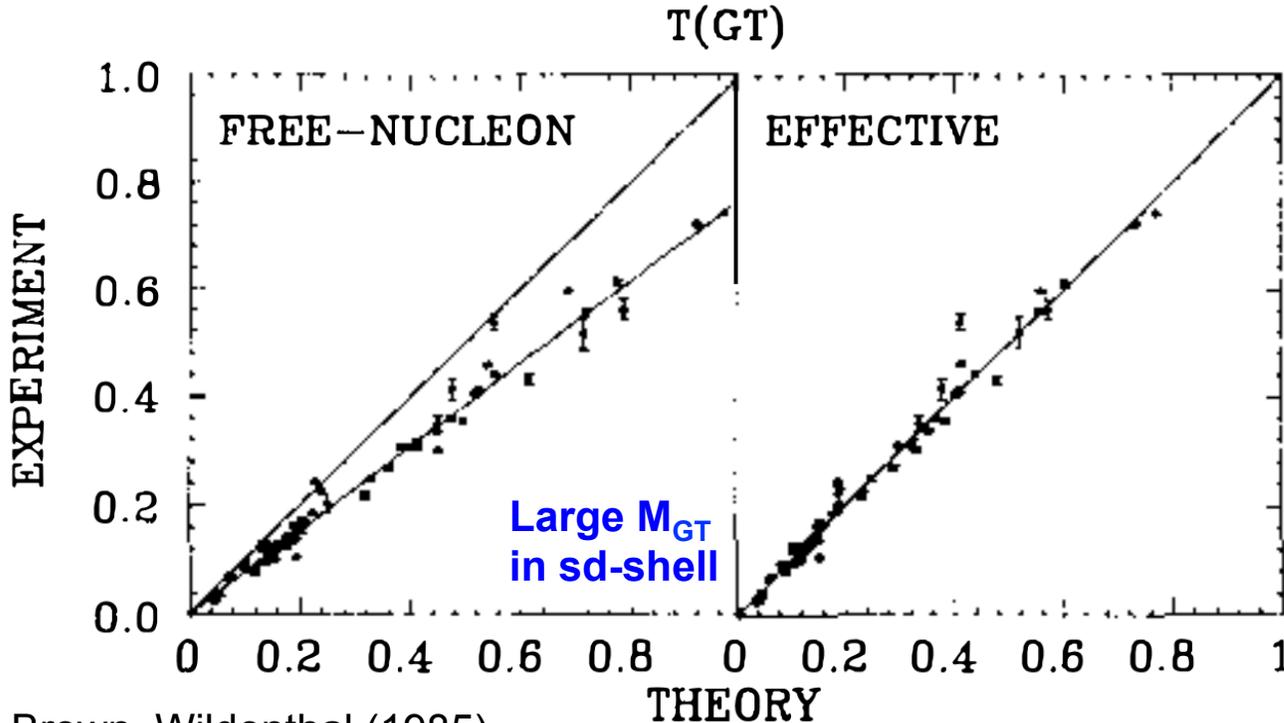
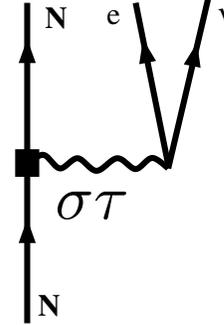


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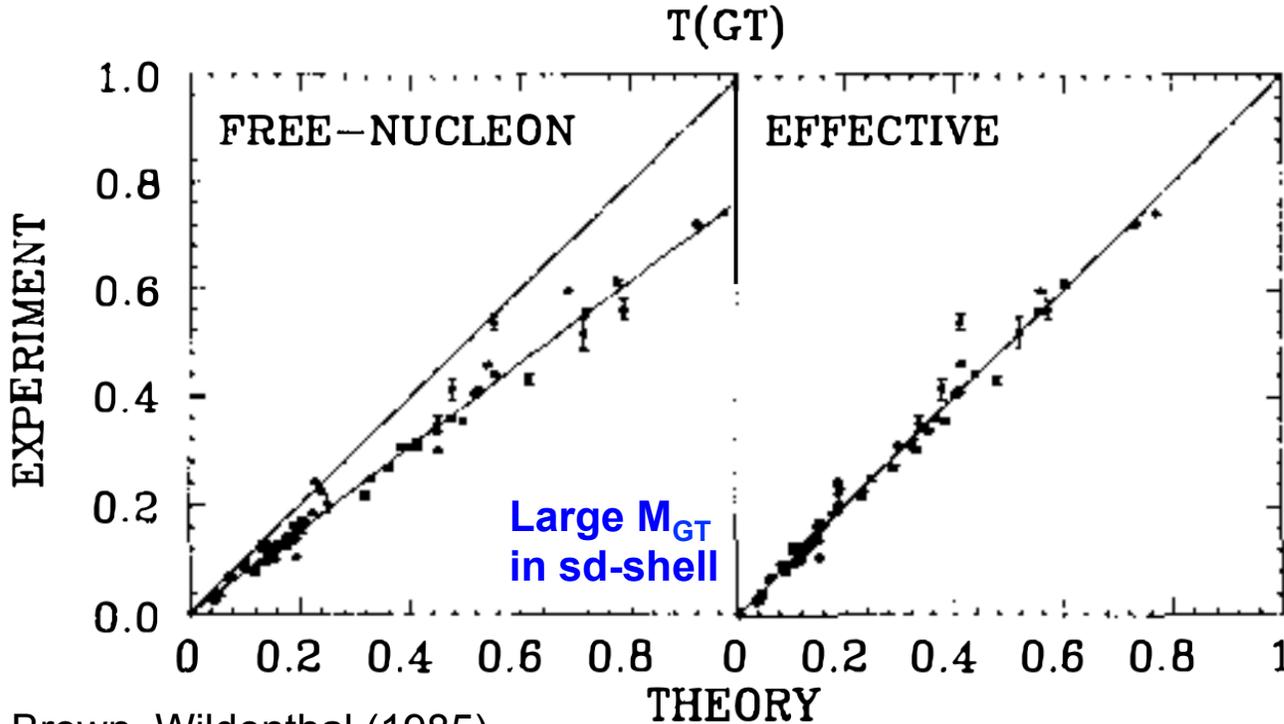
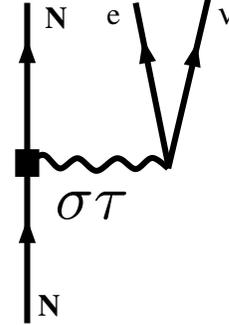
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**What about all the other stuff?**

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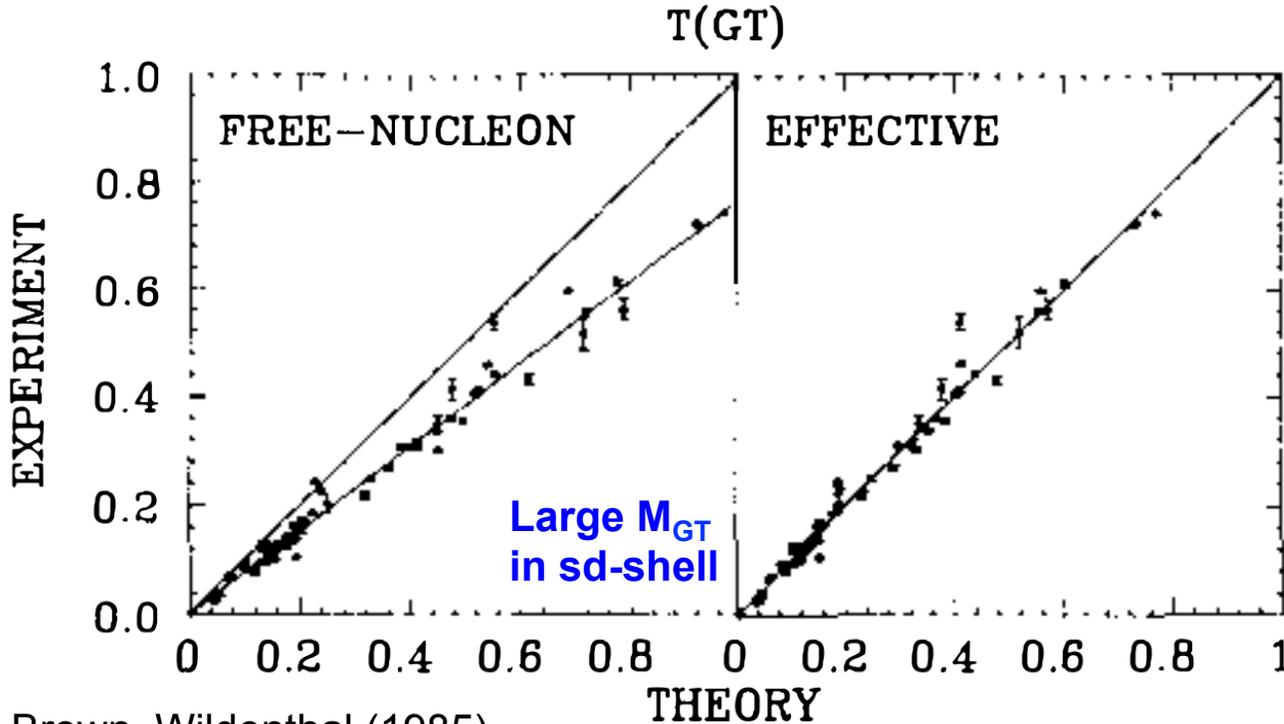
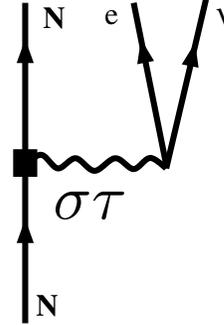
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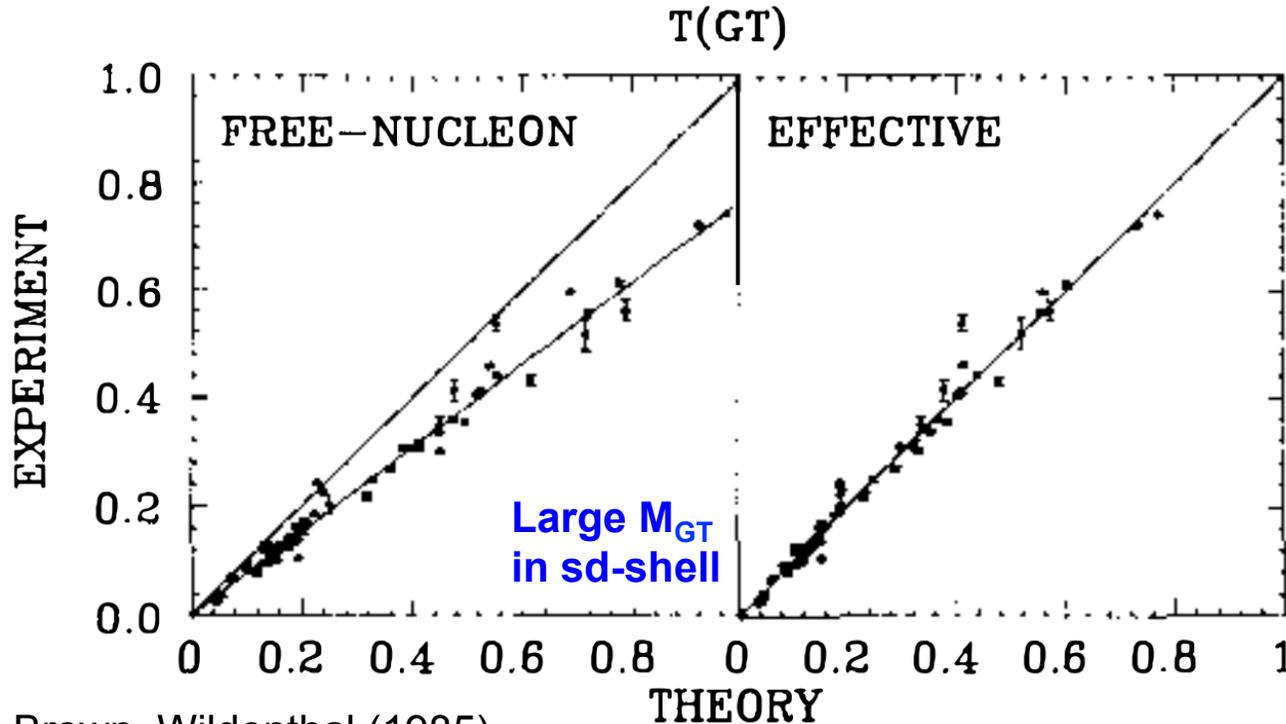
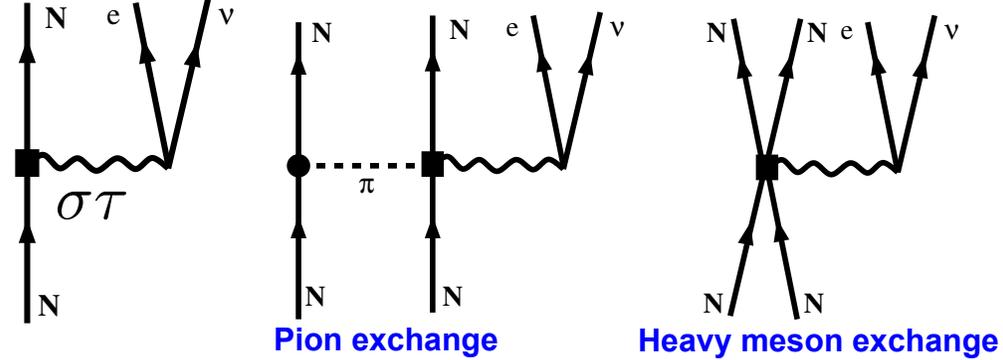
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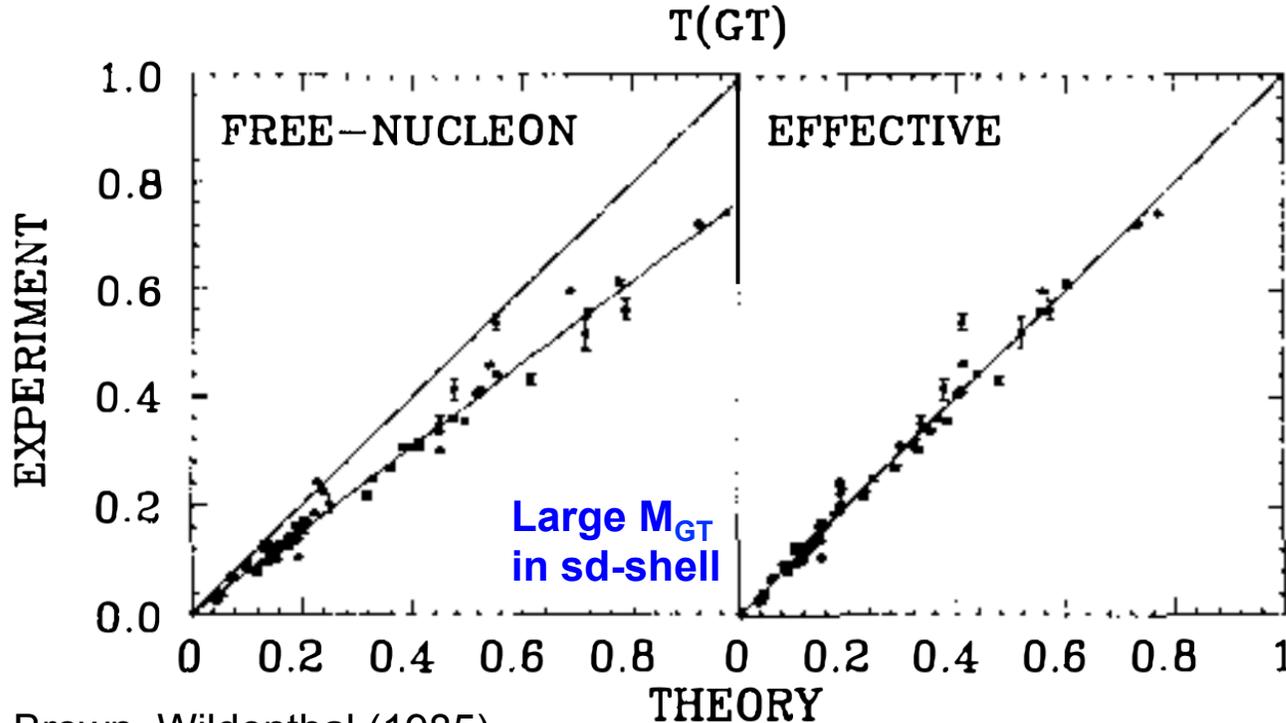
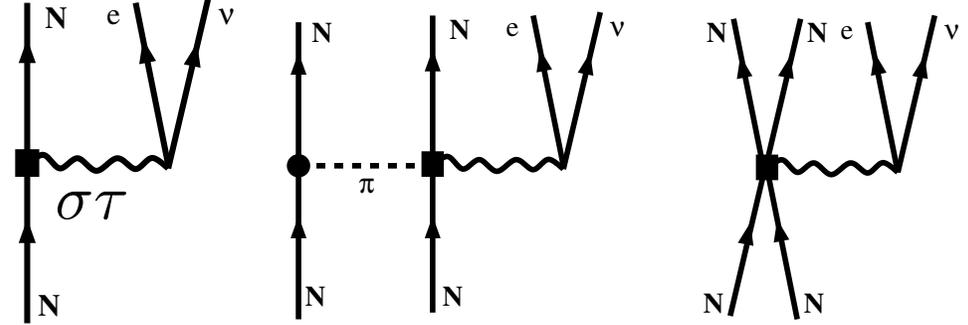
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Brown, Wildenthal (1985)

- Should  $g_A$  be quenched in medium?
- Missing wavefunction correlations
- Renormalized VS operator?
- Neglected two-body currents?
- Model-space truncations?

**Explore in ab initio framework**

## Calculate large GT matrix elements

$$M_{GT} = g_A \langle f | \mathcal{O}_{GT} | i \rangle$$

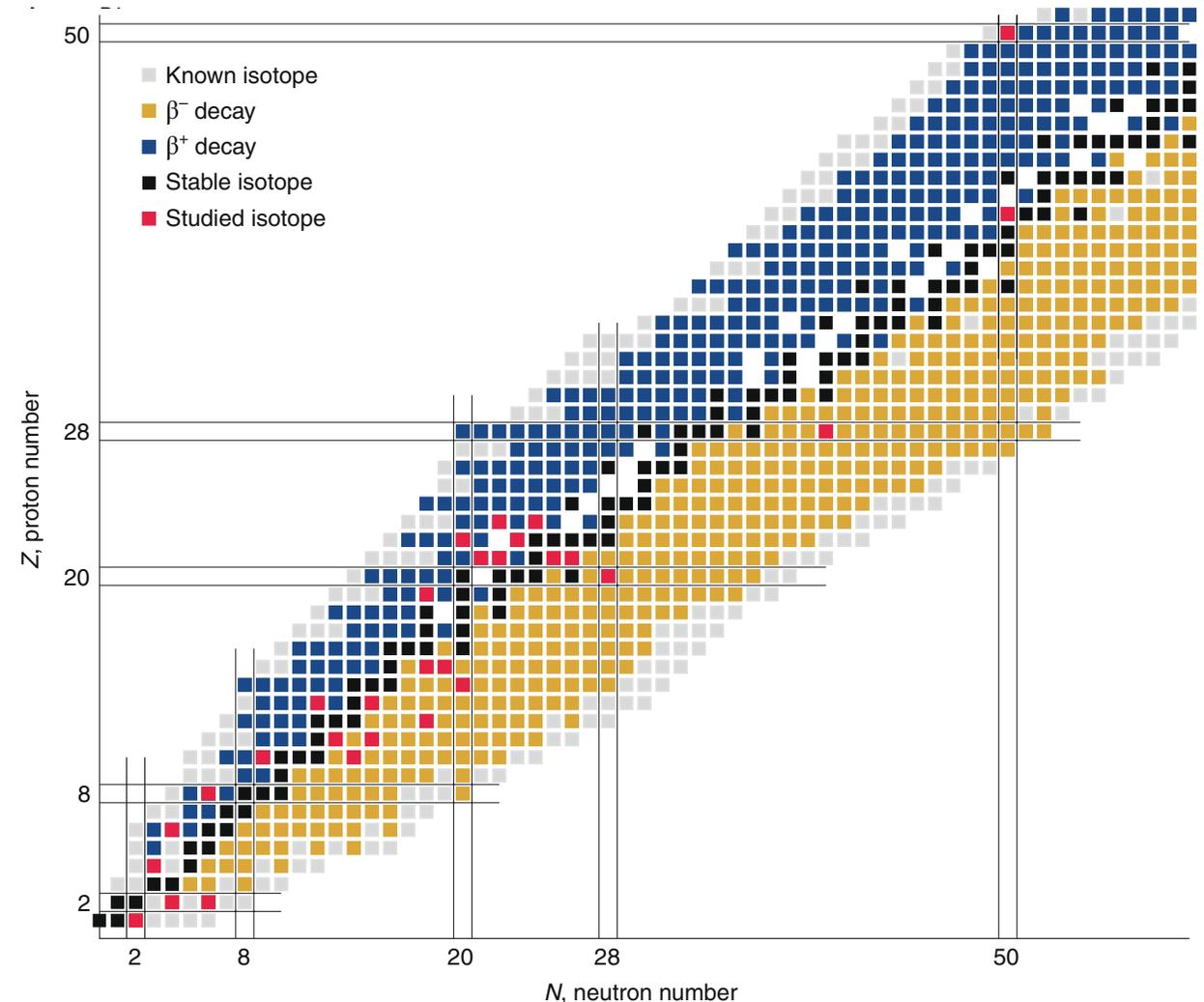
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- Light, medium, and heavy regions
- Benchmark different ab initio methods
- Wide range of NN+3N forces
- Consistent inclusion of 2BC

### NUCLEAR PHYSICS

## Beta decay gets the ab initio treatment

One of the fundamental radioactive decay modes of nuclei is  $\beta$  decay. Now, nuclear theorists have used first-principles simulations to explain nuclear  $\beta$  decay properties across a range of light- to medium-mass isotopes, up to  $^{100}\text{Sn}$ .



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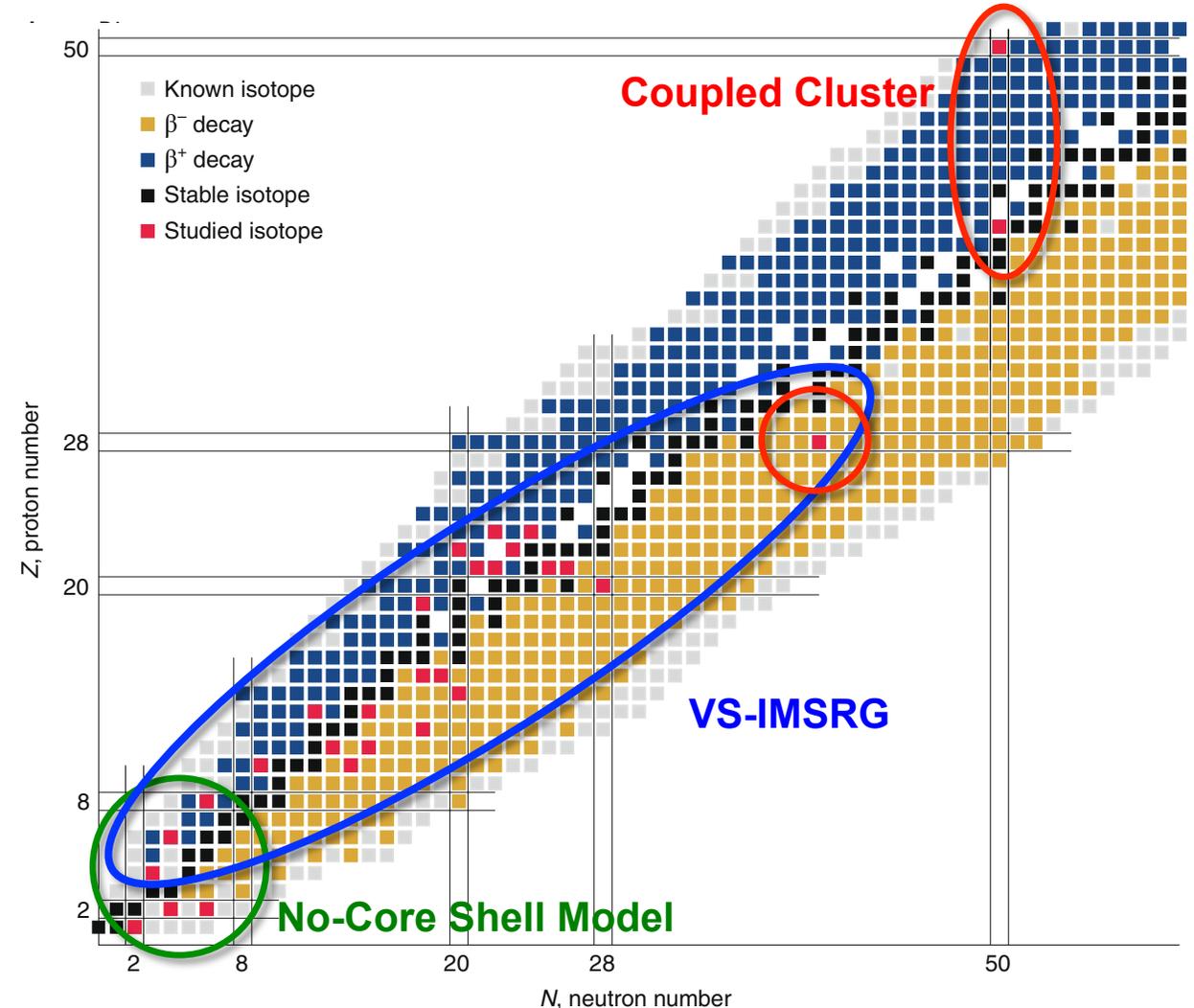
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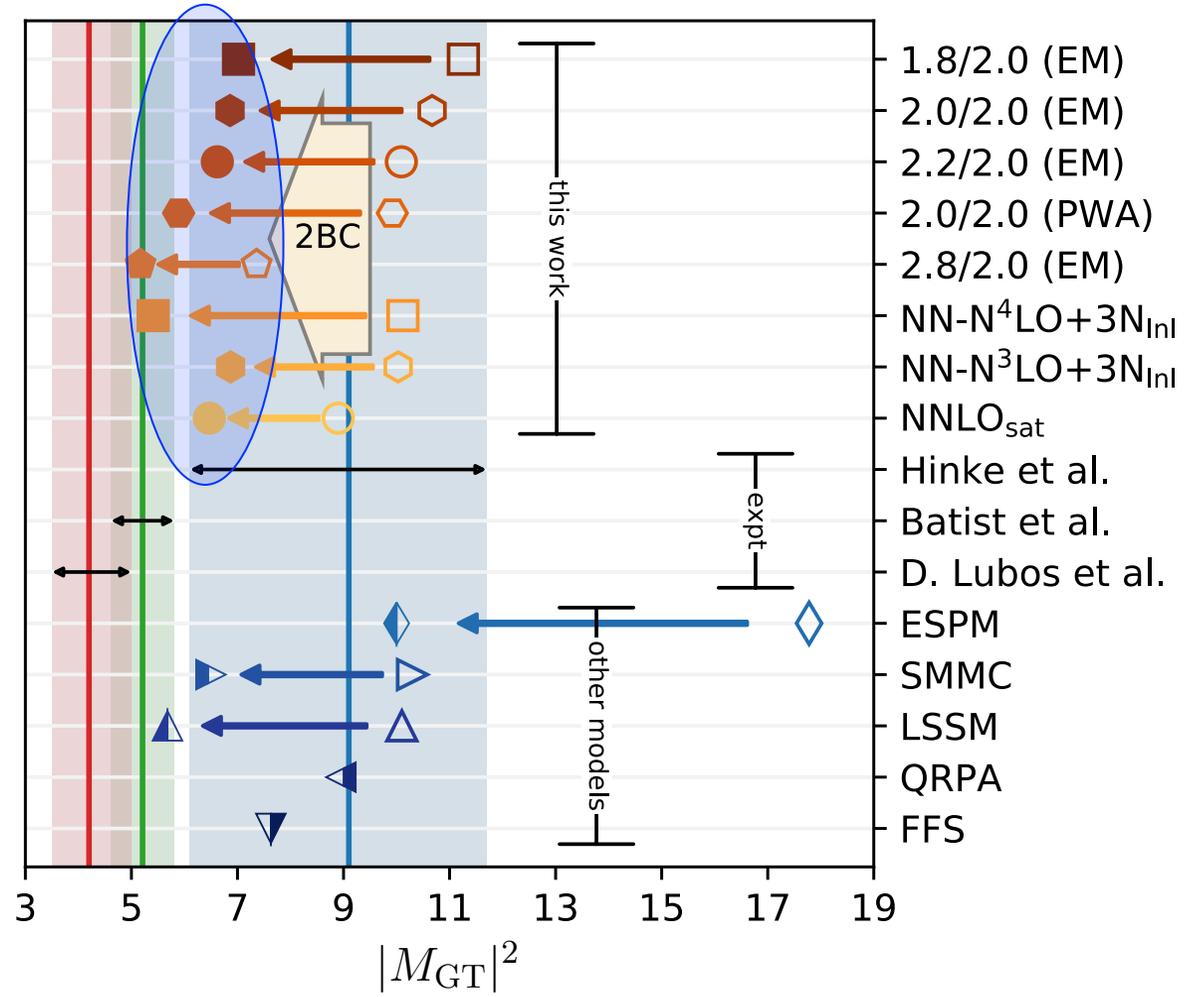
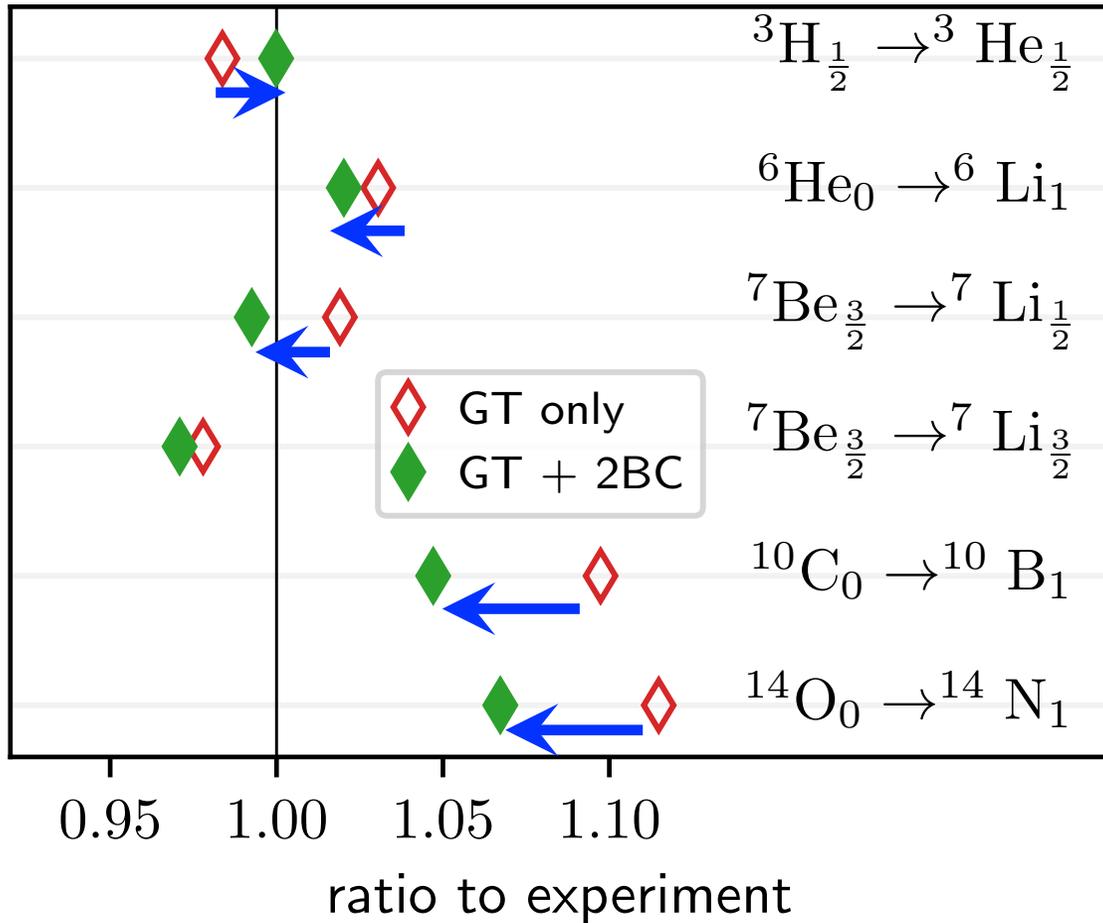
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**NCSM** in light nuclei, **CC** calculations of GT transition in  $^{100}\text{Sn}$  from different forces

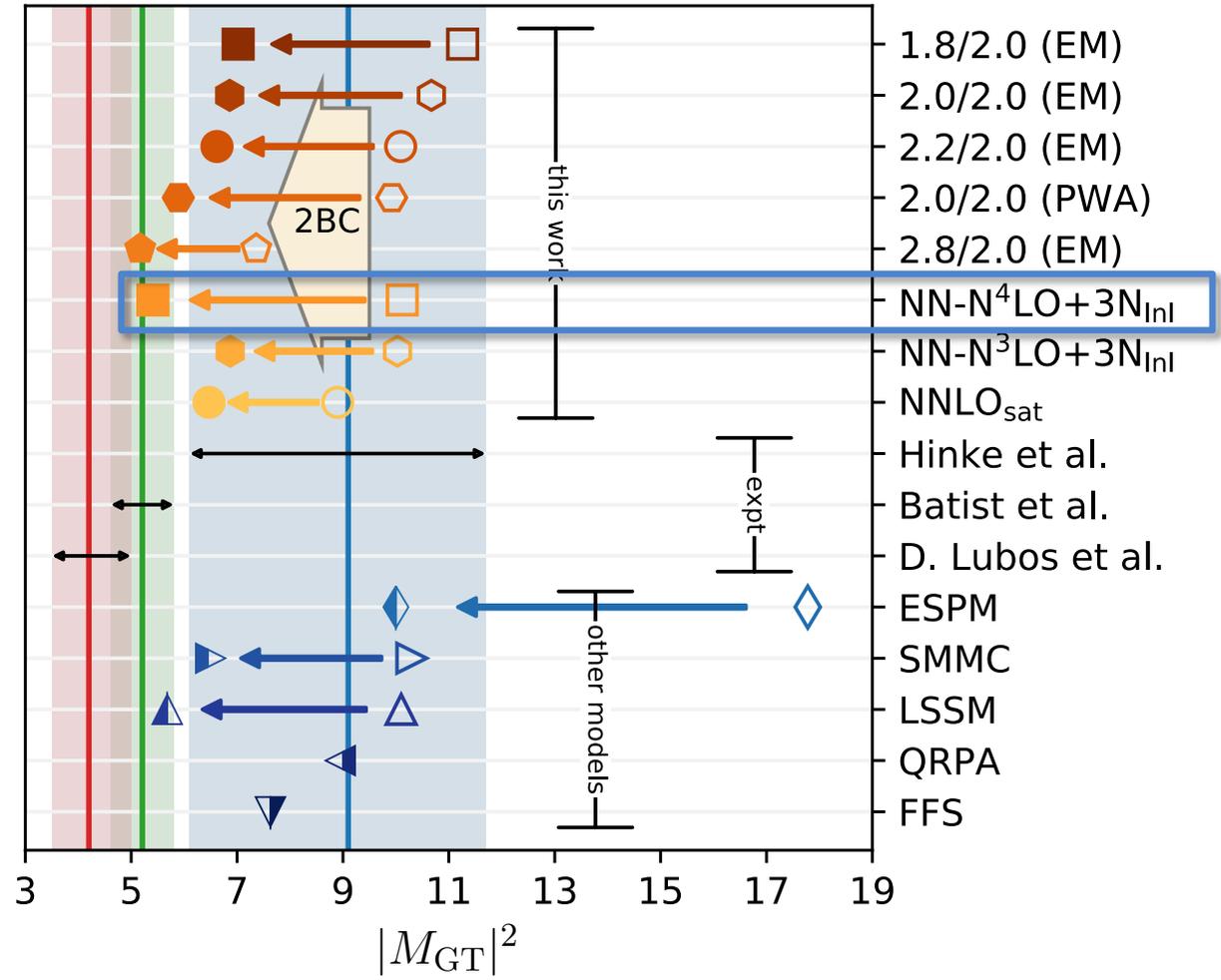
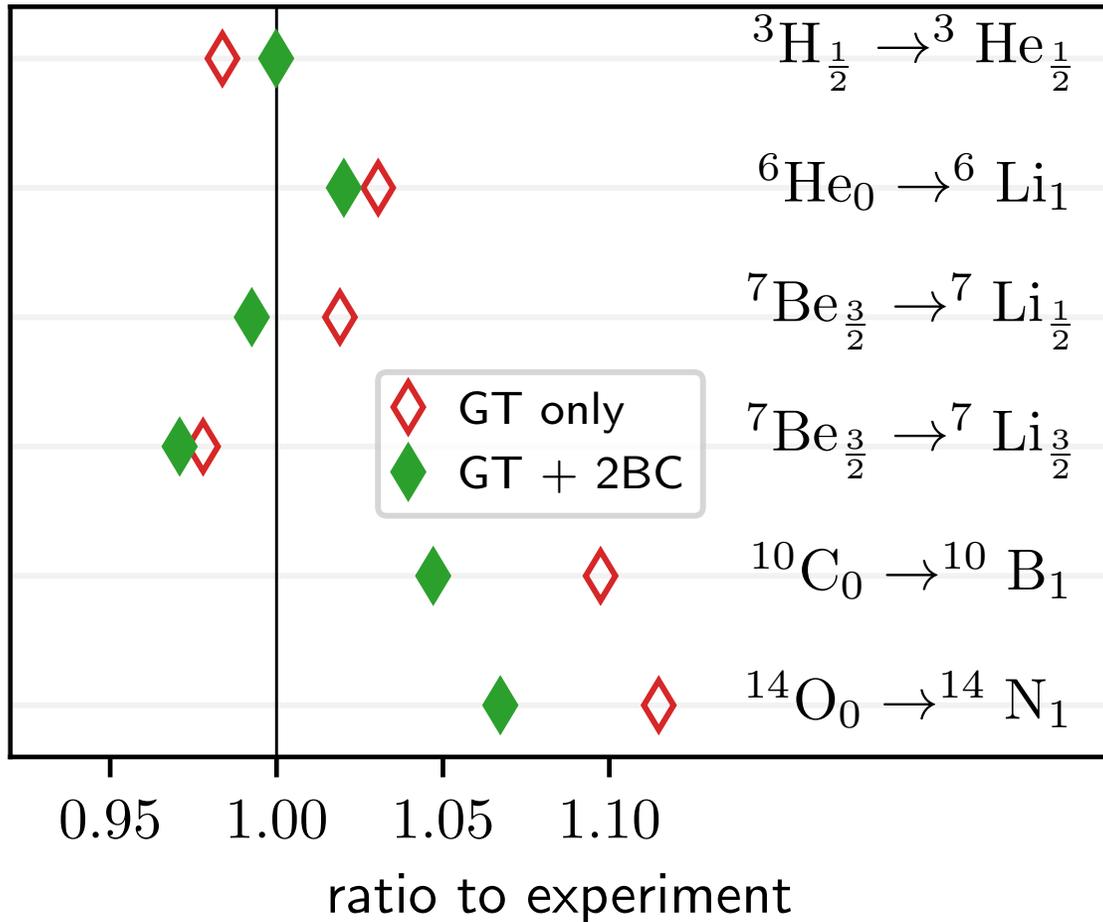


Large quenching effect from correlations

**Addition of 2BC further quenches and reduces spread in results**

Gysbers et al., Nature Phys. (2019)

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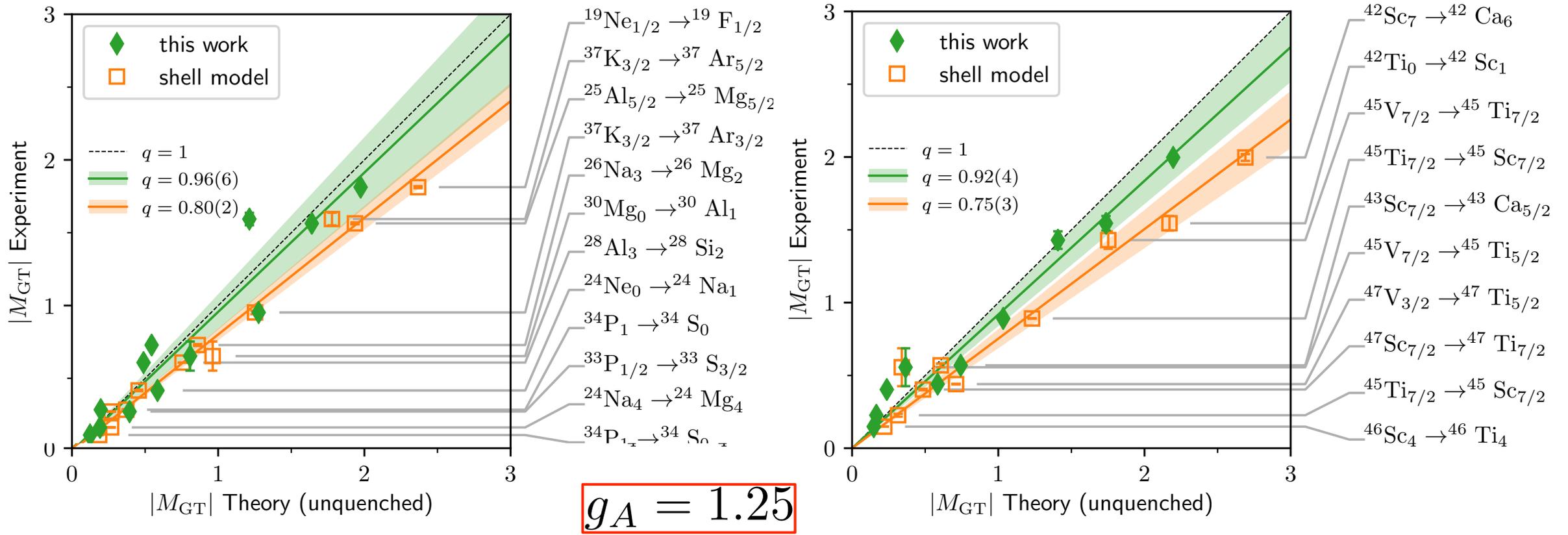
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Gysbers et al., Nature Phys. (2019)

Comparison to standard phenomenological shell model

Ab initio calculations across the chart explain data with free-space  $g_A$



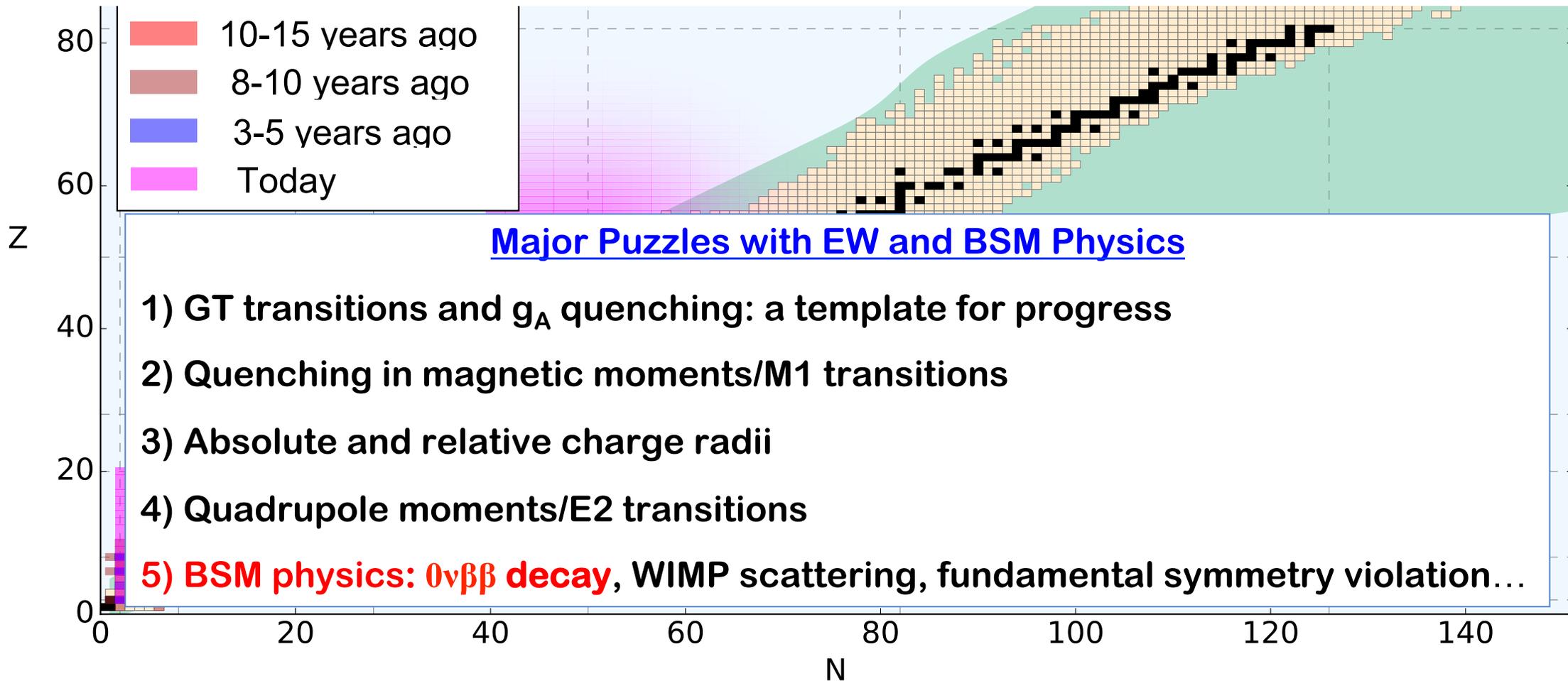
Refine results with improvements in forces and many-body methods Gysbers et al., Nature Phys. (2019)

In progress: muon capture

**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

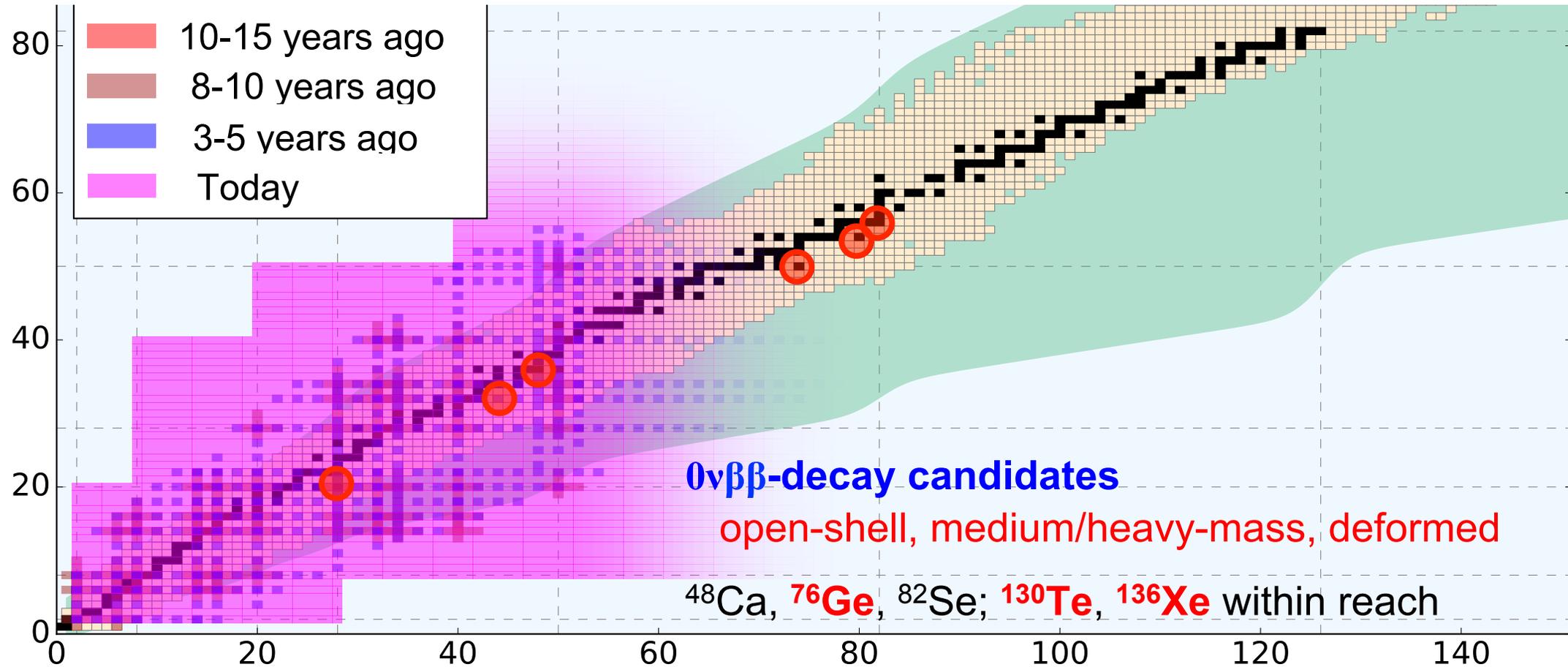
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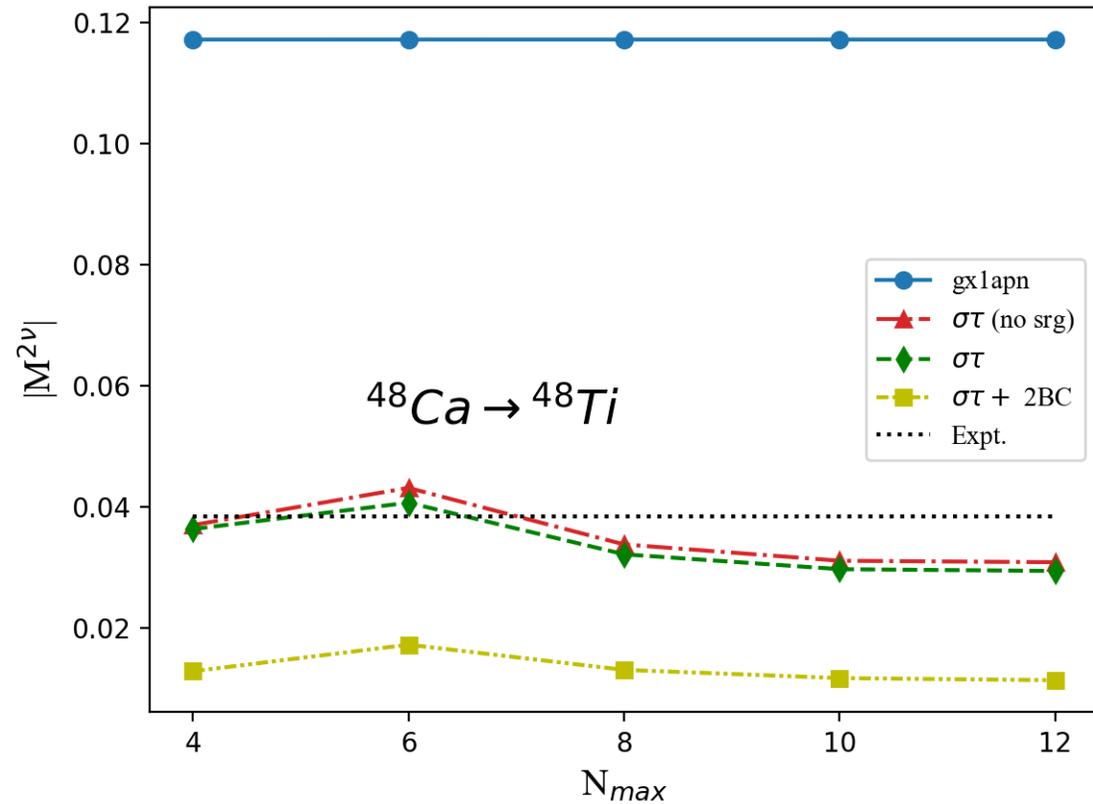
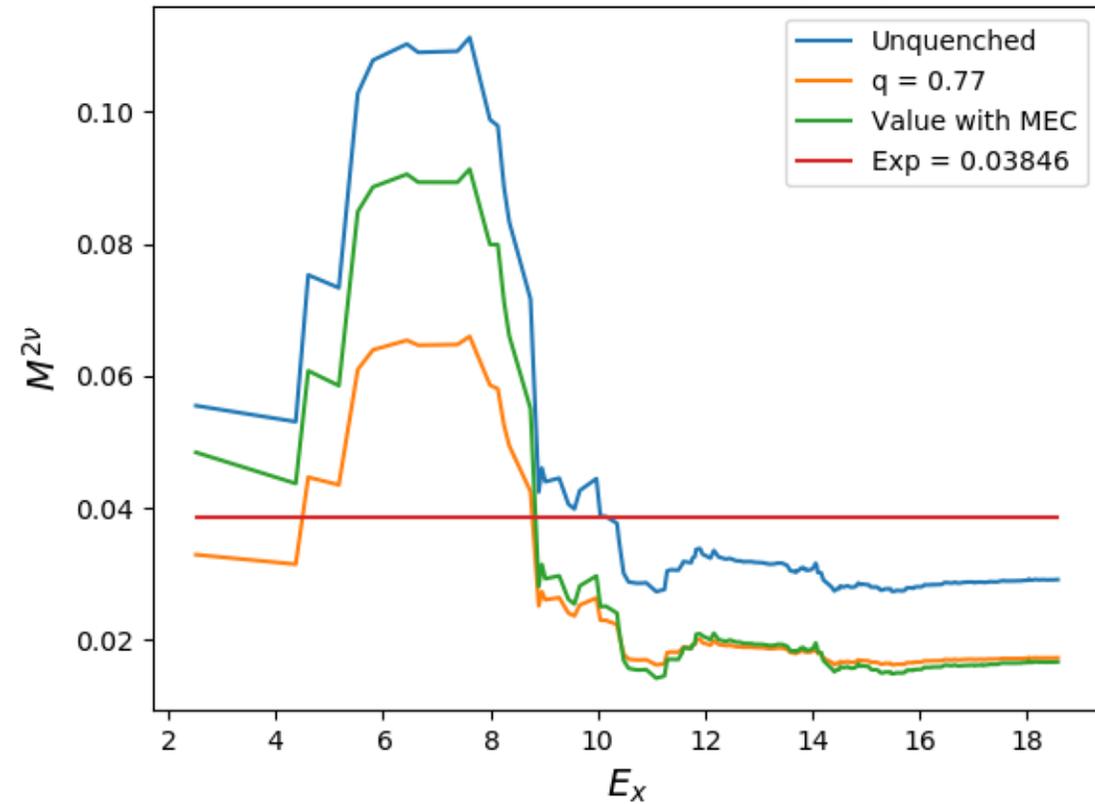
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Consistent many-body wfs/operators from chiral NN+3N forces (**with 2b currents**)

VS-IMSRG 1.8/2.0 (EM)

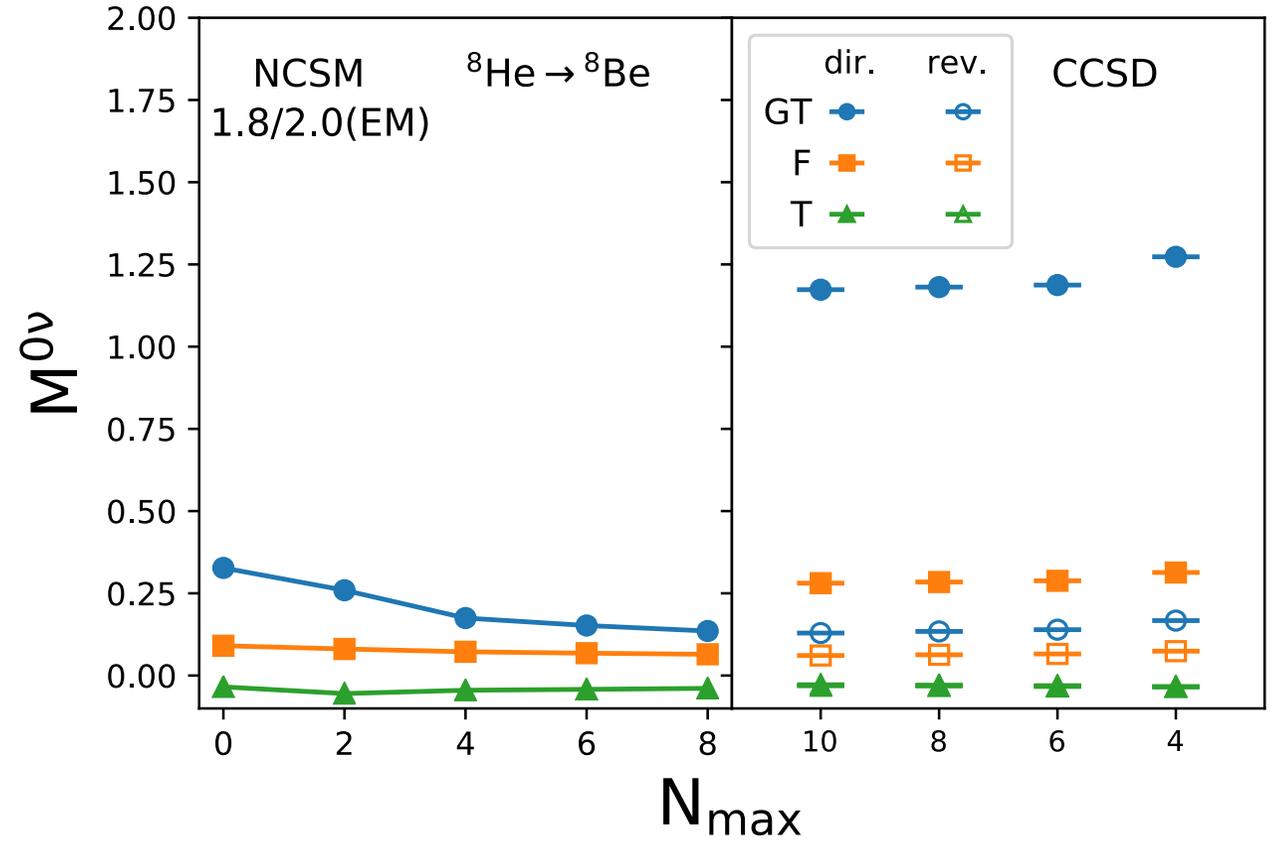
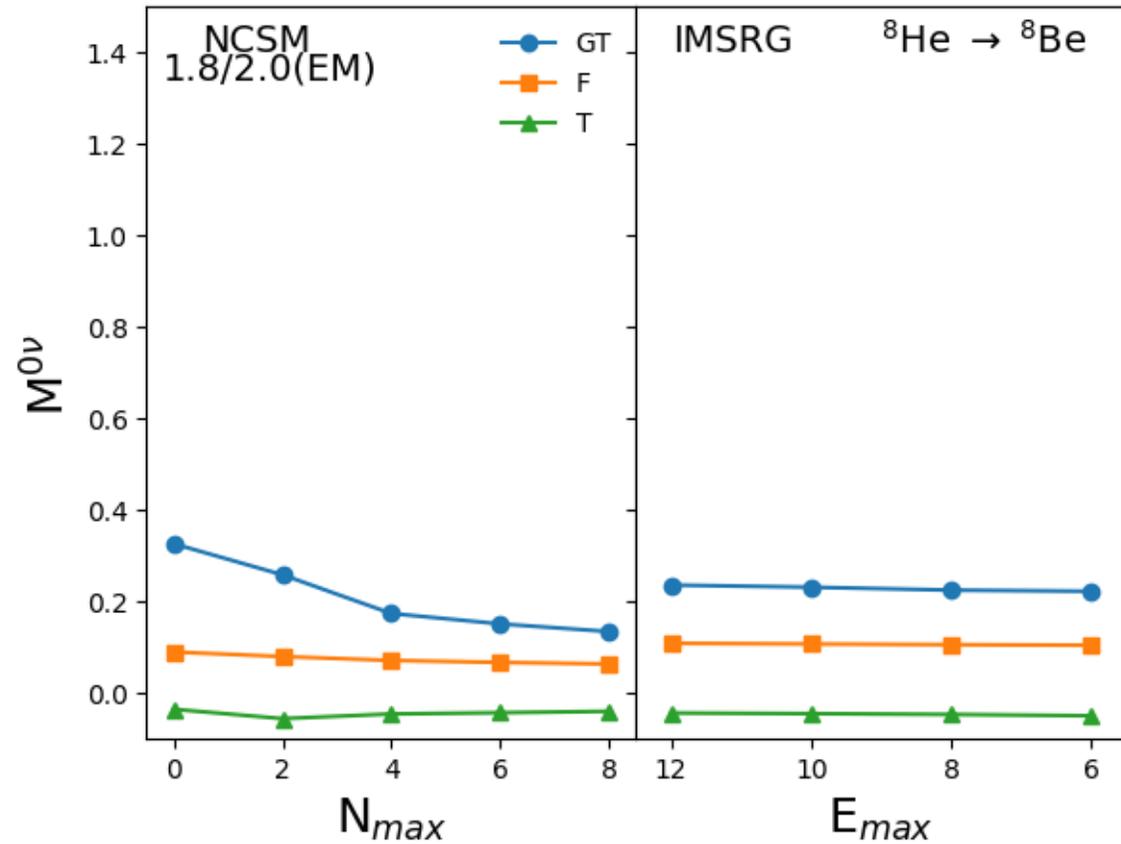


**VS-IMSRG: decrease in final matrix element**

Belley, Payne, Stroberg, JDH, in prep

Potential issues: limited  $1^+$  states, missing IMSRG(3)... benchmarks with CC underway...

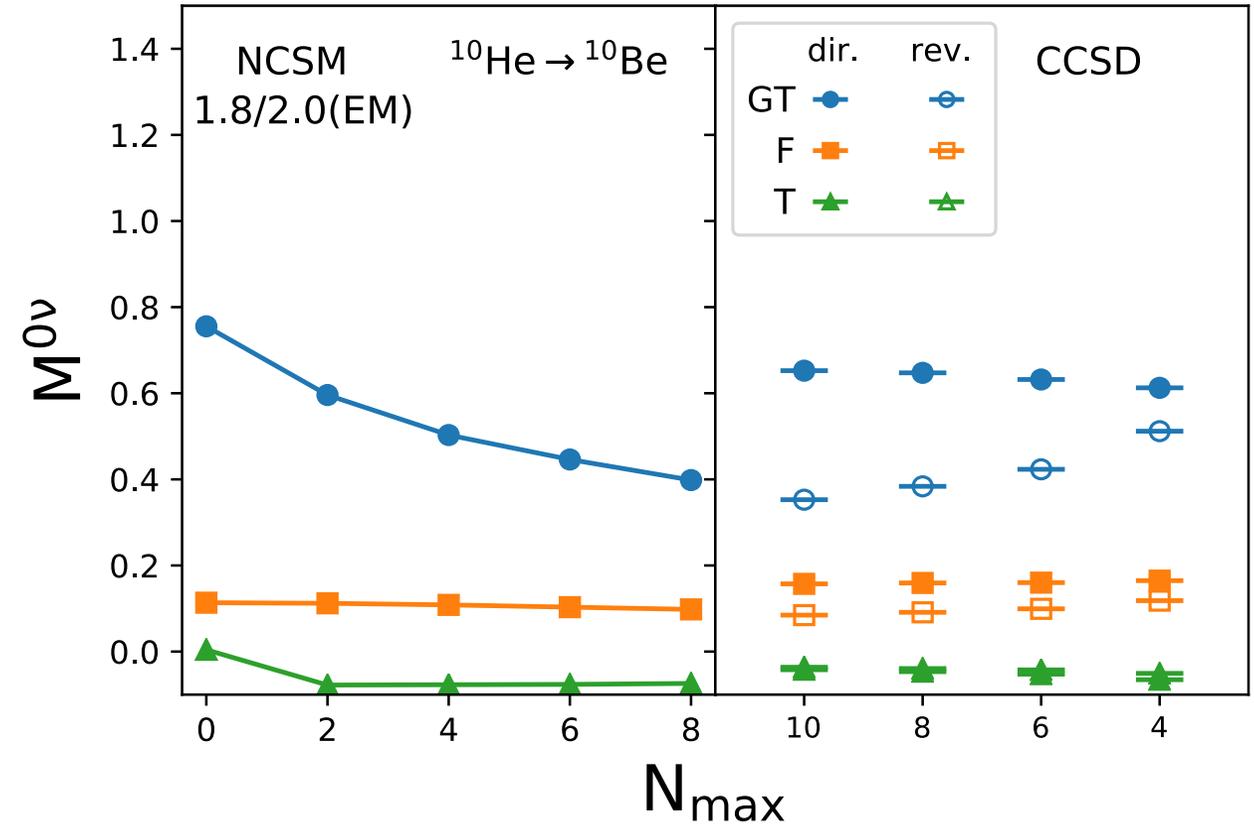
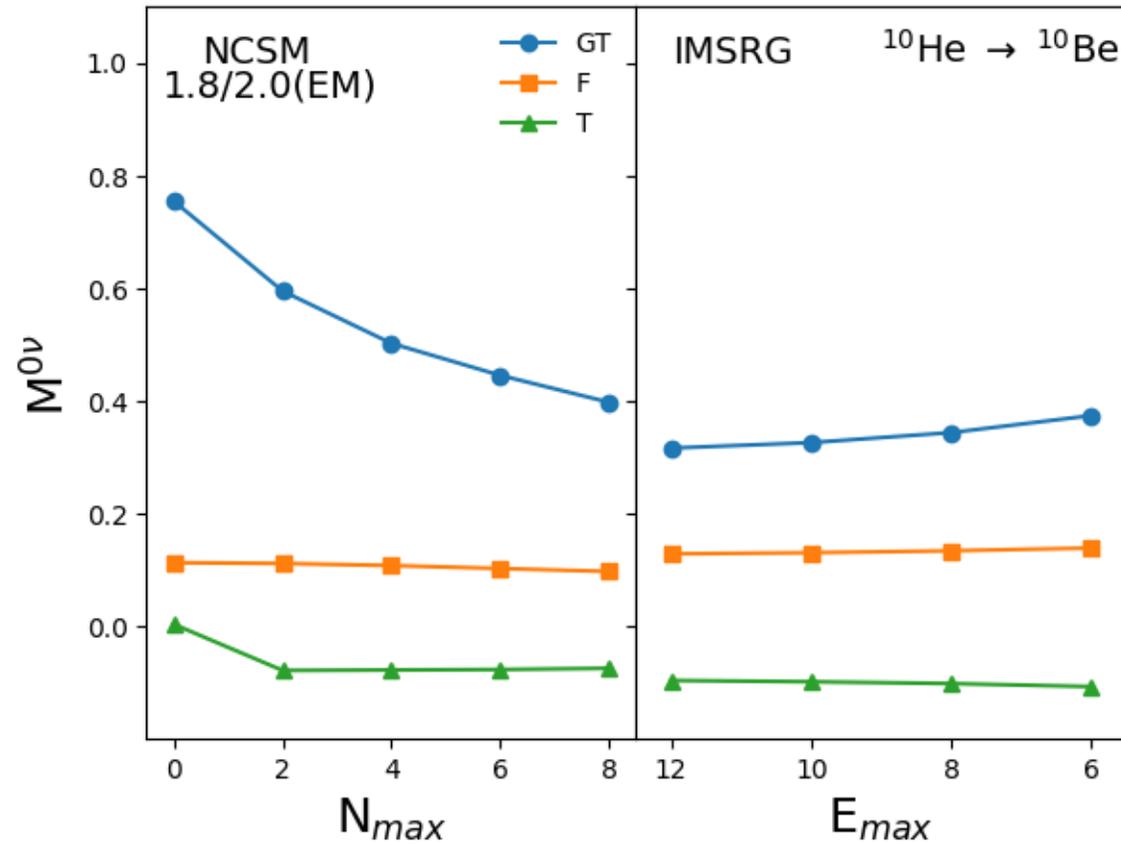
Benchmark with quasi-exact NCSM and CC theory in light systems



**Reasonable/good agreement in all cases!**

Belley, Payne, Stroberg, JDH, in prep

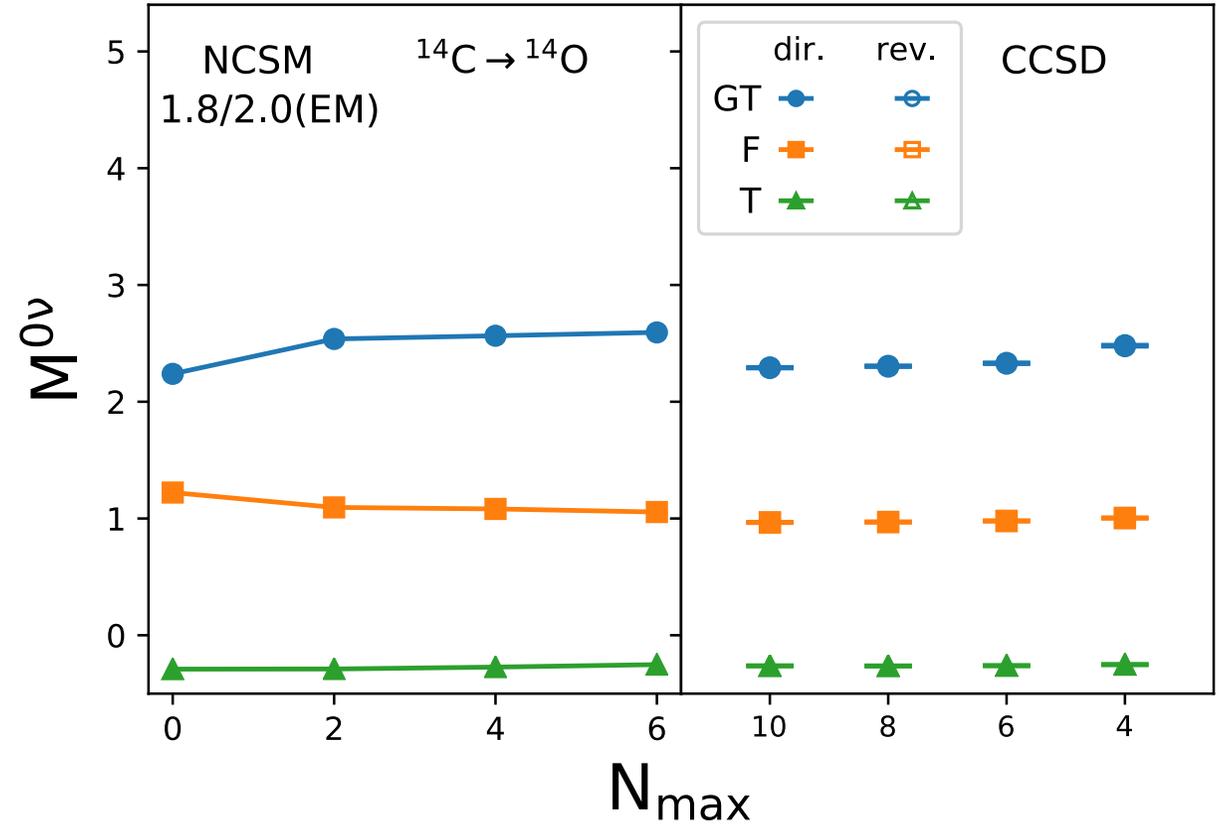
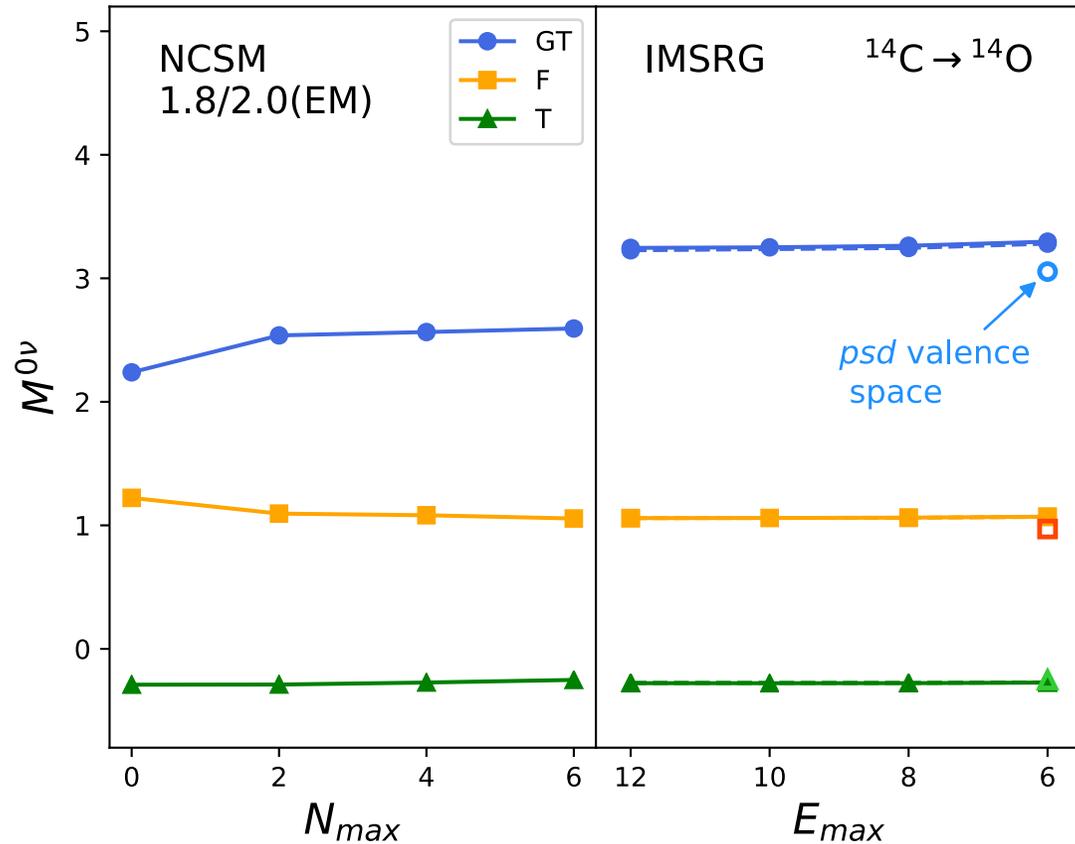
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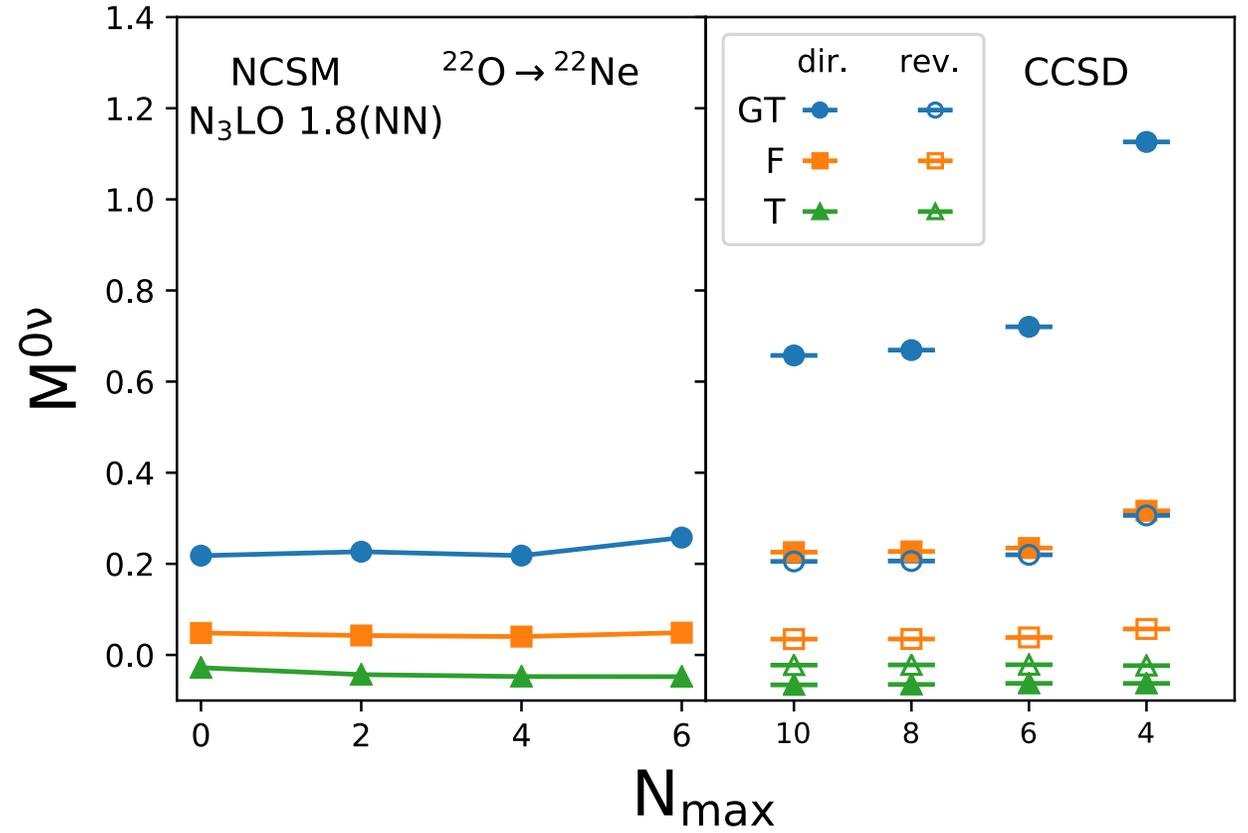
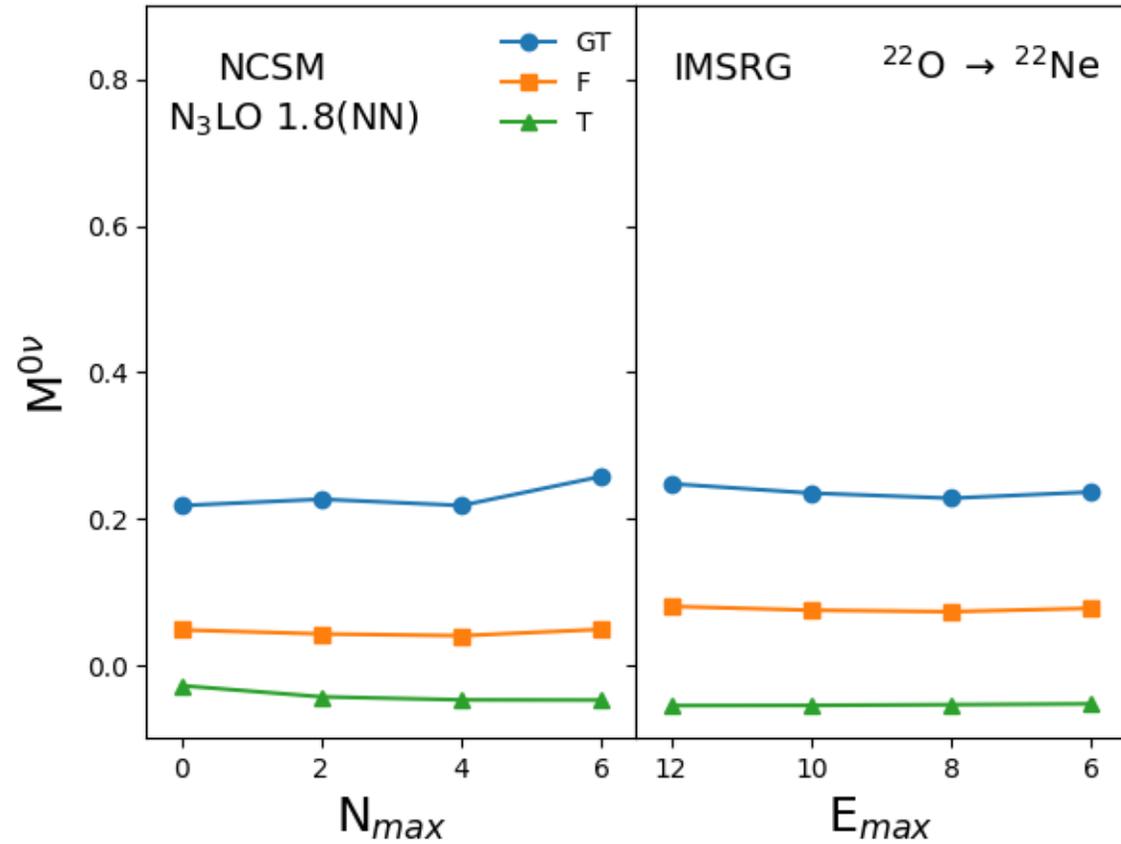
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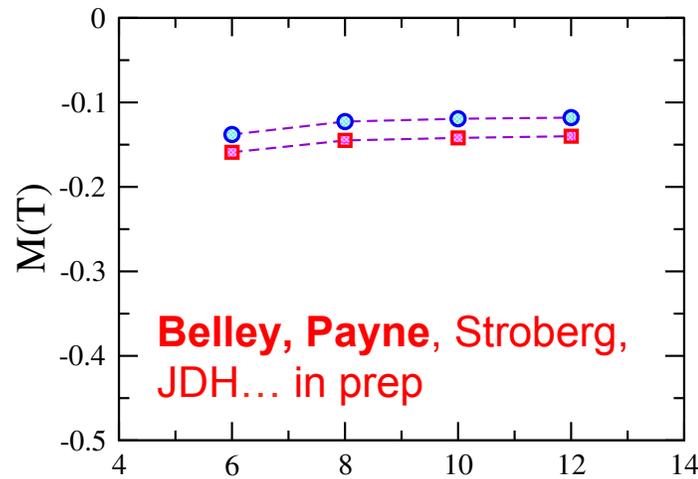
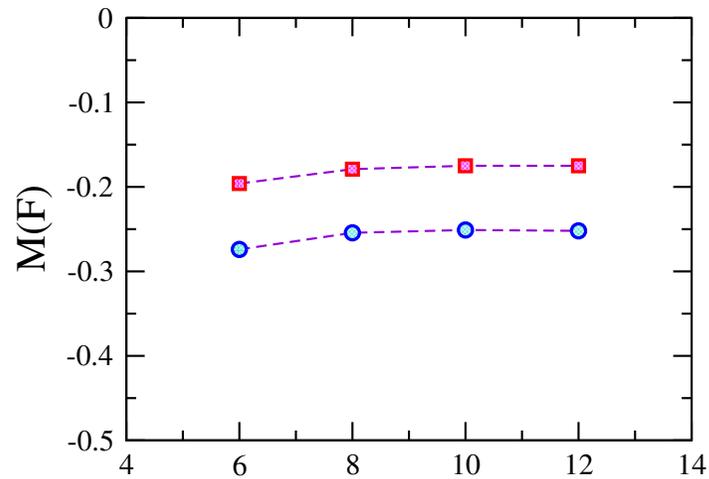
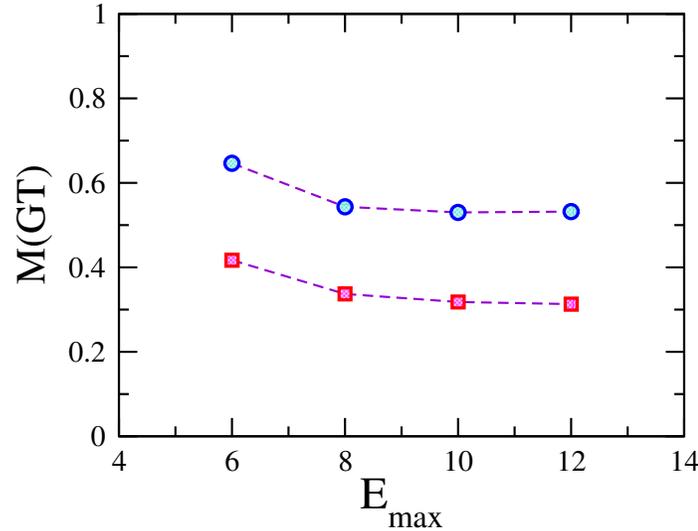
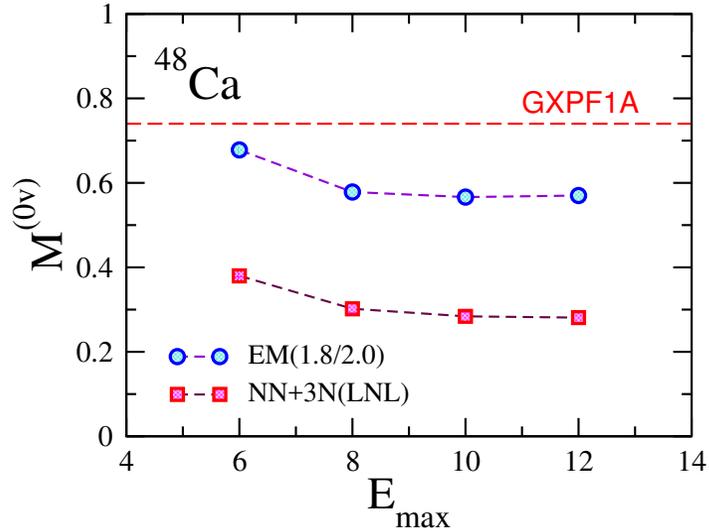
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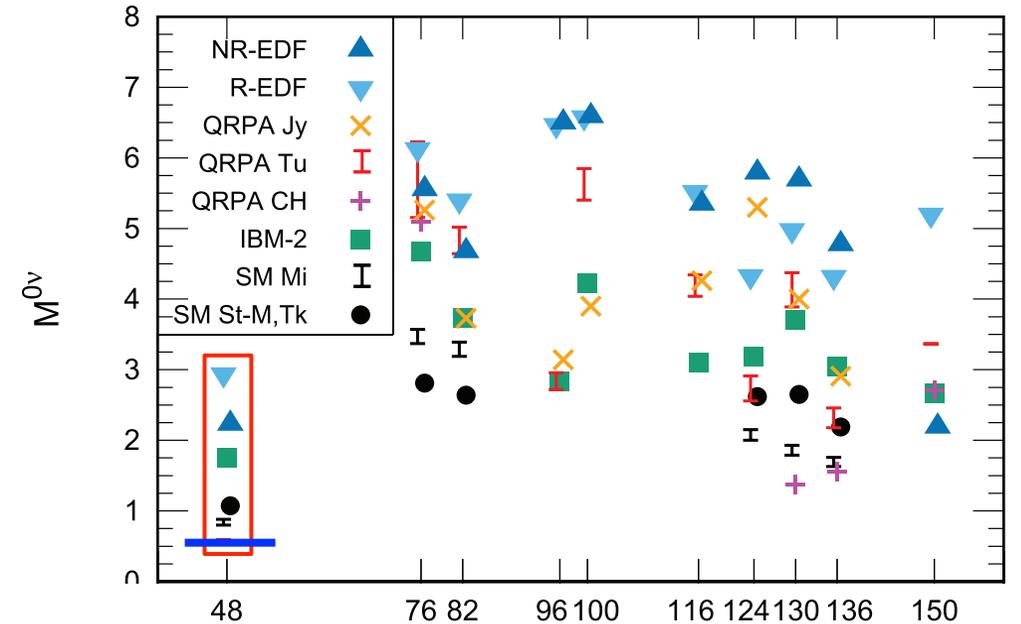
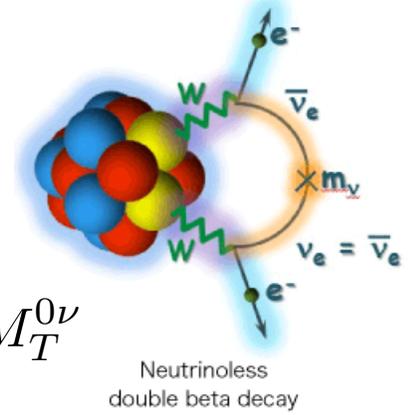
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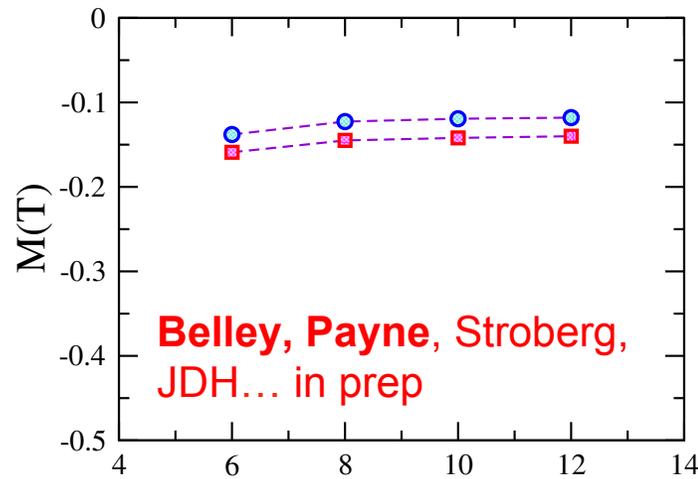
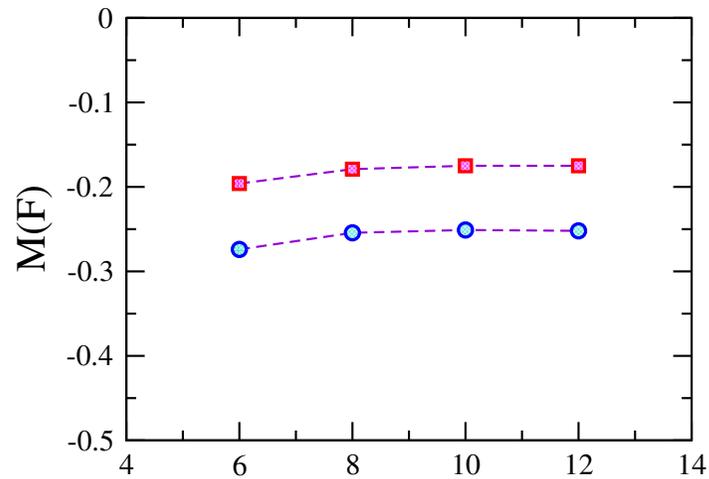
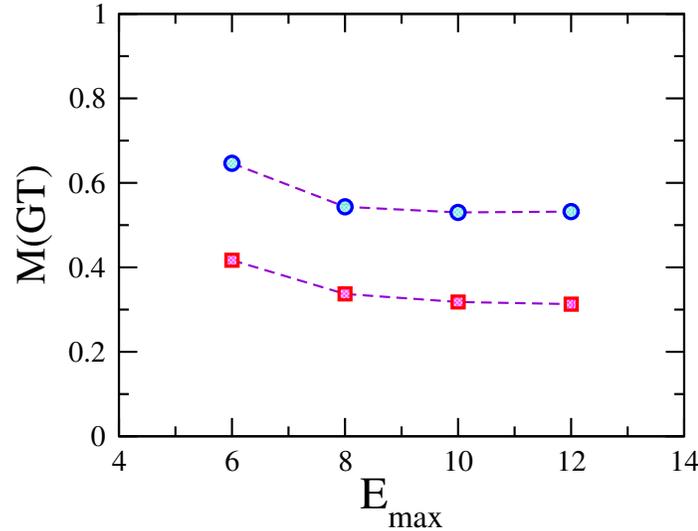
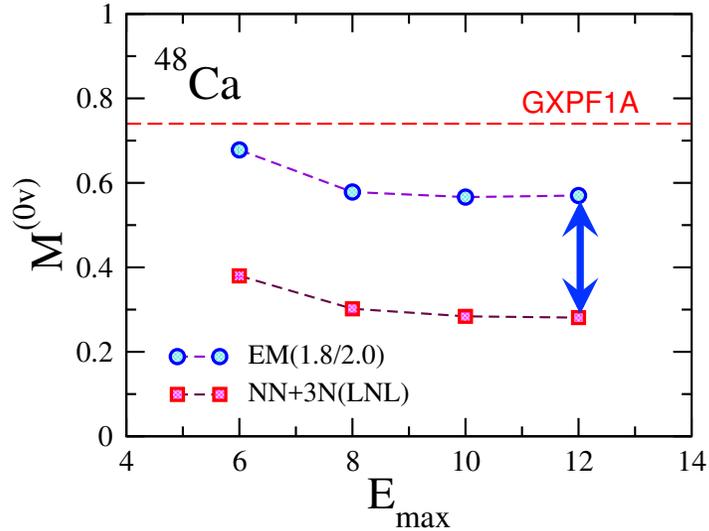
Consistent many-body wfs/operators from chiral NN+3N forces (**no 2b currents**)



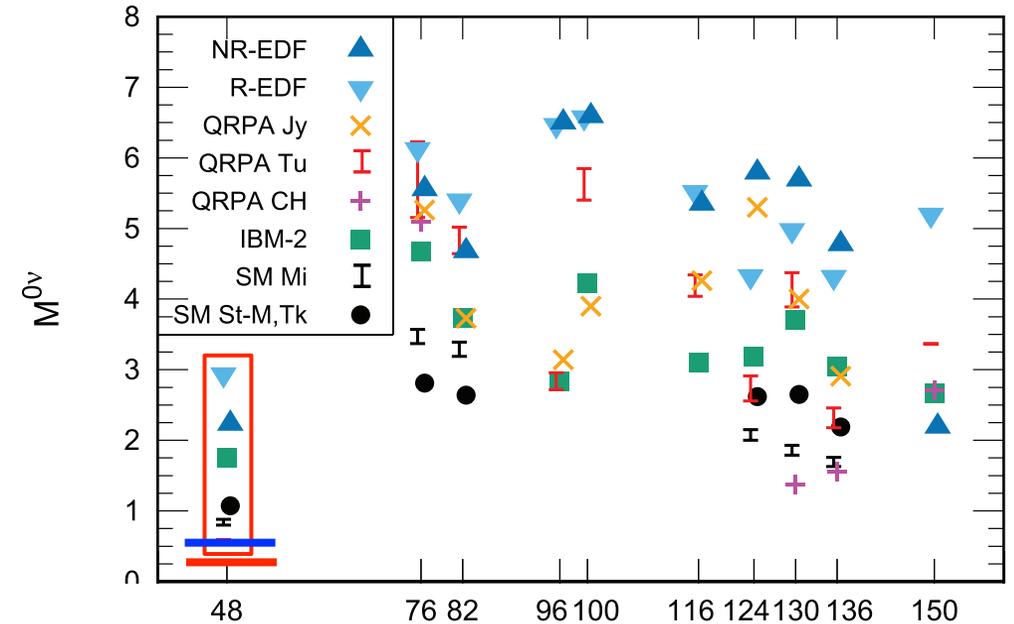
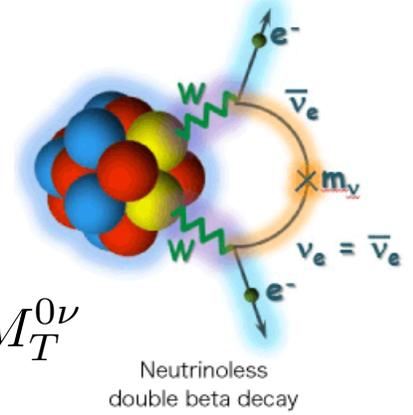
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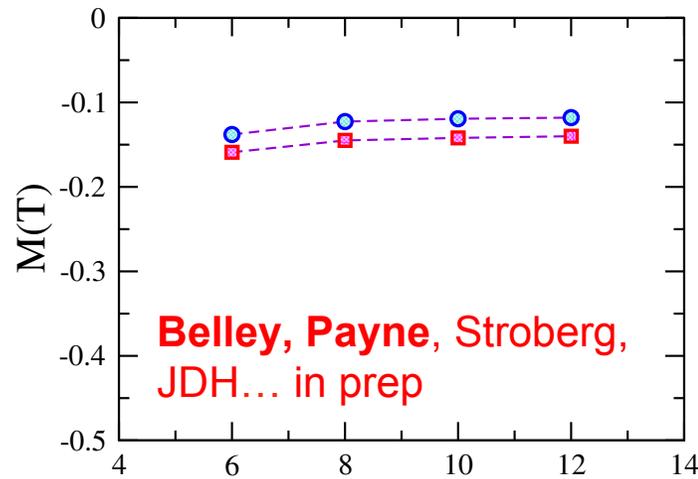
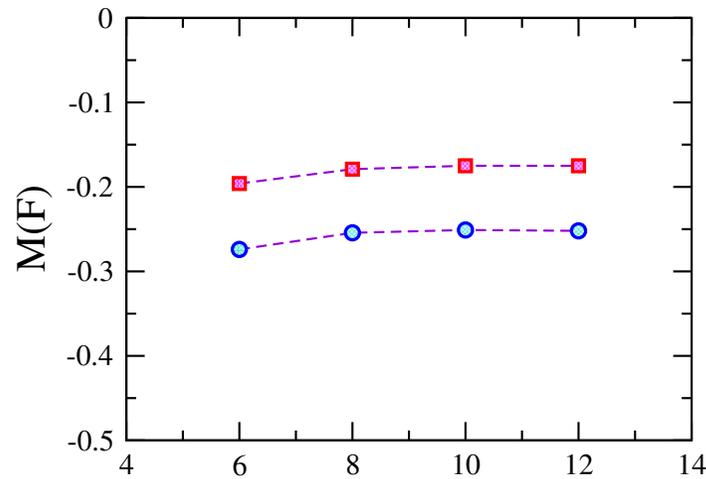
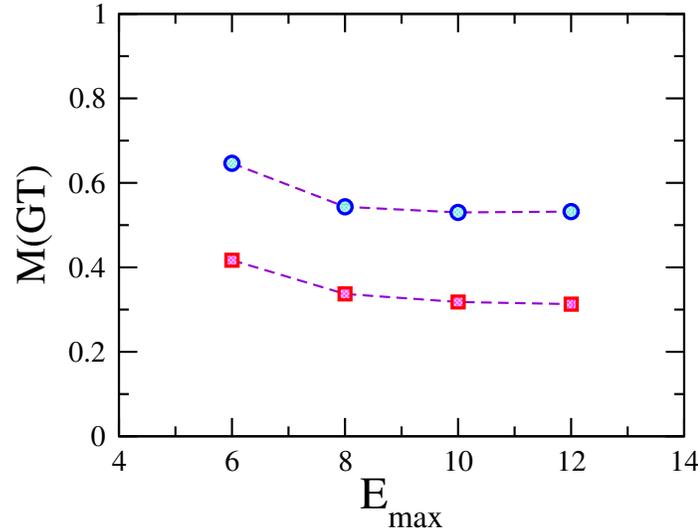
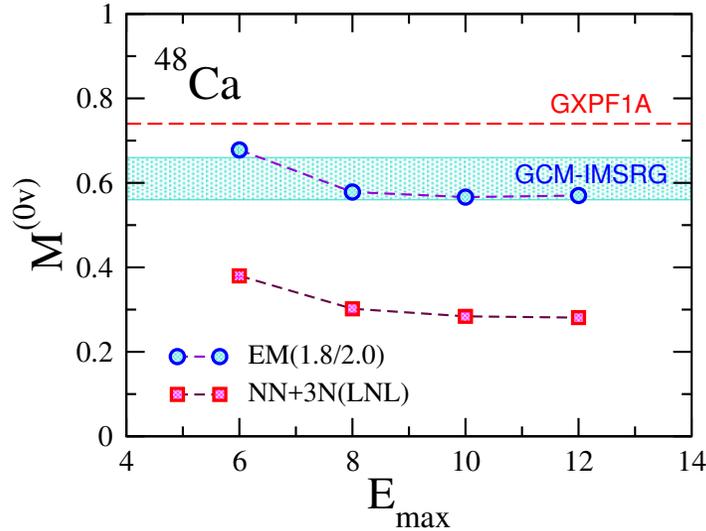
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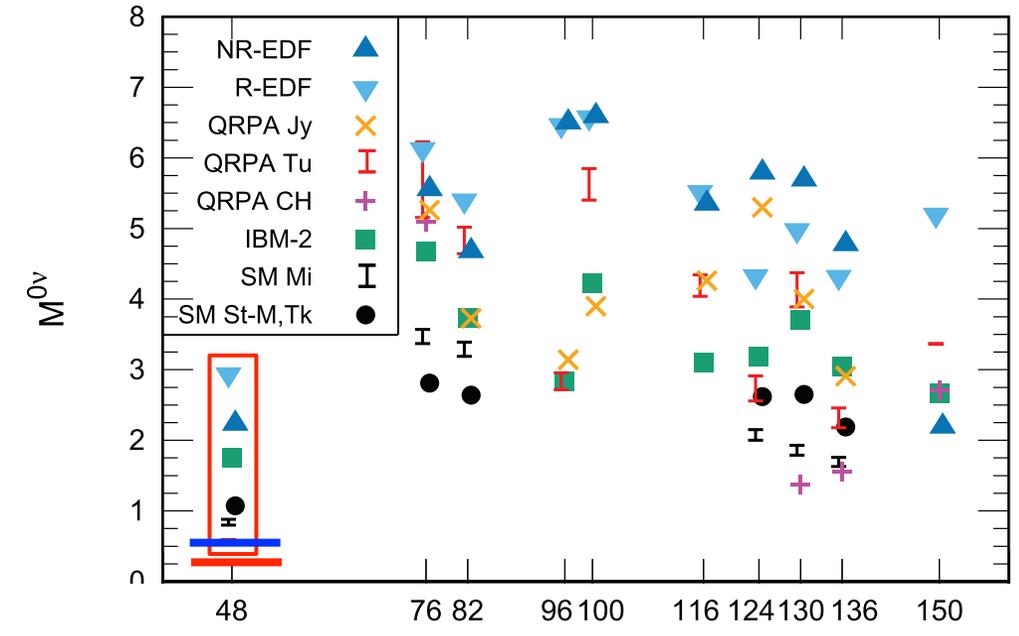
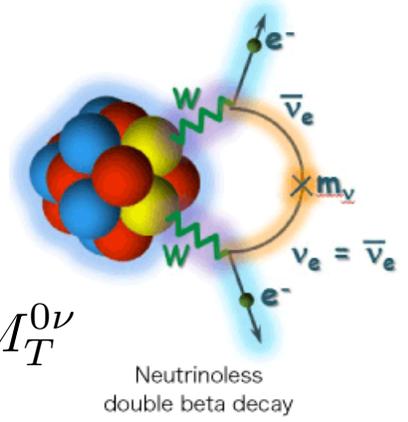
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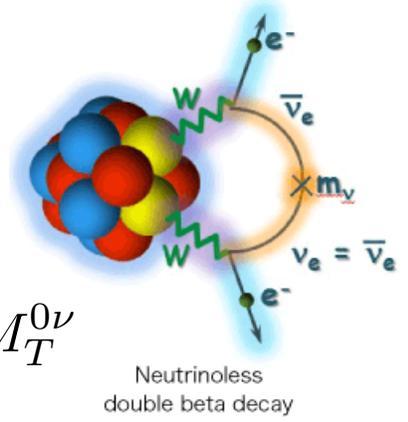


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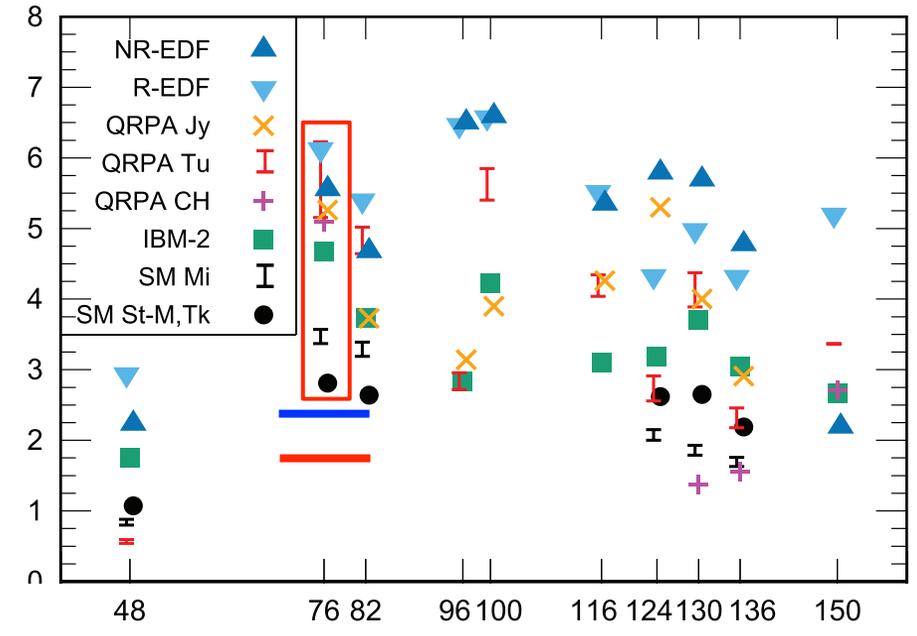
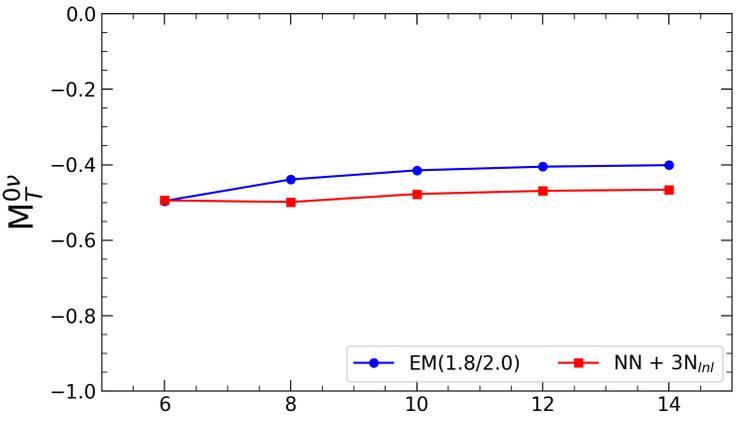
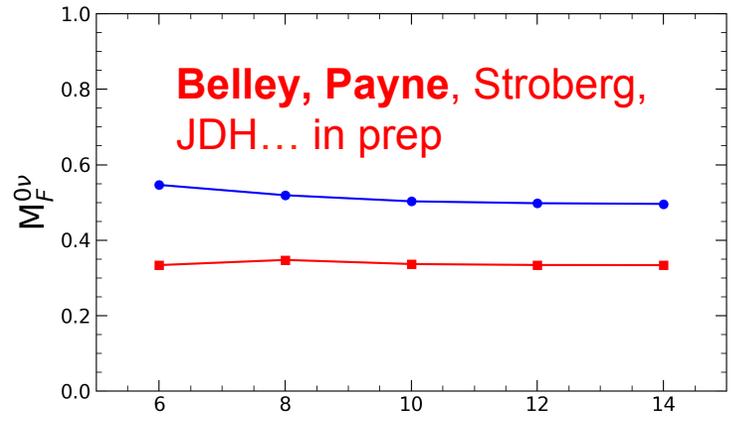
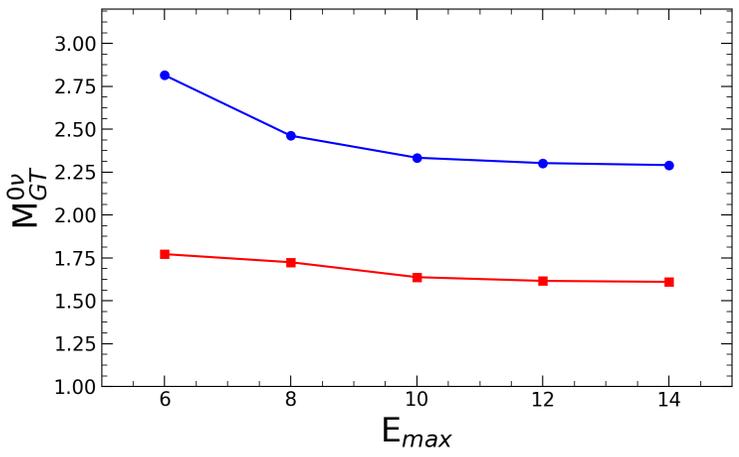
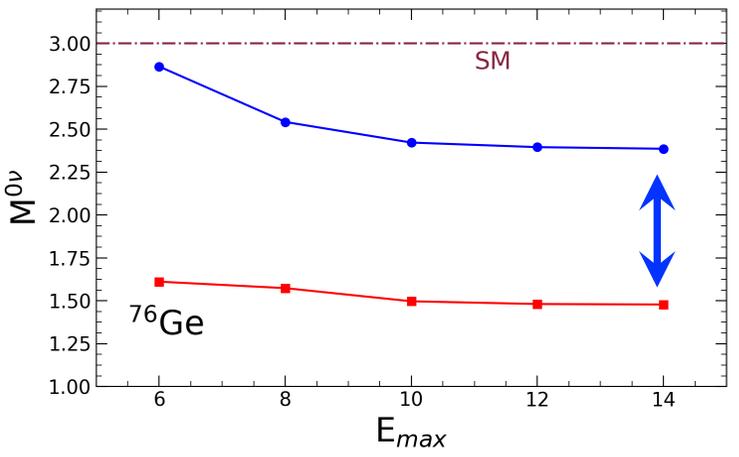


**Good agreement with GCM-IMSRG (tentative)... Further benchmarks underway**

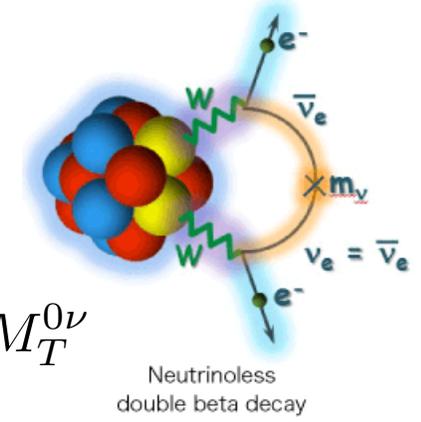
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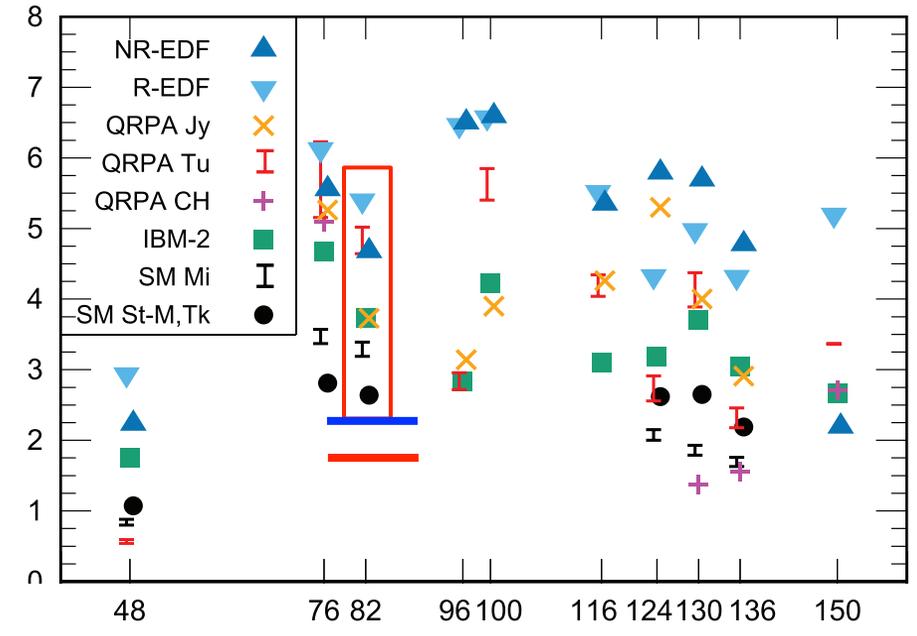
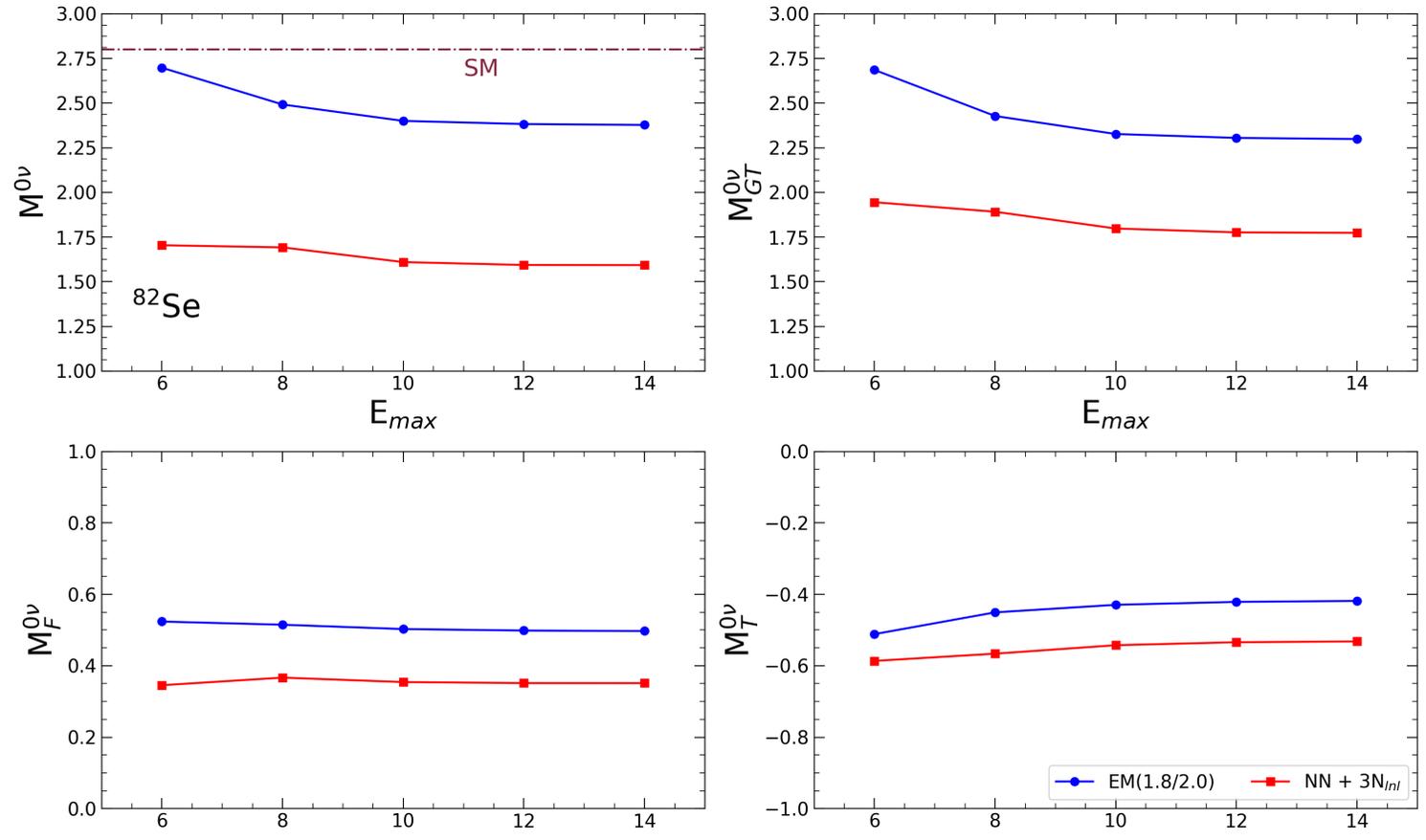
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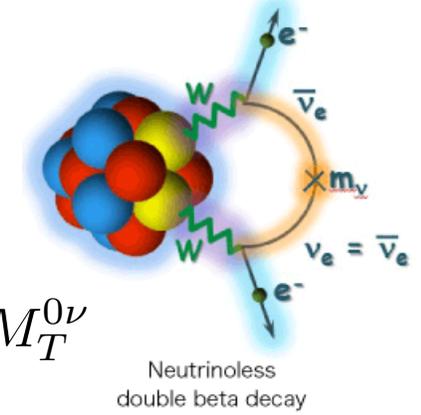


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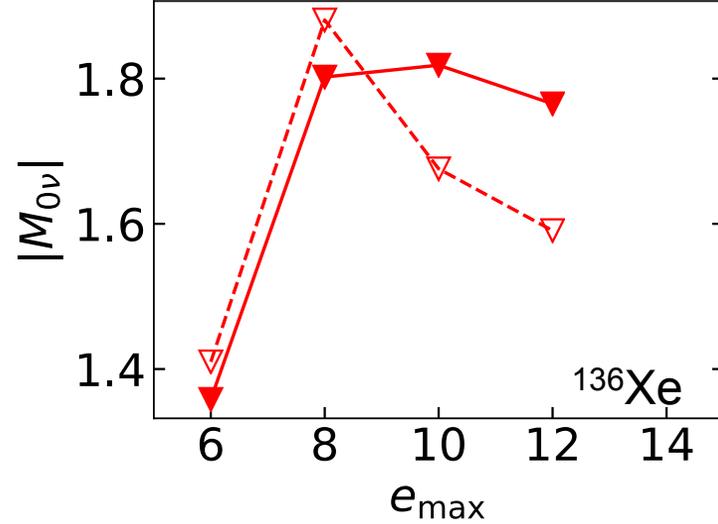
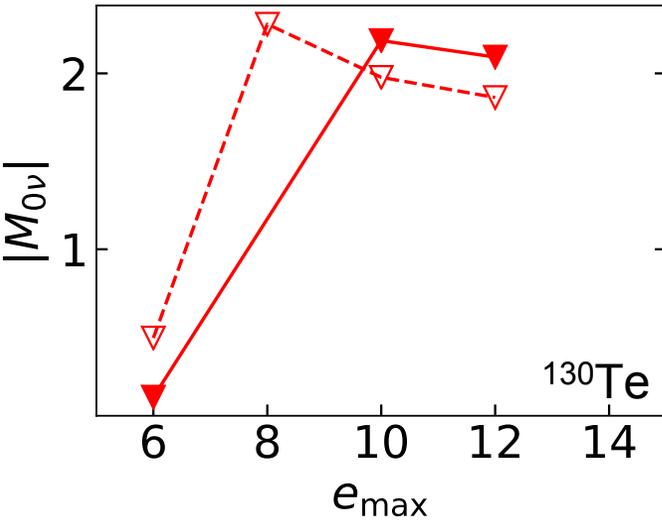


**Results consistently below lowest model predictions...**

Consistent many-body wfs/operators from chiral NN+3N forces (**no 2b currents**)

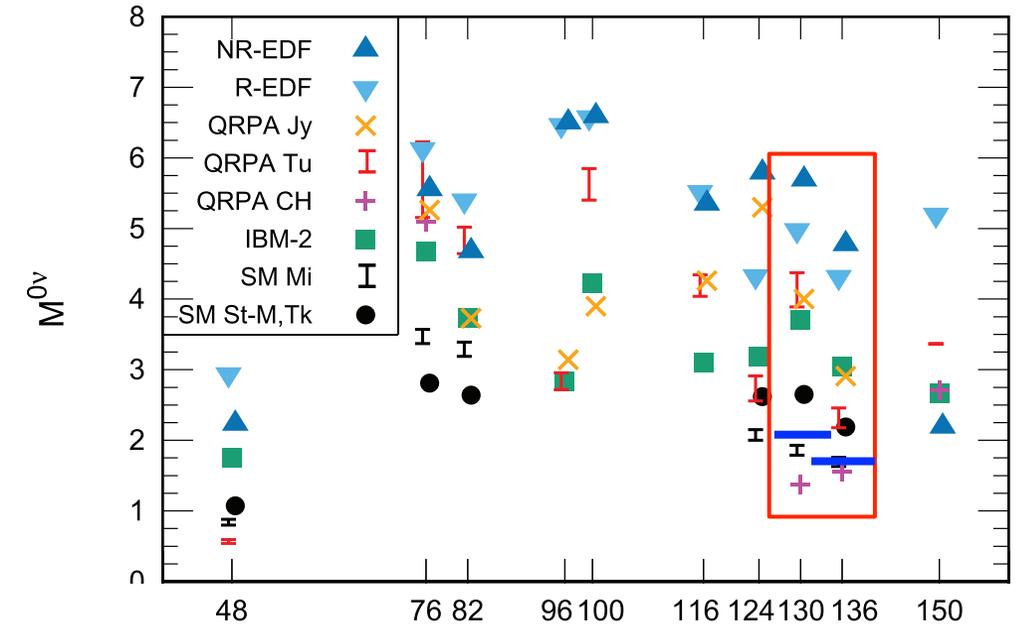


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—▼ EM 1.8/2.0  $e_{3\text{max}} = 16$    
- -▼ EM 1.8/2.0  $e_{3\text{max}} = 14$

Belley, Payne, Stroberg, JDH... in prep

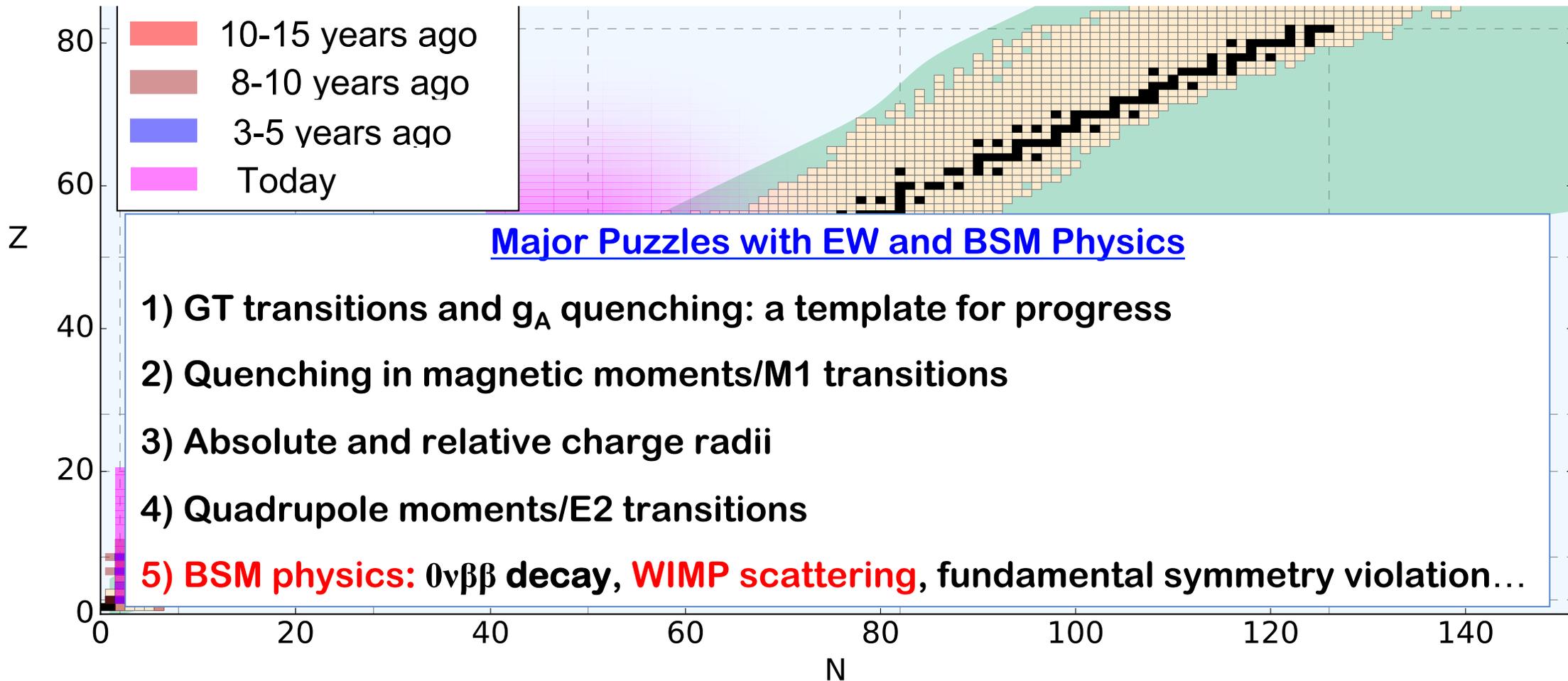


**\*Very Preliminary\*** - results consistently below lowest SM predictions...

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- Nuclear forces, electroweak physics
- Nuclear many-body problem

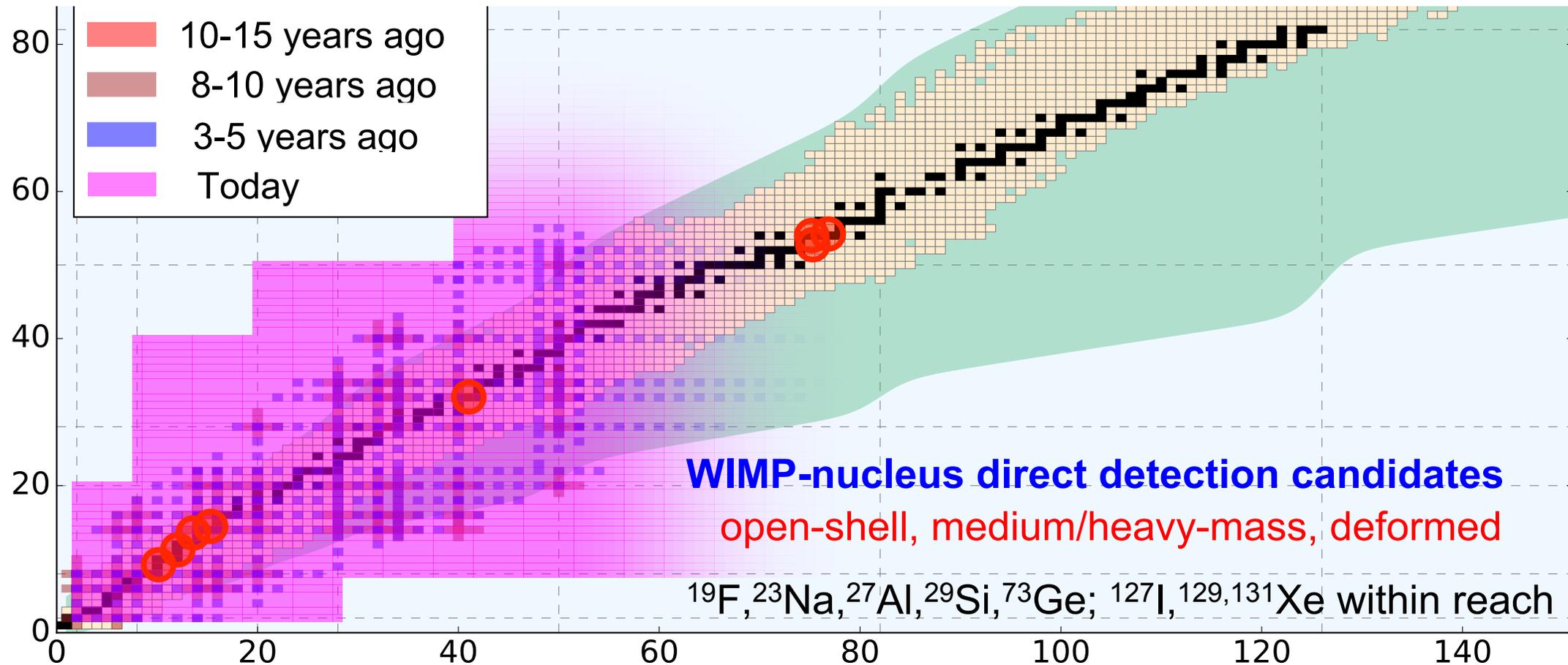
$$H\psi_n = E_n\psi_n$$



**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

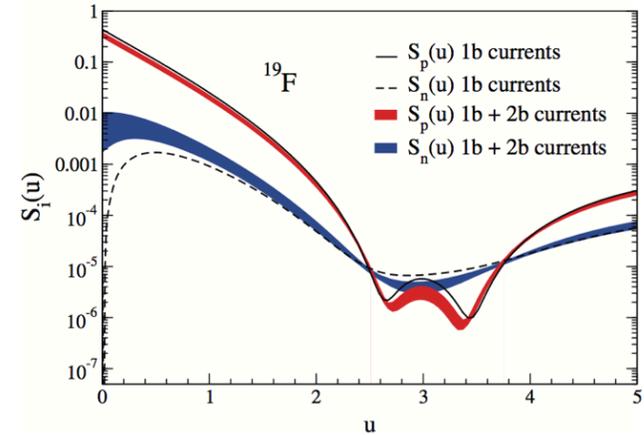
- Nuclear forces, electroweak physics
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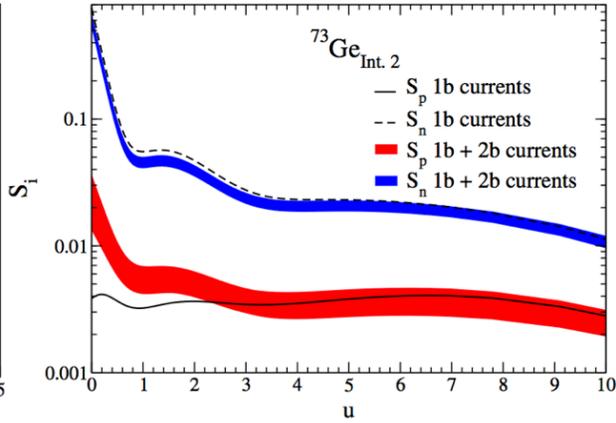


Previous advances: phenomenological wfs + bare operator (**axial currents**)

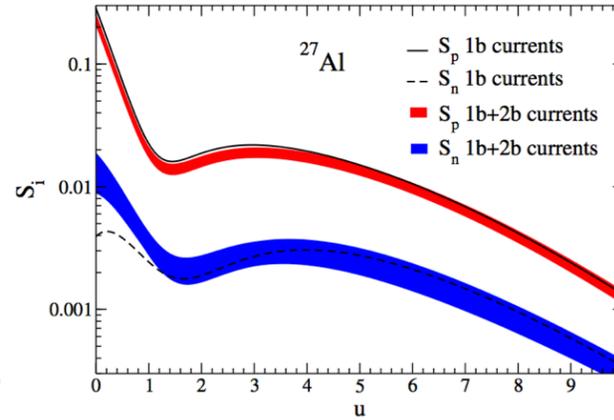
$$S_A(p) = \sum_{L \geq 0} |\langle J_f || \mathcal{L}_L || J_i \rangle|^2 + \sum_{L \geq 0} \left( |\langle J_f || \mathcal{T}_L^{\text{el}} || J_i \rangle|^2 + |\langle J_f || \mathcal{T}_L^{\text{mag}} || J_i \rangle|^2 \right)$$



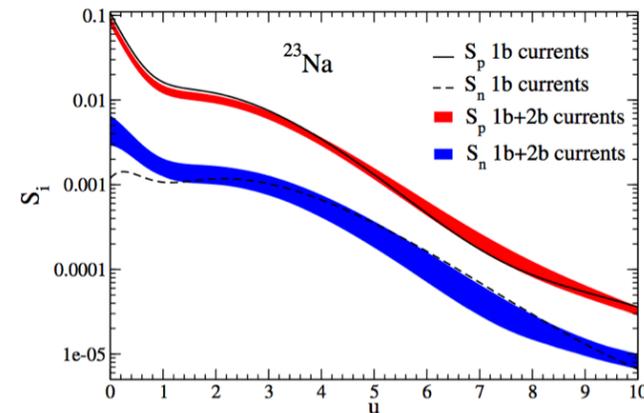
PICASSO, COUPP, SIMPLE



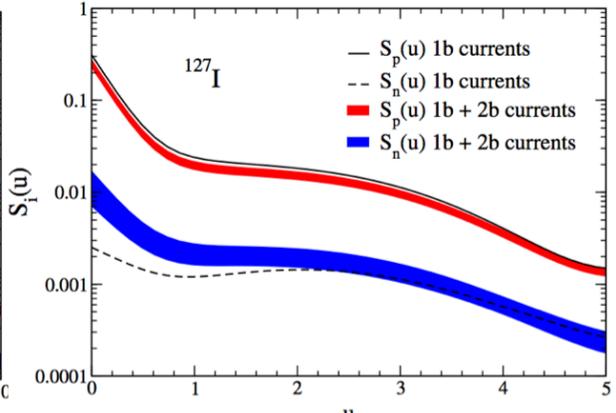
CDMS, EDELWEISS, EURECA



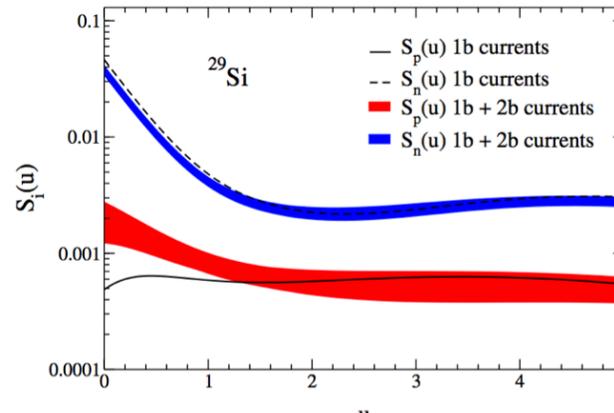
CRESST



DAMA, ANAIS, DM-Ice



DAMA, ANAIS, DM-Ice, KIMS

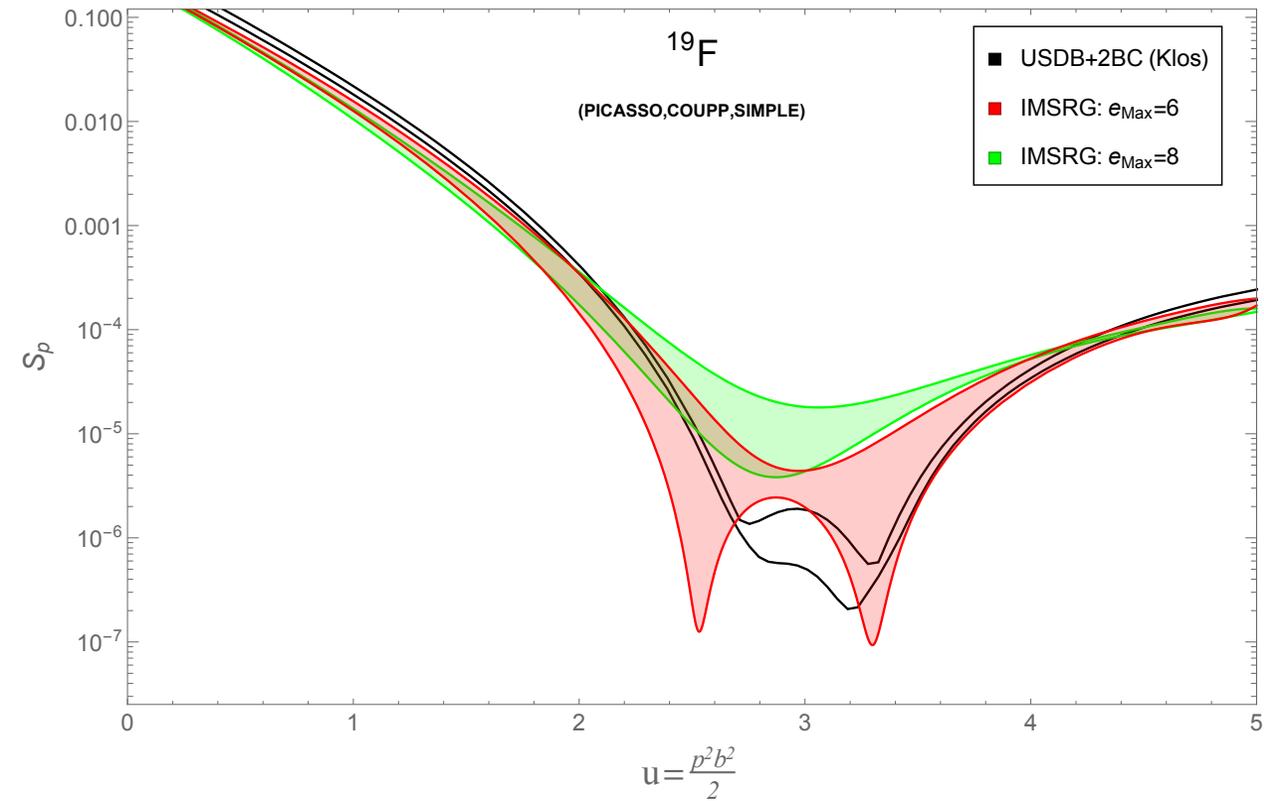
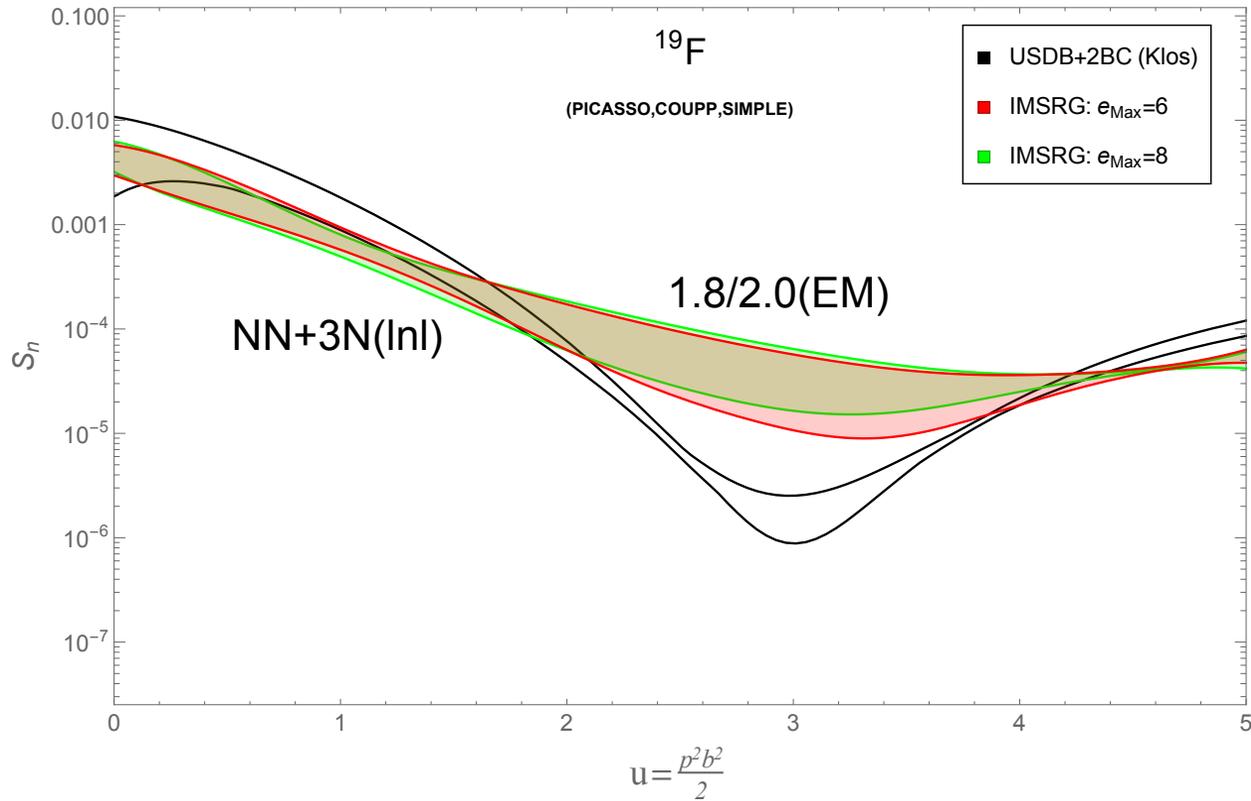


CDMS-II

Klos et al, PRD (2013)

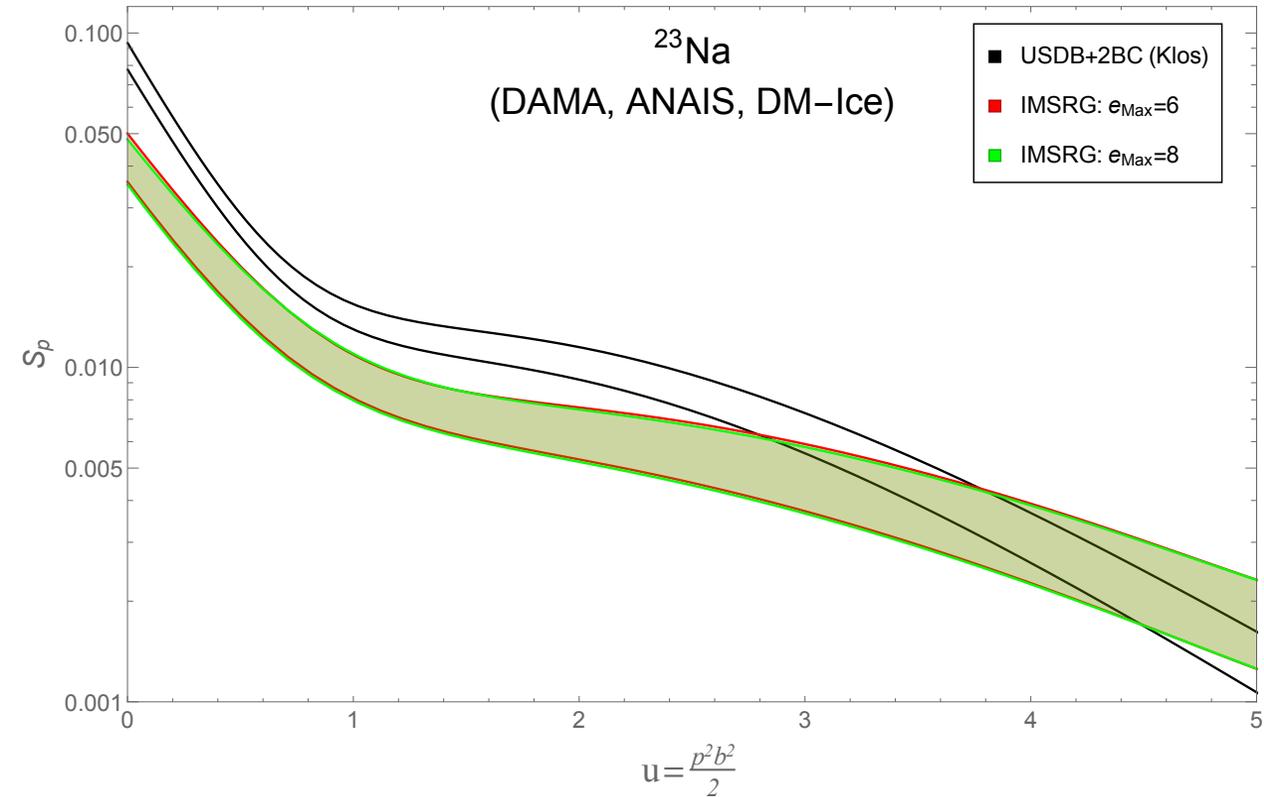
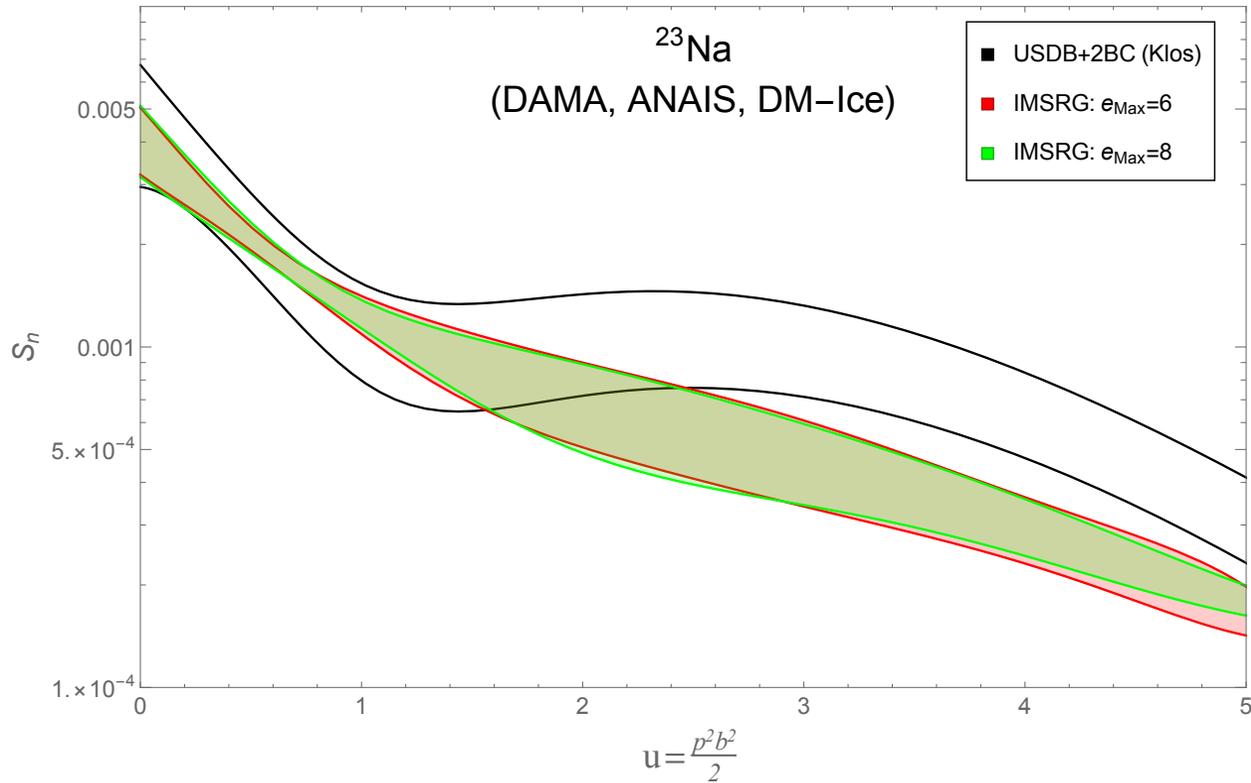
Ab initio: Consistent many-body wfs/operators from chiral NN+3N forces + 2B currents

Two NN+3N interactions: 1.8/2.0(EM), NN+3N(LNL)



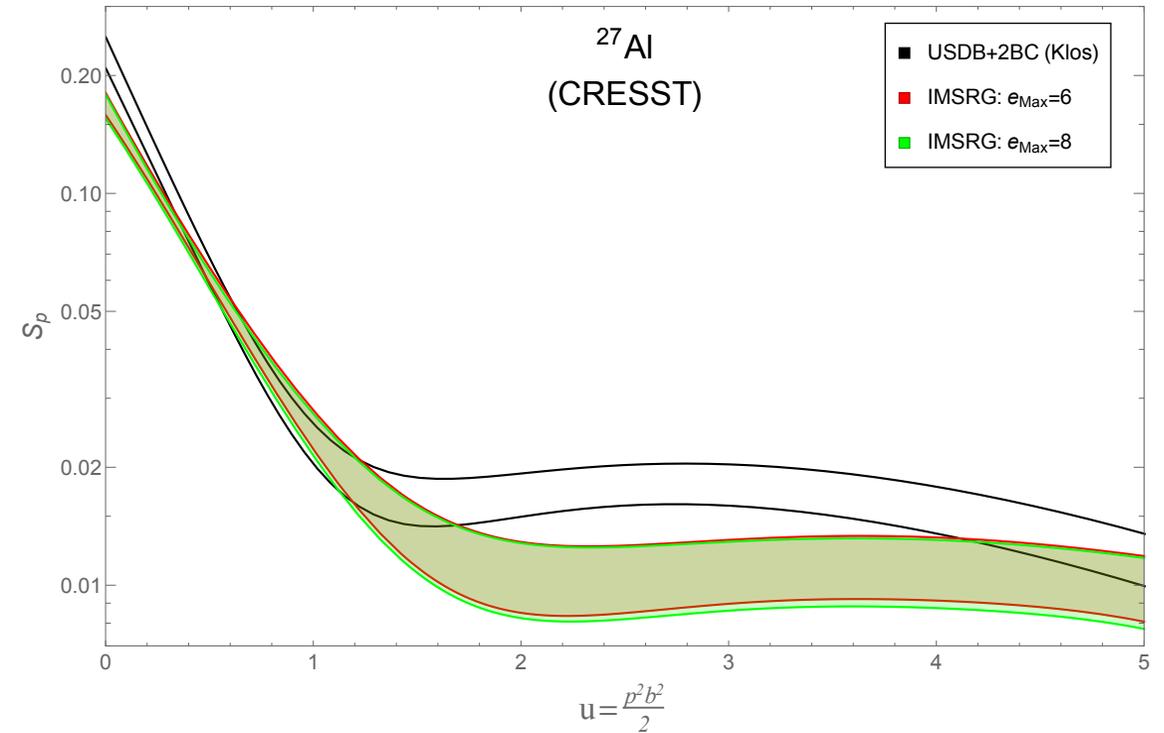
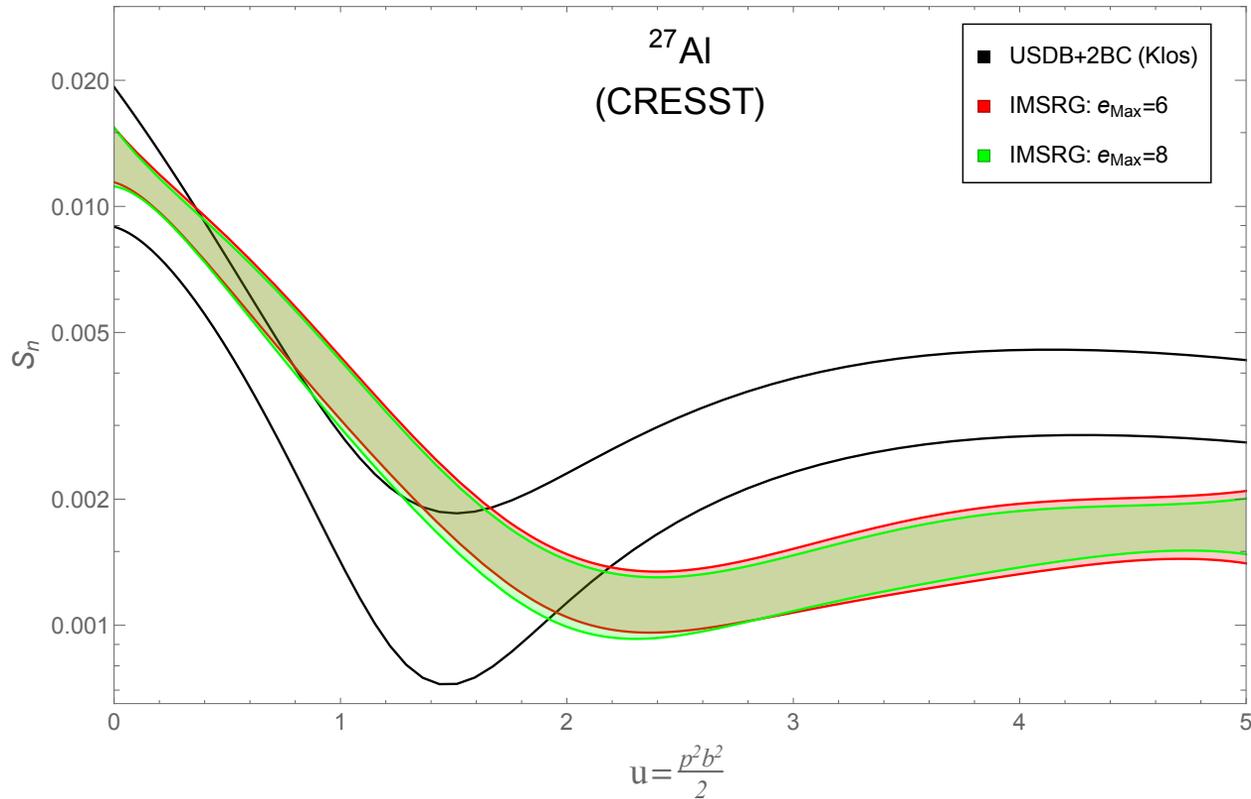
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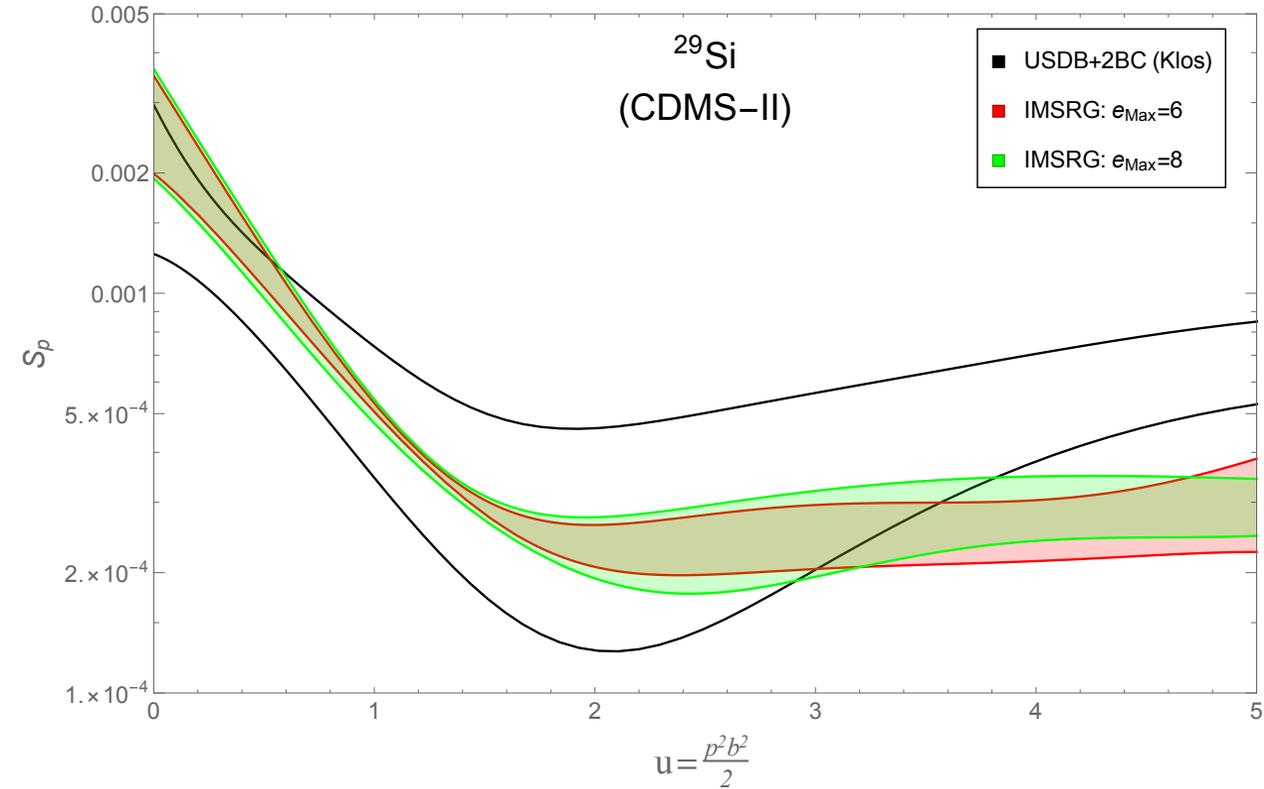
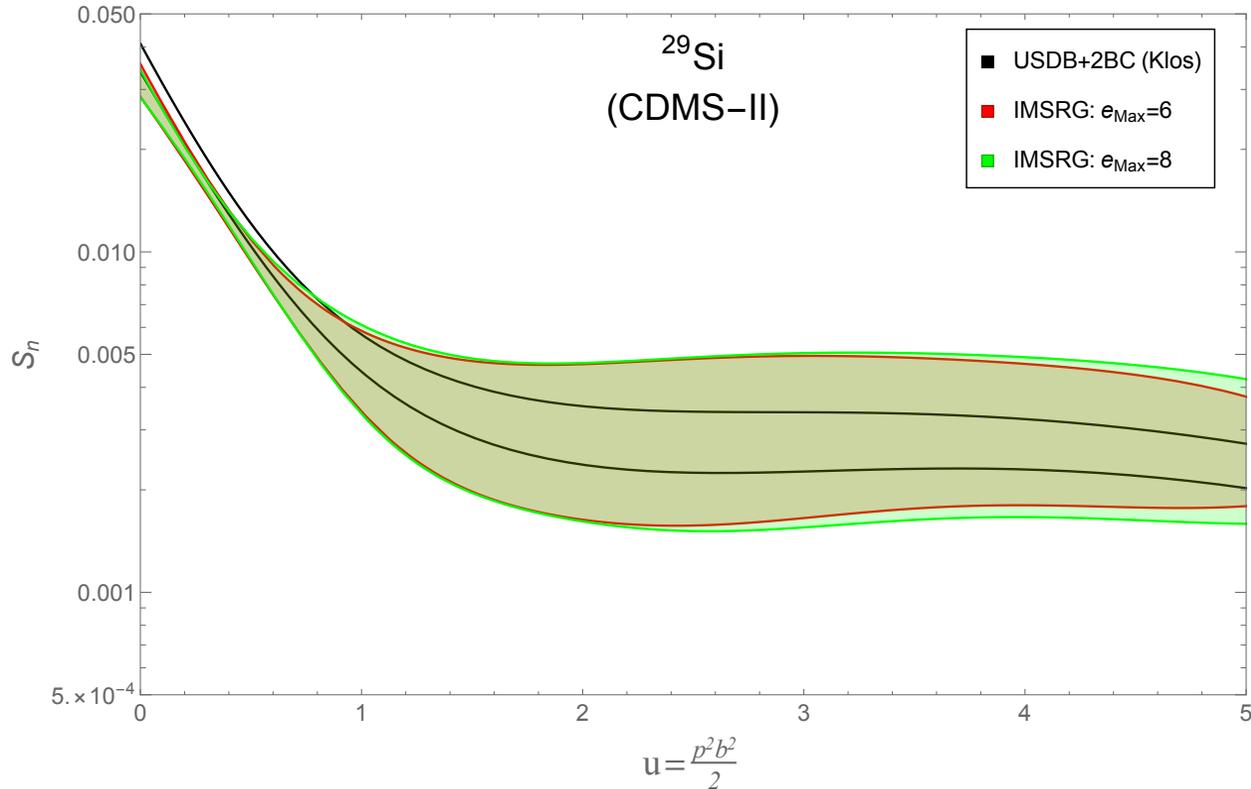
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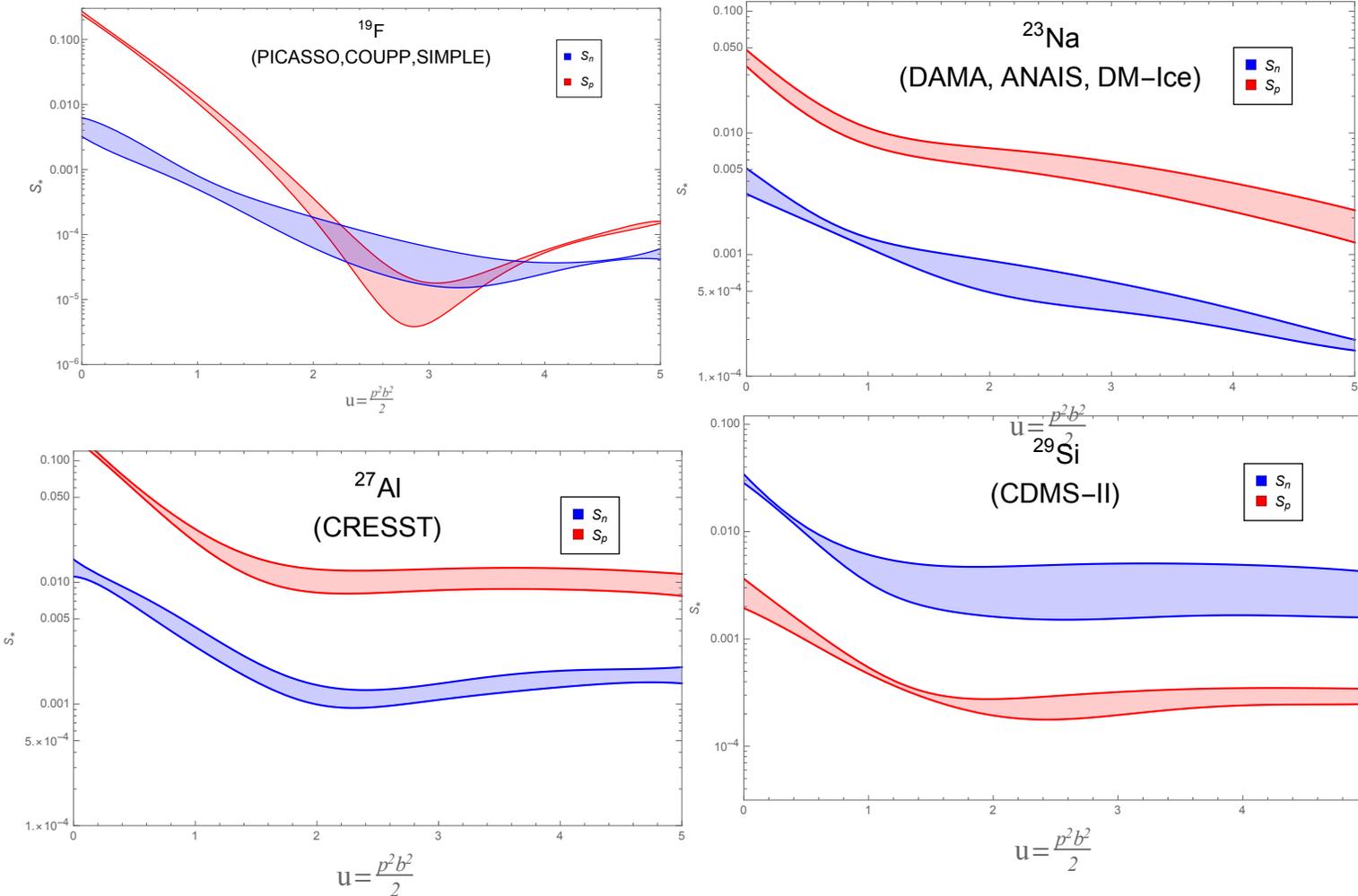
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Two NN+3N interactions: 1.8/2.0(EM), NN+3N(LNL)



Padua, Leutheusser, Stroberg, JDH, in prep.

In progress: all nuclear targets to Xe, Spin Independent

Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

## Nuclear Structure

Development of forces and currents<sup>1</sup>

Dripline predictions for medium-mass

Evolution of magic numbers from masses, radii, spectroscopy, EM transitions: <sup>78</sup>Ni

Multi-shell theory:

Island of inversion<sup>2</sup>

Forbidden decays<sup>3</sup>

Atomic systems<sup>4</sup>

## Fundamental Symmetries/BSM Physics

Effective electroweak operators: GT quenching

Effective  $0\nu\beta\beta$  decay operator<sup>5</sup>

WIMP-Nucleus scattering<sup>6</sup>

Superallowed Fermi transitions<sup>7</sup>

Symmetry-violating moments [molecules]<sup>8</sup>

## Outstanding issues

Controlled IMSRG(3) approximation\*

E2 operators/collectivity problematic

Understand discrepancies with CC

Quantify uncertainties



S. R. Stroberg\*

T. Miyagi<sup>2,3,4,7,8</sup>

C. Gwak<sup>3,8</sup>

D. Livermore<sup>4</sup>

G. Tenkila<sup>4</sup>

A. Belley<sup>5</sup>

C. Payne<sup>5</sup>

J. Padua<sup>6</sup>

S. Leutheusser<sup>6</sup>



T. Morris

G. Hagen

T. Papenbrock



TECHNISCHE  
UNIVERSITÄT  
DARMSTADT

A. Schwenk



東京大学

THE UNIVERSITY OF TOKYO

J. Menéndez



H. Hergert

S. Bogner



THE UNIVERSITY  
of NORTH CAROLINA  
at CHAPEL HILL

J. Engel



J. Simonis<sup>1</sup>



Massachusetts  
Institute of  
Technology

R. F. Garcia-Ruiz<sup>8</sup>



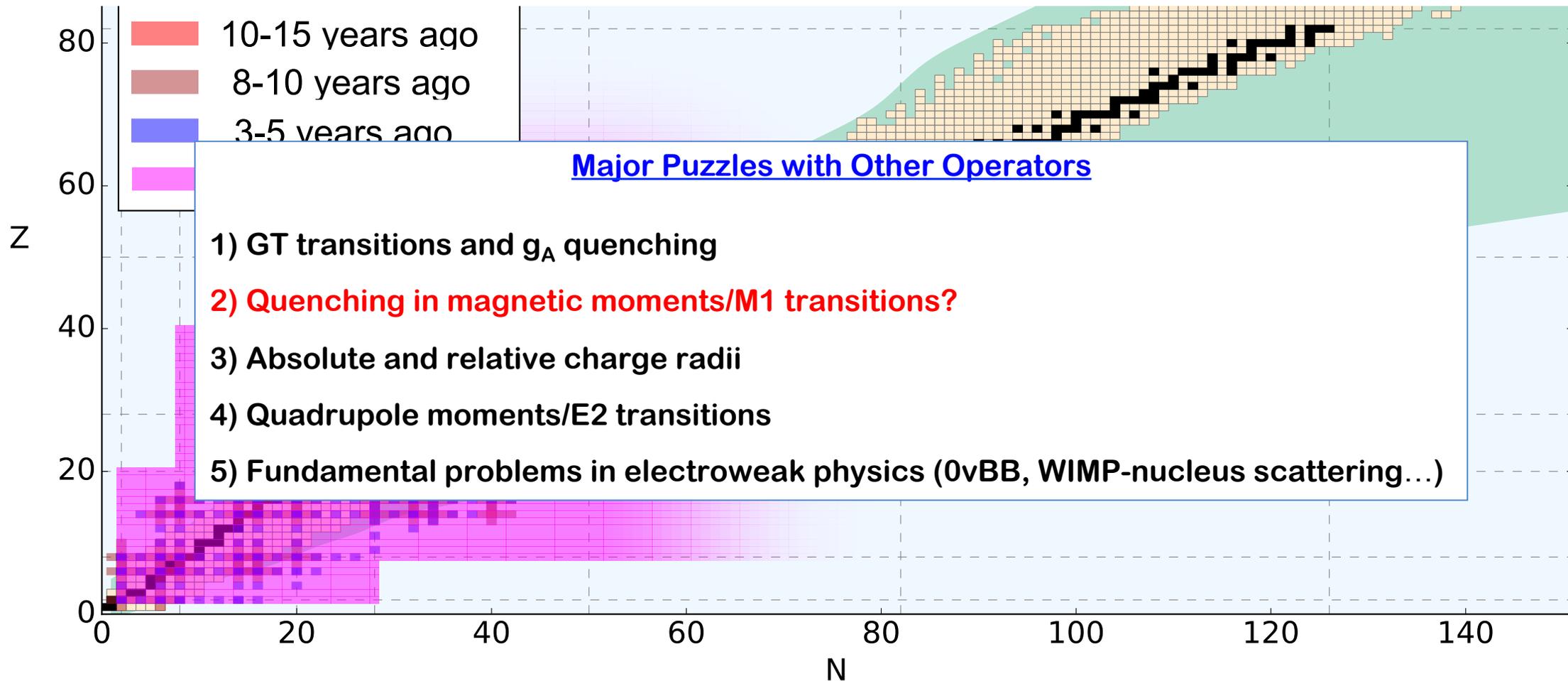
M. Martin<sup>7</sup>

K. G. Leach

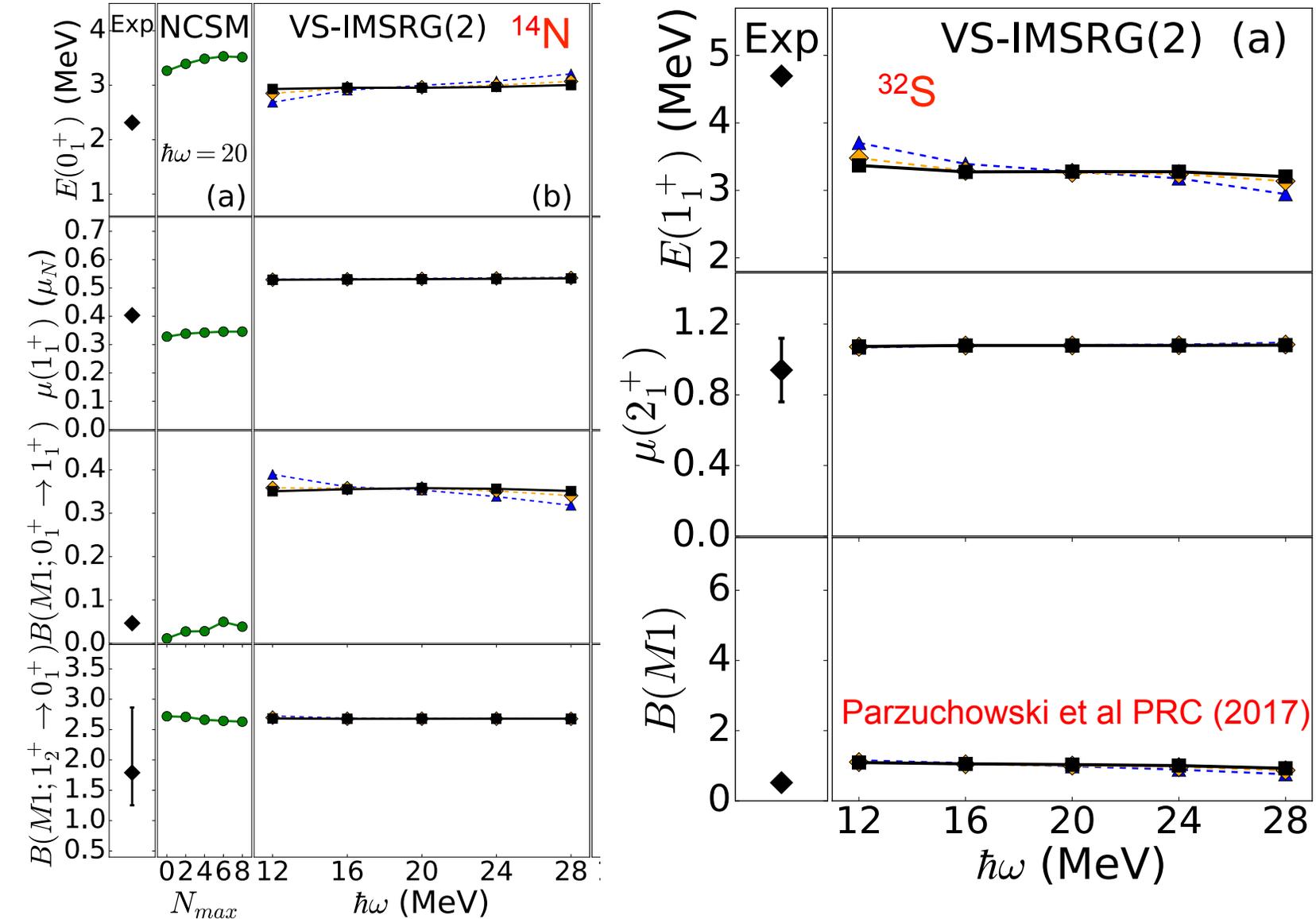
**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem

$$H\psi_n = E_n\psi_n$$



Similar effects expected as in GT quenching: renormalized operator + 2BC ~0.75-0.8



Reasonable experimental agreement: additional quenching needed

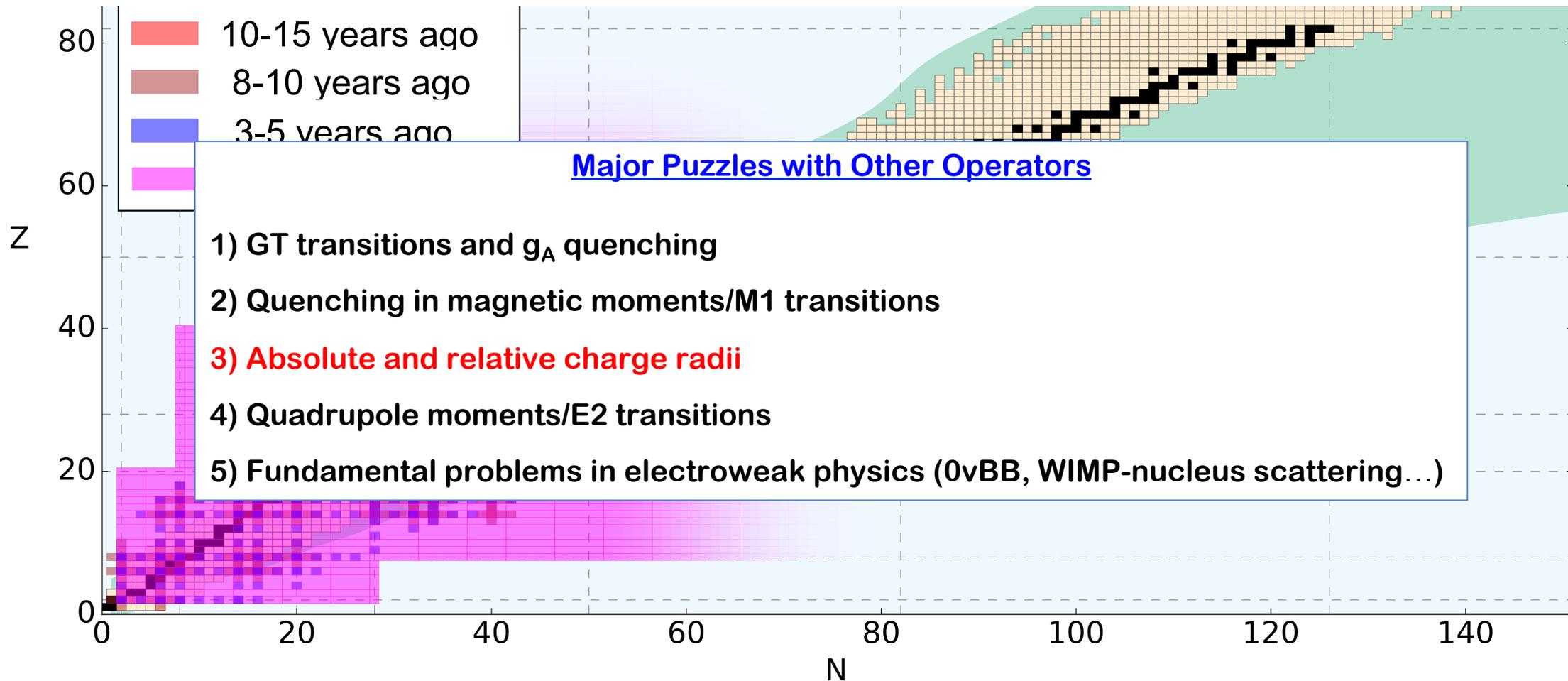
No inclusion of 2BC yet - developments underway...

Parzuchowski et al PRC (2017)

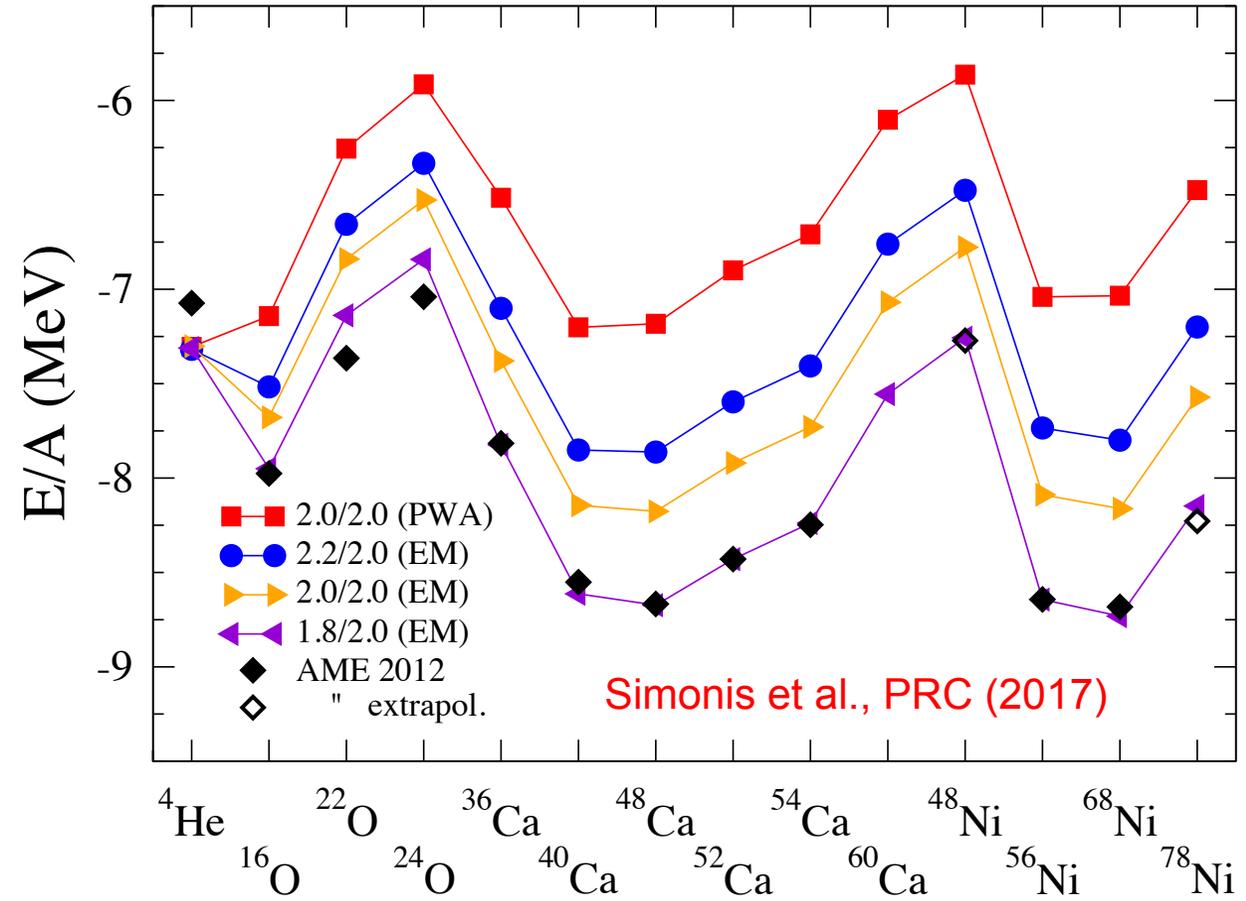
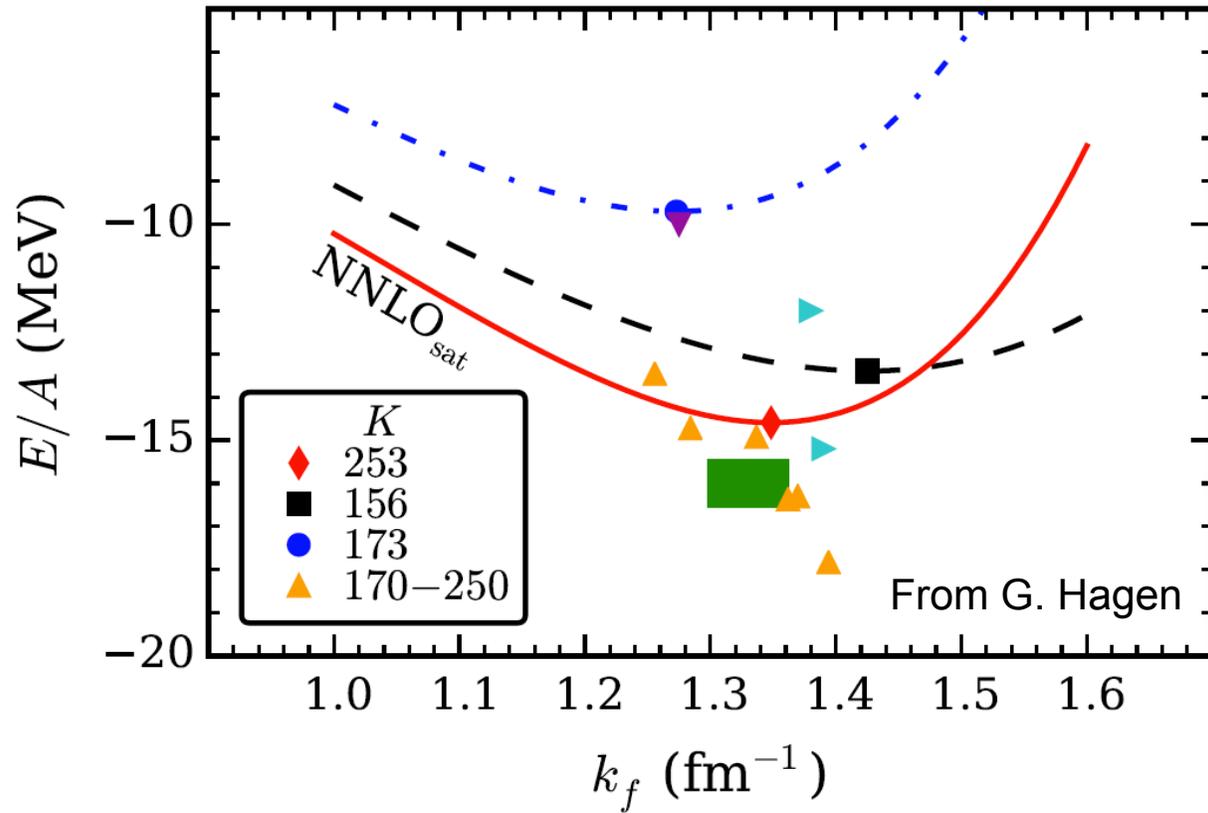
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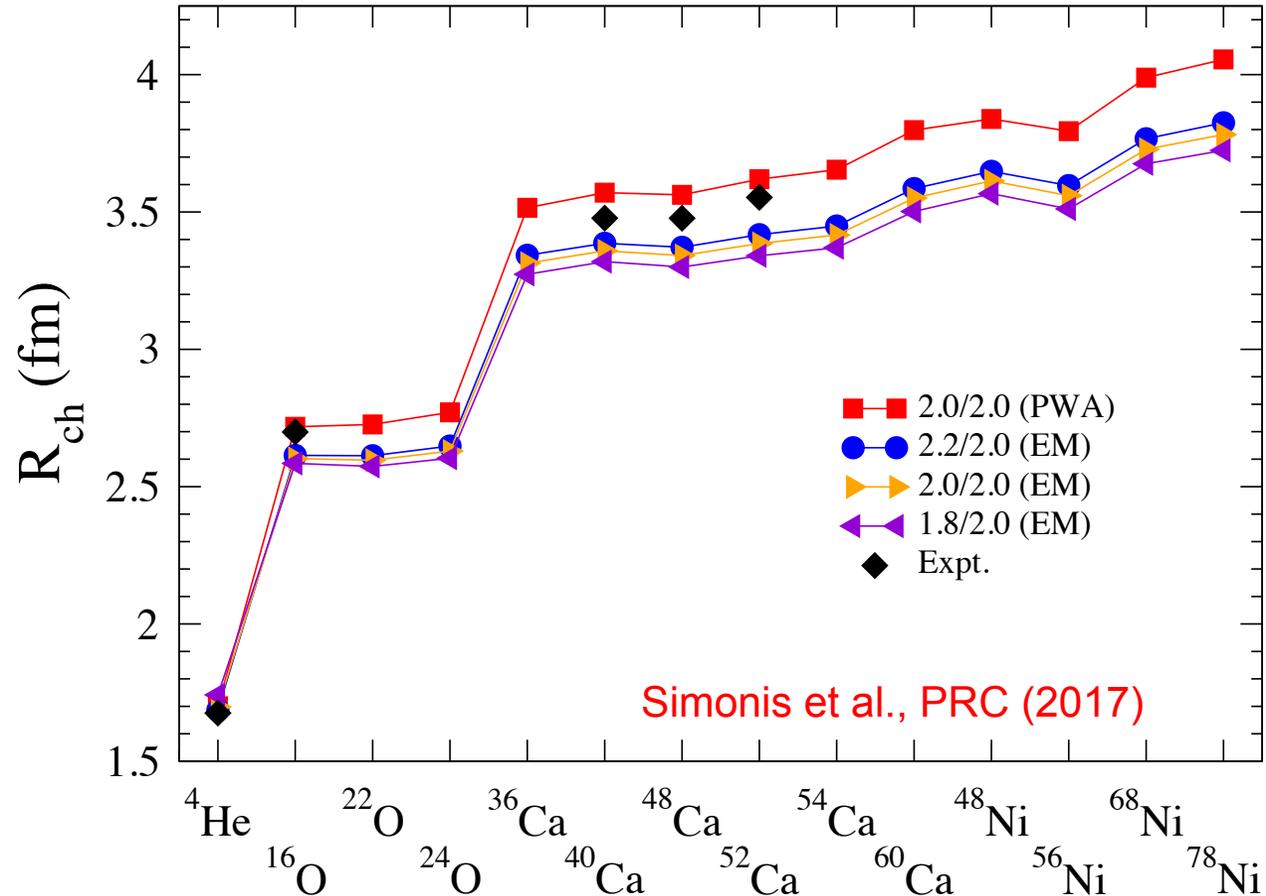
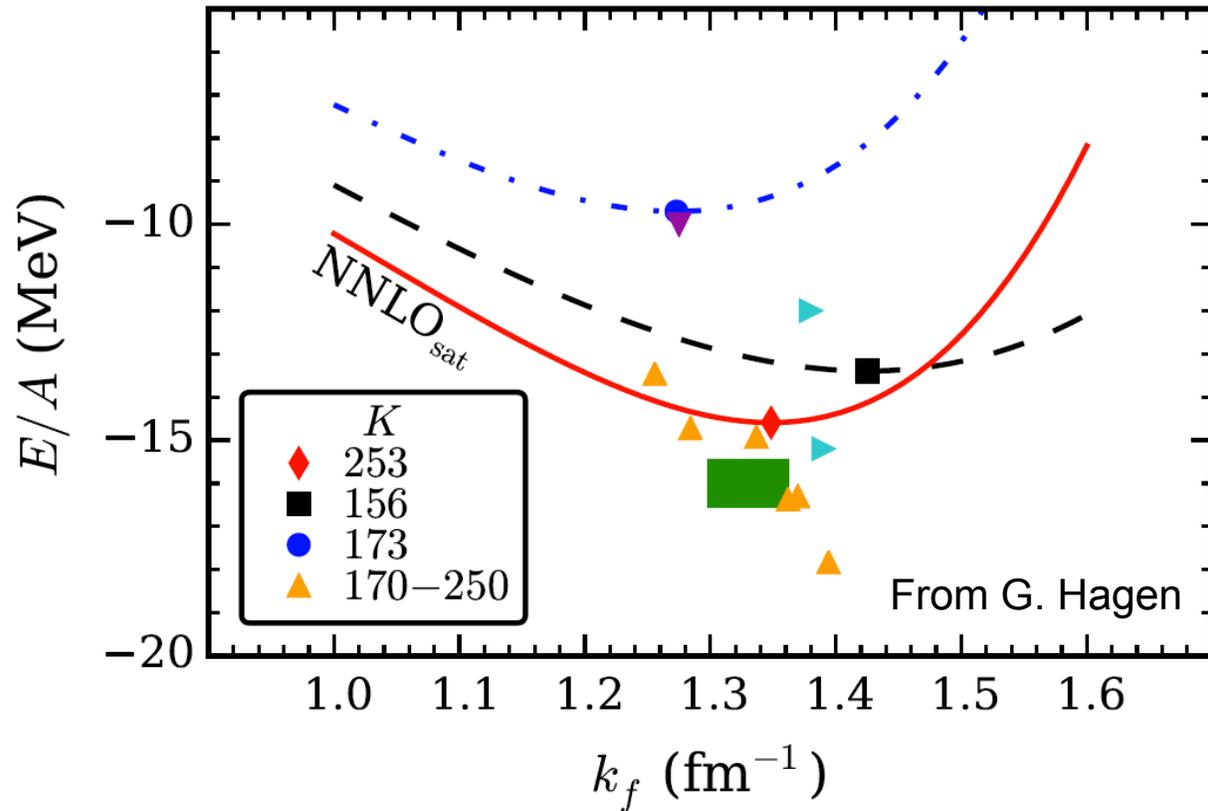
## NN+3N force with good reproduction of ground-state energies



**1.8/2.0 (EM) reproduces ground-state energies through  $^{78}\text{Ni}$**

Slight underbinding for neutron-rich oxygen

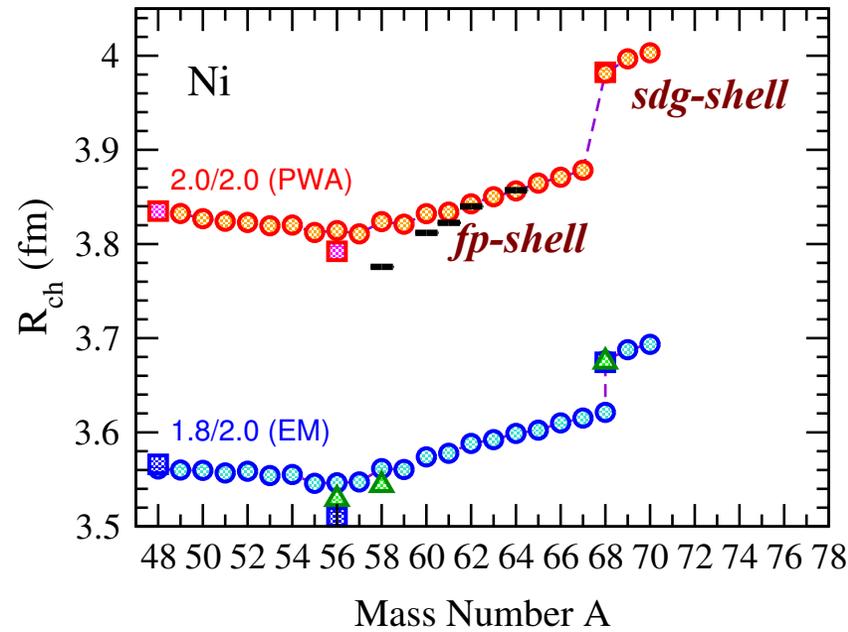
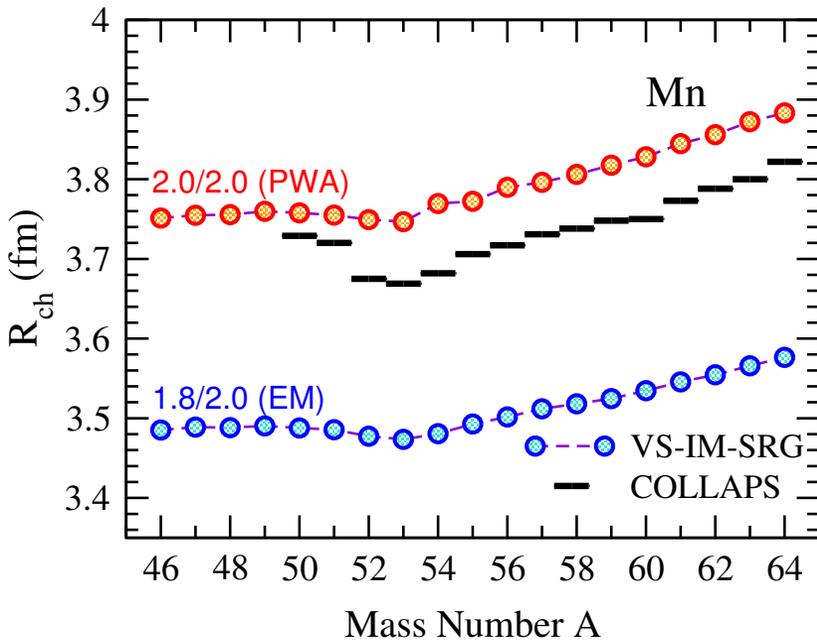
NN+3N force with good reproduction of ground-state energies (but poor radii)



Description of radii depends on saturation density

No interactions reproduces perfectly total charge radii

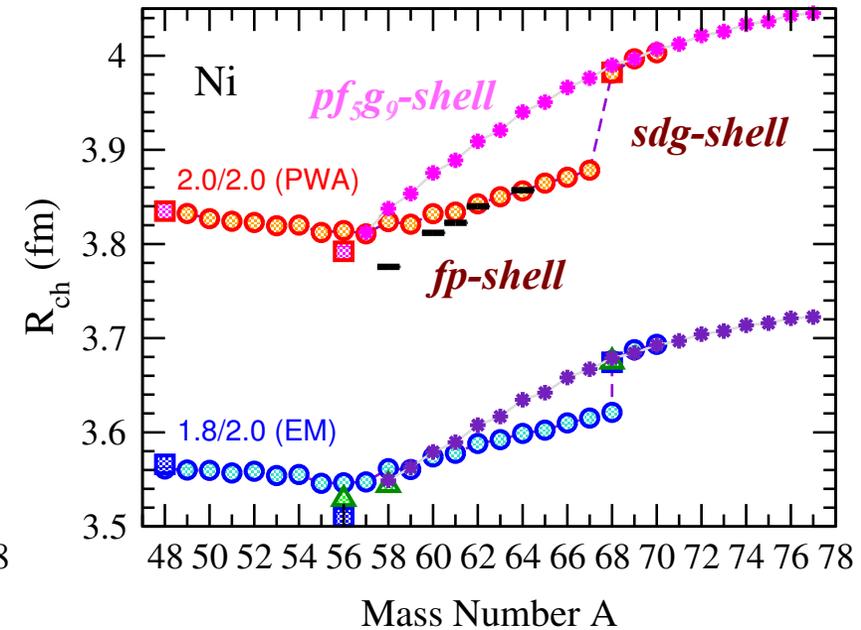
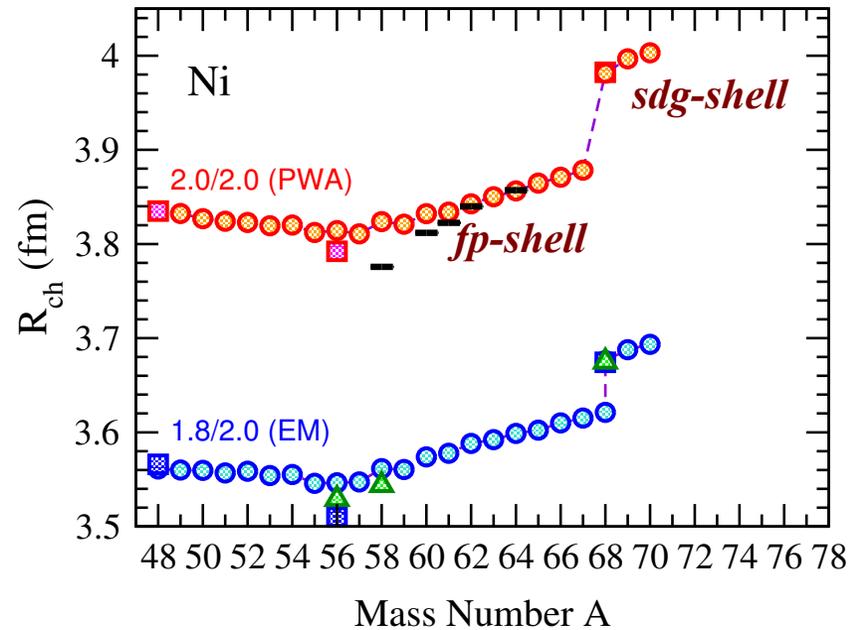
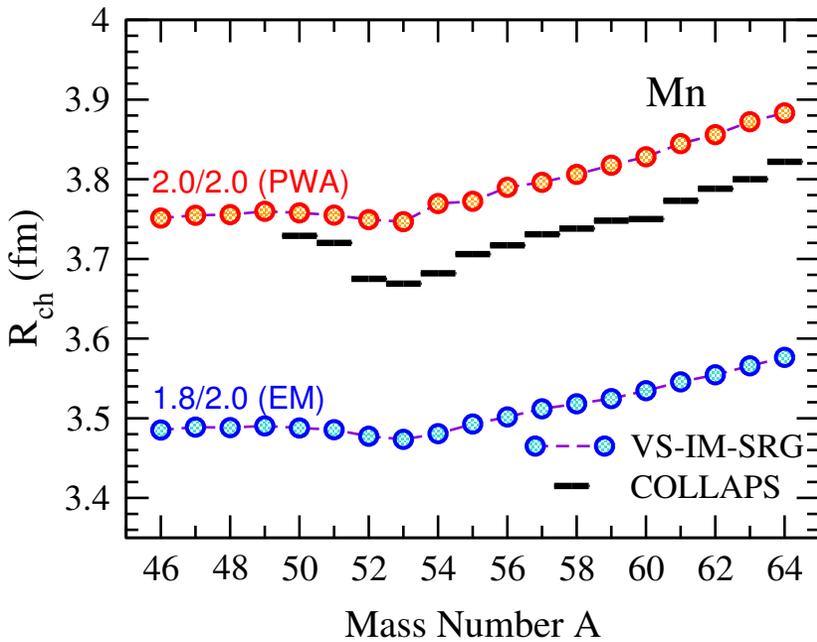
Study charge radii across isotopic chains:  $\langle R^2 \rangle = \langle \Phi_0 | \tilde{R}^2 | \Phi_0 \rangle + \langle \Phi_{\text{SM}} | \tilde{R}^2 | \Phi_{\text{SM}} \rangle$



2.0/2.0 (PWA) “best” results: overpredicts experiment, less pronounced trends

Clear discrepancy at  $^{68}\text{Ni}$ : benchmark against CC and GGF in progress

Study charge radii across isotopic chains:  $\langle R^2 \rangle = \langle \Phi_0 | \tilde{R}^2 | \Phi_0 \rangle + \langle \Phi_{\text{SM}} | \tilde{R}^2 | \Phi_{\text{SM}} \rangle$

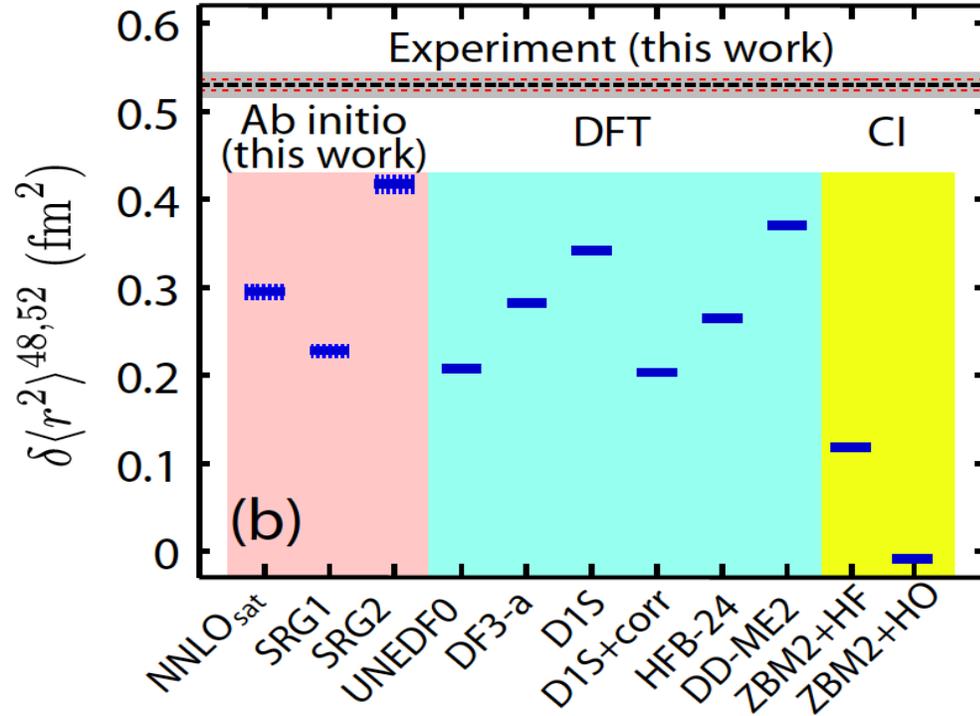
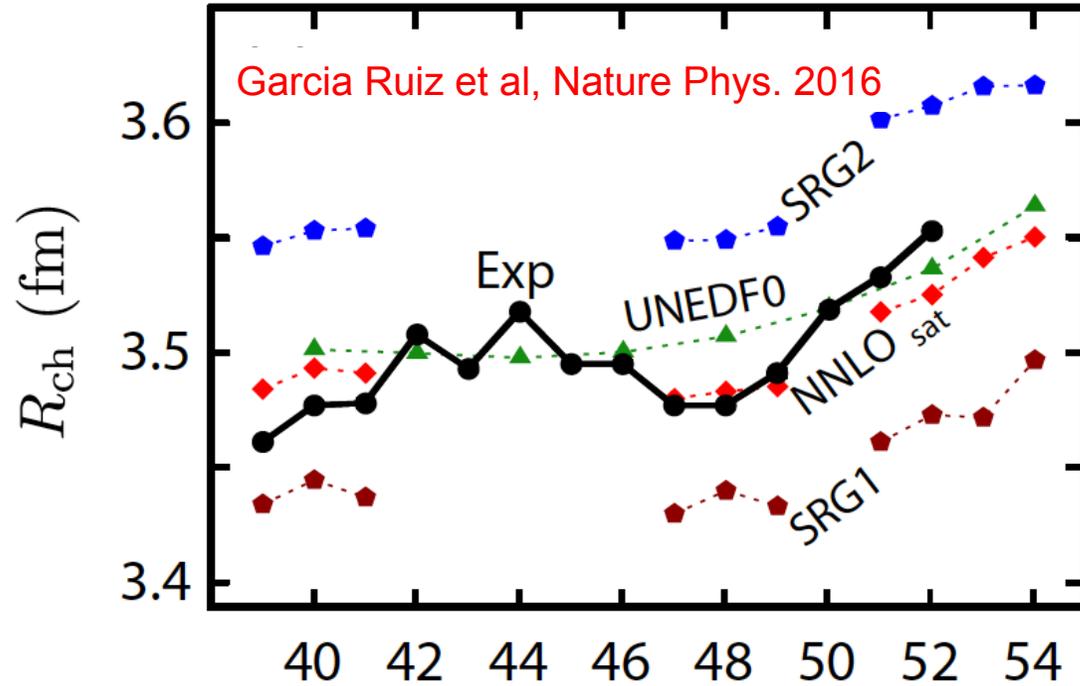


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Clear discrepancy at  $^{68}\text{Ni}$ : benchmark against CC and GGF in progress

Multi-shell VS-IMSRG in progress...

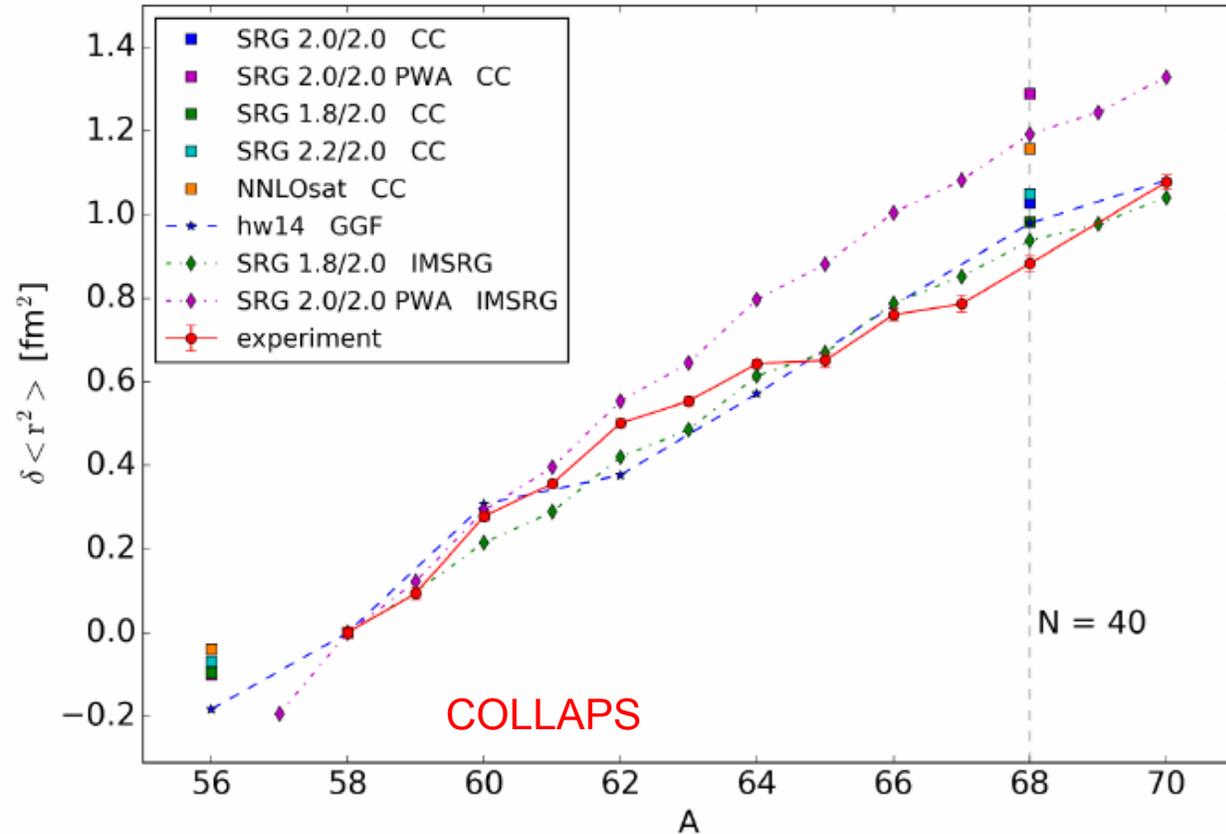
Charge radii of  $^{49-52}\text{Ca}$  measured from laser spectroscopy at COLLAPS, CERN



**Unexpected increase in charge radius questions magicity of  $^{52}\text{Ca}$**

Theory underestimates this increase – challenge for future

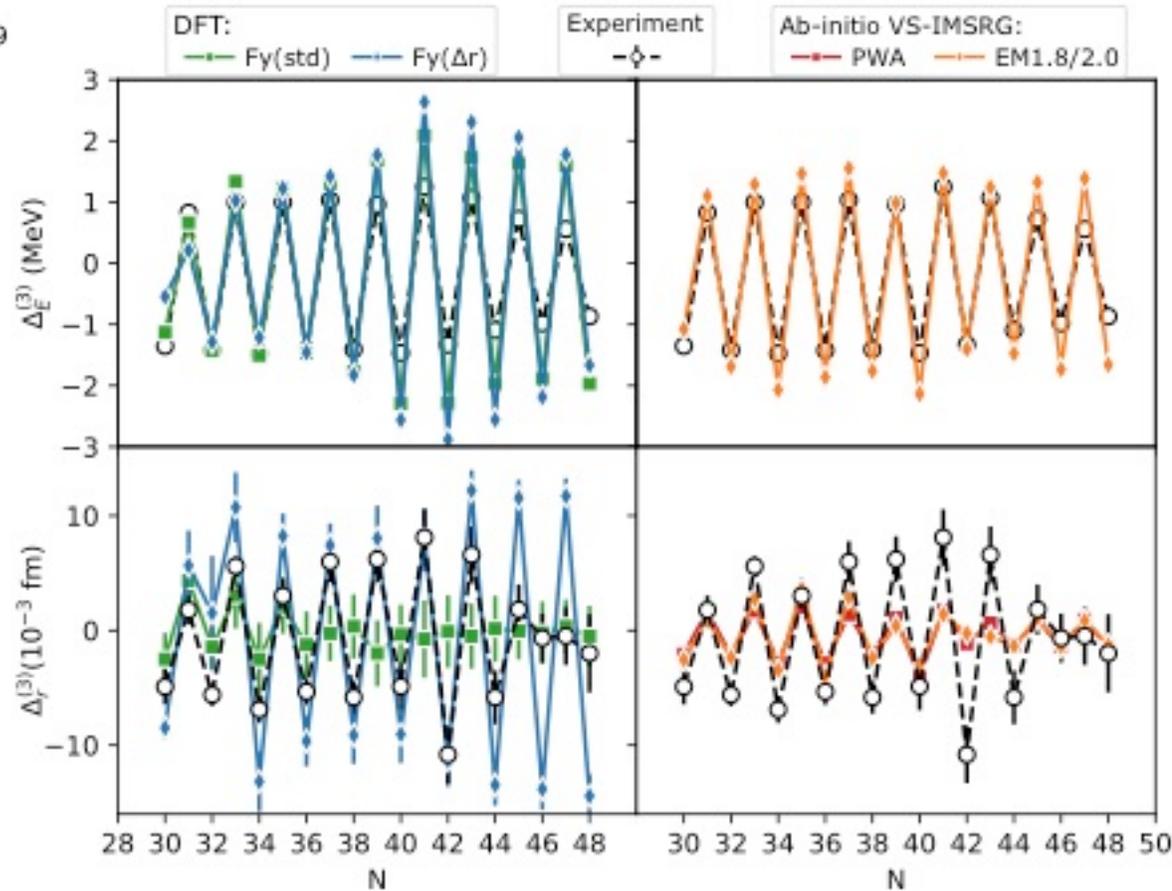
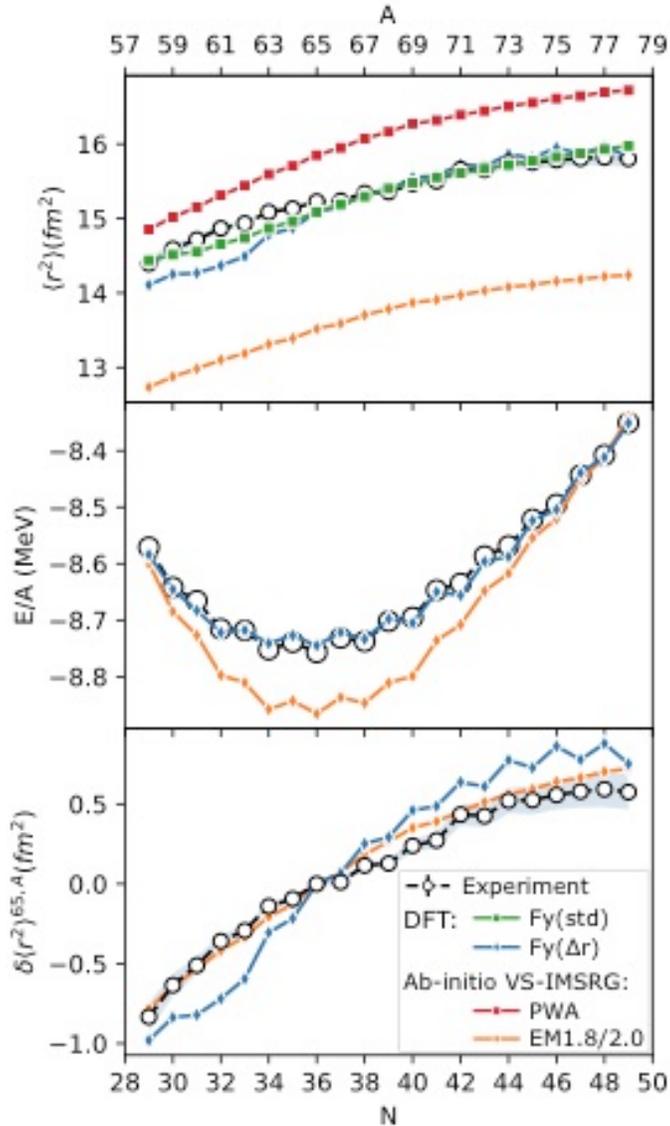
Study charge radii across isotopic chains:  $\langle R^2 \rangle = \langle \Phi_0 | \tilde{R}^2 | \Phi_0 \rangle + \langle \Phi_{\text{SM}} | \tilde{R}^2 | \Phi_{\text{SM}} \rangle$



Study radii normalized to reference (as measured in laser spec. experiments)

1.8/2.0(EM) reproduces trends more accurately in Ni isotopes

Study charge radii across isotopic chains:  $\langle R^2 \rangle = \langle \Phi_0 | \tilde{R}^2 | \Phi_0 \rangle + \langle \Phi_{SM} | \tilde{R}^2 | \Phi_{SM} \rangle$



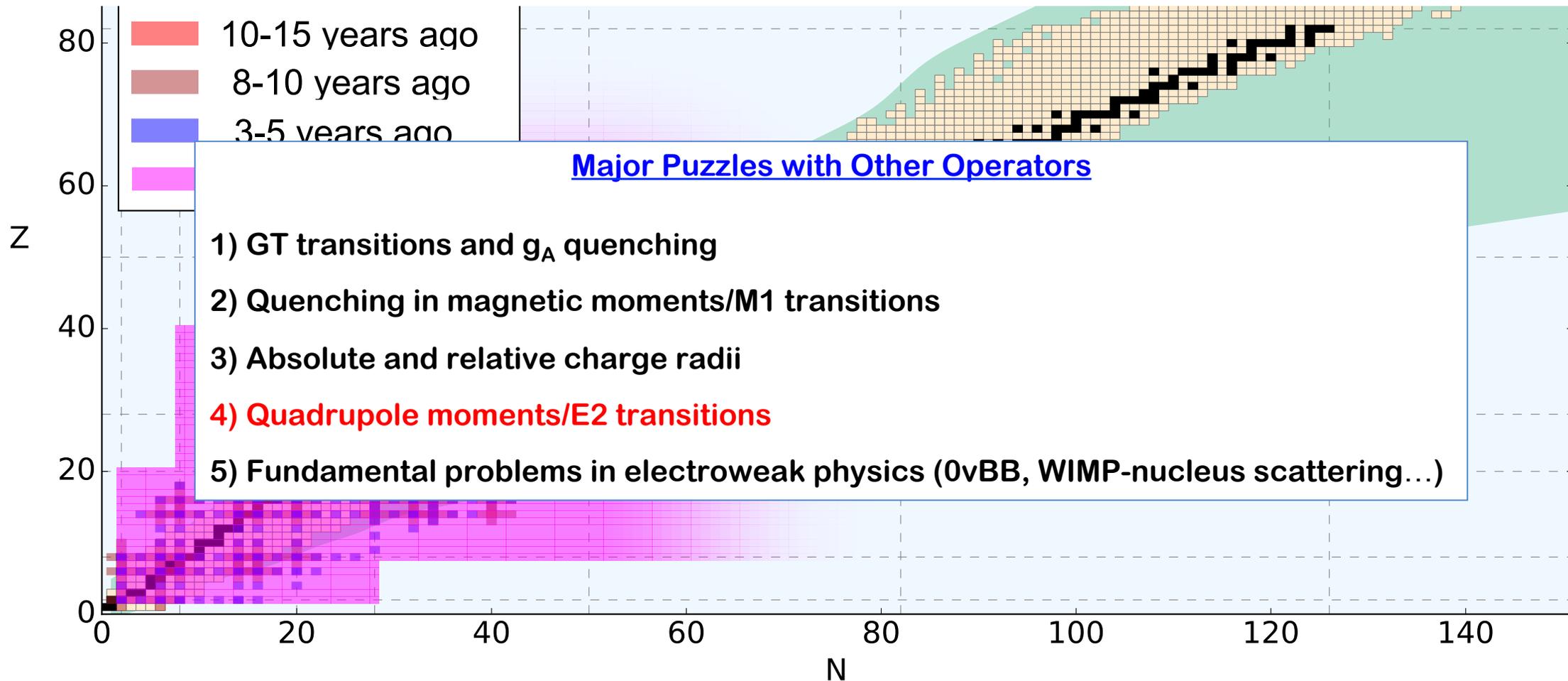
R.P. de Groote et al., Nat. Phys. (2020)

Cu isotopes, odd-even staggering reproduced, but still deficient  
 Competitive with DFT fit to reproduce odd-even staggering in region

**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem

$$H\psi_n = E_n\psi_n$$

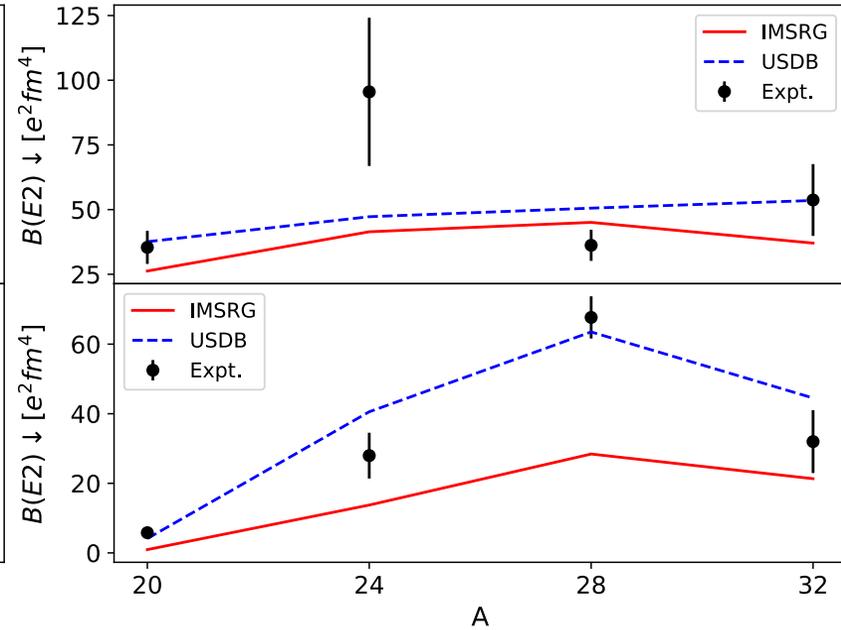
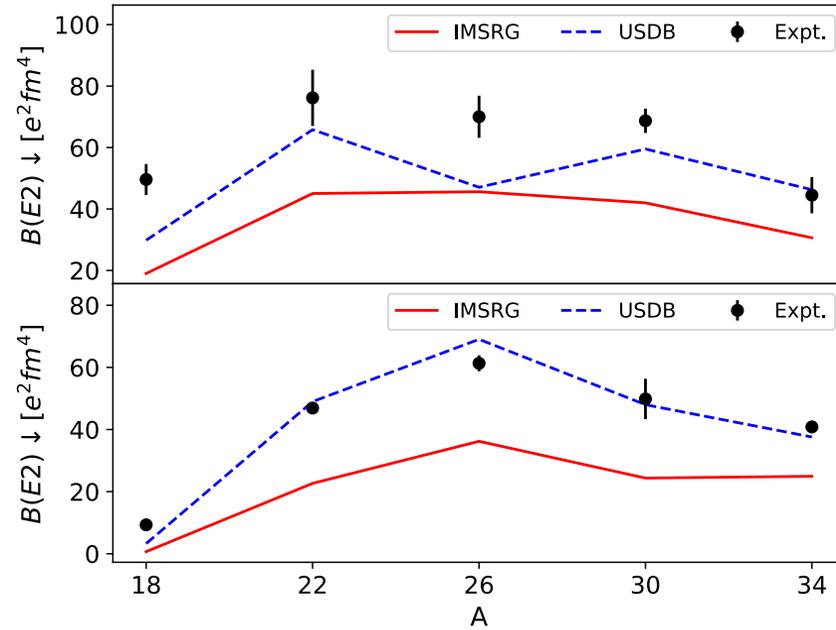
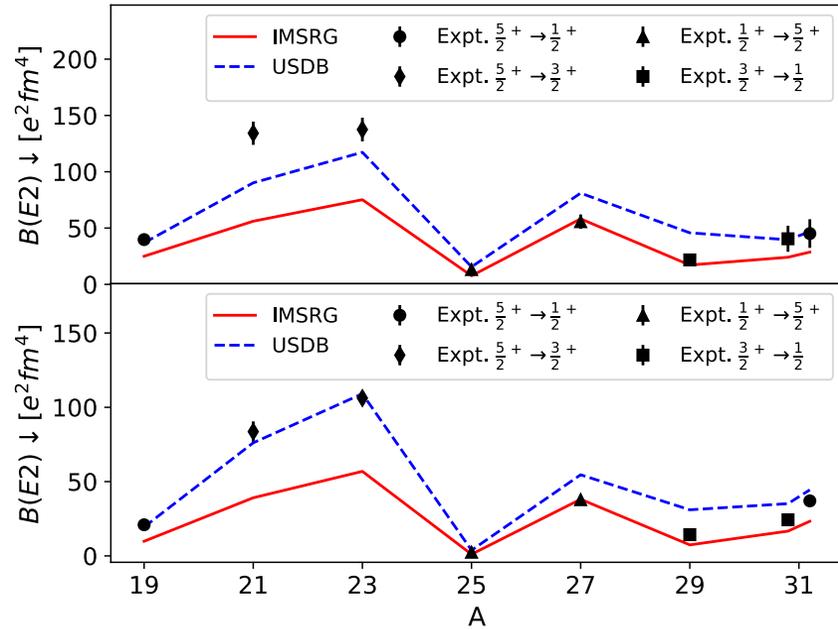


## Study charge E2 transitions across sd-shell

$$T_z = \pm \frac{1}{2}$$

$$T_z = \pm 1$$

$$T_z = \pm \frac{3}{2}$$

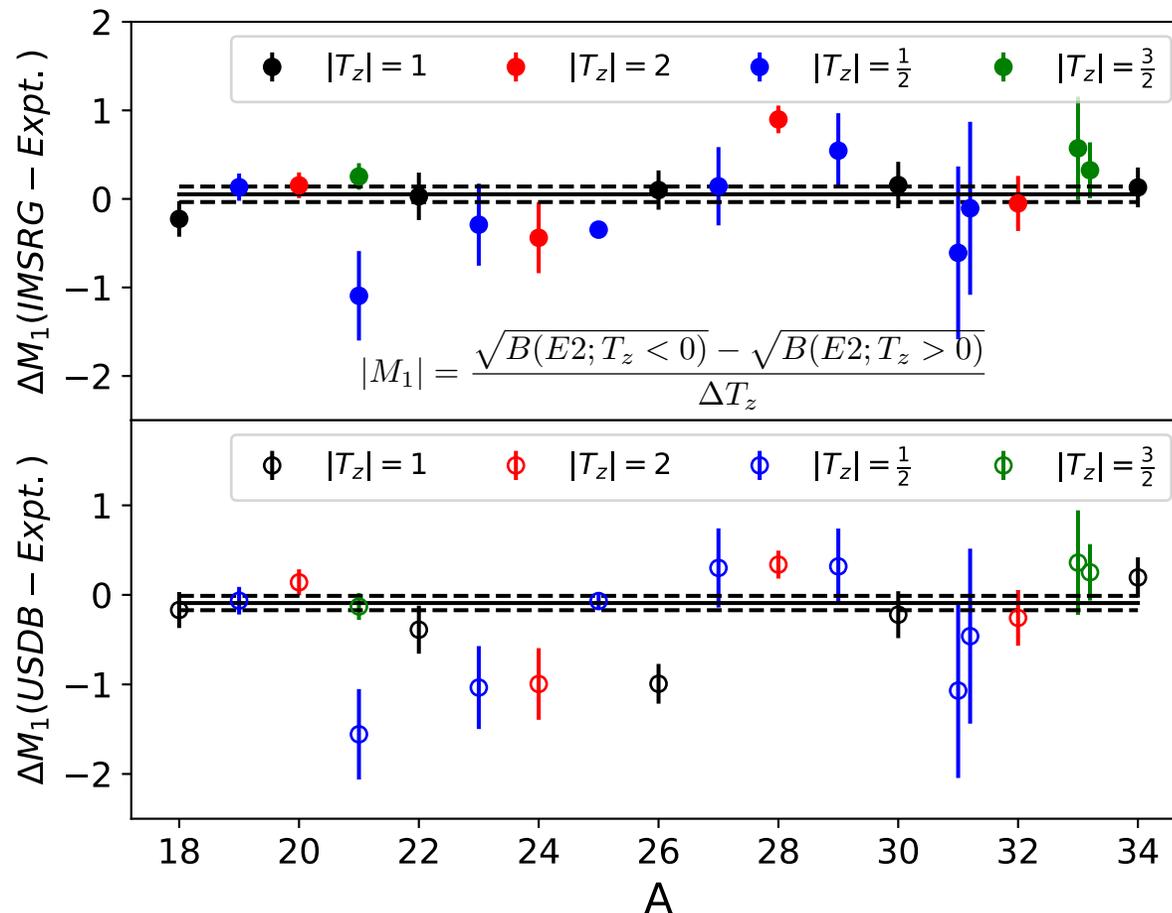
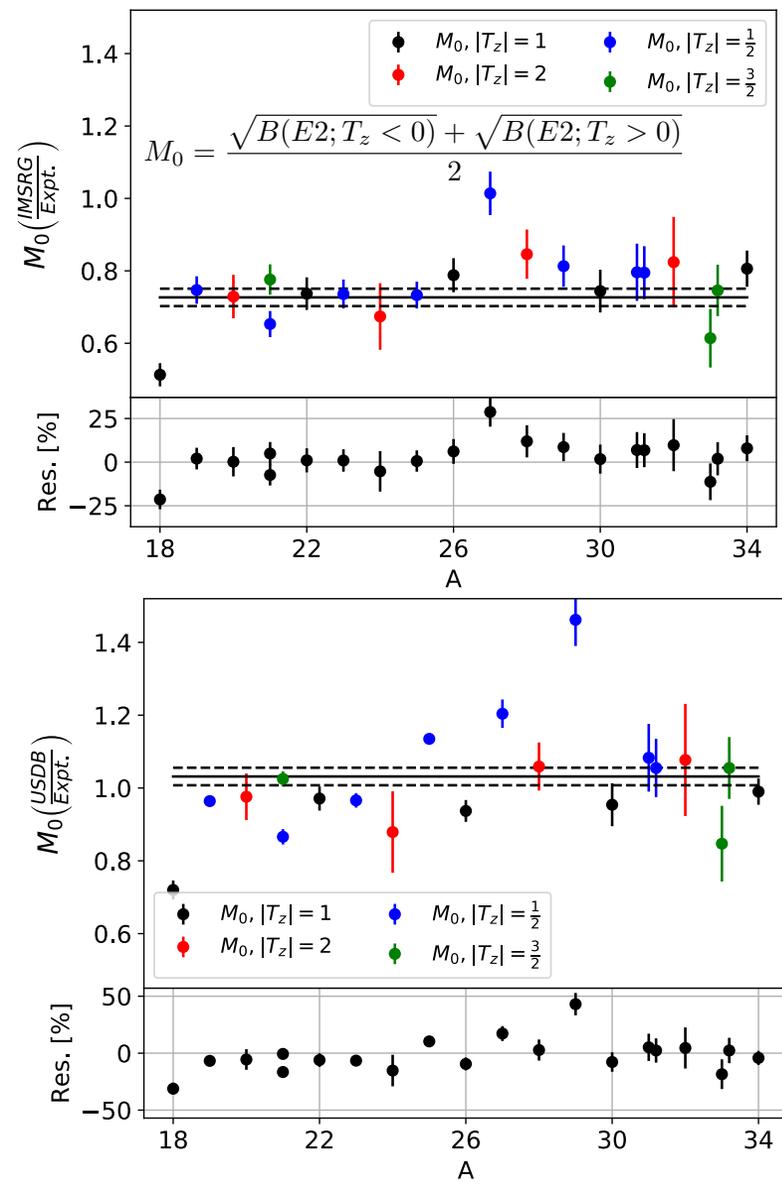


USDB with effective charges typically reproduces absolute values well

VS-IMSRG (**no effective charges**) typically underpredicts experiment

Trends well reproduced in both...

Study charge E2 transitions across sd-shell: IS ( $M_0$ ) and IV ( $M_1$ )

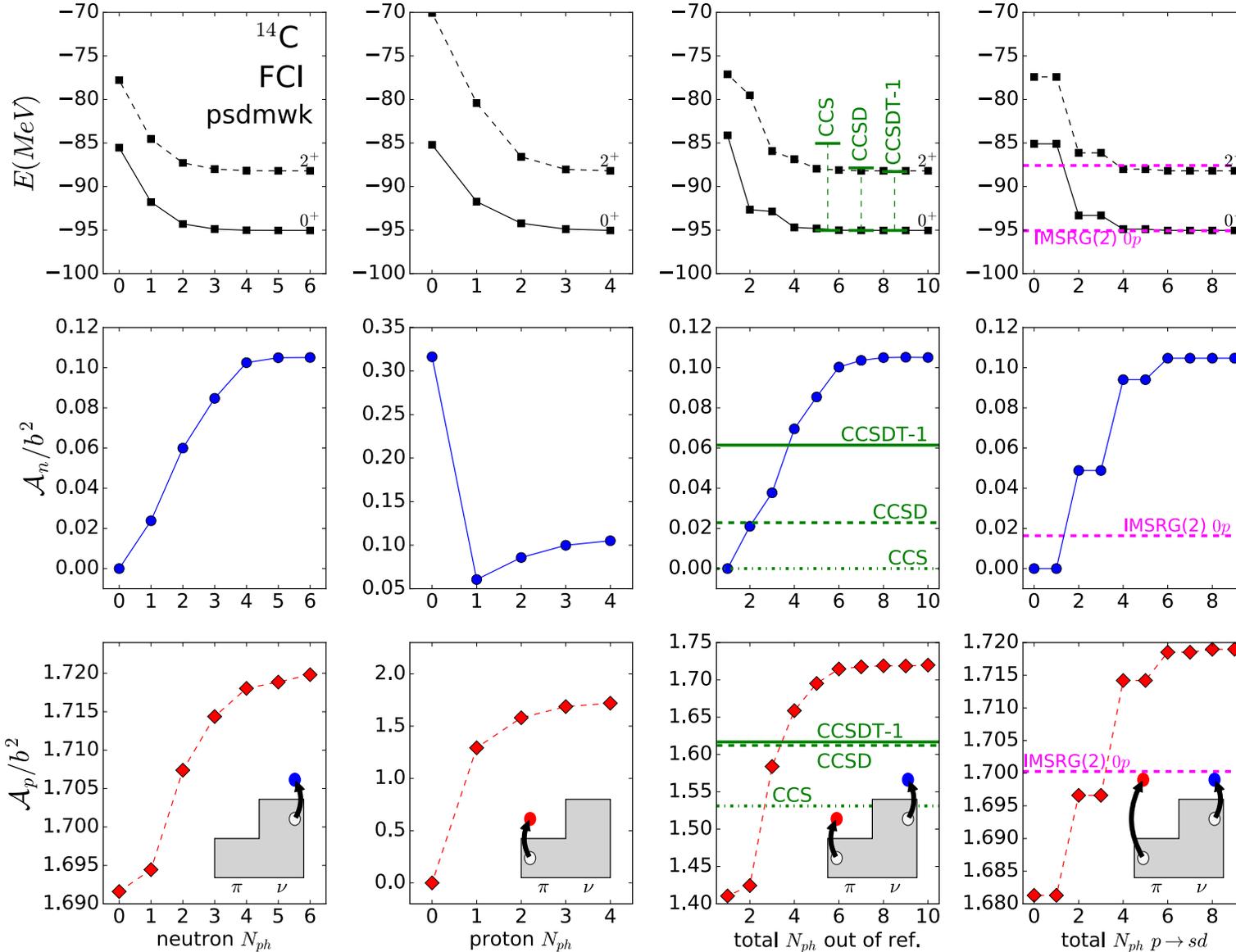


IS: USDB good agreement, VS-IMSRRG systematically small

IV: Both agree well

Deficiencies in IS only

Perform CC and VS-IMSRG calculations of  $^{14}\text{C}$  in toy psd space with phenomenological potential



Energies well converged all around

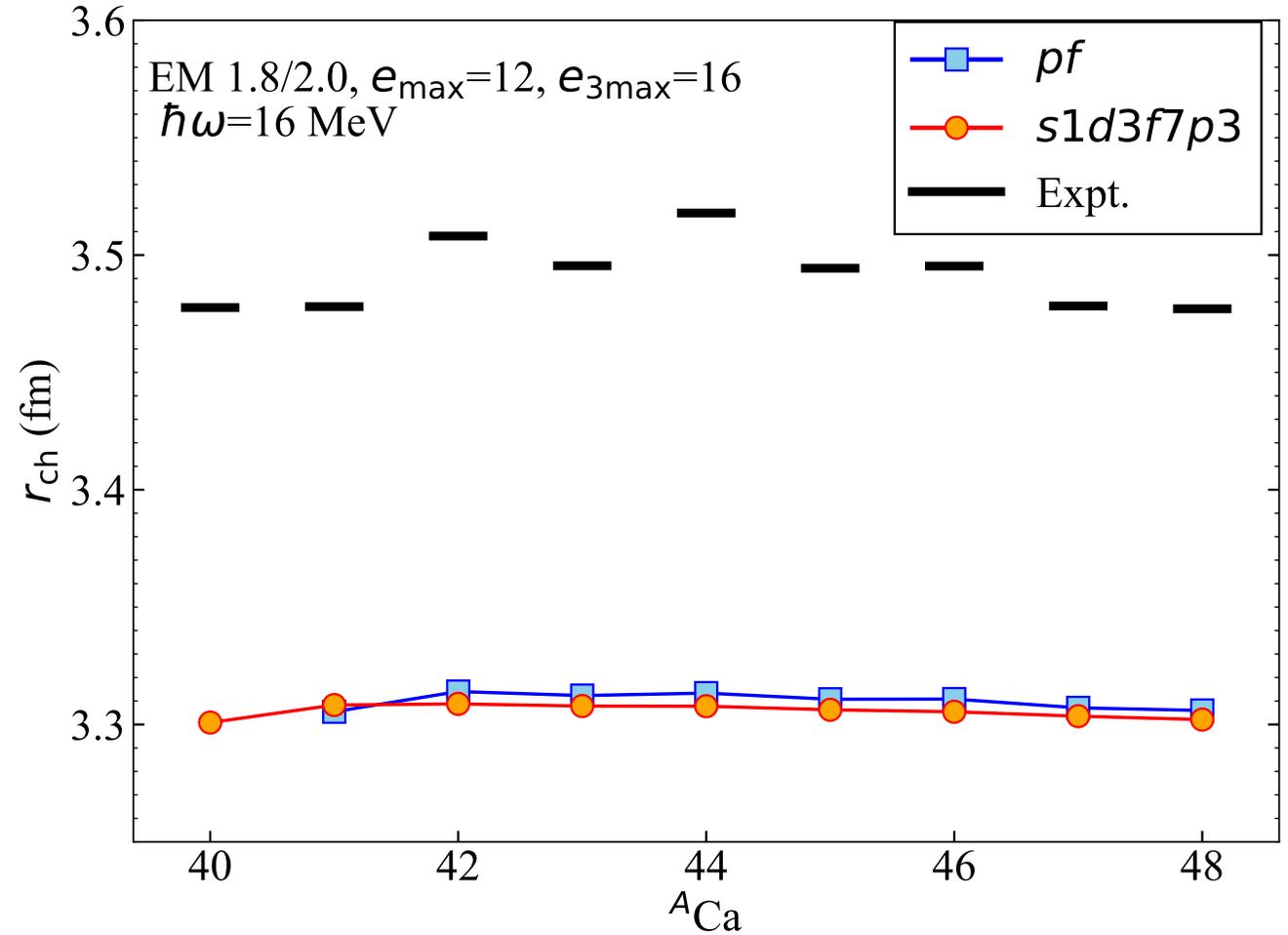
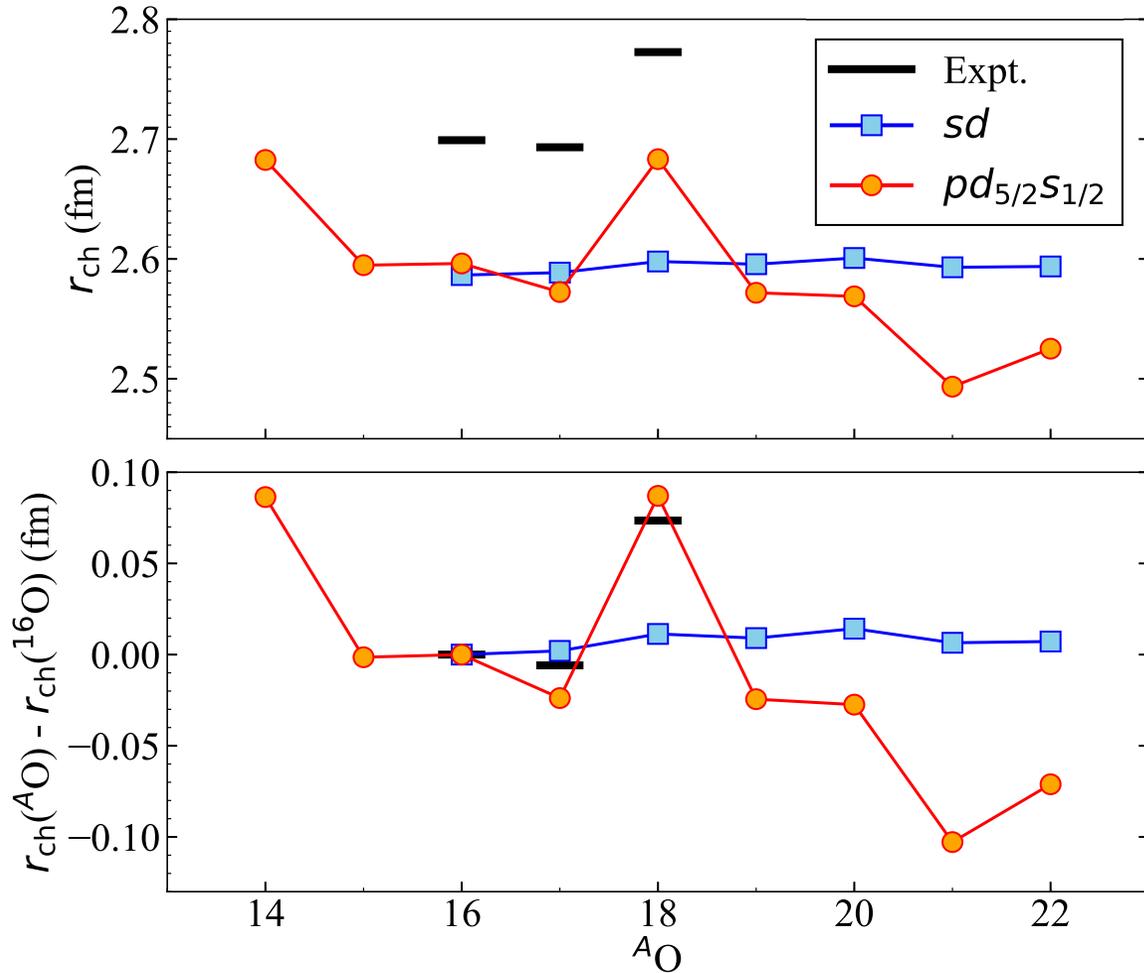
p/n amplitudes increase with p/h ex.

Only converged at 6-8 Nph

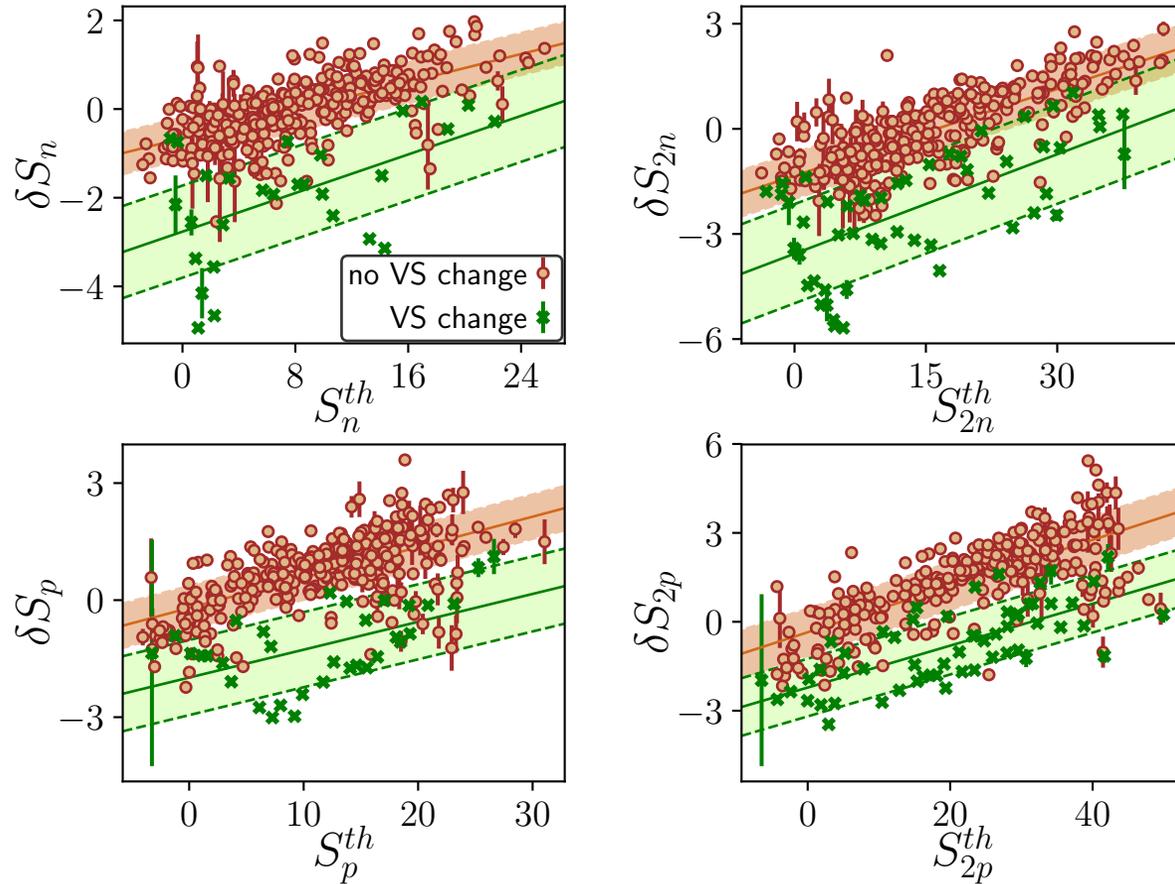
Not possible to capture in CC/IMSRG

Improved trends across oxygen isotopes with  $pd5s1$  space!

Calcium... not so much...



**Defect 2: Incomplete convergence near threshold** – clear trend in residuals



$$\delta \mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$

JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

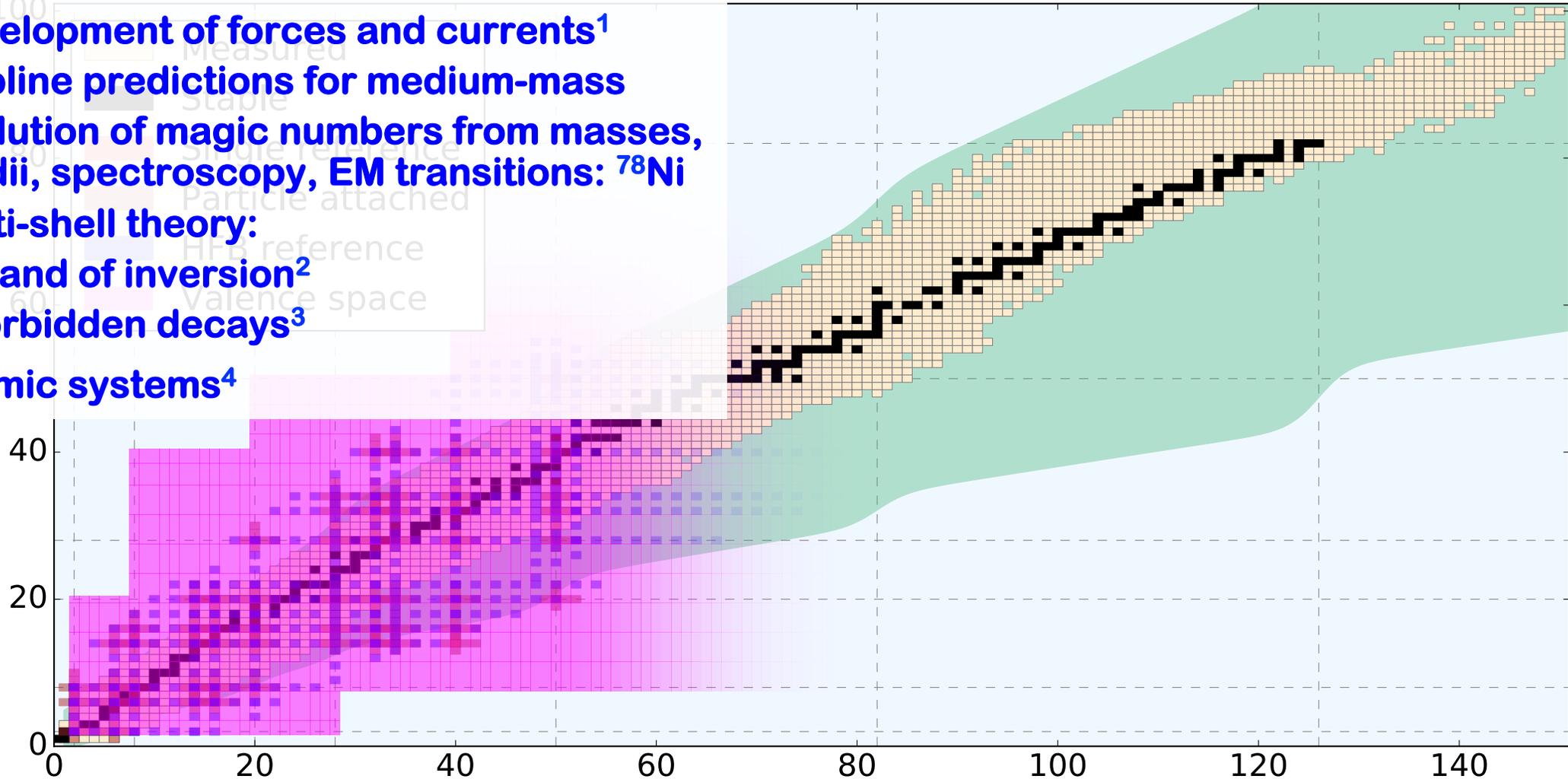
Separate trends for VS change and no change

Correct VS-IMSRG results with linear fit of residuals

Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

## Nuclear Structure

- Development of forces and currents<sup>1</sup>
- Dripline predictions for medium-mass
- Evolution of magic numbers from masses, radii, spectroscopy, EM transitions: <sup>78</sup>Ni
- Multi-shell theory:
  - Island of inversion<sup>2</sup>
  - Forbidden decays<sup>3</sup>
- Atomic systems<sup>4</sup>



Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

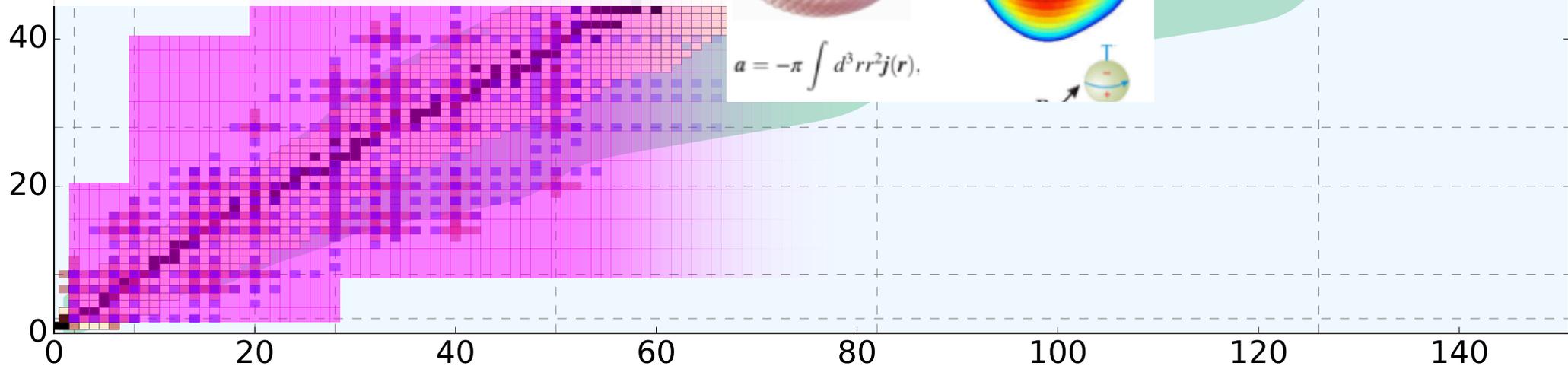
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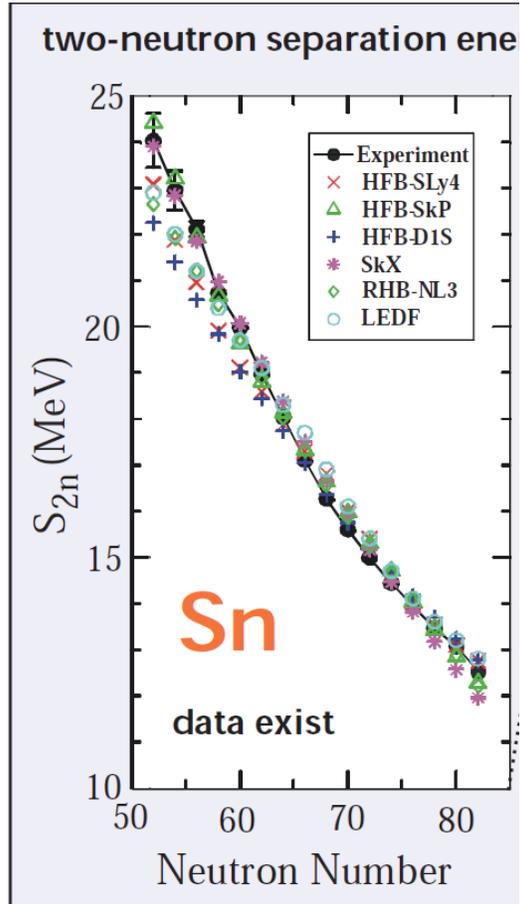
## Atomic systems<sup>4</sup>

## Fundamental Symmetries/BSM Physics

- Effective electroweak operators: GT quenching
- Effective  $0\nu\beta\beta$  decay operator<sup>5</sup>
- WIMP-Nucleus scattering<sup>6</sup>
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- Symmetry-violating moments [molecules]<sup>8</sup>

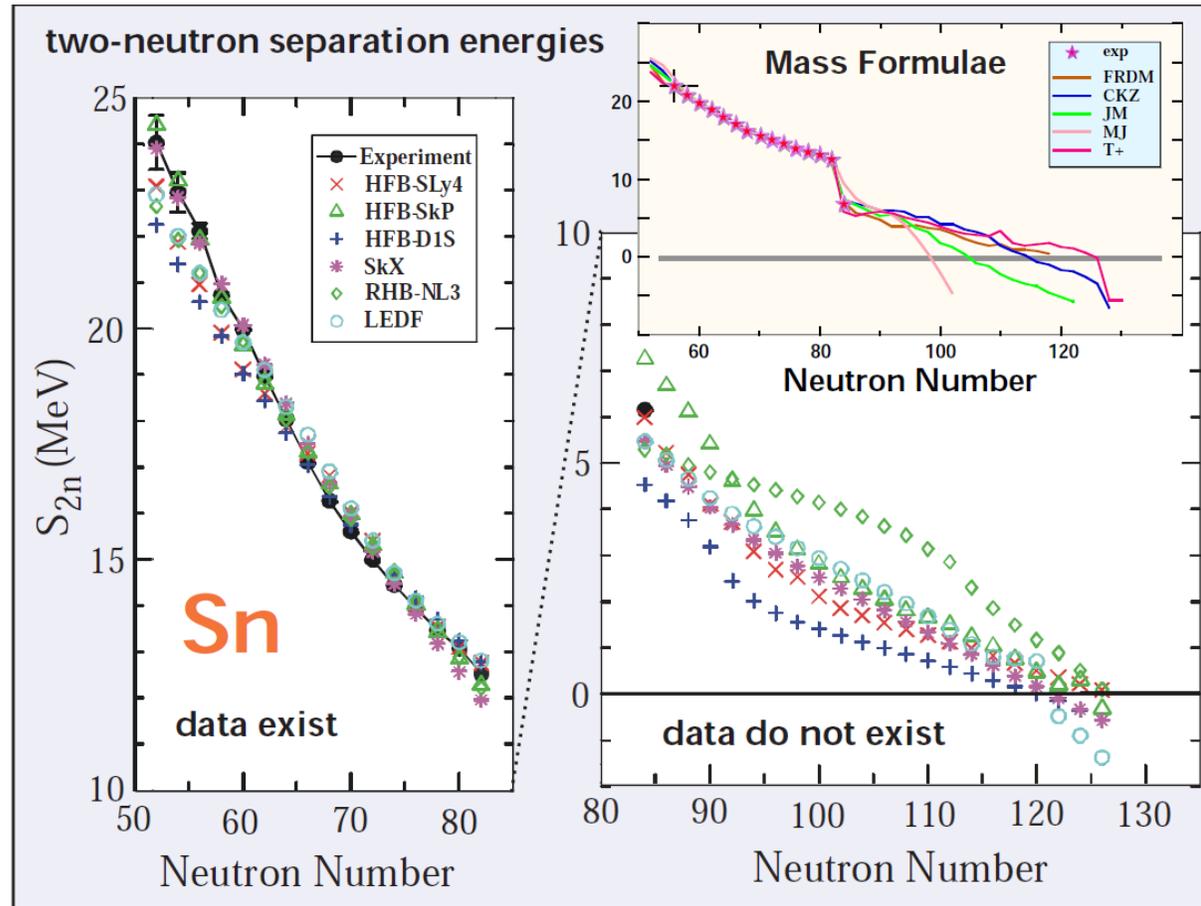


How well can nuclear models motivate experiments, predict beyond data?



Work well where informed  
by data

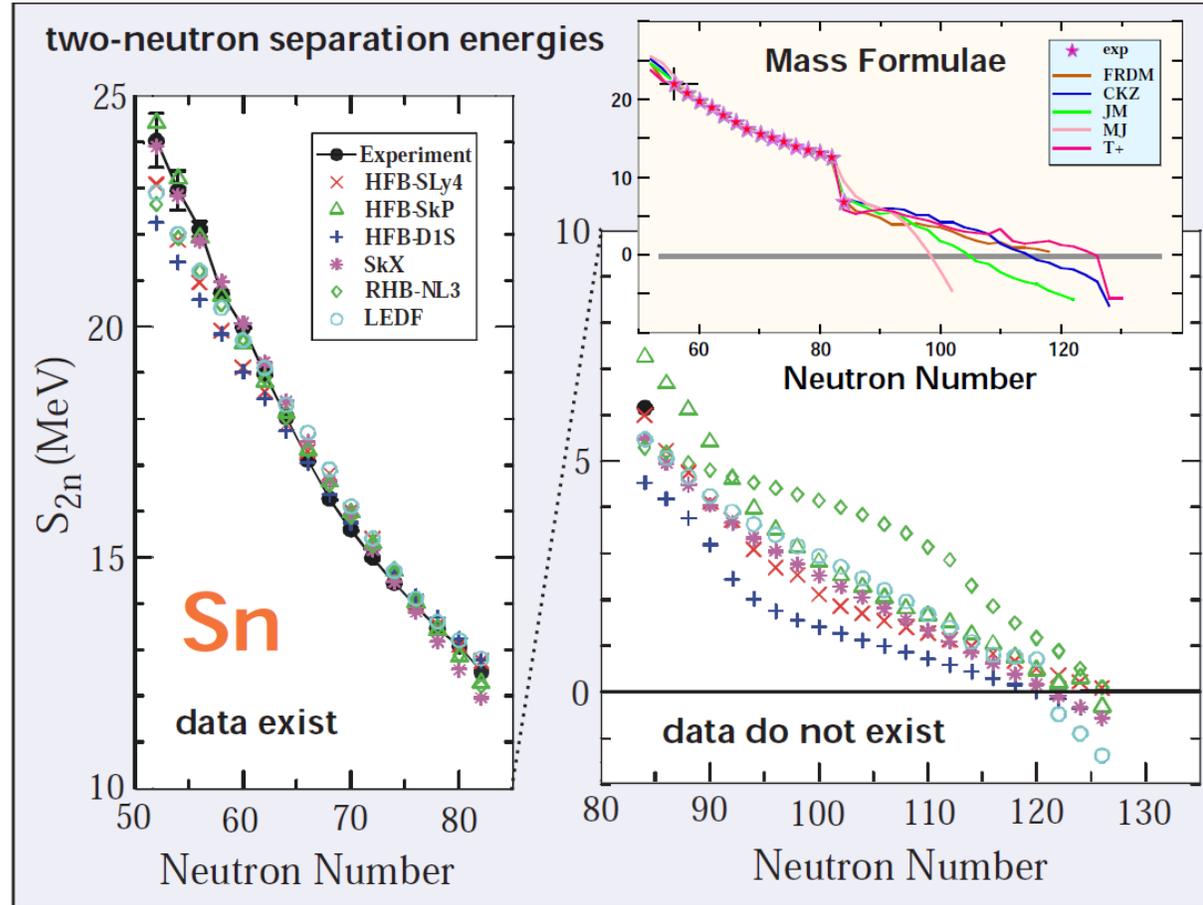
How well can nuclear models motivate experiments, predict beyond data?



Models can extrapolate unreliably

Spread in results  $\neq$  meaningful uncertainty

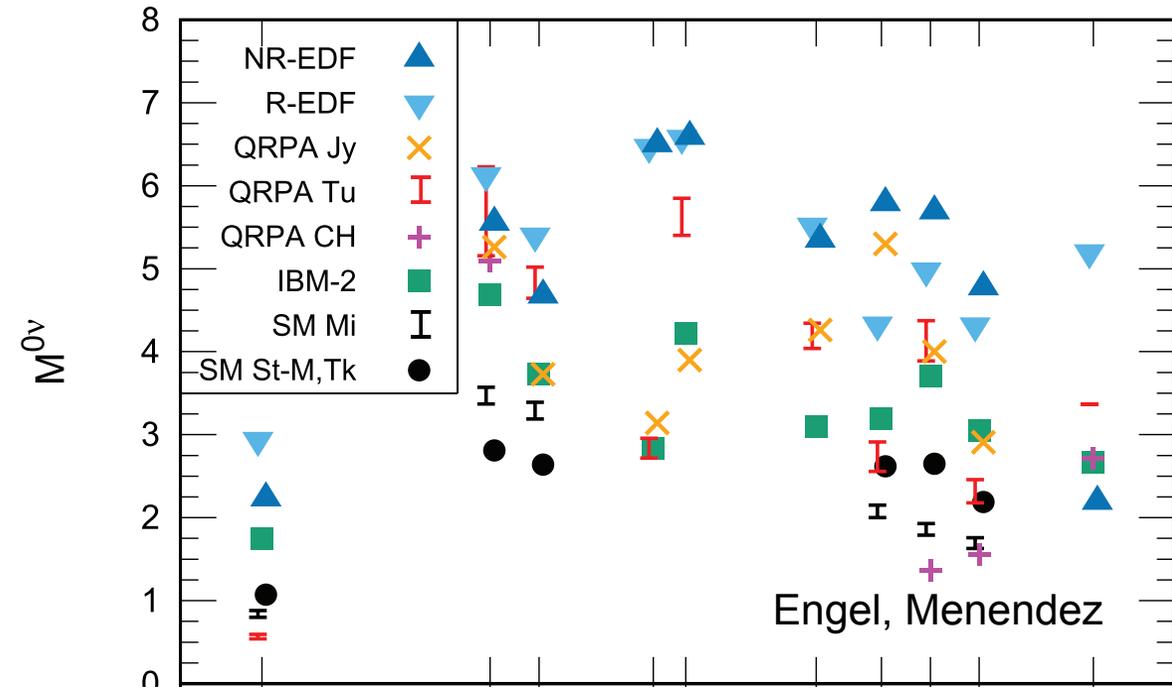
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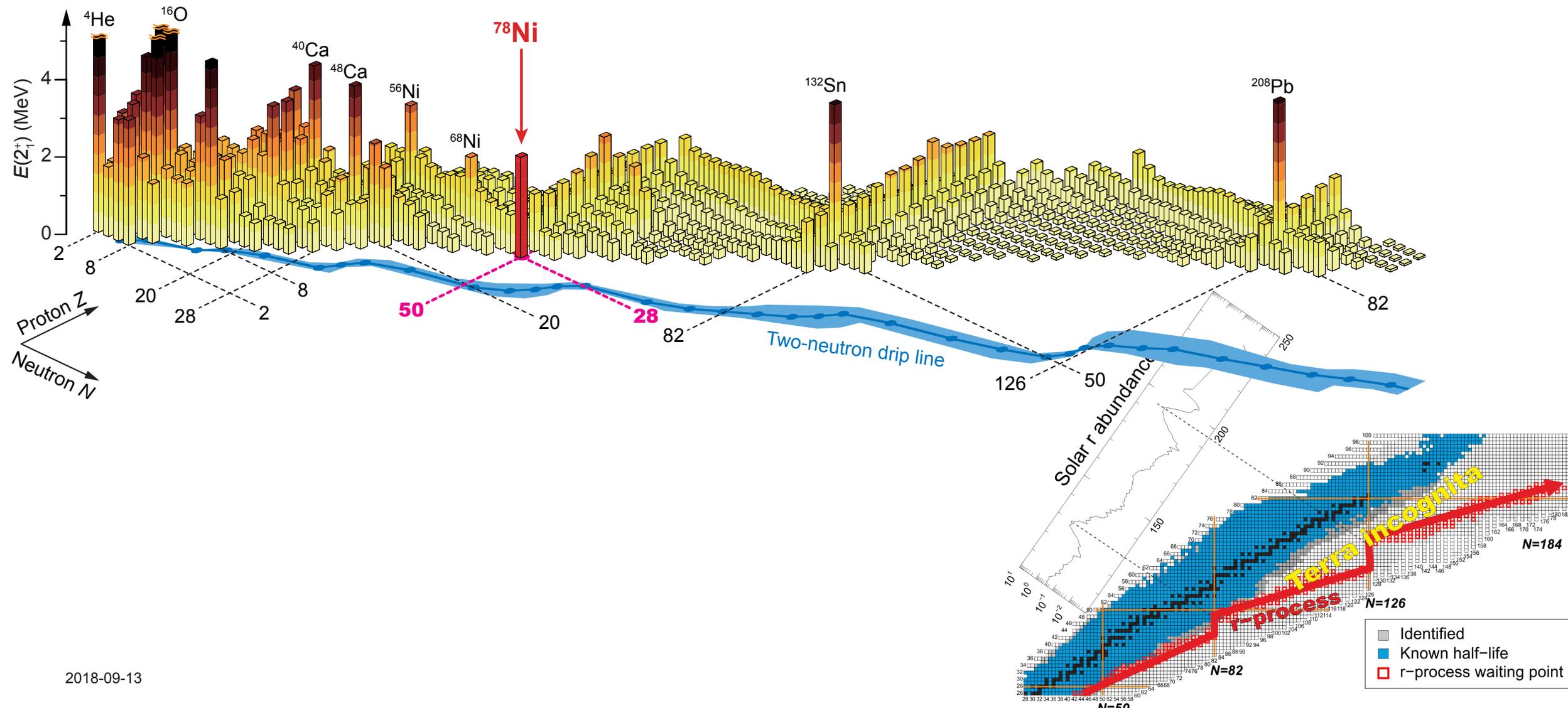
Models can extrapolate unreliably

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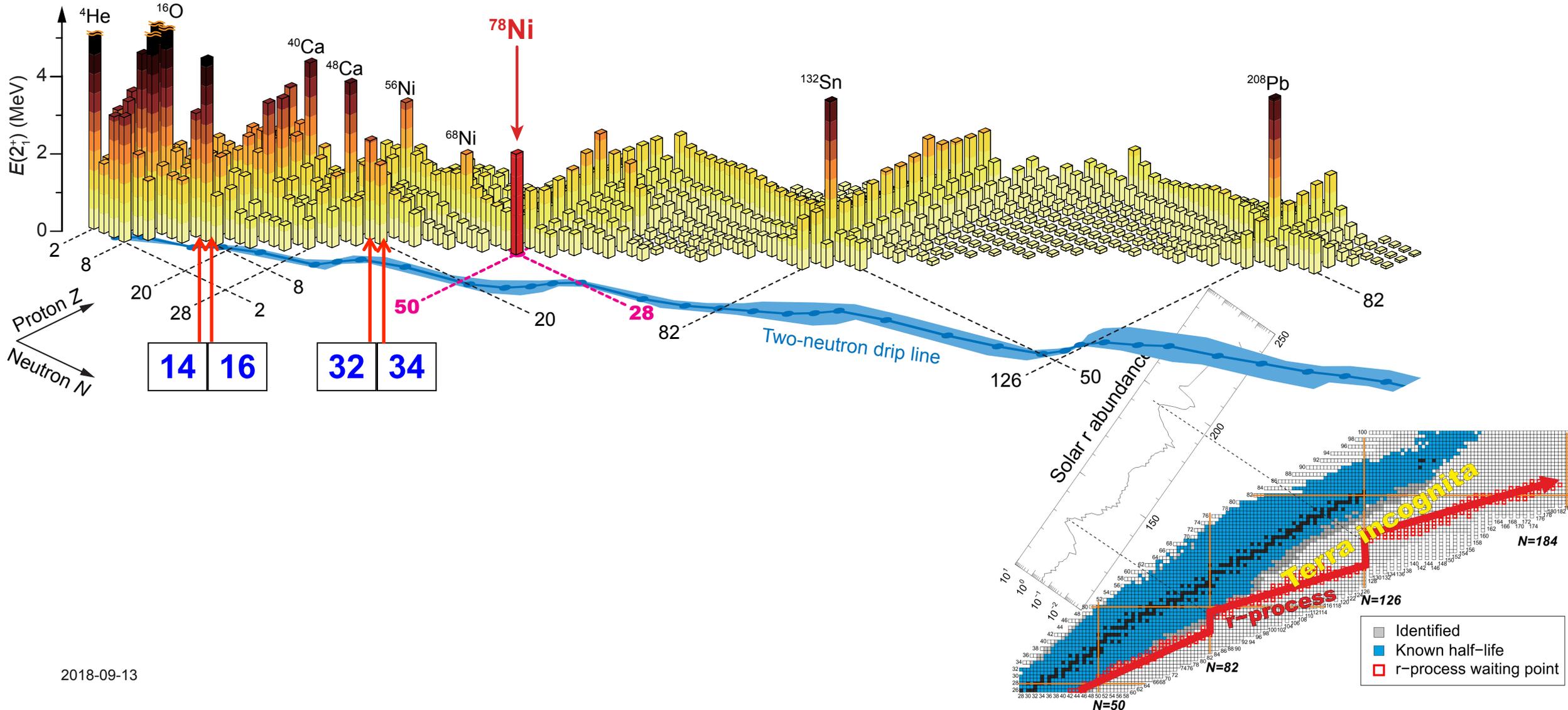
Analogous picture in  $0\nu\beta\beta$  decay



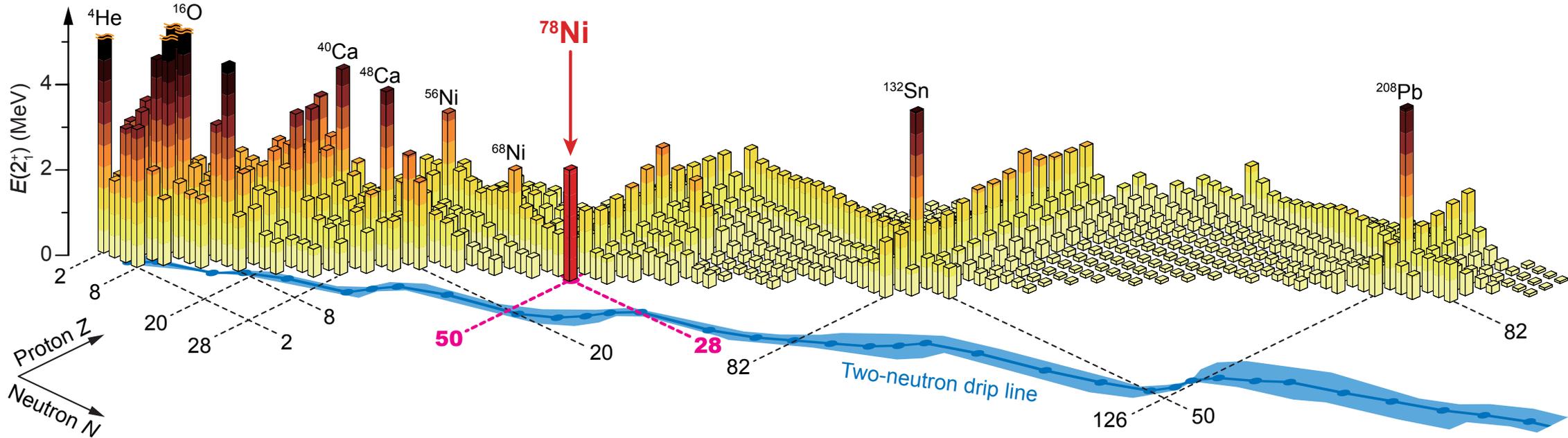
**Magic numbers:** pillars of nuclear structure, vital for r-process nucleosynthesis



Magic numbers: pillars of nuclear structure, **novel evolution in exotic nuclei**



**Magic numbers:** pillars of nuclear structure, novel evolution in exotic nuclei

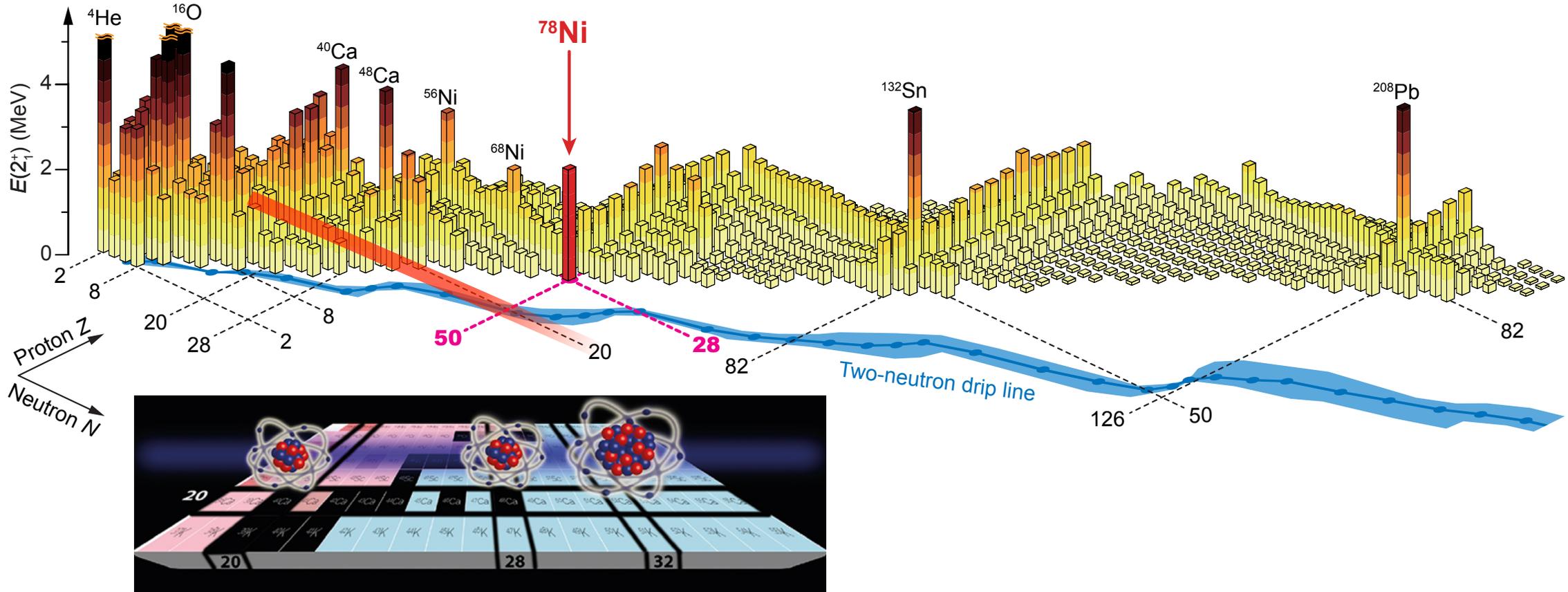


## Signatures of Magic Numbers

- Sharp decrease in separation energy (masses)
- Elevated first excited  $2+$  energy (spectroscopy)
- Tightly bound (decreased radii)

**Must observe all signatures – many experiments (and calculations) needed!**

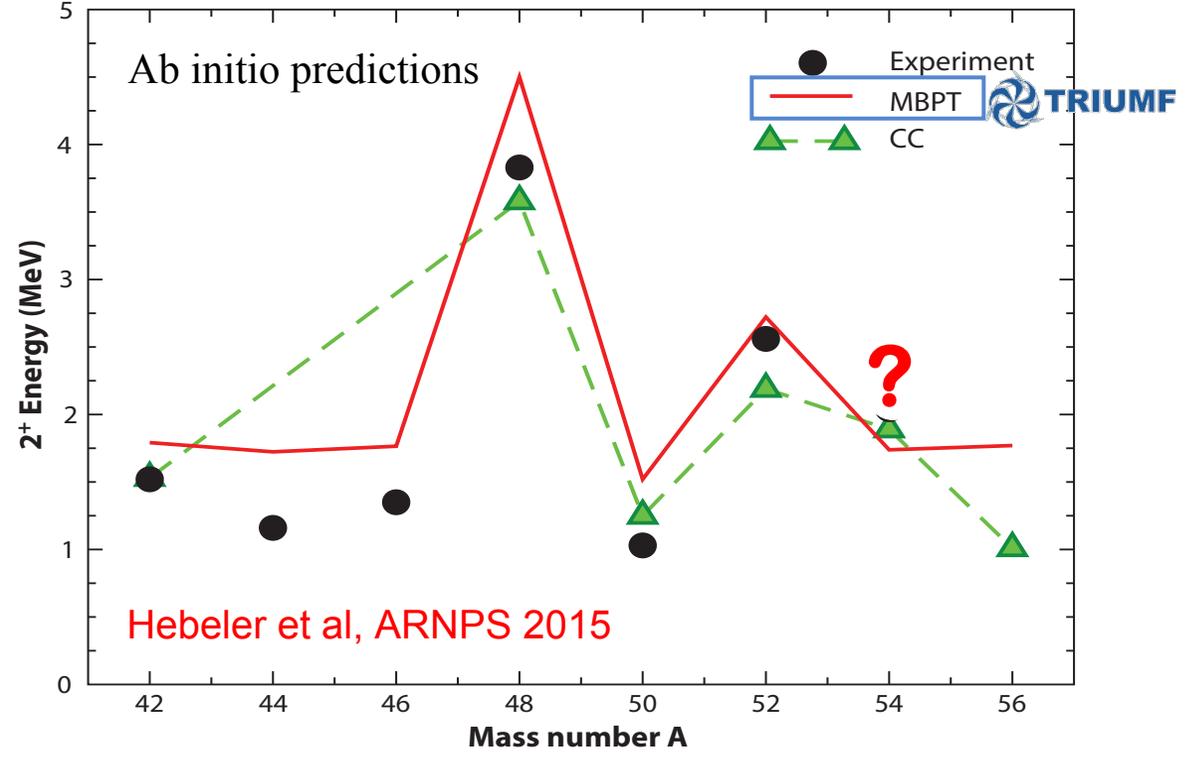
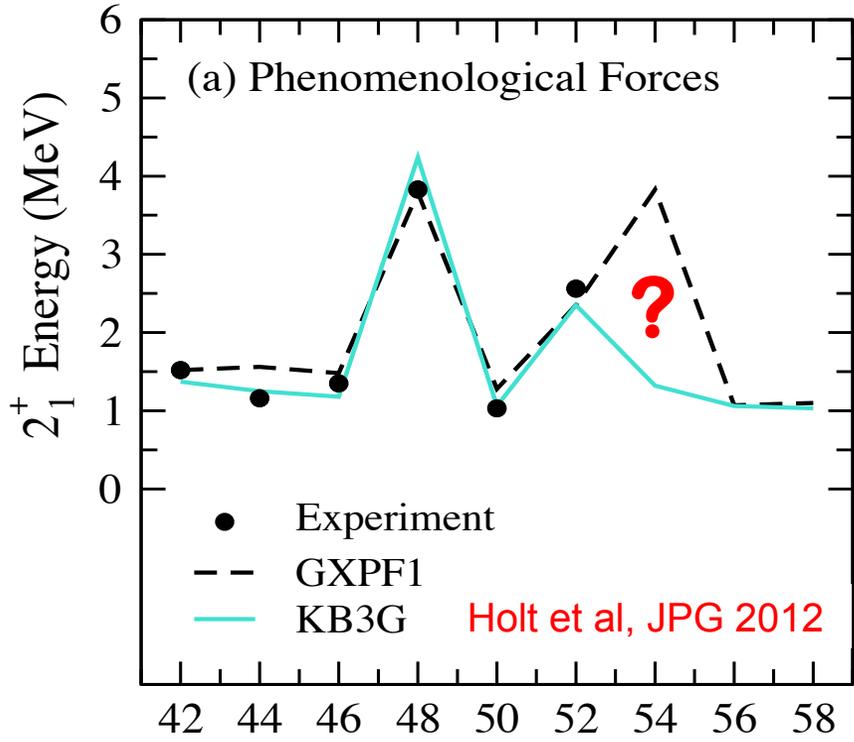
**Magic numbers:** pillars of nuclear structure, novel evolution in exotic nuclei



**Highlight of TRIUMF theory and experiment:**

Discovery and evolution of new N=32,34 magic numbers in calcium region

**2013** potentially new magic numbers from  $2^+$  energies:  $N=32,34$



## Phenomenological Models

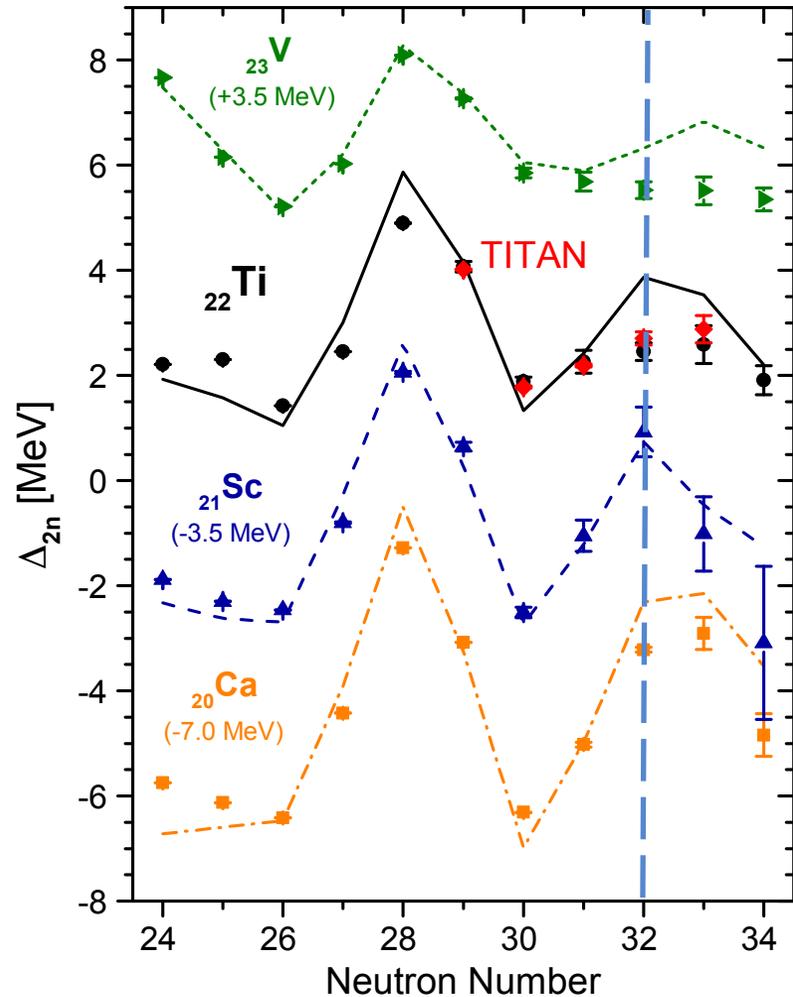
Reproduce magic  $N=28,32$ ; discrepancy at  $N=34$  (beyond data)

## Ab initio theories

Predict all magic numbers; **consistent at  $N=34$**

Further questions: how do magic numbers evolve with proton number?

## Current frontier of measurements and theory



### New TITAN Measurements of Ti masses

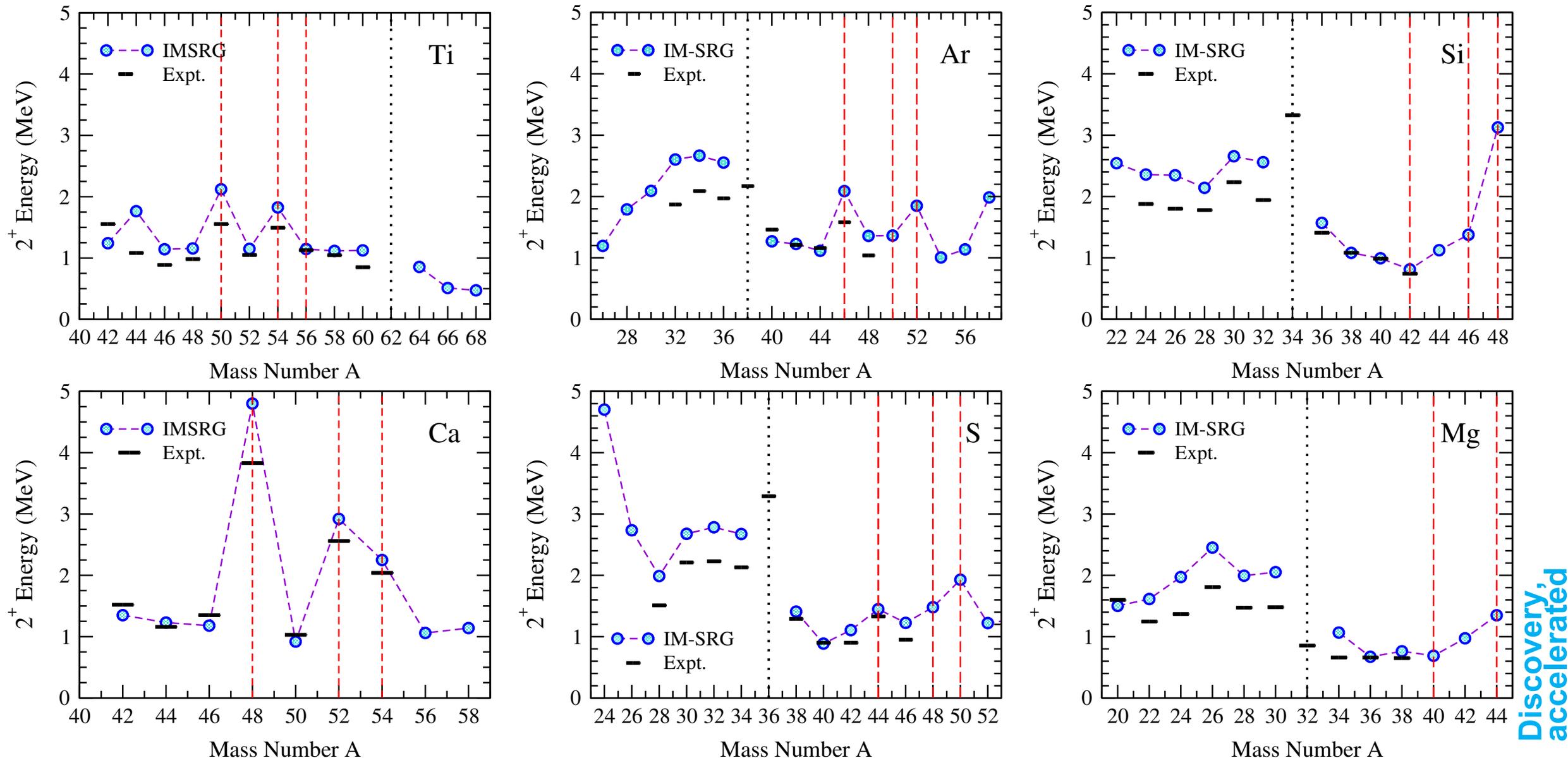
Probe “dawning” of N=32 magic number

### Ab Initio from NN+3N

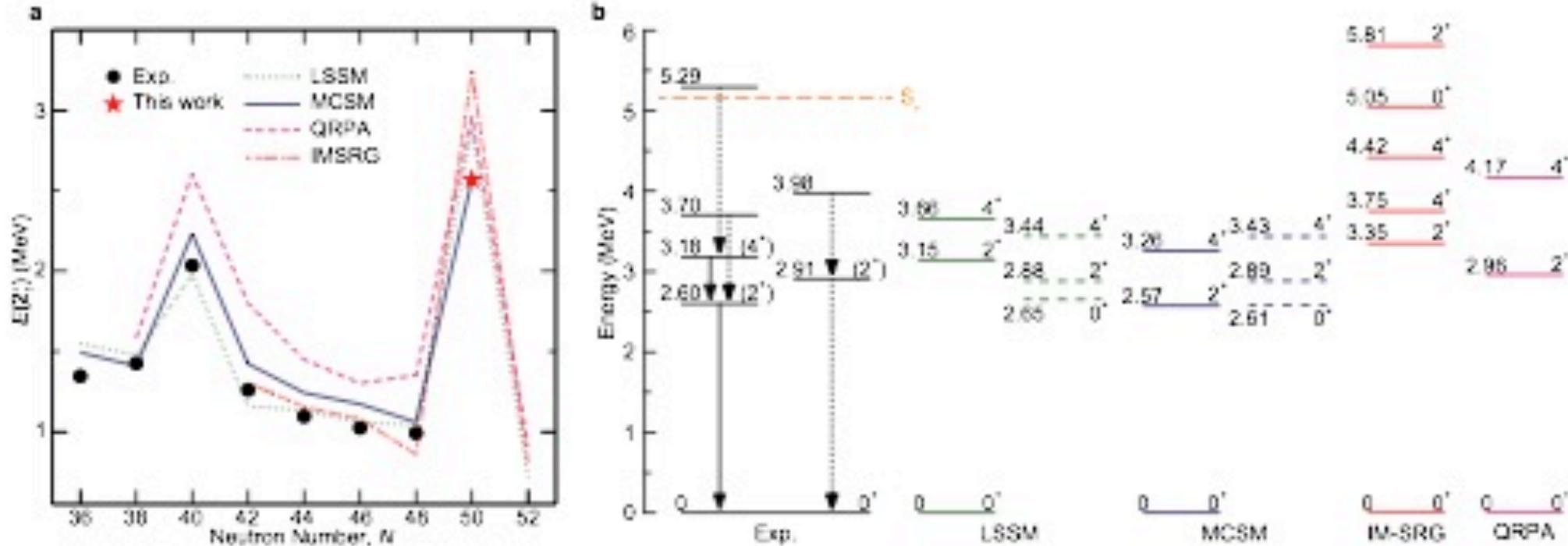
Generally good agreement, but predicts appearance too early

**Future: Evolution to be measured in Ar, Cl**

Ab initio predictions from above calcium towards oxygen – **persistence of N=34**



New measurement at RIKEN  $2^+$  energy in  $^{78}\text{Ni}$  – clear peak compared to  $^{76}\text{Ni}$

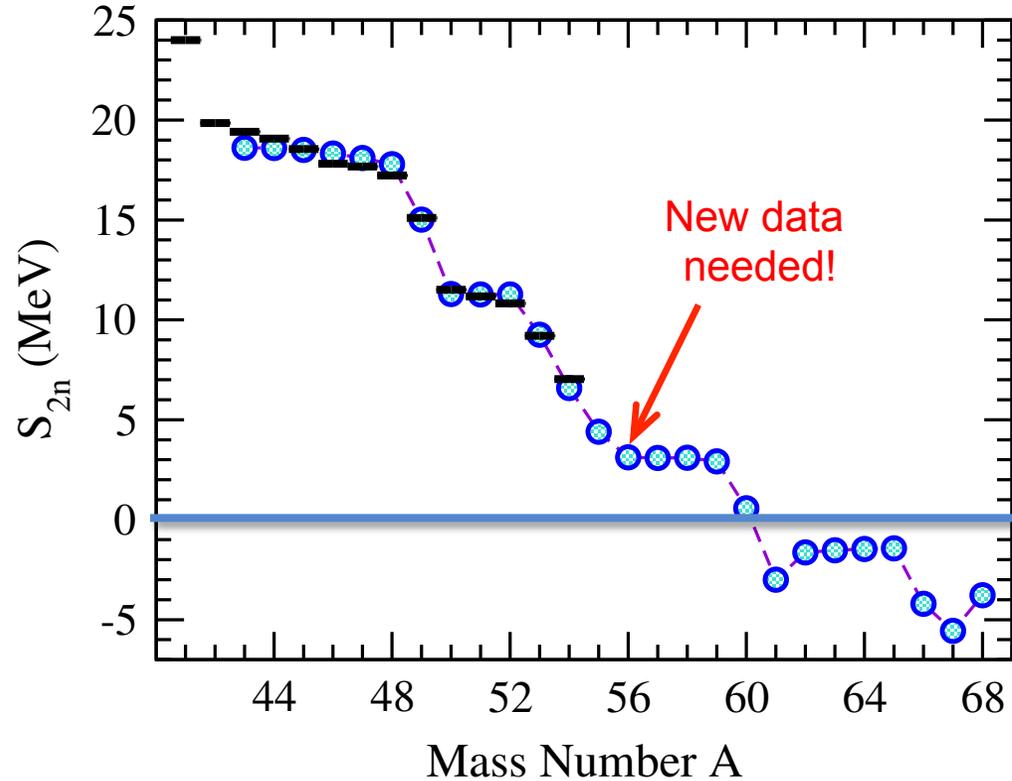


Peak wrt neighboring systems well predicted by IMSRG (also phenomenology)

**First evidence for the (double) magicity of  $^{78}\text{Ni}$ !**

**2013-2018** impressive series of experiments; ideal example of theory/exp overlap

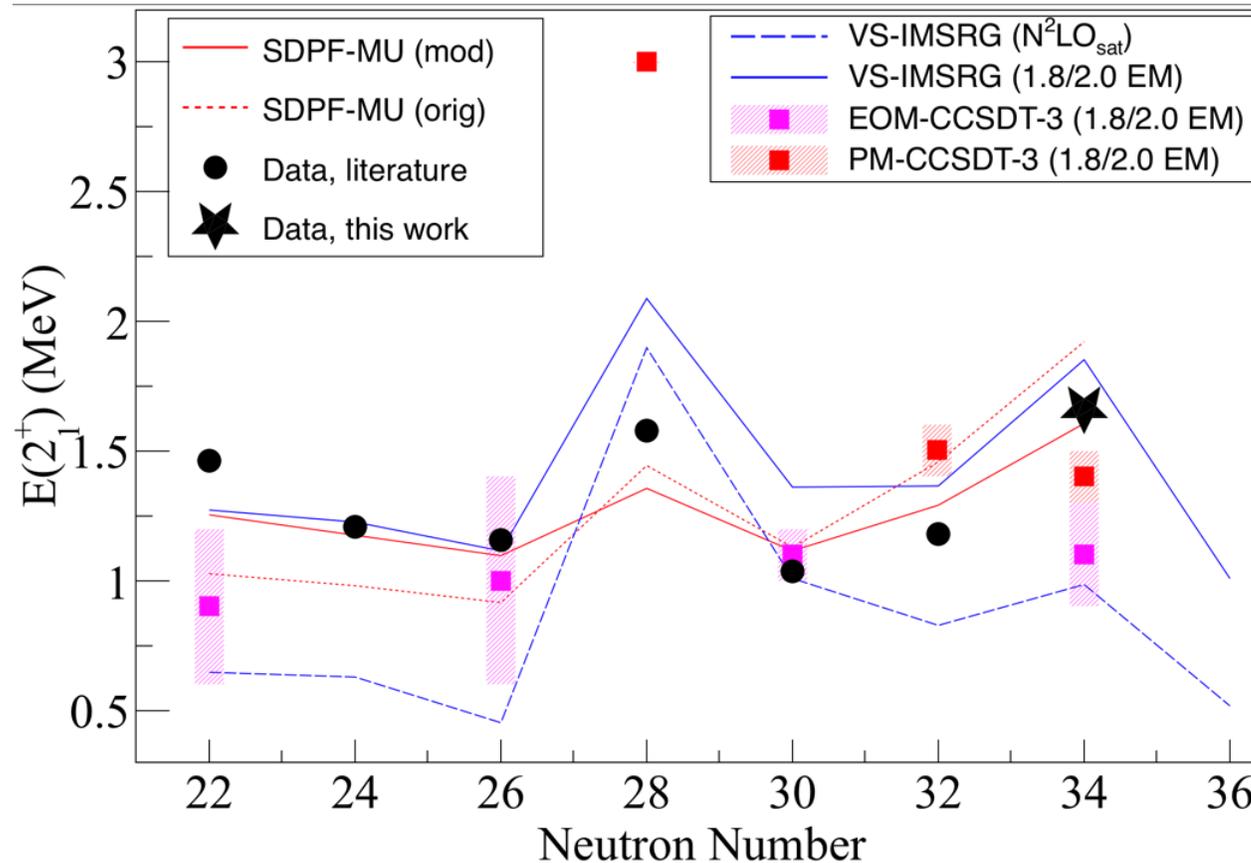
Story continues at ???



**2017:**

**Updated ab initio theory predicts shell closure**

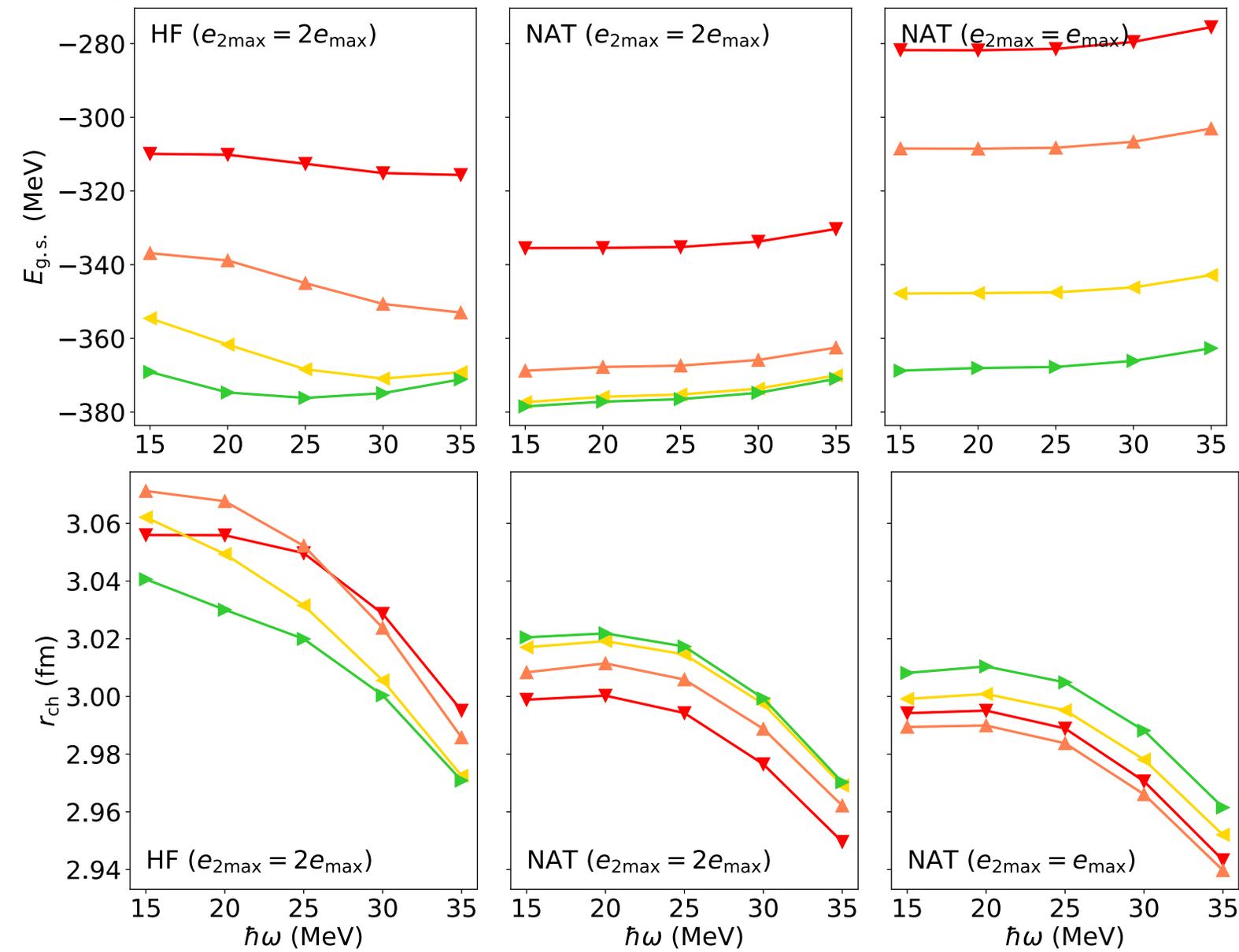
**New measurement at RIKEN:**  $2^+$  energy in  $^{52}\text{Ar}$  – clear peak at N=34



Agreement with IMSRG and other ab initio predictions (coupled cluster theory)

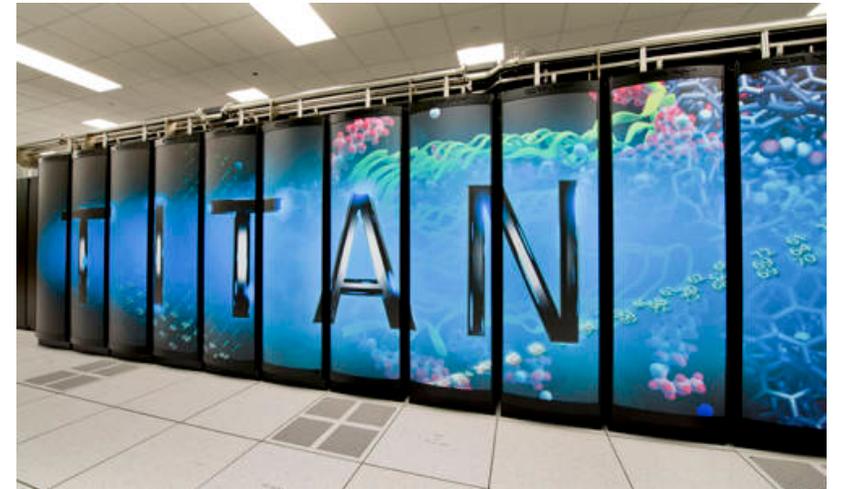
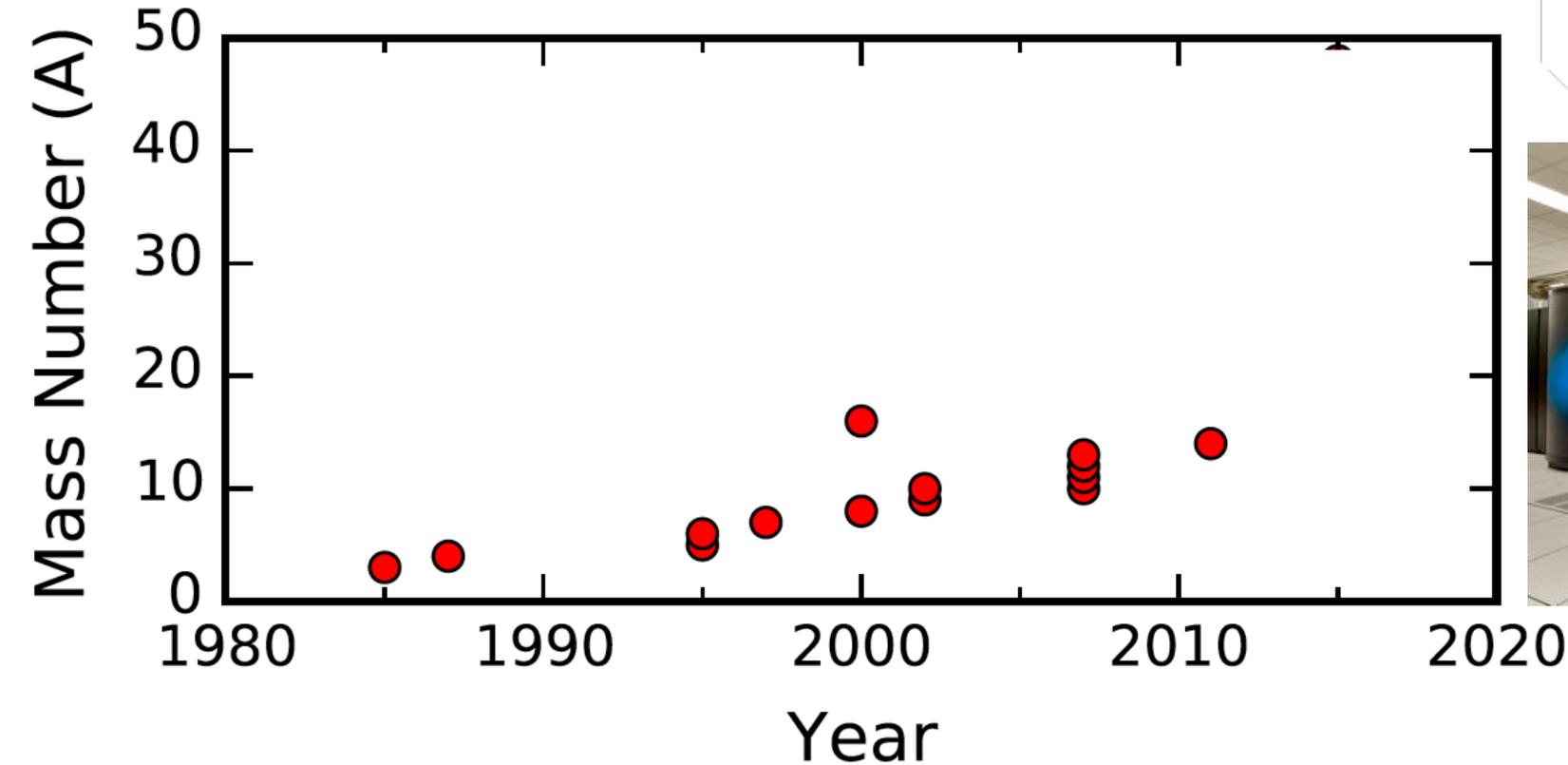
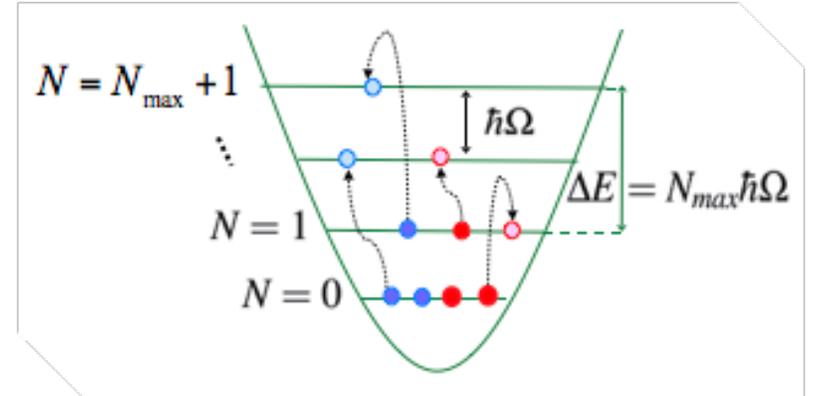
**First evidence for persistence of N=34 magic number away from calcium!**

They work! Next, test in VS formulation...



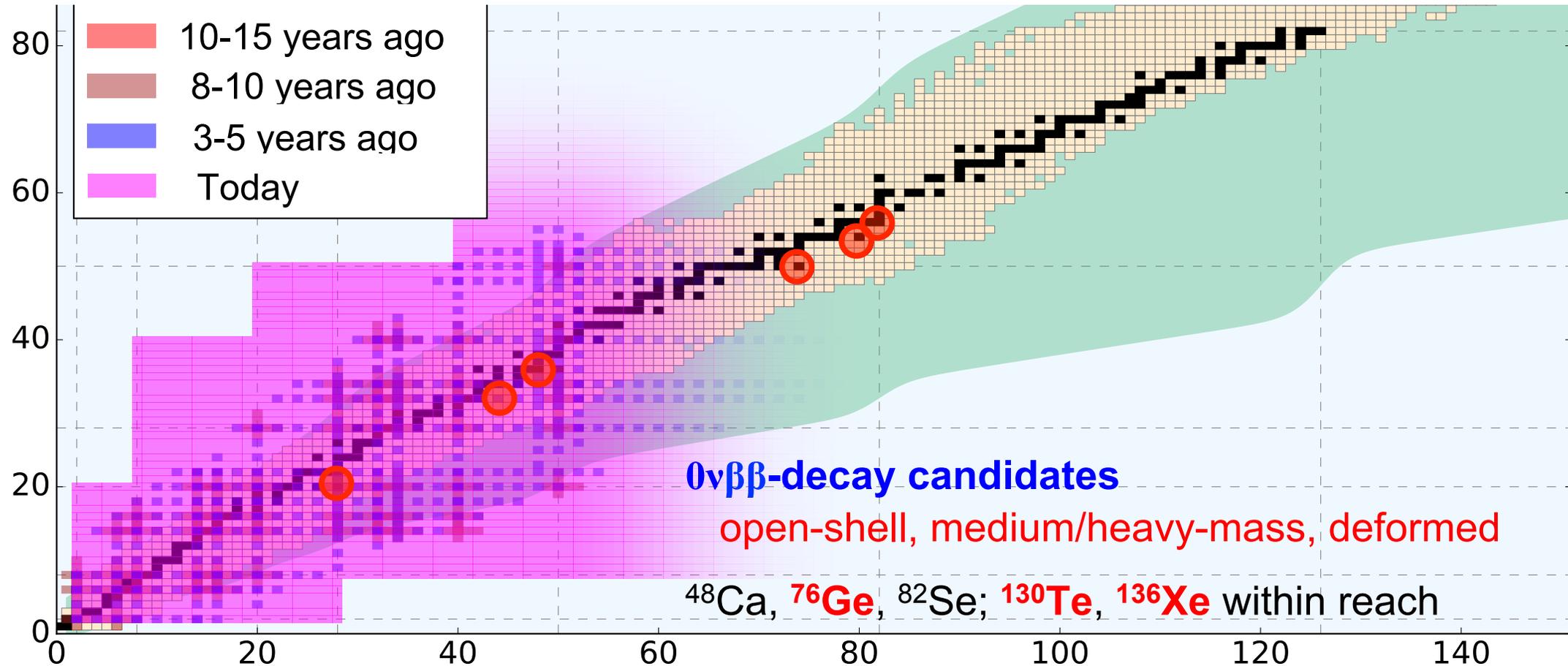
Moore's law: exponential growth in computing power

Methods for light nuclei (QMC, NCSM) scale exponentially with mass

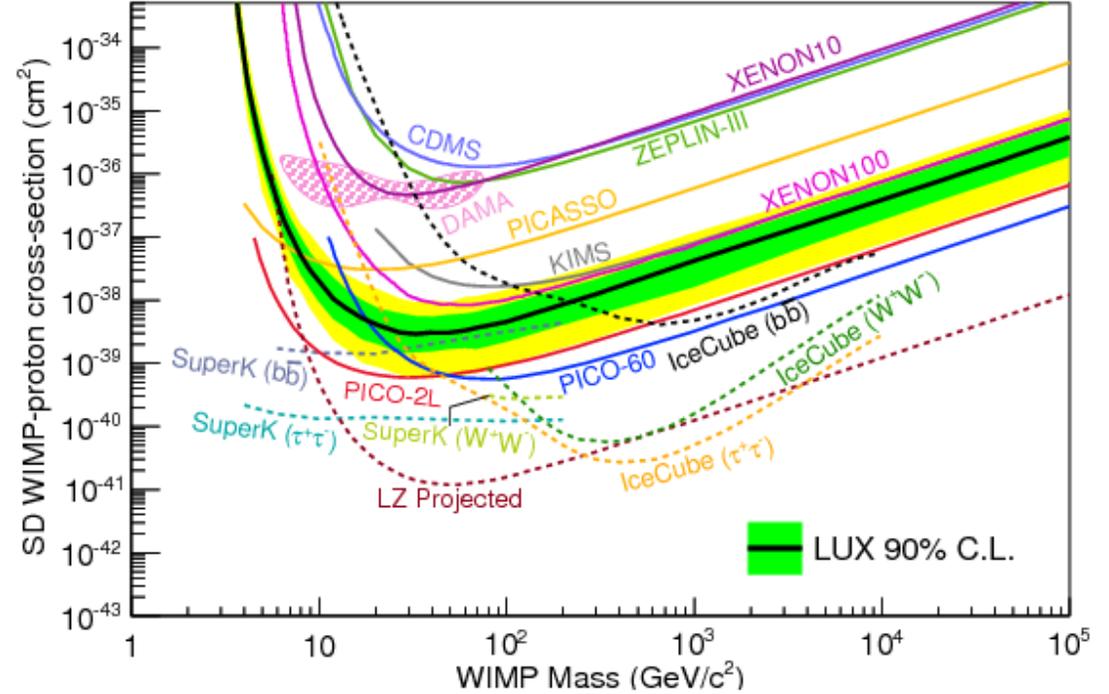
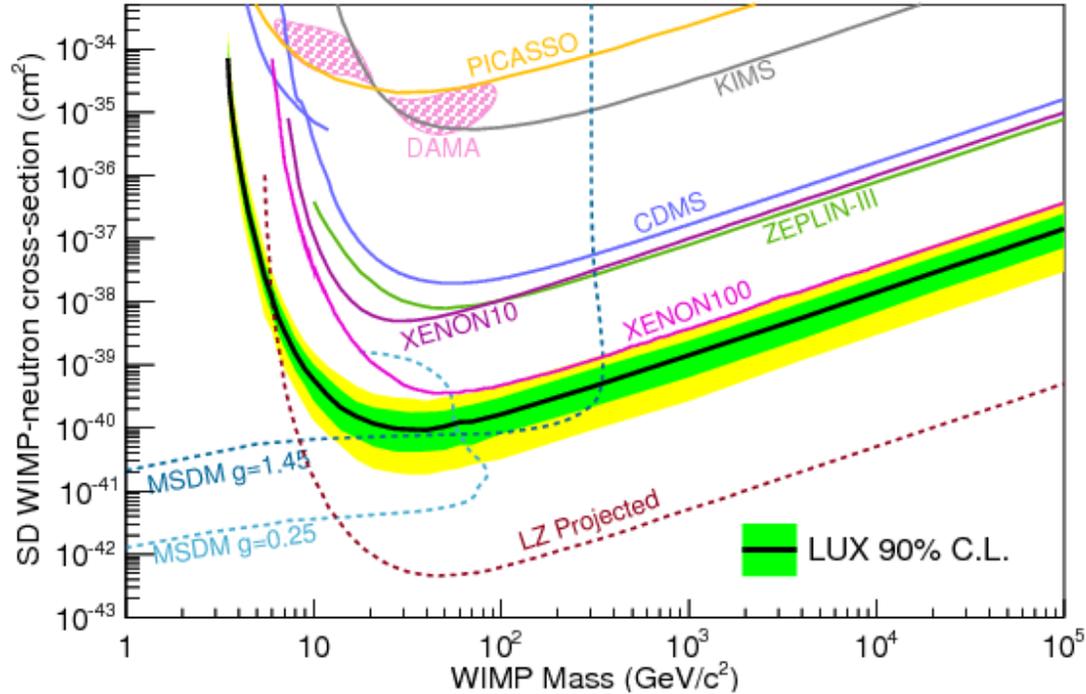


**Aim of modern nuclear theory:** Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- Nuclear many-body problem



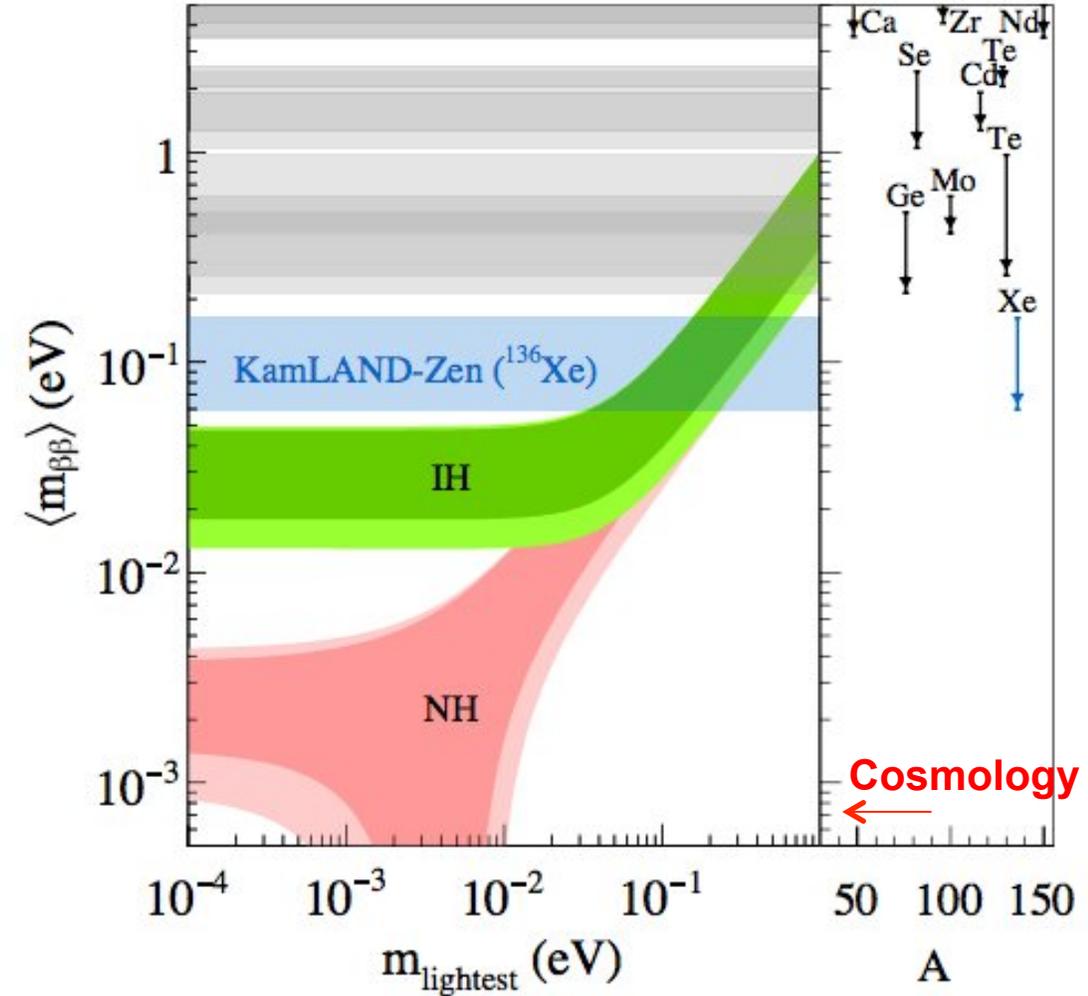
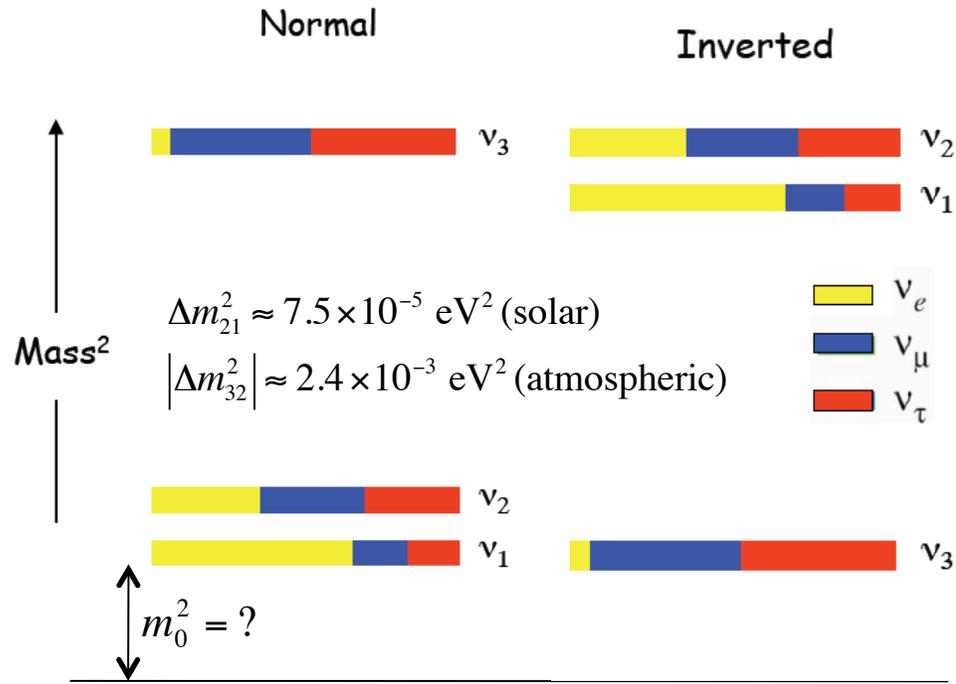
Exclusion plots for WIMP-nucleon total cross section: spin-dependent (axial) currents



Differential cross section: compare results from different target nuclei

$$\frac{d\sigma}{dp^2} = \frac{8G_F^2}{(2J_i + 1)v^2} S_A(p)$$

Progress in large-scale searches pushing towards **IH**



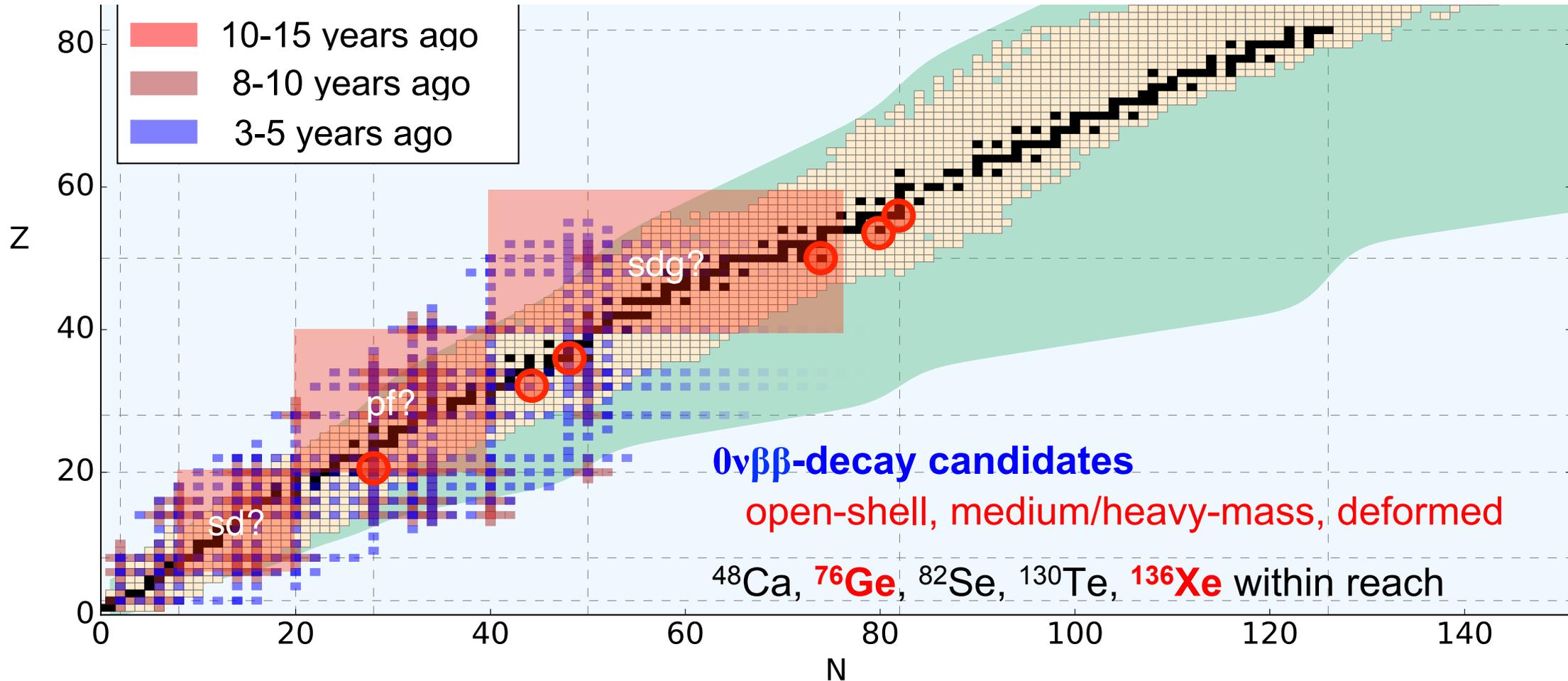
$$\left(T_{1/2}^{0\nu\beta\beta}\right)^{-1} = G^{0\nu} \left(M^{0\nu}\right)^2 \langle m_{\beta\beta} \rangle^2 \quad \langle m_{\beta\beta} \rangle = \left| \sum_{i=1}^3 U_{ei} m_i \right|$$

Uncertainty from **Nuclear Matrix Element**; bands do not represent rigorous uncertainties

Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

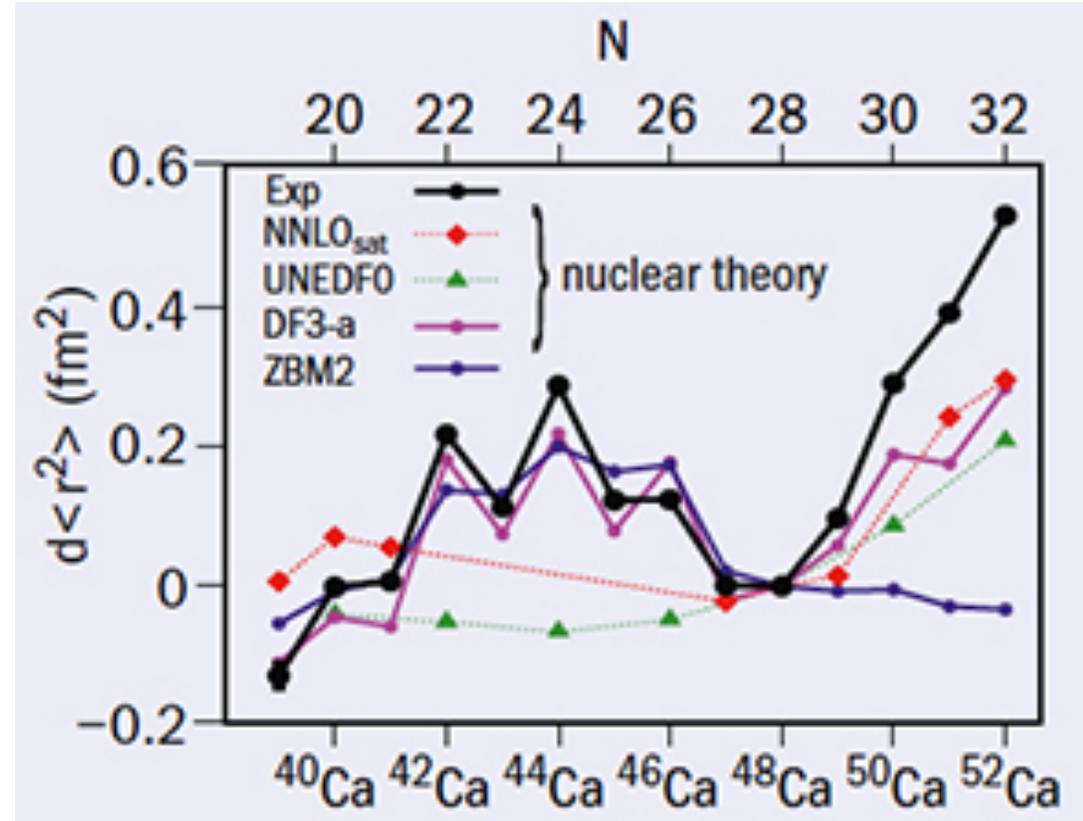
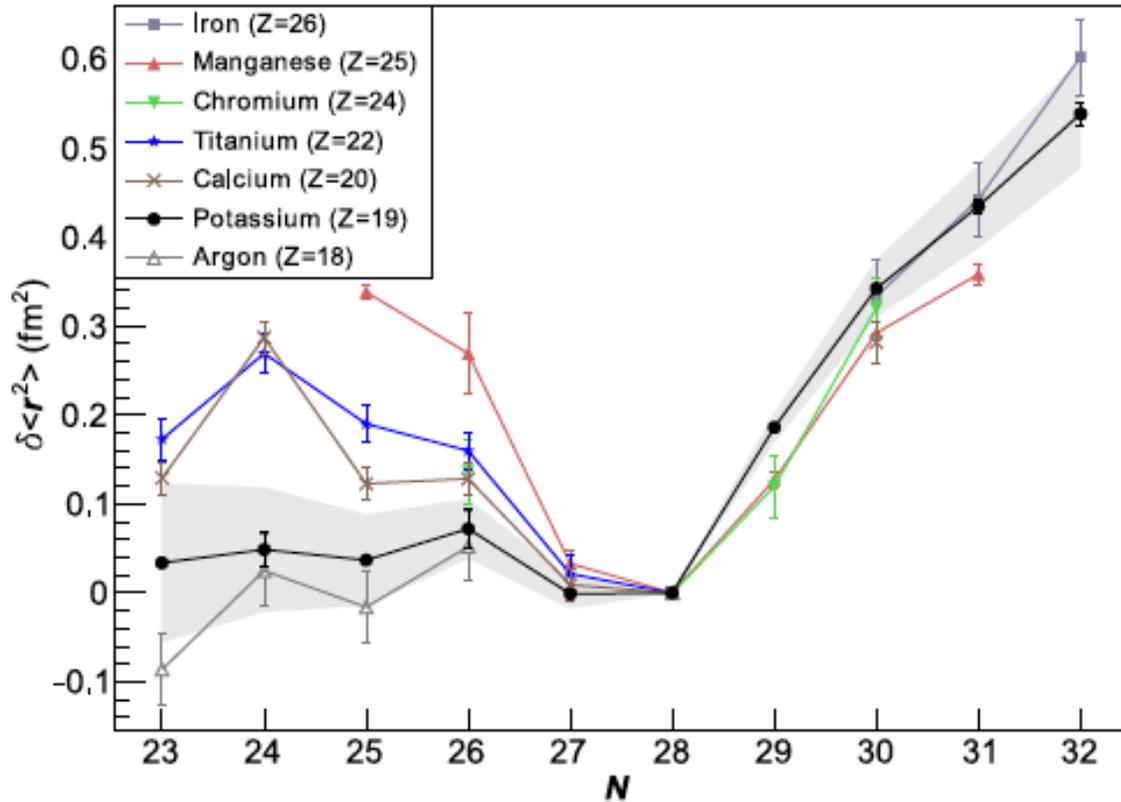
- Nuclear forces, electroweak physics
- **Nuclear many-body problem**

$$H\psi_n = E_n\psi_n$$



Charge radii of  $^{49,51,52}\text{Ca}$ , obtained from laser spectroscopy experiments at COLLAPS, CERN

**Unexpected large increase in charge radius questions the magicity of  $^{52}\text{Ca}$**



Theoretical models all underestimate the charge radius

Ab-initio calculations reproduce the trend of charge radii

“The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. **Thus one hopes to obtain knowledge of the nuclear forces.** If the forces are known, one should, in principle, **be able to calculate deductively the properties of individual nuclei.** **Only after this has been accomplished can one say that one completely understands nuclear structure...**

–*M. Goeppert-Mayer, Nobel Lecture*



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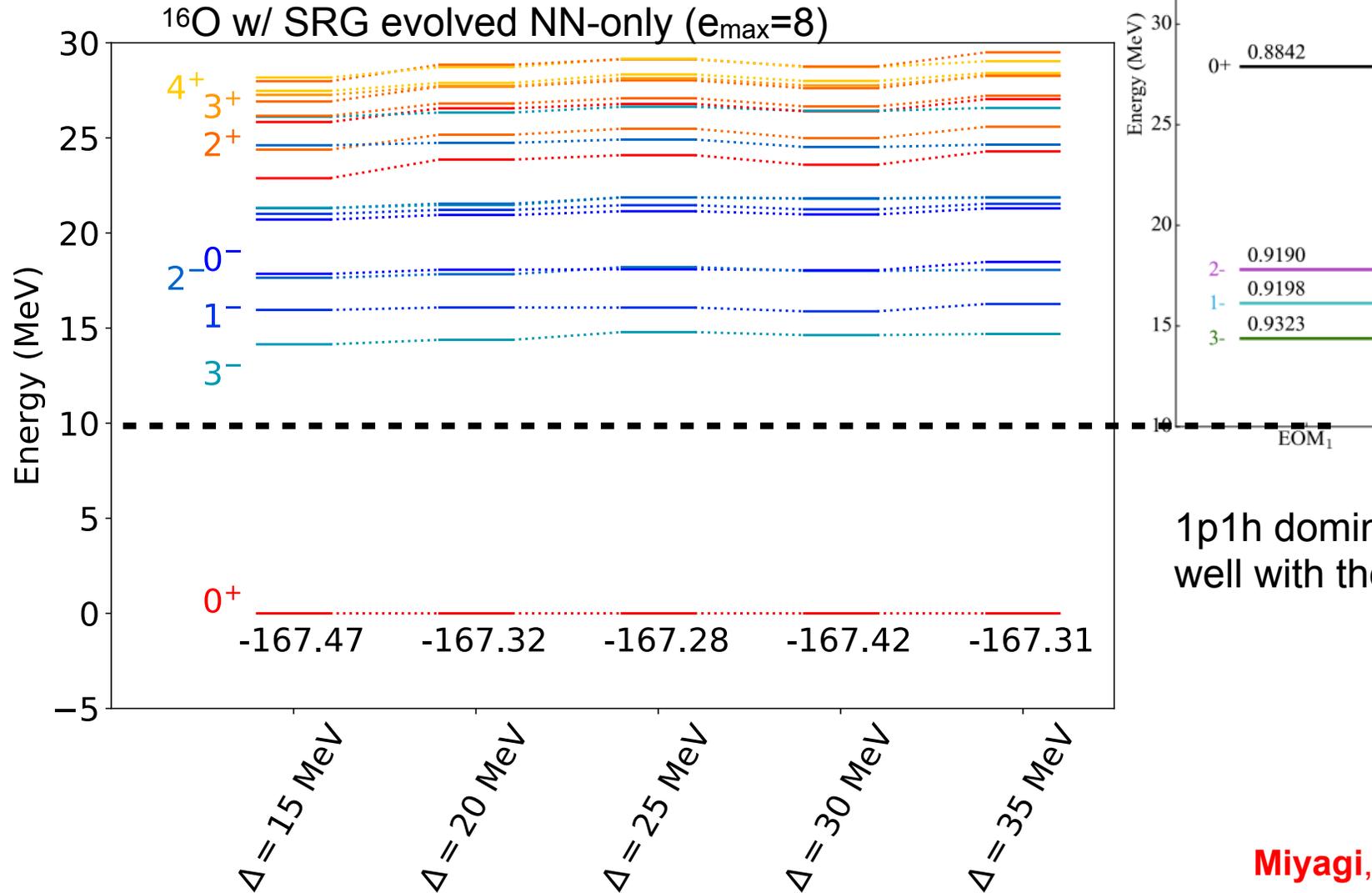
–*M. Goepfert-Mayer, Nobel Lecture*

*Ab initio* approach vs. *phenomenological models*

To date, nuclear physics largely phenomenological



# Comparison with EOM method

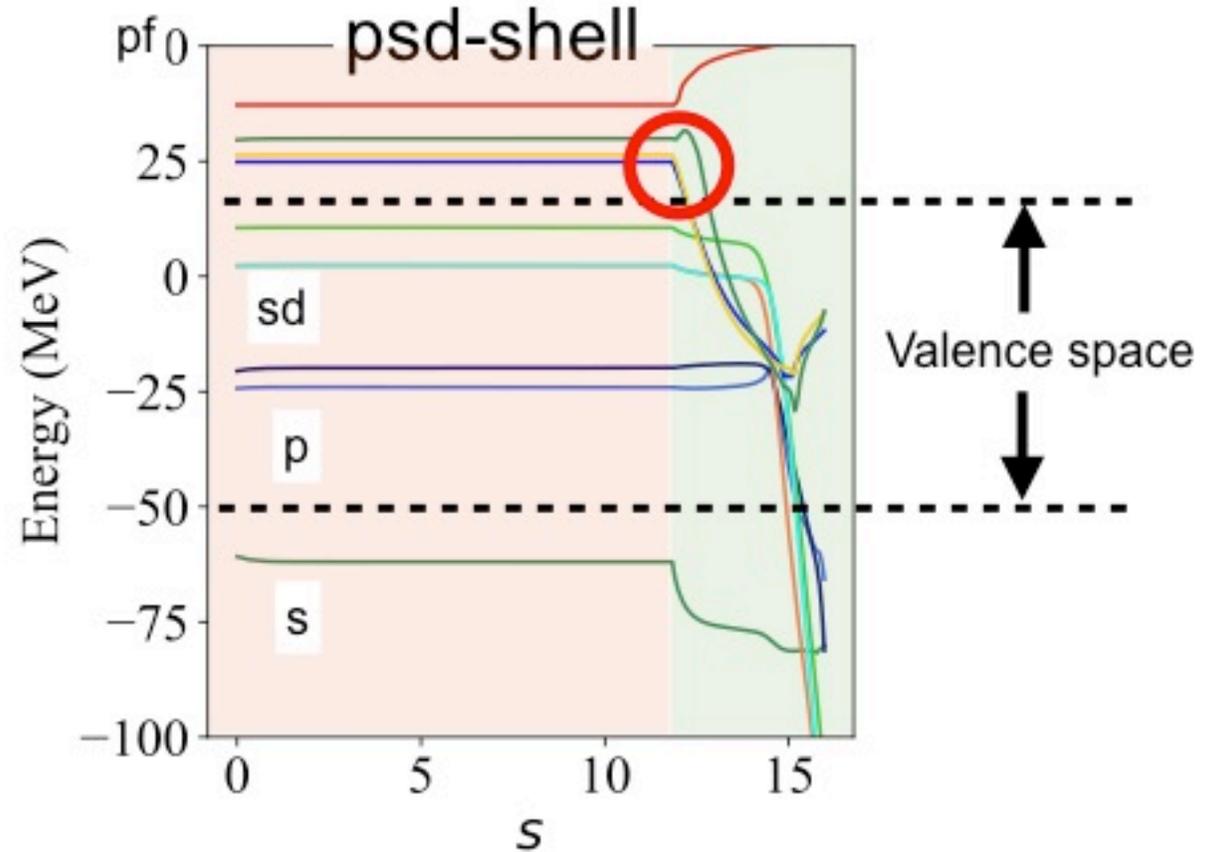


1p1h dominant lowest 3-, 1-, 2- agree well with the EOM-IMSRG results.

Miyagi, Stroberg, JDH... in prep

- Flow of single-particle energies

- At the very beginning of valence-decoupling flow, some of pf-shell orbits come down.
- Intuitively, we expect that P- and Q-space single particle energies do not mix.
- At the beginning of the flow, the slope of single-particle energies ( $df/ds$ ) seems to be crucial.



Moore's law: exponential growth in computing power

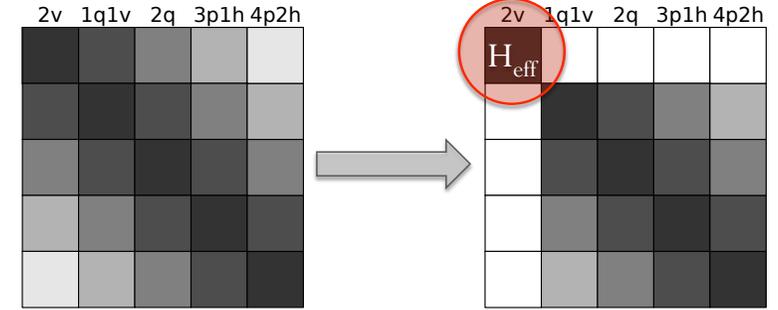
Methods for light nuclei (QMC, NCSM) scale exponentially with mass

Polynomial scaling methods developed (CC, IMSRG, SCGF...)

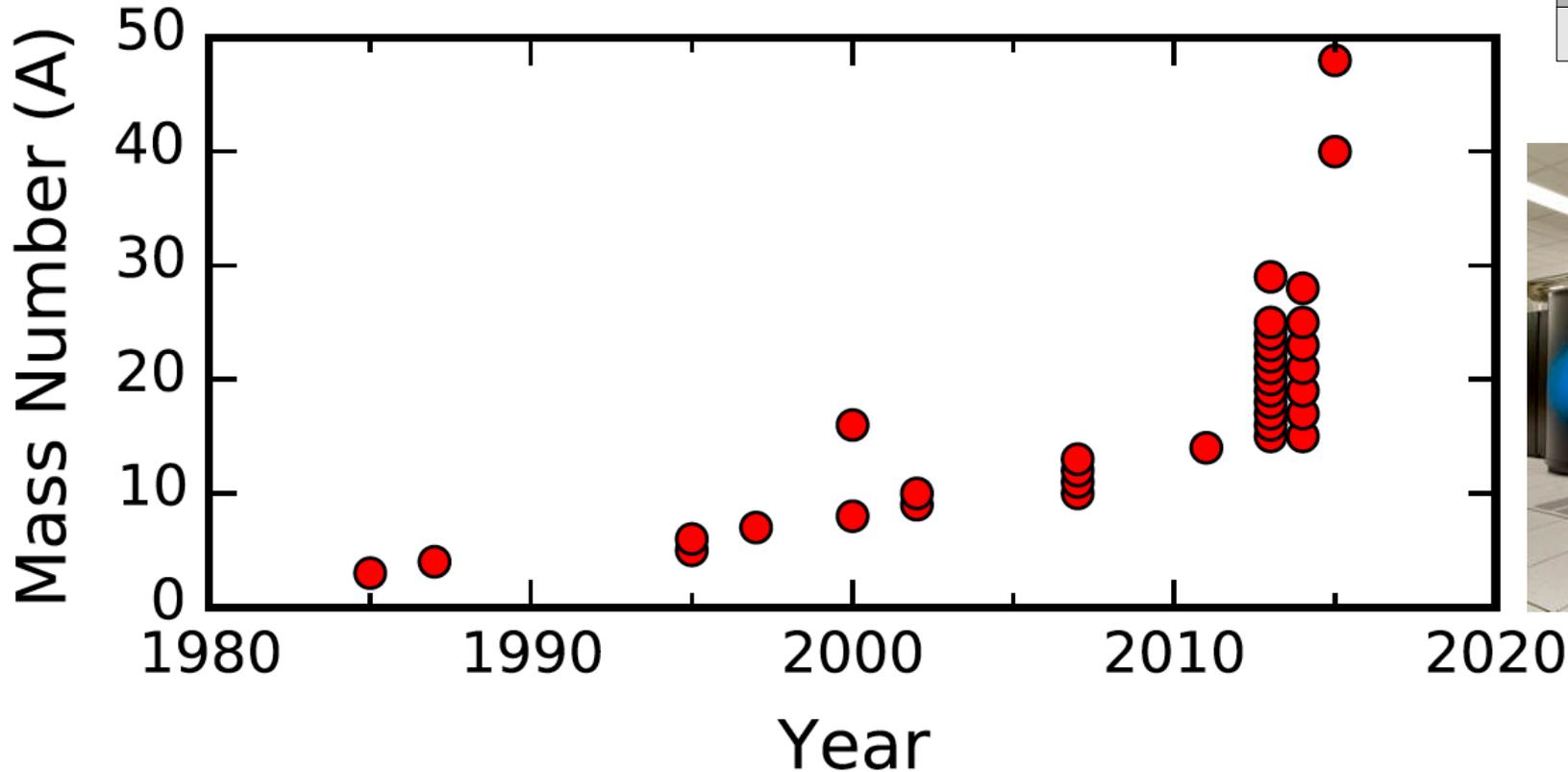
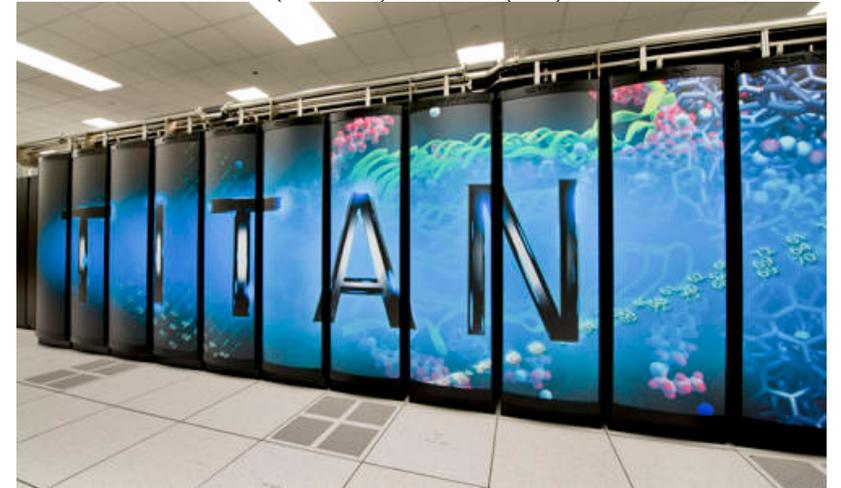
**Explosion in limits of ab initio theory**



**2019:  $A > 100$**

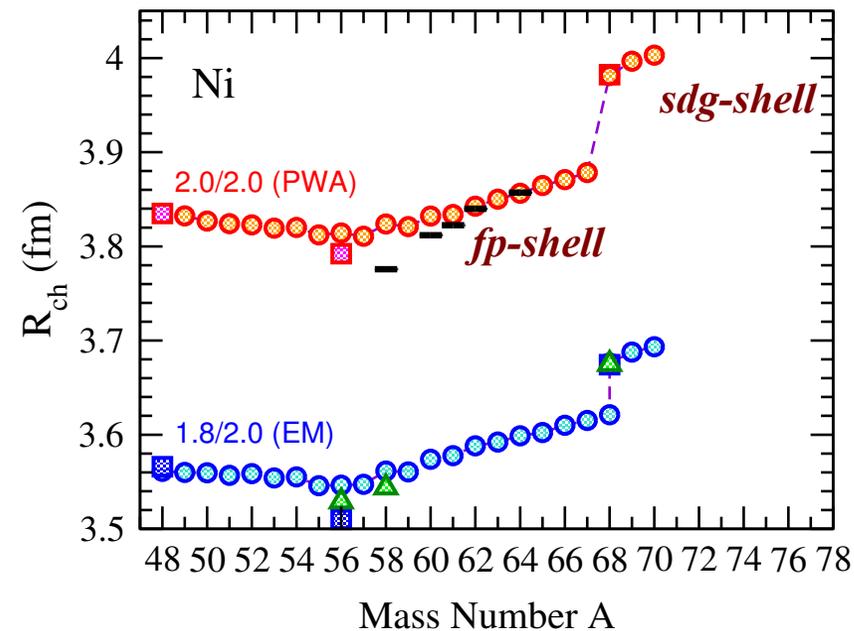
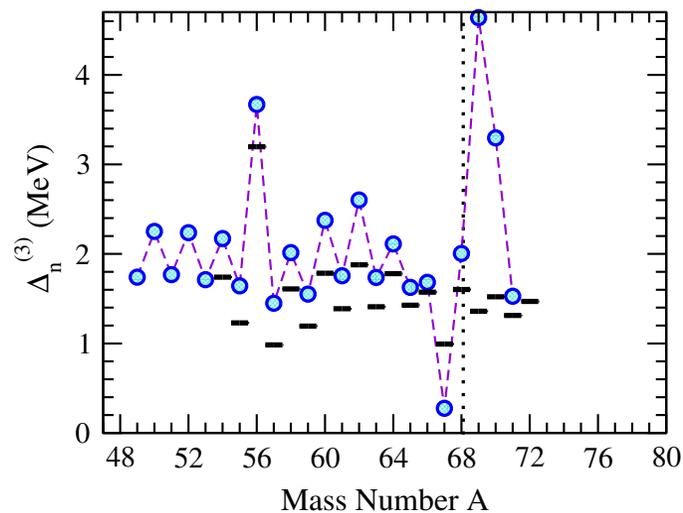
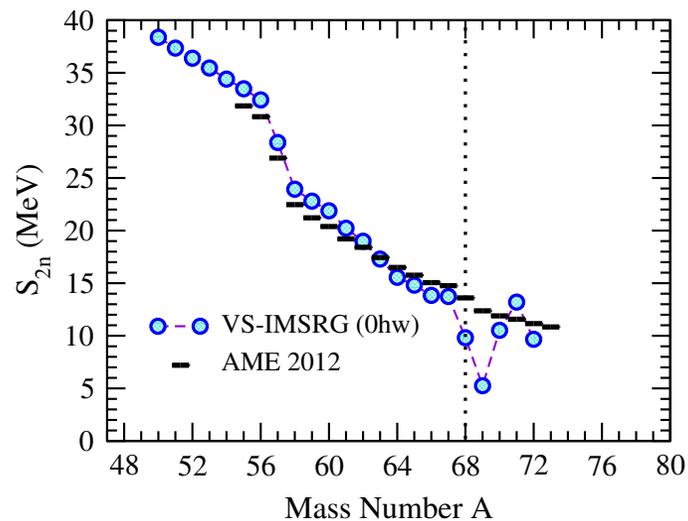
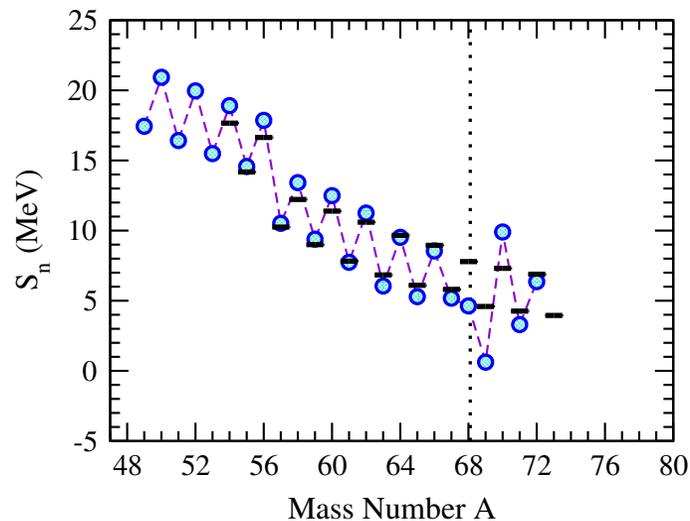
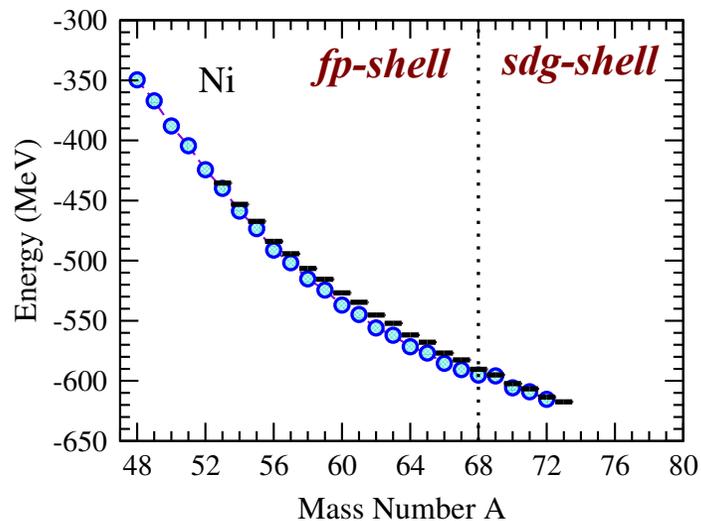


$$H(s=0) \rightarrow H(\infty)$$

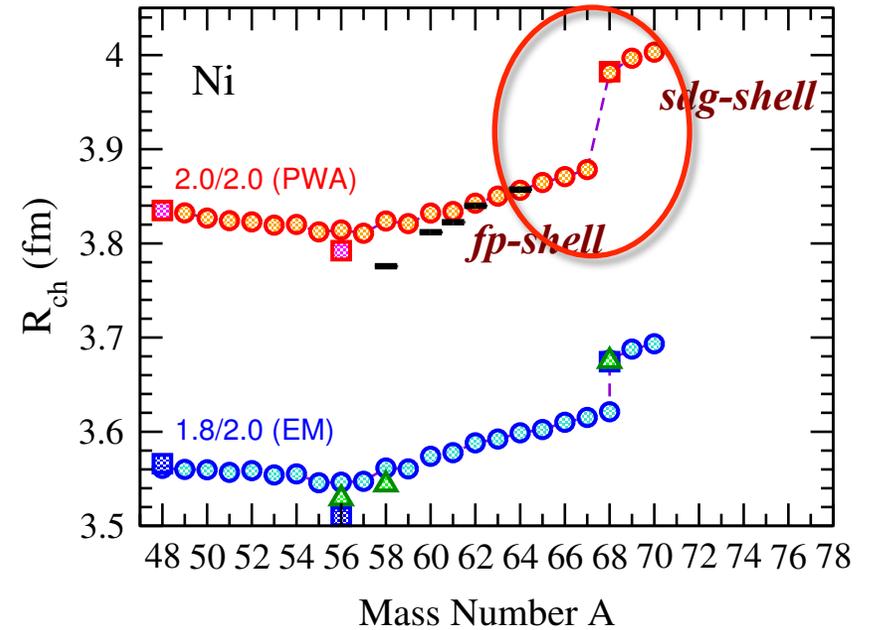
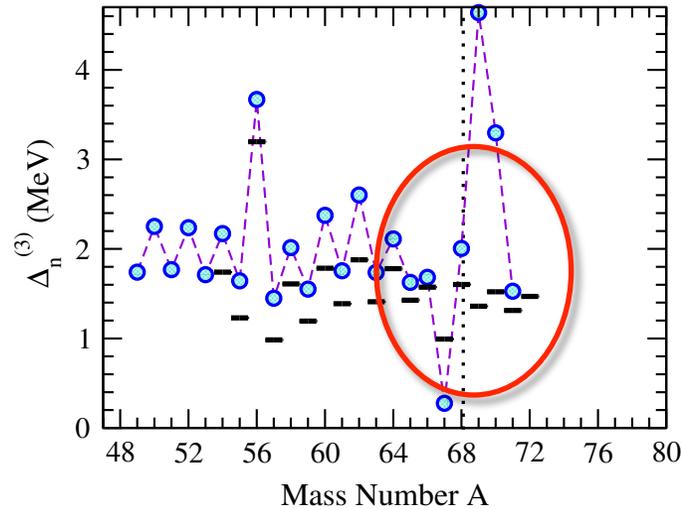
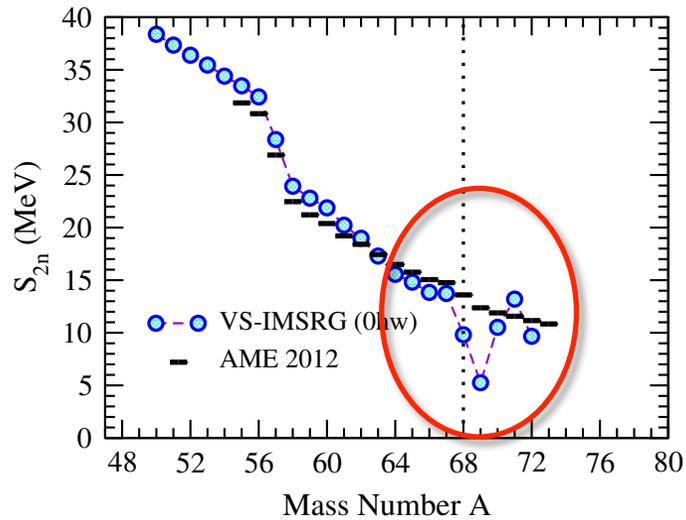
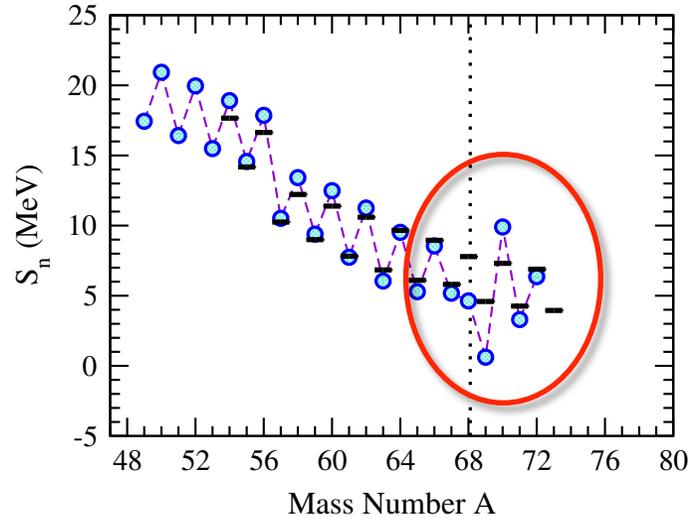
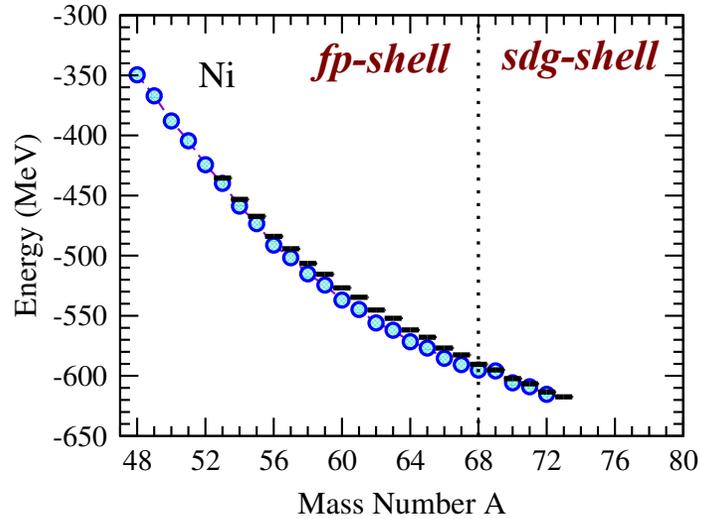




## Defect 1: Clear artifacts when changing valence spaces

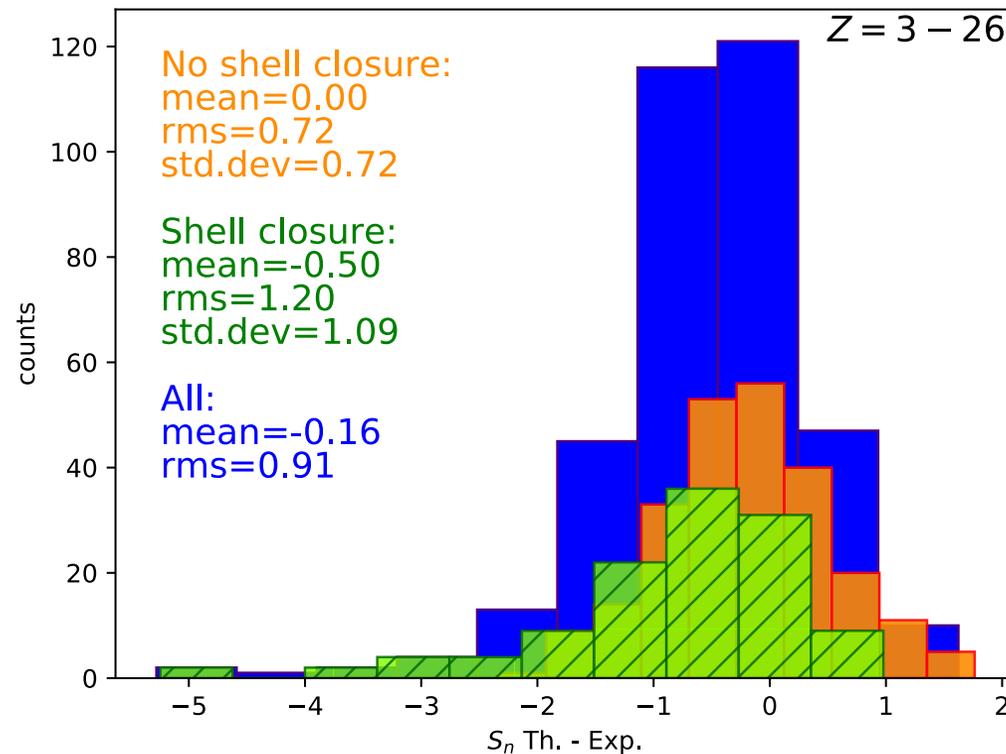
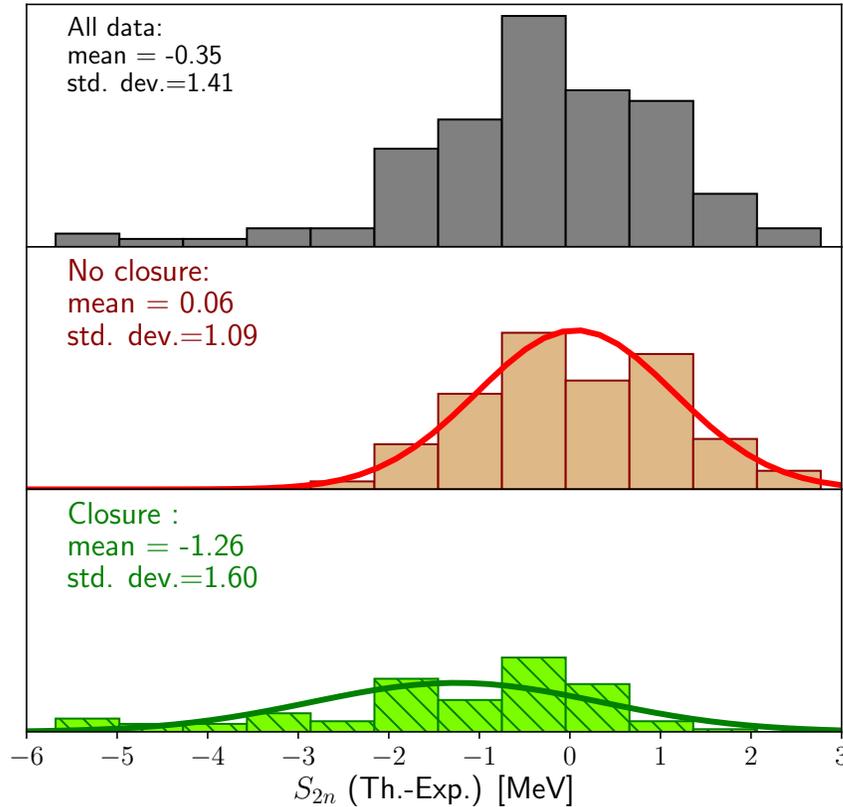


## Defect 1: Clear artifacts when changing valence spaces



Potential errors at shell closures from changing valence spaces

Differentiate between “closure” and “no closure” cases



$$\delta \mathcal{O} \equiv \mathcal{O}^{(th)} - \mathcal{O}^{(exp)}$$

JDH, Stroberg, Schwenk, Simonis,  
arXiv:1905.10475

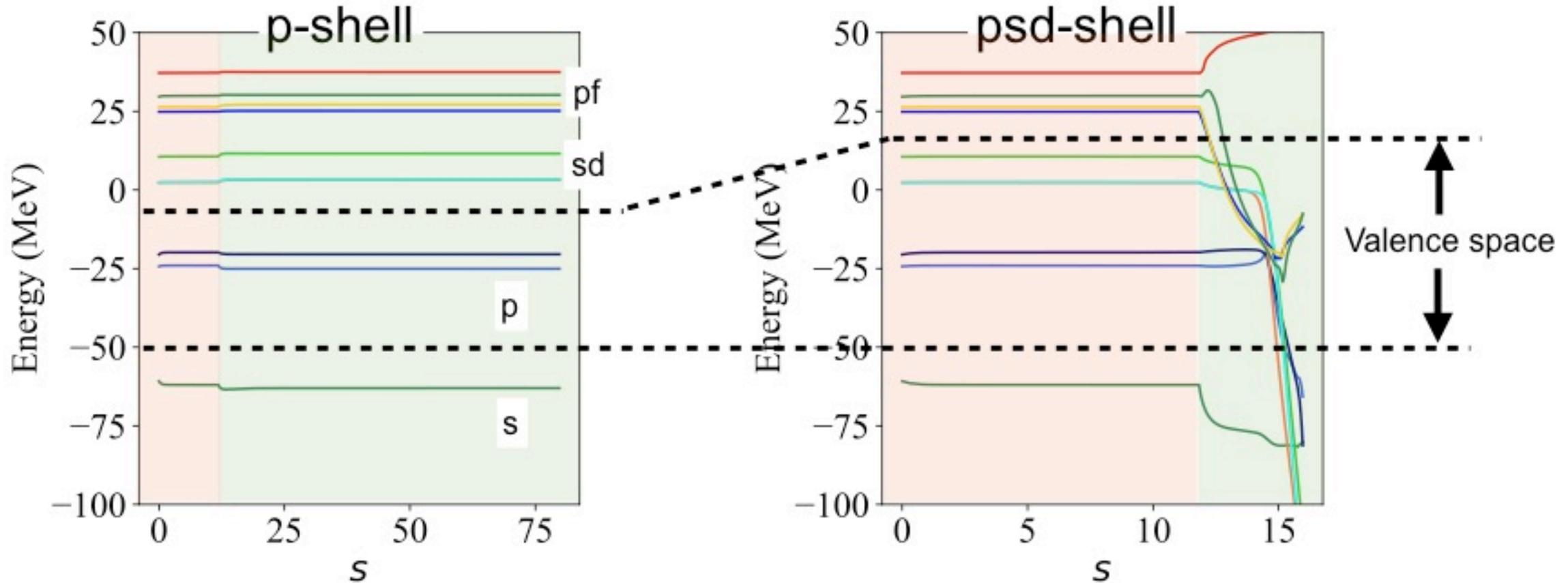
**Distributions approximately Gaussian**

Non closed shells approximately centered at 0; rms approximately 1MeV

Essential for many applications: island of inversion, forbidden transitions, heavier beta decay cases

**IMSRG typically fails!**

- Flow of single-particle energies



Proposed fix: modify generator to give constant shift to energy denominator

**Never have negative energy denominators if on order of hw...**

K. Suzuki, Prog. Theor. Phys. **58**, 1064 (1977).

N. Tsunoda, K. Takayanagi, M. Hjorth-Jensen, and T. Otsuka, Phys. Rev. C **89**, 024313 (2014).

$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212}}$$

$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234}}$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$



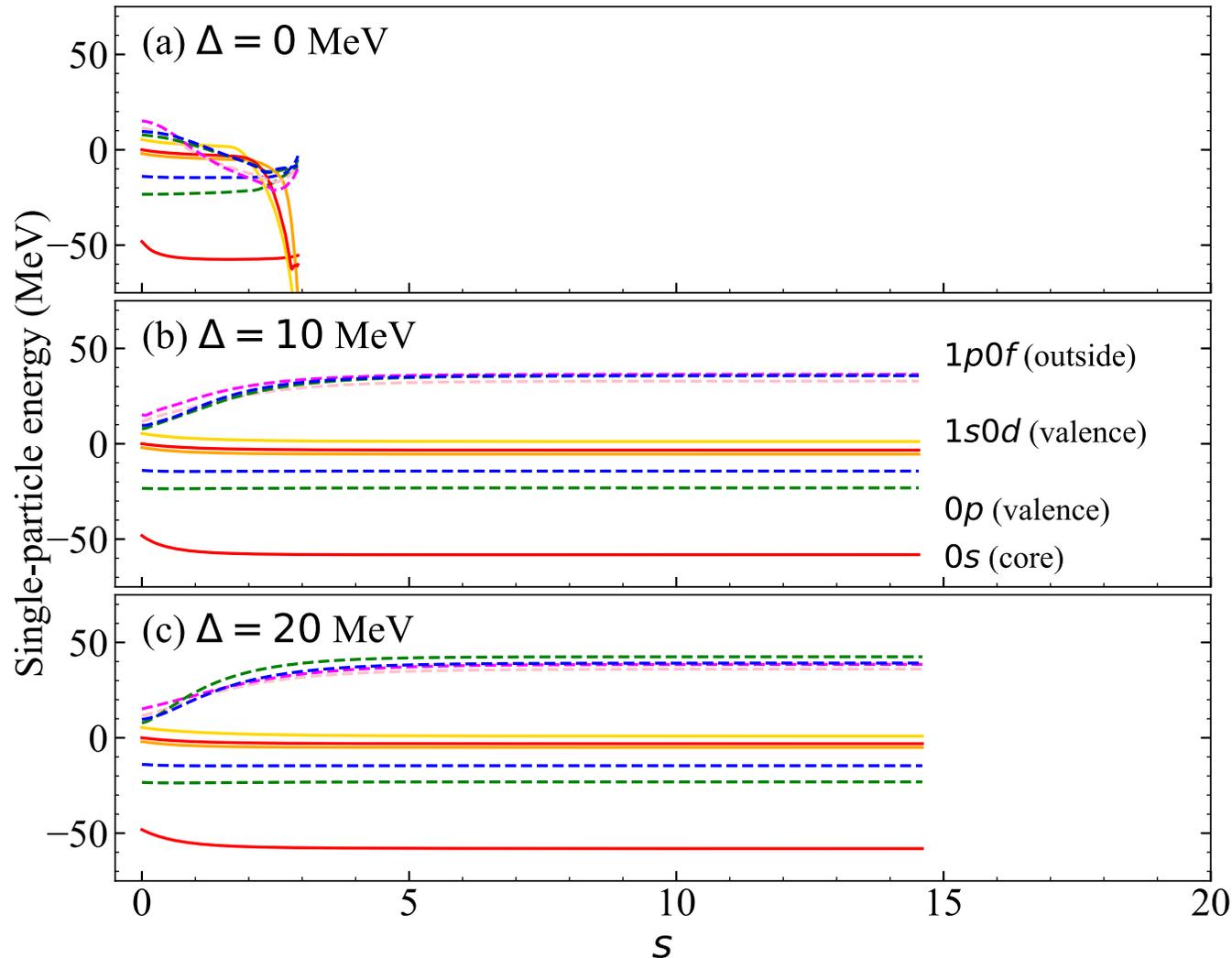
$$\eta_{12} = \frac{f_{12}}{f_{11} - f_{22} + \Gamma_{1212} + \Delta}$$

$$\eta_{1234} = \frac{\Gamma_{1234}}{f_{11} + f_{22} - f_{33} - f_{44} + A_{1234} + \Delta}$$

$$A_{1234} = \Gamma_{1212} + \Gamma_{3434} - \Gamma_{1313} - \Gamma_{2424} - \Gamma_{1414} - \Gamma_{2323}$$

Proposed fix: modify generator to give constant shift to energy denominator

**Never have negative energy denominators if on order of  $\hbar\omega$ ...**



“The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. **Thus one hopes to obtain knowledge of the nuclear forces.** If the forces are known, one should, in principle, **be able to calculate deductively the properties of individual nuclei.** **Only after this has been accomplished can one say that one completely understands nuclear structure...**

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*Ab initio* approach vs. *phenomenological models*

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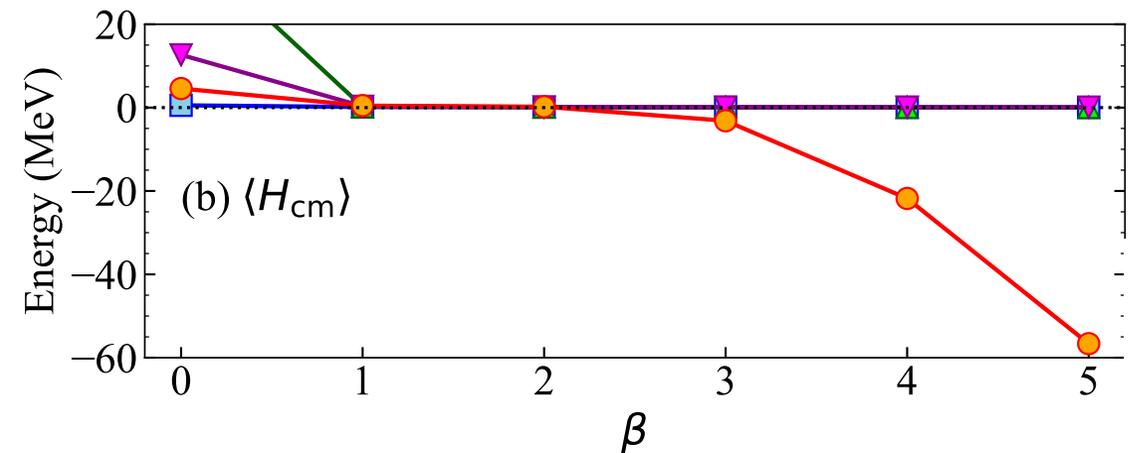
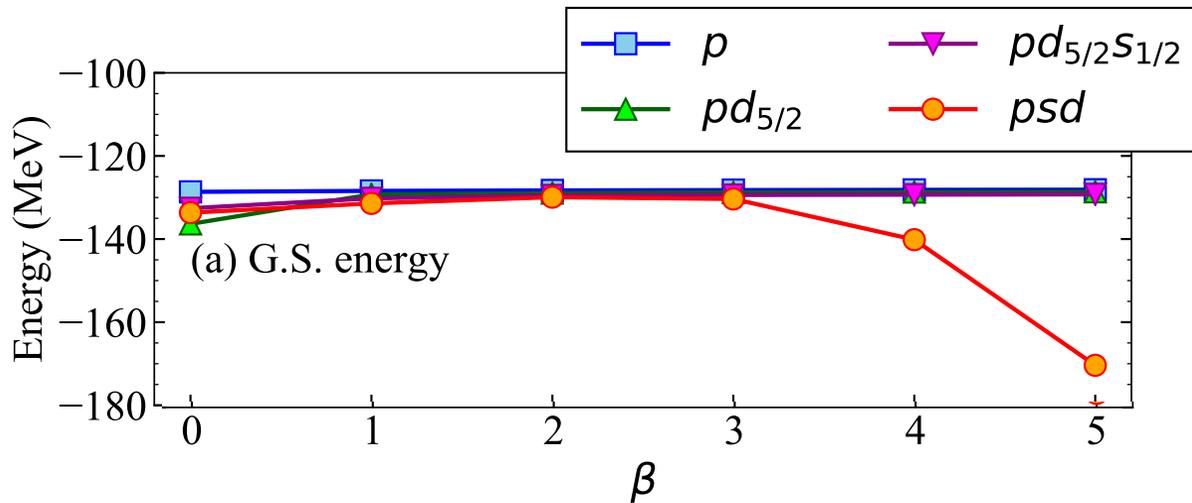


- So far, we added the center-of-mass Hamiltonian at the shell-model calculation stage:

$$H \longrightarrow H_{\text{VS}} + \beta H_{\text{cm}} \longrightarrow \text{energies}$$

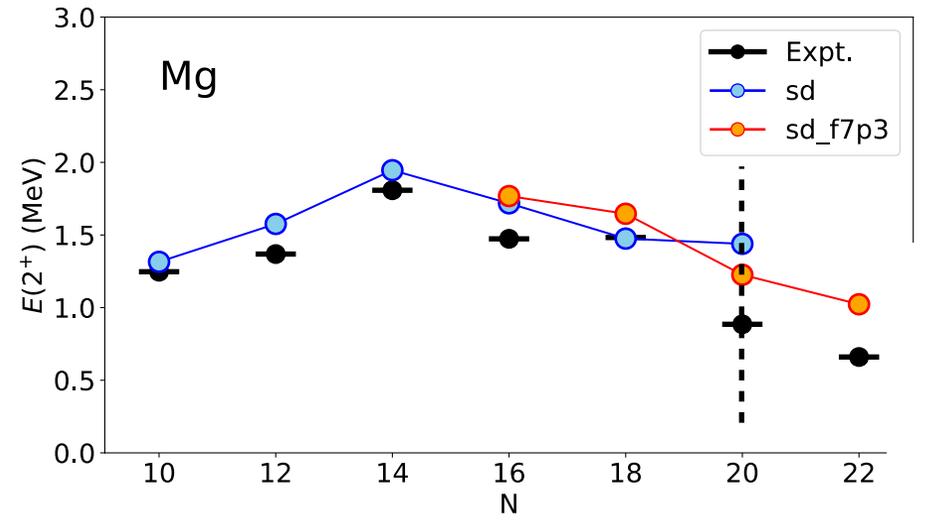
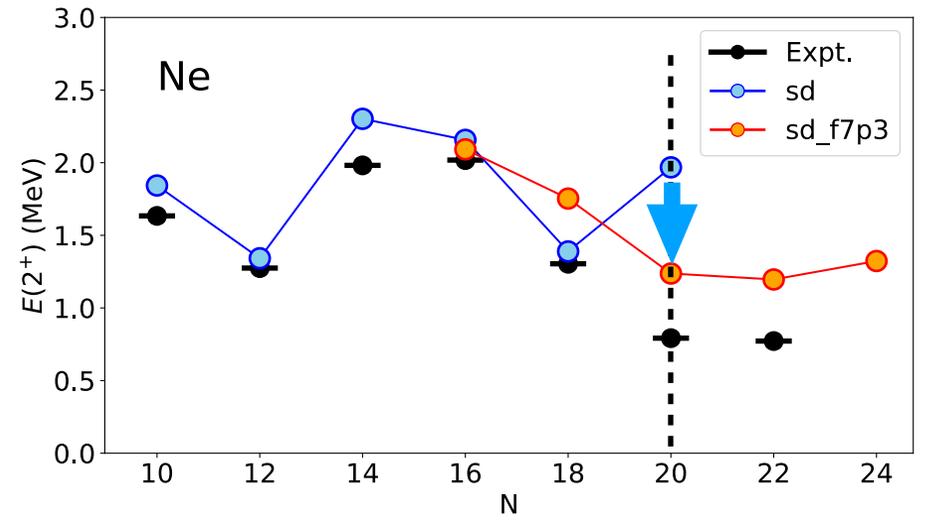
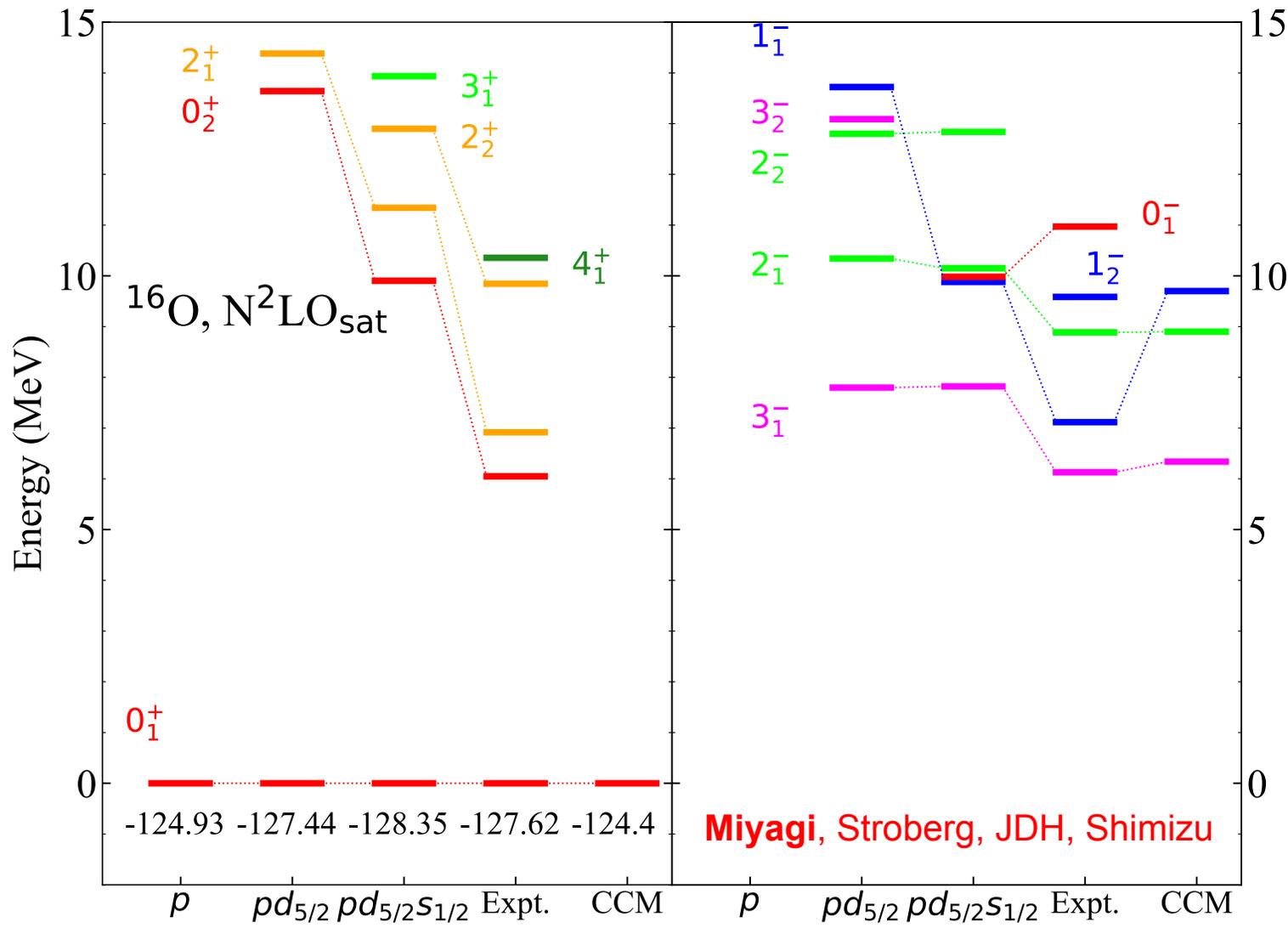
- But,  $H_{\text{VS}}$  is no longer represented in HO basis. We should add  $H_{\text{cm}}$  from the beginning:

$$H + \beta H_{\text{cm}} \longrightarrow H_{\text{VS}} \longrightarrow \text{energies}$$

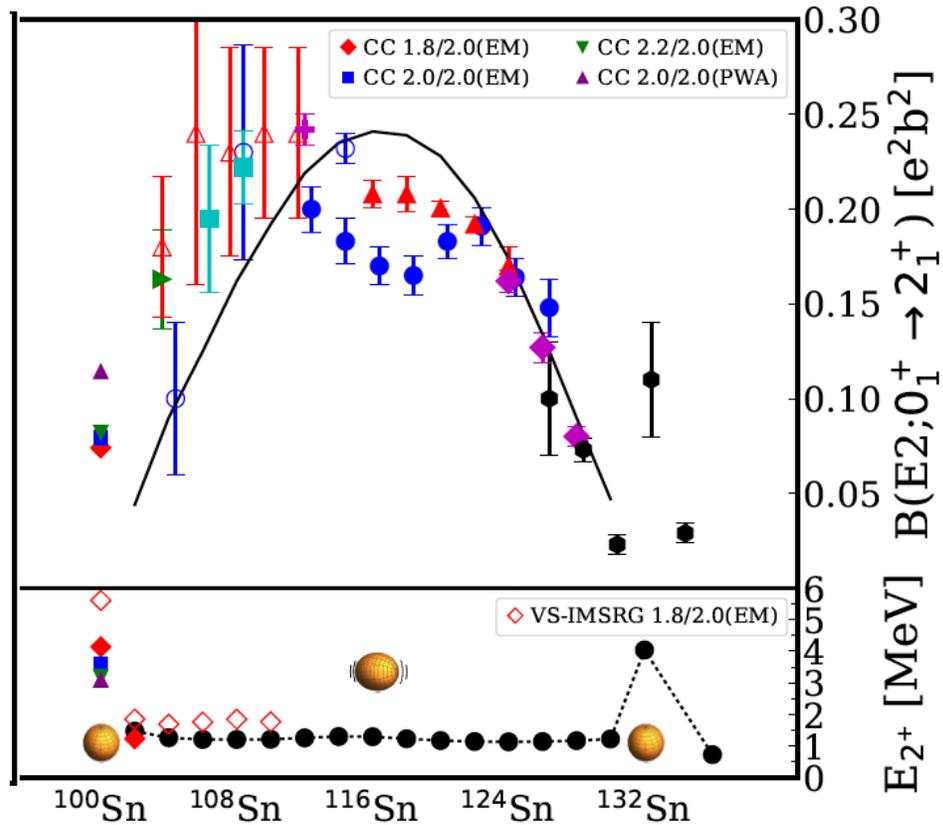


With selected orbitals, free of CoM contamination

## Excited states in $^{16}\text{O}$ , Island of Inversion

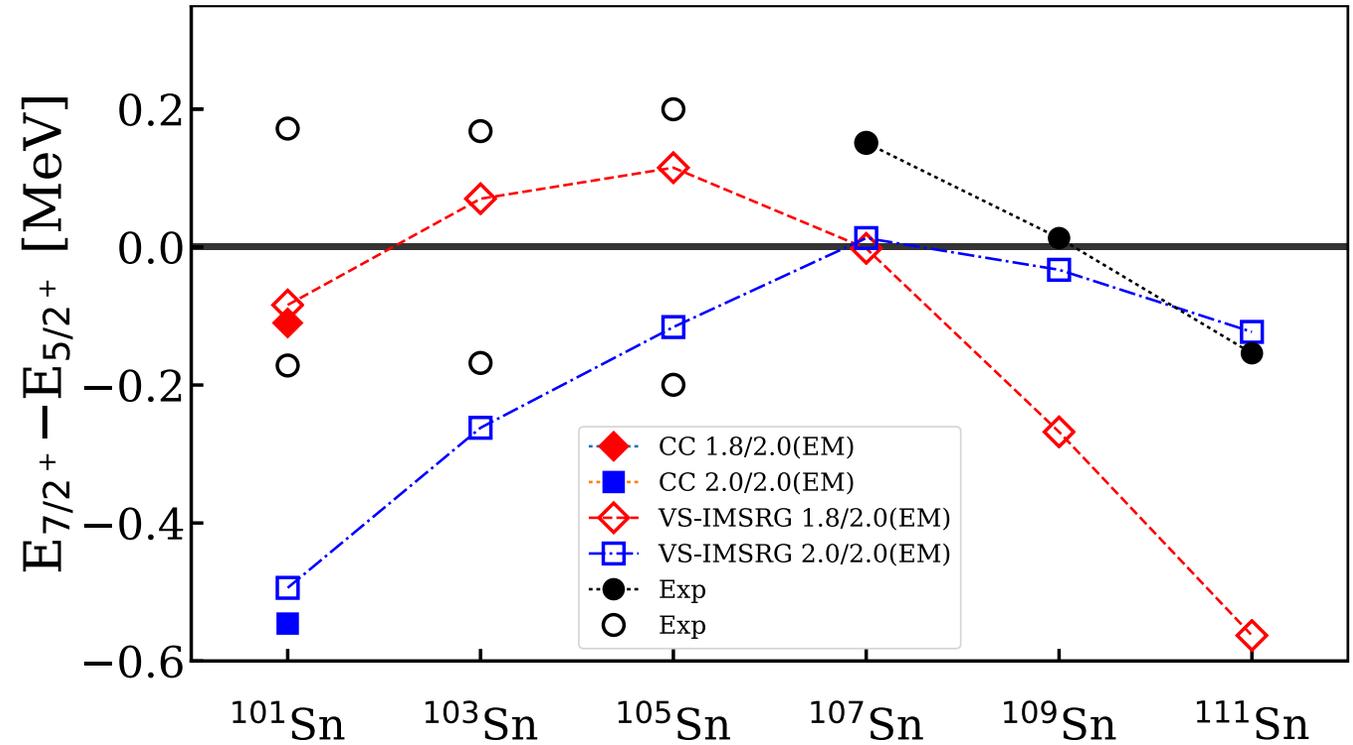


Extend ab initio to heavy-mass region: magicity of  $^{100}\text{Sn}$ , controversial level ordering in  $^{101}\text{Sn}$



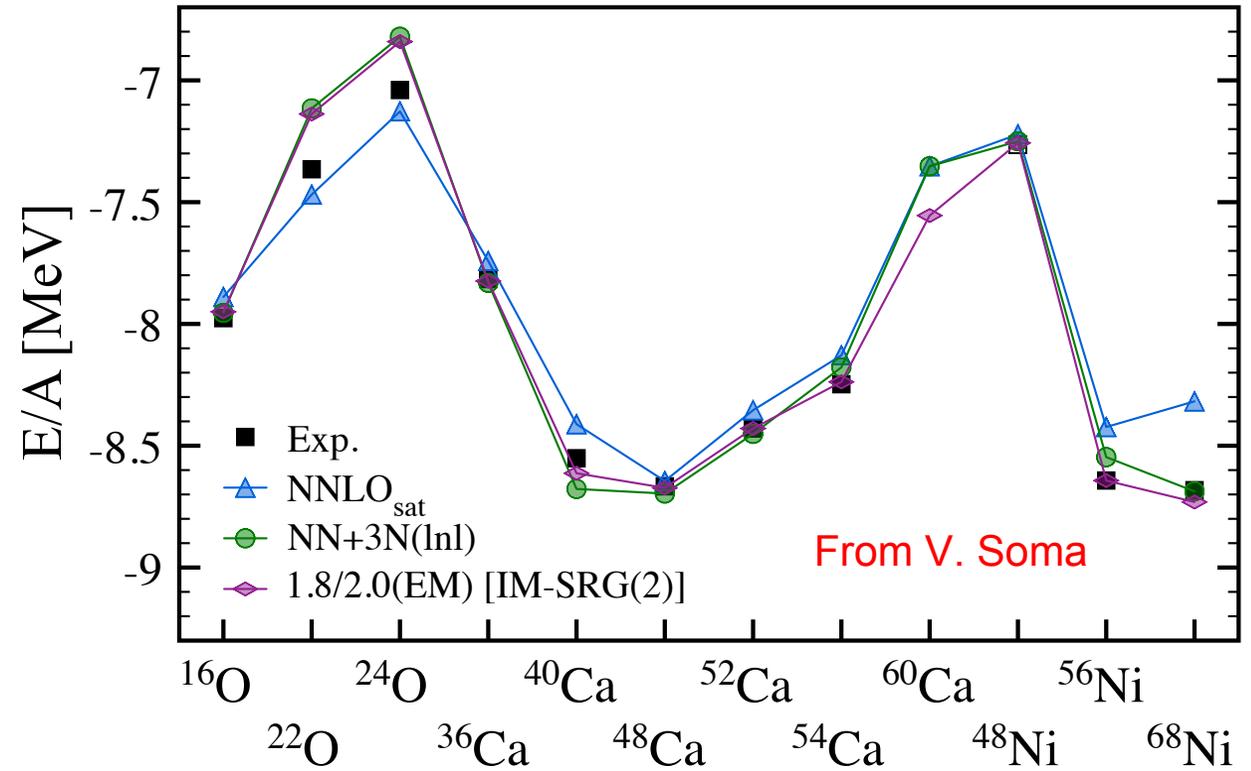
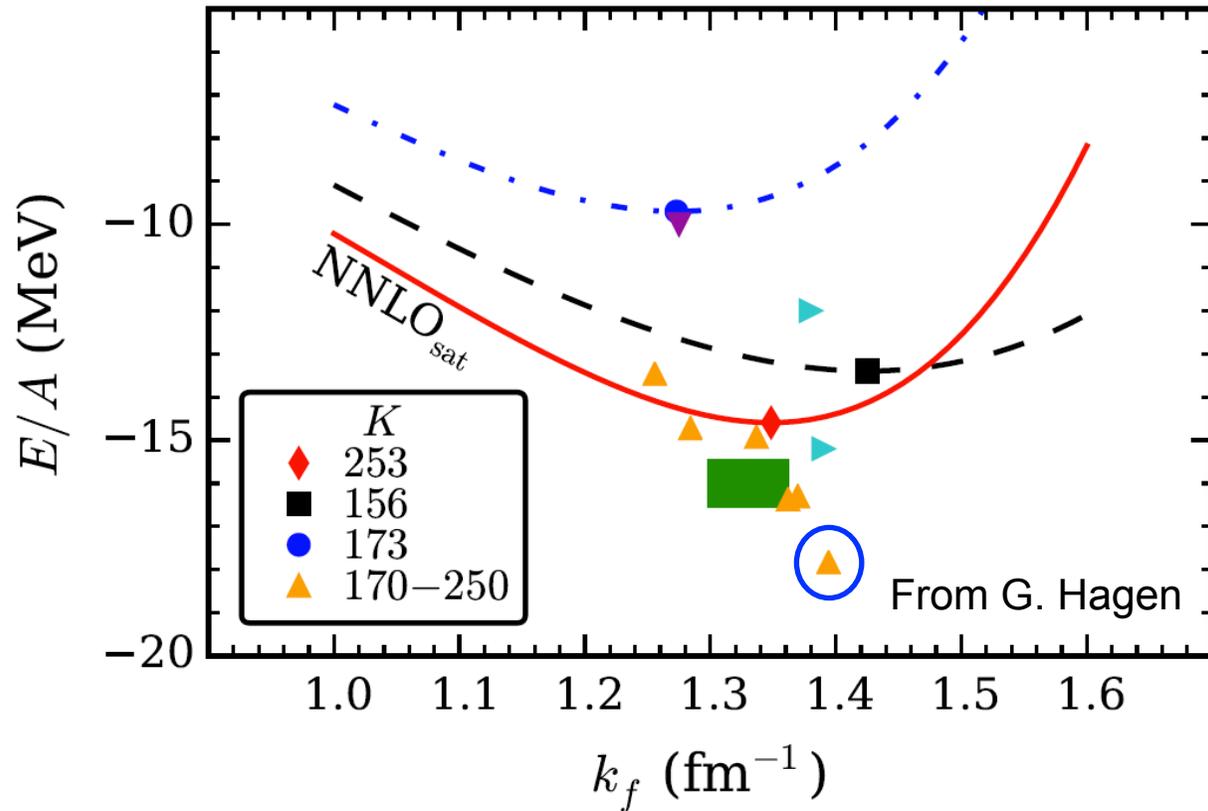
Predicts doubly magic nature from  $2^+$  energies and  $B(E2)$  systematics

Morris et al., PRL (2018)



Both calculations predict  $5/2^+$  ground state

## NN+3N force with good reproduction of ground-state energies



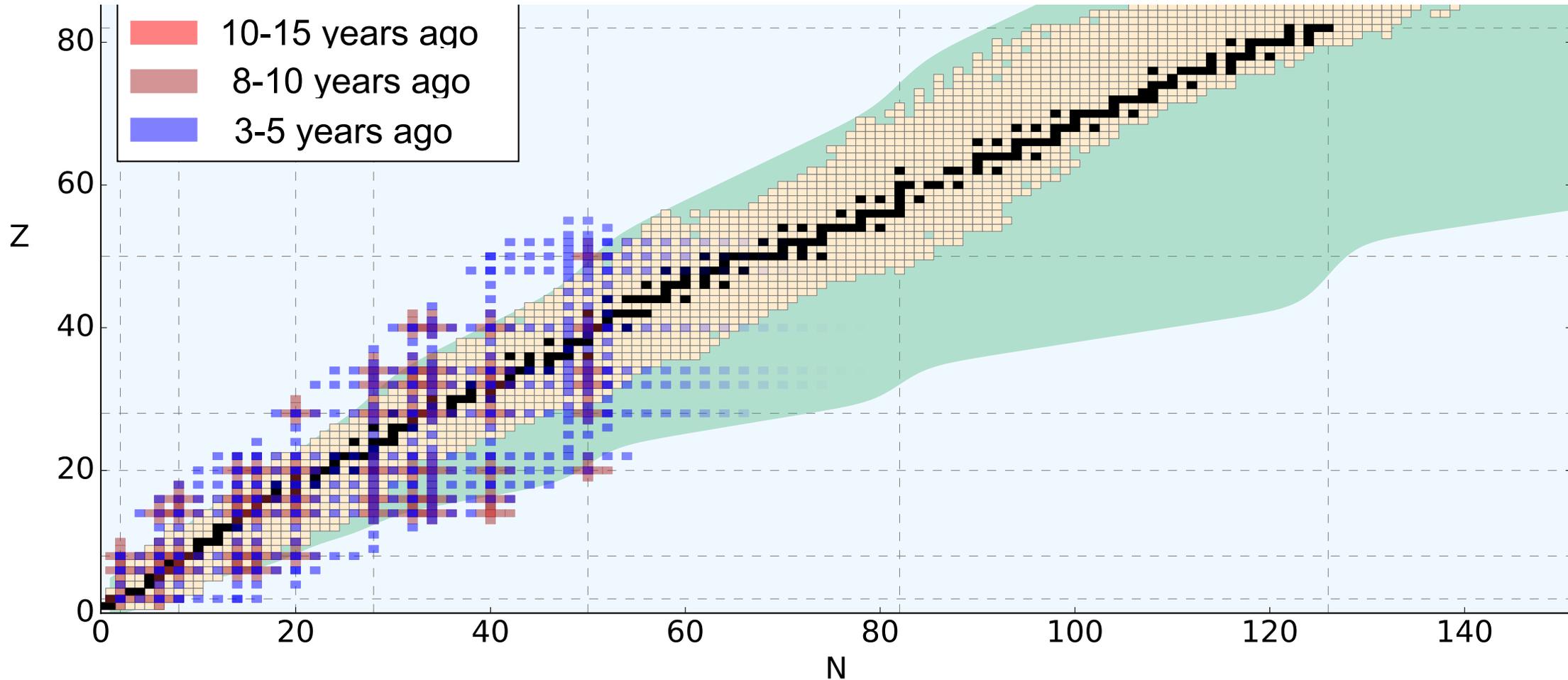
1.8/2.0 (EM), new LNL potential reproduce ground-state energies through  $^{78}\text{Ni}$

$NNLO_{sat}$ , typically underbinds

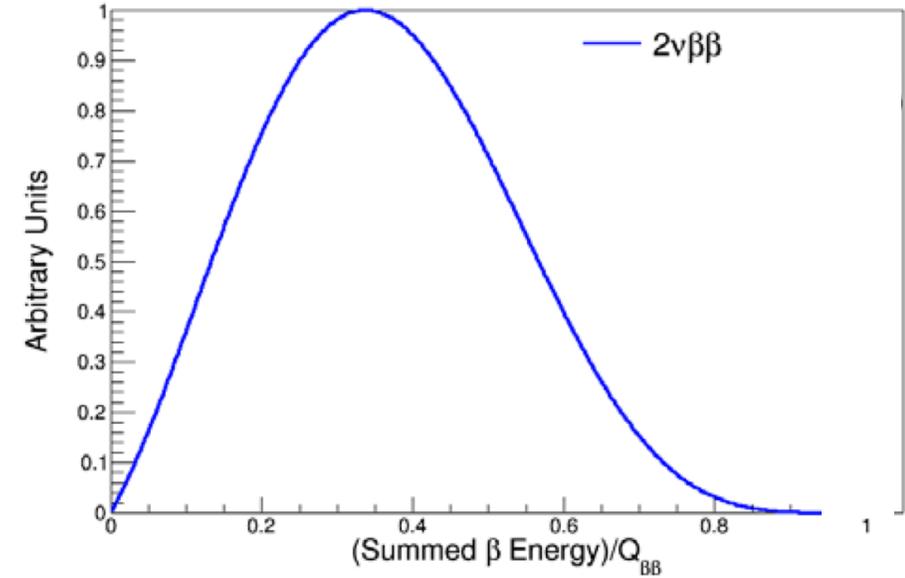
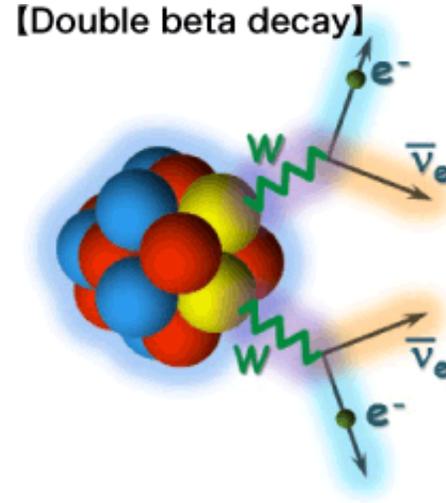
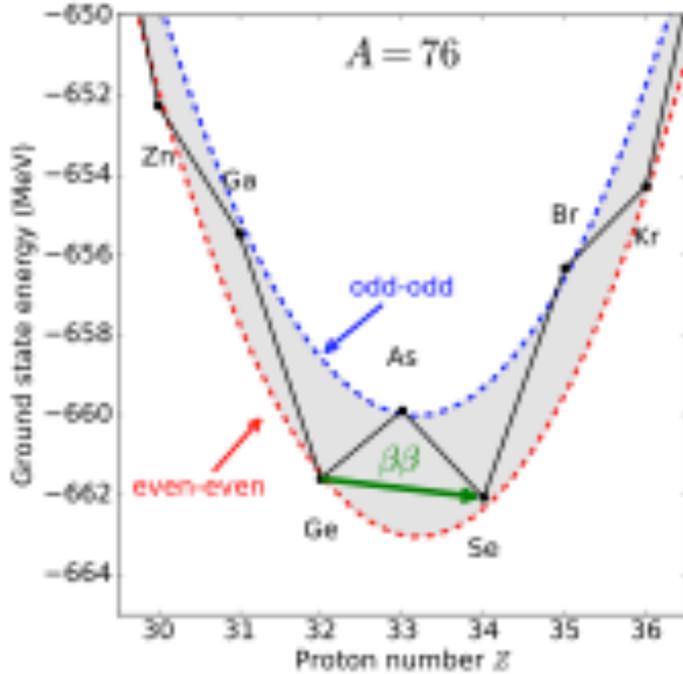
Aim of modern nuclear theory: Develop unified *first-principles* picture of structure and reactions

- Nuclear forces, electroweak physics
- **Nuclear many-body problem**

$$H\psi_n = E_n\psi_n$$



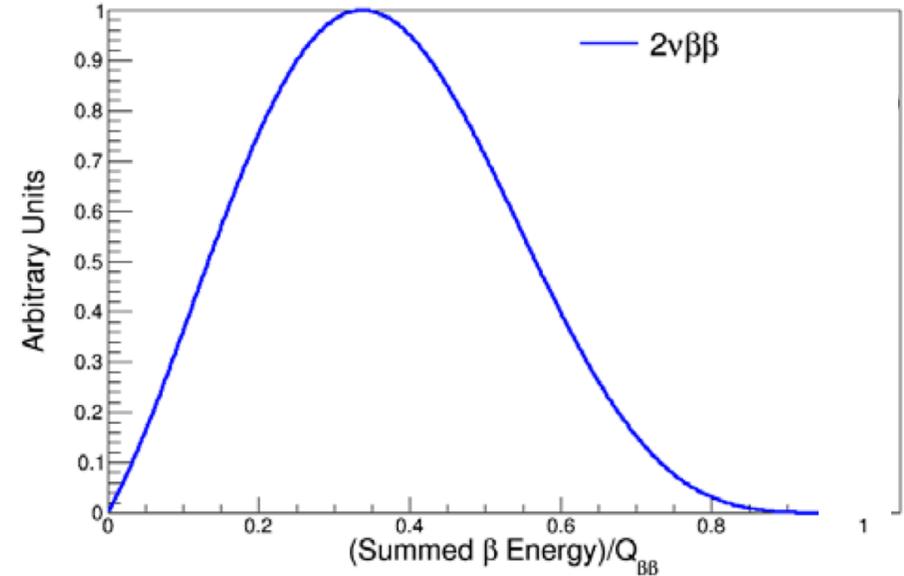
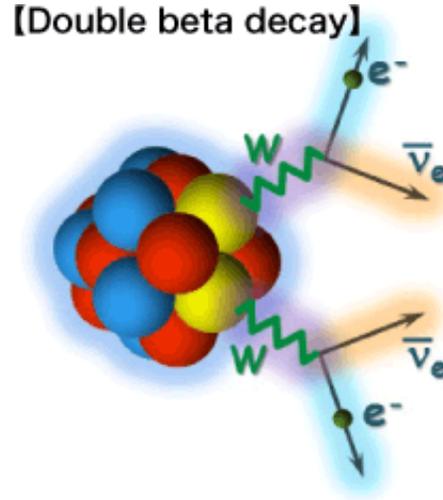
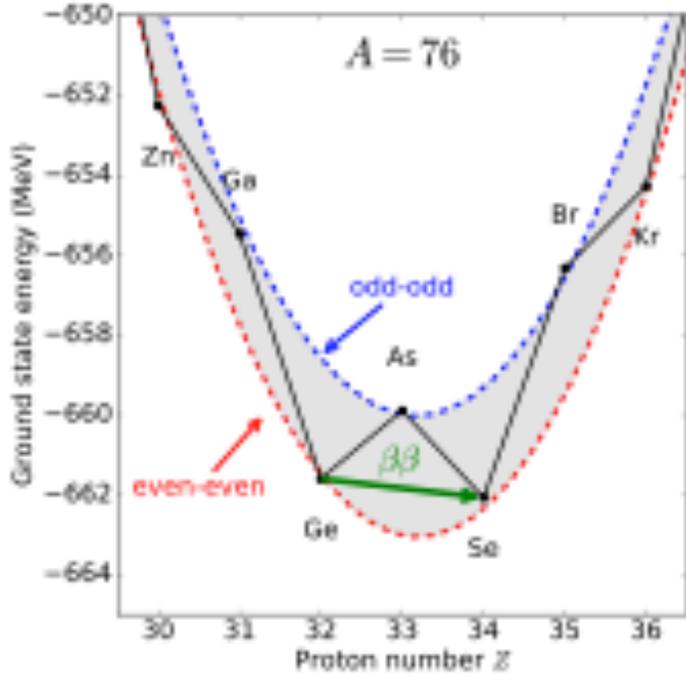
In rare cases beta decay is energetically forbidden – simultaneous beta decays



2<sup>nd</sup>-order weak process allowed by standard model

$$\left(T_{1/2}^{2\nu\beta\beta}\right)^{-1} = G^{2\nu}(Q_{\beta\beta}, Z) |M^{2\nu}|^2$$

In rare cases beta decay is energetically forbidden – simultaneous beta decays



Observed in ~15 nuclei

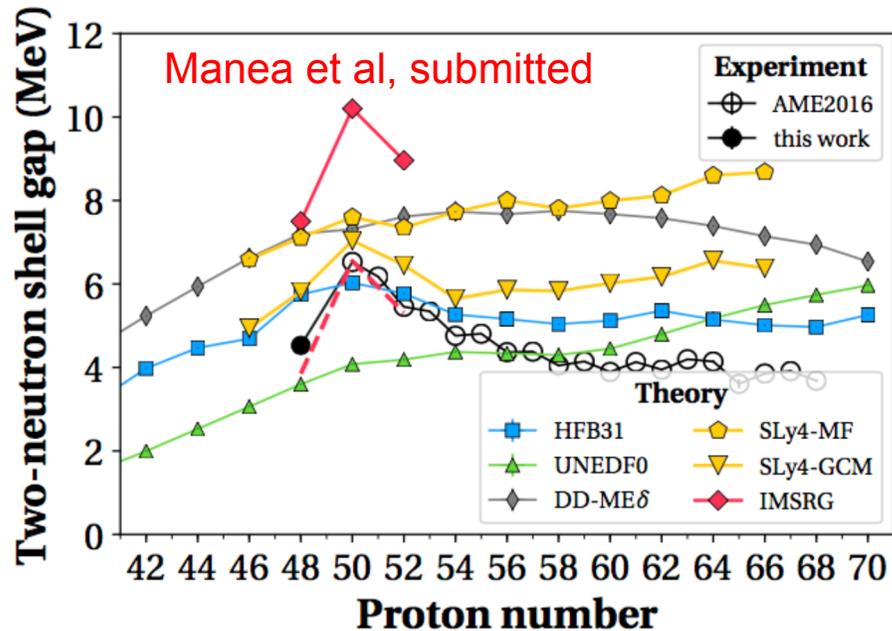
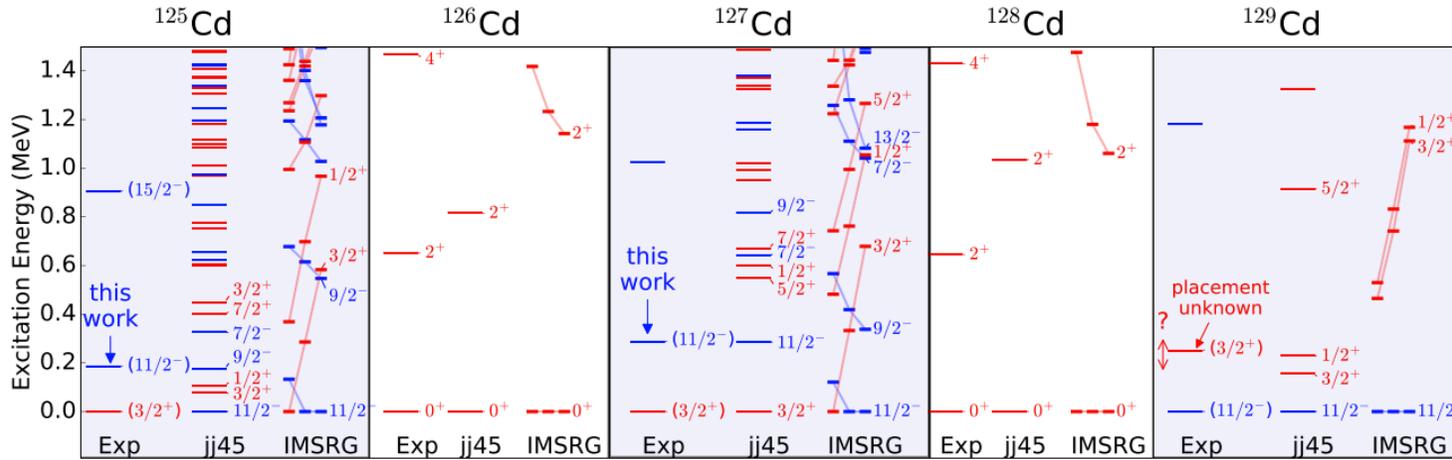
2<sup>nd</sup>-order weak process allowed by standard model

$$\left(T_{1/2}^{2\nu\beta\beta}\right)^{-1} = G^{2\nu}(Q_{\beta\beta}, Z) |M^{2\nu}|^2$$

Lifetimes ~ 10<sup>20</sup> years: **governed by NME**

Isotope	$T_{1/2}(2\nu)$ (years)	Isotope	$T_{1/2}(2\nu)$ (years)
<sup>48</sup> Ca	$4.4^{+0.6}_{-0.5} \times 10^{19}$	<sup>116</sup> Cd	$(2.8 \pm 0.2) \times 10^{19}$
<sup>76</sup> Ge	$(1.5 \pm 0.1) \times 10^{21}$	<sup>128</sup> Te	$(1.9 \pm 0.4) \times 10^{24}$
<sup>82</sup> Se	$(0.92 \pm 0.07) \times 10^{20}$	<sup>130</sup> Te	$(6.8^{+1.2}_{-1.1}) \times 10^{20}$
<sup>96</sup> Zr	$(2.3 \pm 0.2) \times 10^{19}$	<sup>150</sup> Nd	$(8.2 \pm 0.9) \times 10^{18}$
<sup>100</sup> Mo	$(7.1 \pm 0.4) \times 10^{18}$	<sup>150</sup> Nd- <sup>150</sup> Sm(0 <sub>1</sub> <sup>+</sup> )	$1.33^{+0.45}_{-0.26} \times 10^{20}$
<sup>100</sup> Mo- <sup>100</sup> Ru(0 <sub>1</sub> <sup>+</sup> )	$5.9^{+0.8}_{-0.6} \times 10^{20}$	<sup>238</sup> U	$(2.0 \pm 0.6) \times 10^{21}$

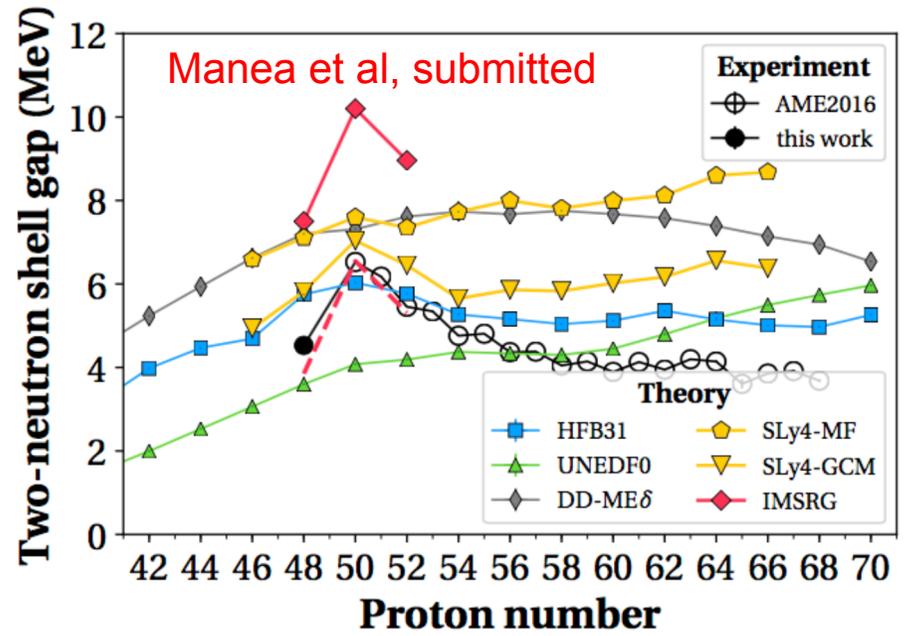
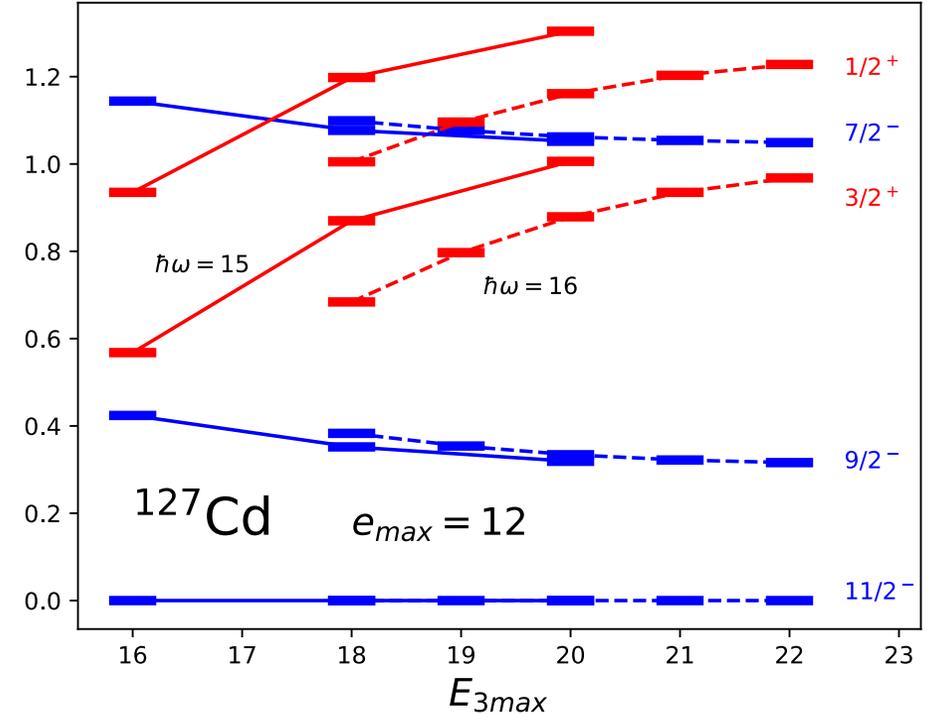
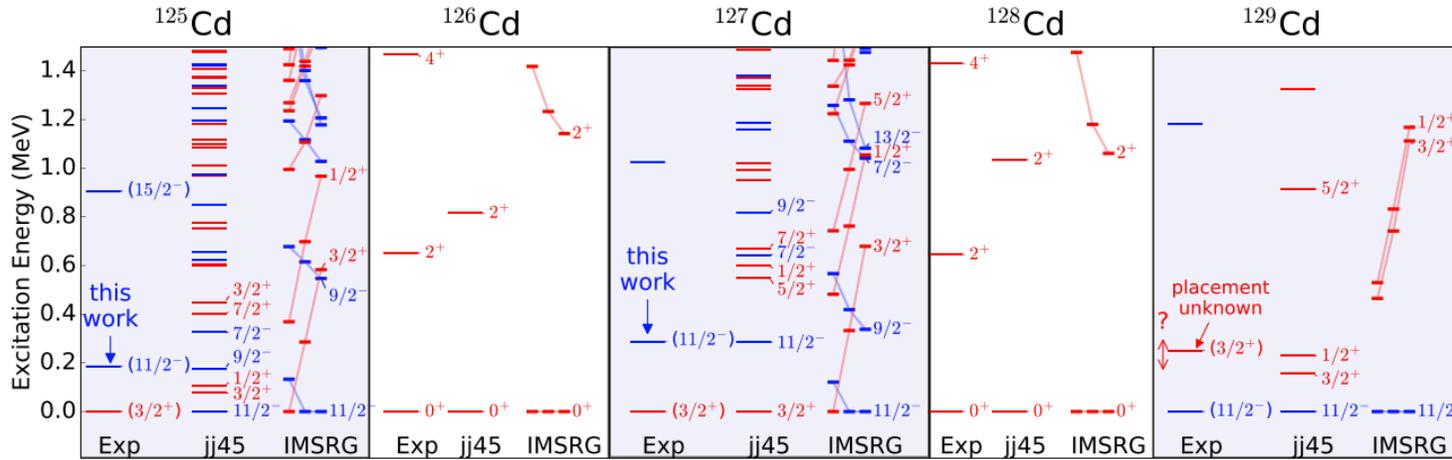
Size of N=70 gap clearly not converged wrt E3max – for neutron-rich Sn, In, Cd...



Lascar et al PRC (2017)

Resorted to unreliable extrapolations...

Size of N=70 gap clearly not converged wrt E3max – for neutron-rich Sn, In, Cd...



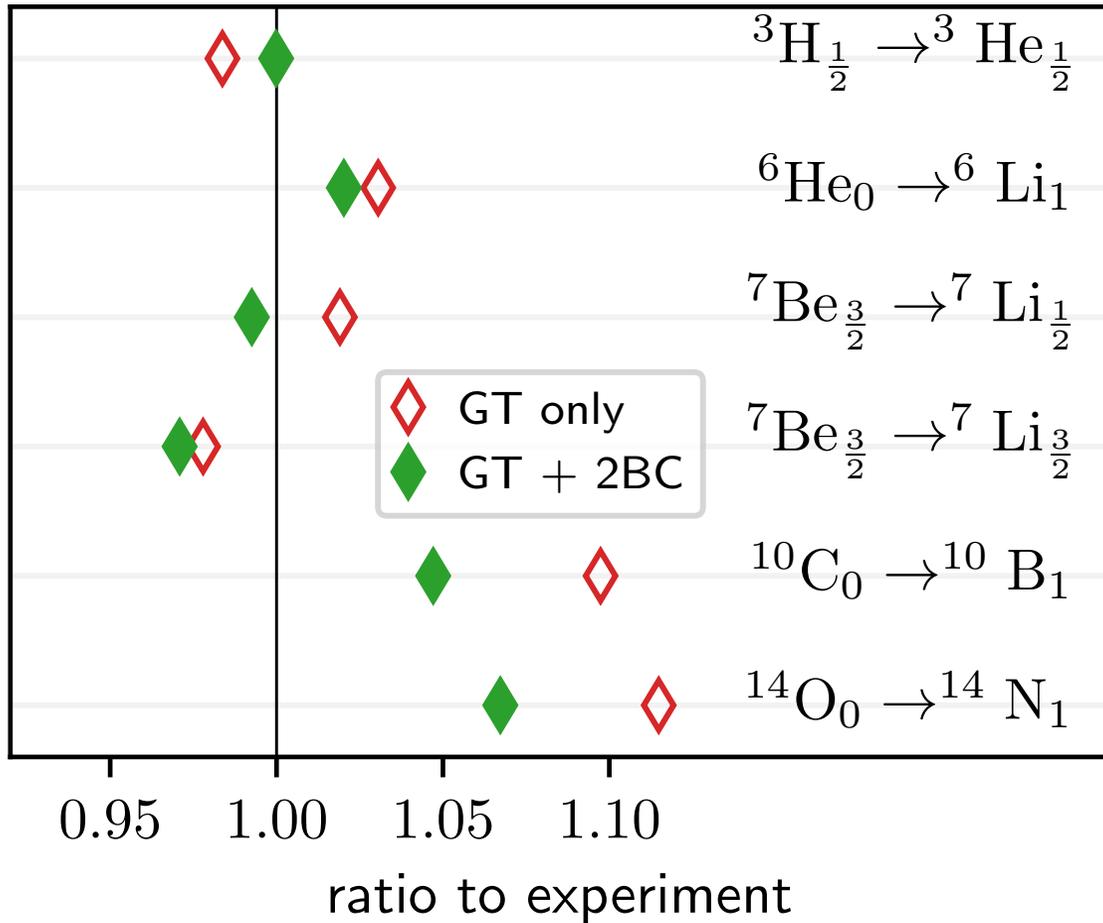
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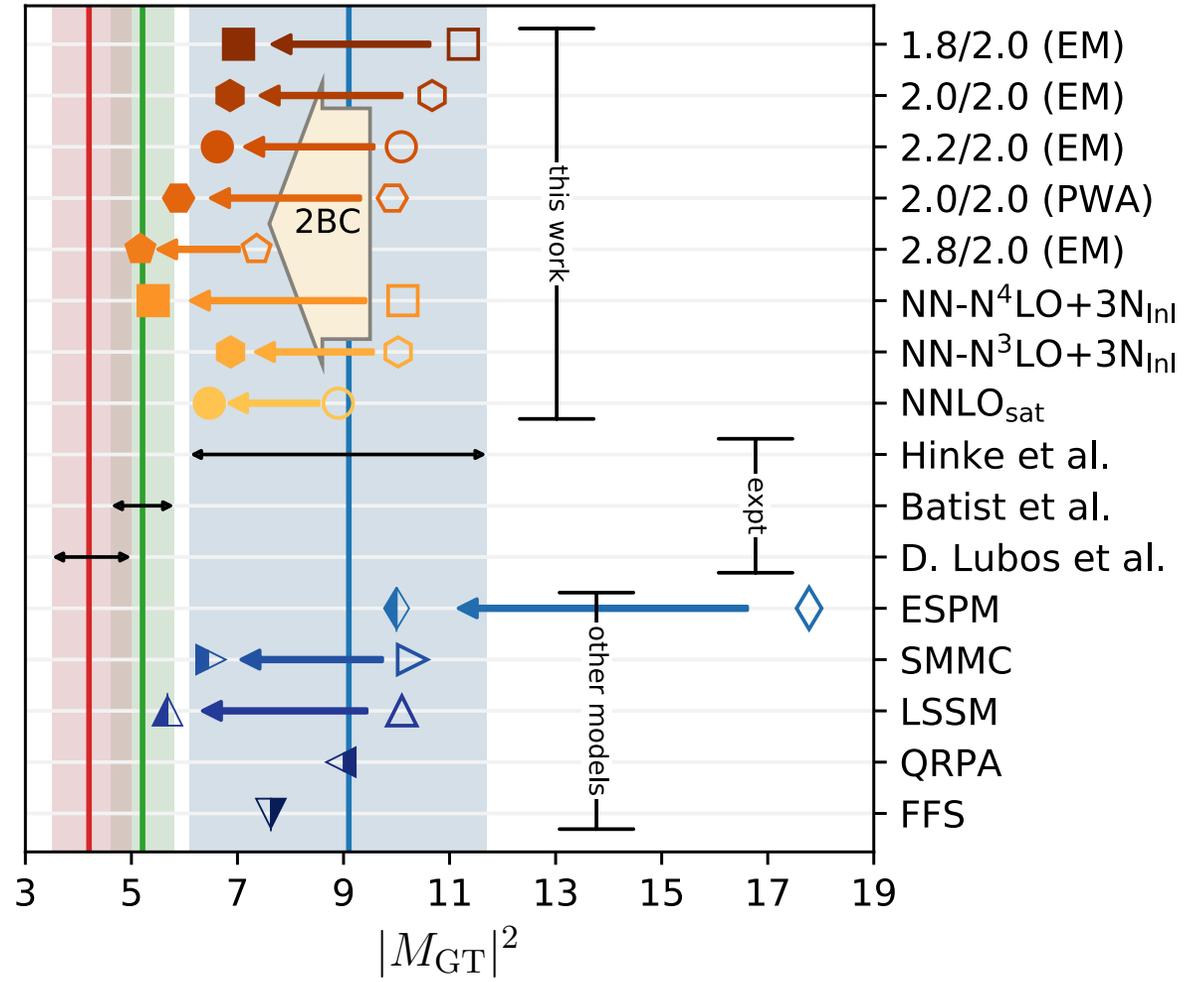
**New capabilities: converged spectra in N=82 region!**

Explore new physics near  $^{132}\text{Sn}$ !

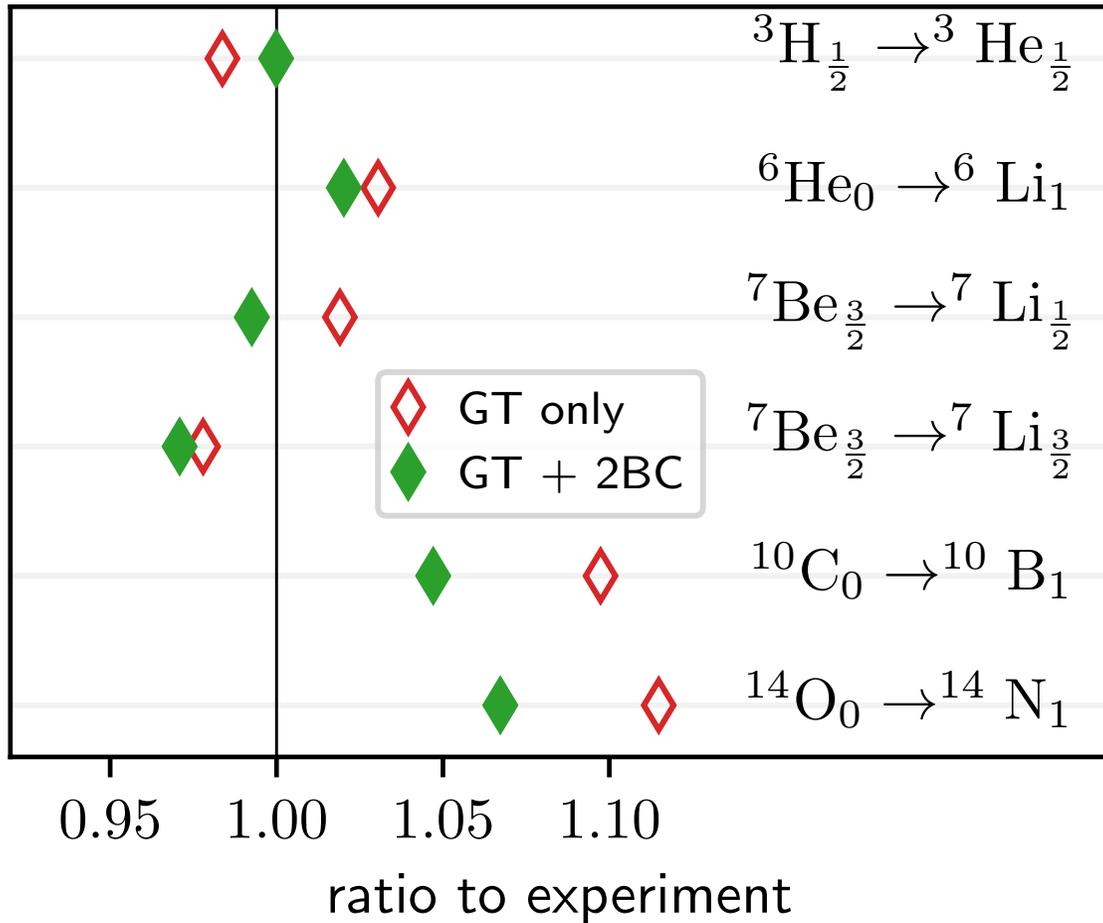
**NCSM** in light nuclei, **CC** calculations of GT transition in  $^{100}\text{Sn}$  from different forces



Large quenching effect from correlations

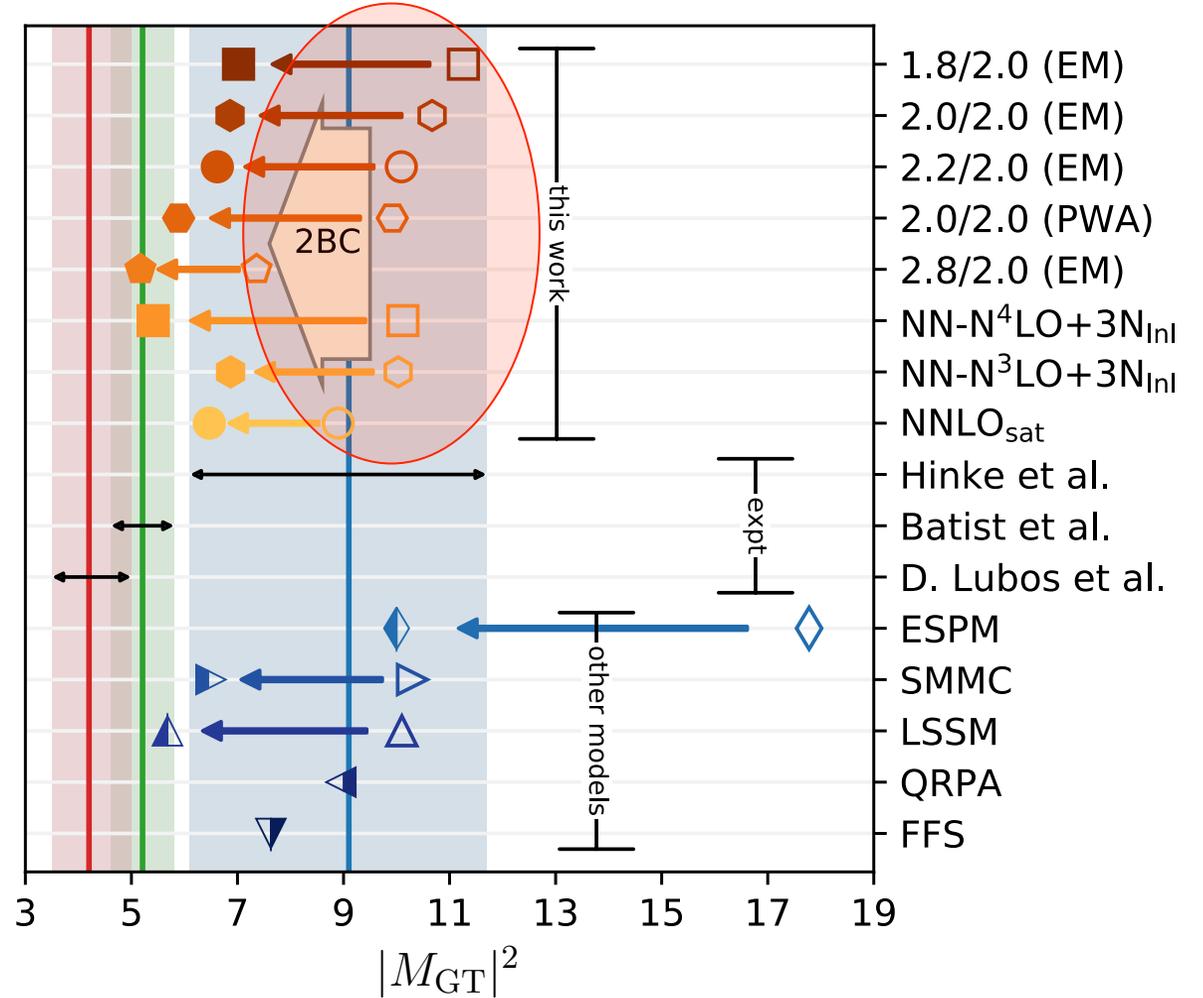


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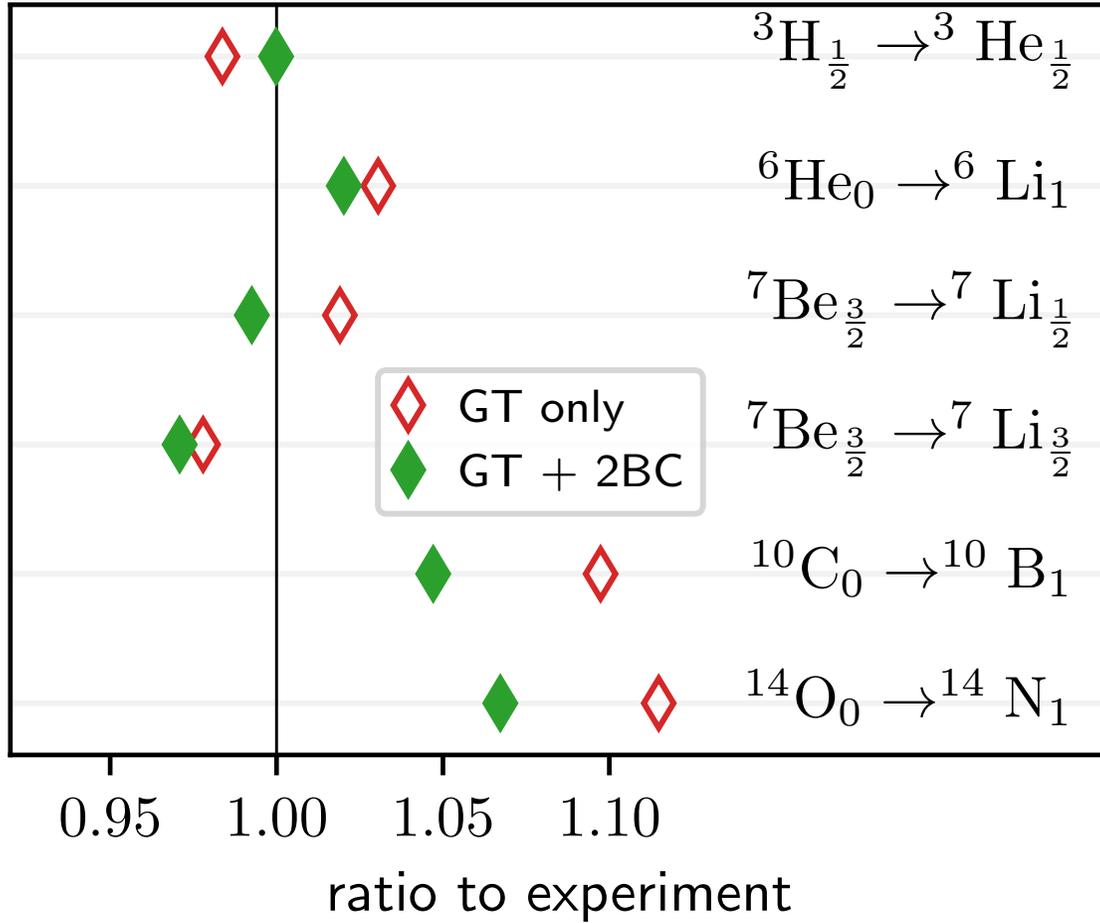
Large quenching effect from correlations

**Without 2B currents, large spread in results**

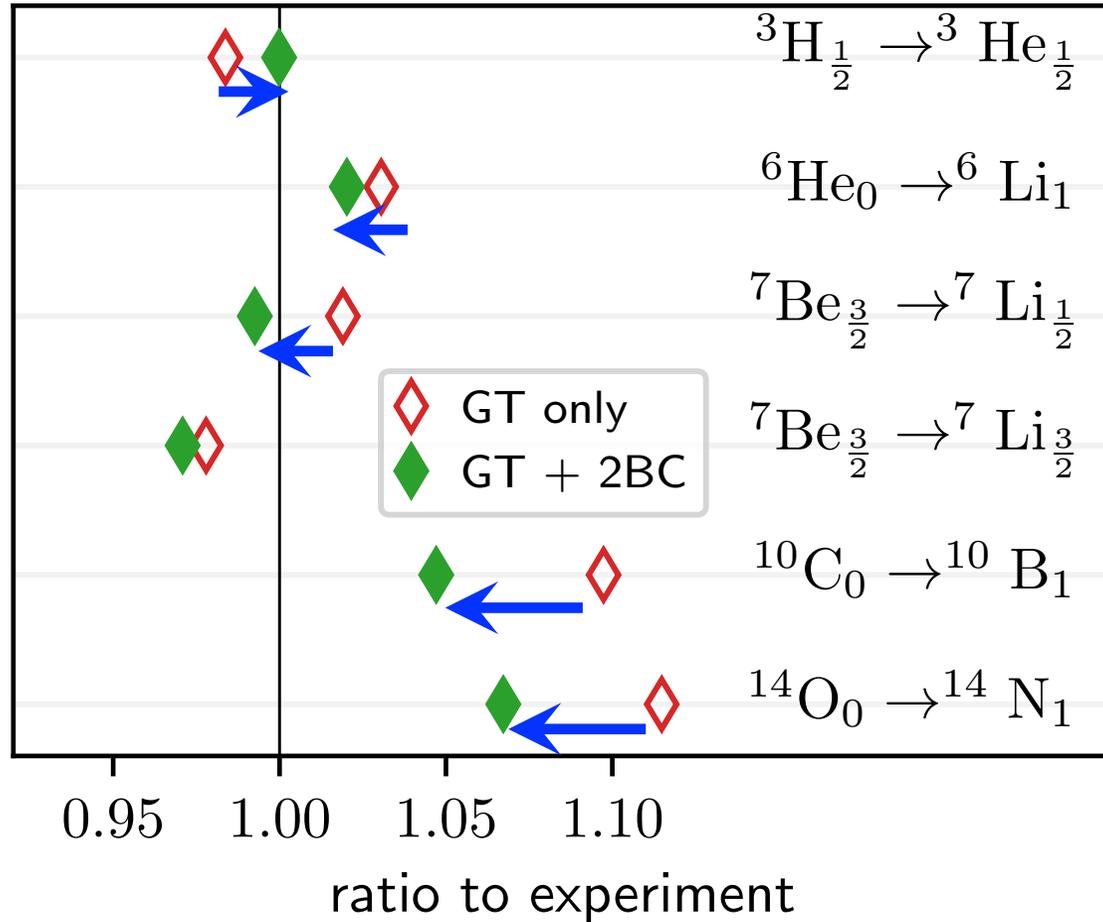


Gysbers et al., Nature Phys. (2019)

## NCSM in light nuclei



## NCSM in light nuclei



**2BC provide modest quenching in most cases**

## Convergence and method benchmarks of VS-IMSRG GT transitions

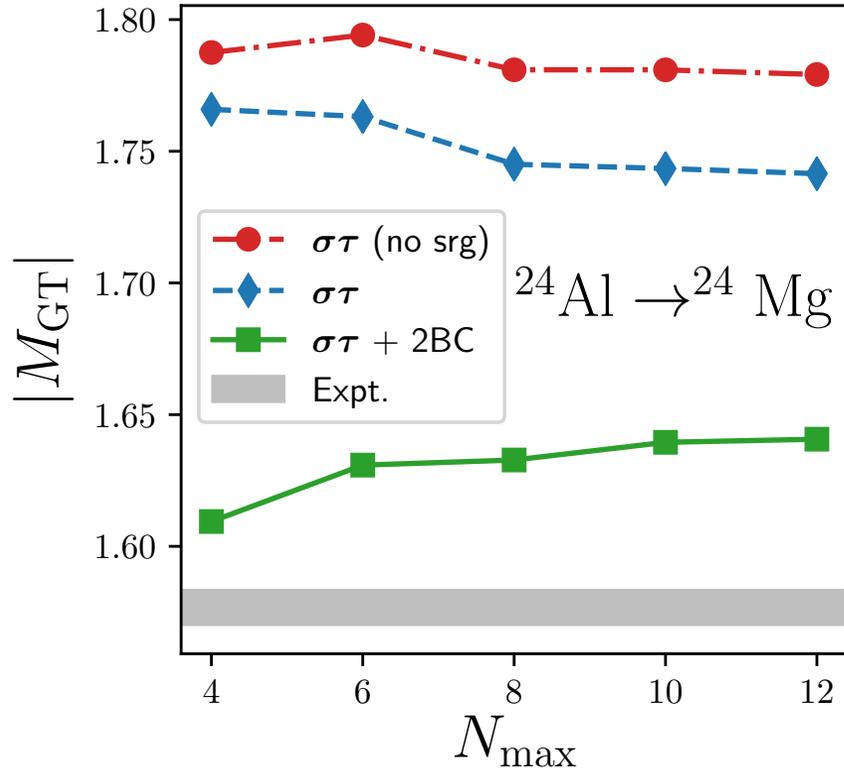


TABLE IV. Gamow Teller (GT) transition strength in  $^{10}\text{C}$  to the first  $1_1^+$  in  $^{10}\text{B}$  for the NN- $\text{N}^4\text{LO} + 3\text{N}_{\text{Inl}}$  interaction calculated in the VS-IMSRG(2) and NCSM approaches.

Method	$ M_{\text{GT}}(\sigma\tau) $	$ M_{\text{GT}} $
VS-IMSRG(2)	1.94	1.88
NCSM	2.01	1.92

TABLE III. Gamow Teller (GT) transition strength in  $^{14}\text{O}$  to the second  $1_2^+$  in  $^{14}\text{N}$  for the  $\text{NNLO}_{\text{sat}}$  and NN- $\text{N}^4\text{LO} + 3\text{N}_{\text{Inl}}$  interactions calculated in the EOM-CCSD, EOM-CCSDT-1, VS-IMSRG, and NCSM approaches.

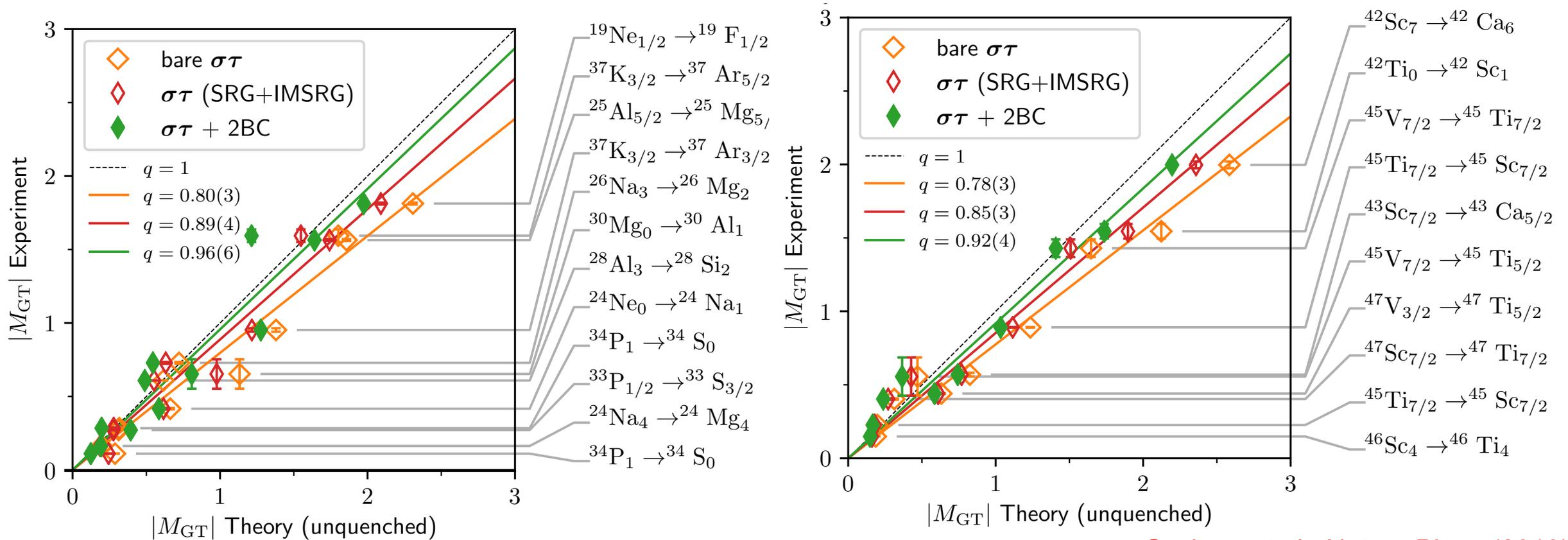
Interaction	$\text{NNLO}_{\text{sat}}$		$\text{NN-}\text{N}^4\text{LO}+3\text{N}_{\text{Inl}}$	
	$ M_{\text{GT}}(\sigma\tau) $	$ M_{\text{GT}} $	$ M_{\text{GT}}(\sigma\tau) $	$ M_{\text{GT}} $
EOM-CCSD	2.15	2.08	2.26	2.06
EOM-CCSDT-1	1.77	1.69	1.97	1.86
VS-IMSRG(2)	1.72	1.76	1.83	1.83
NCSM	1.80	1.69	1.86	1.78

**Well converged and good agreement with other ab initio methods**

Ab initio calculations of **large** GT transitions in *sd*, *pf* shells

Bare operator similar to phenomenological shell model

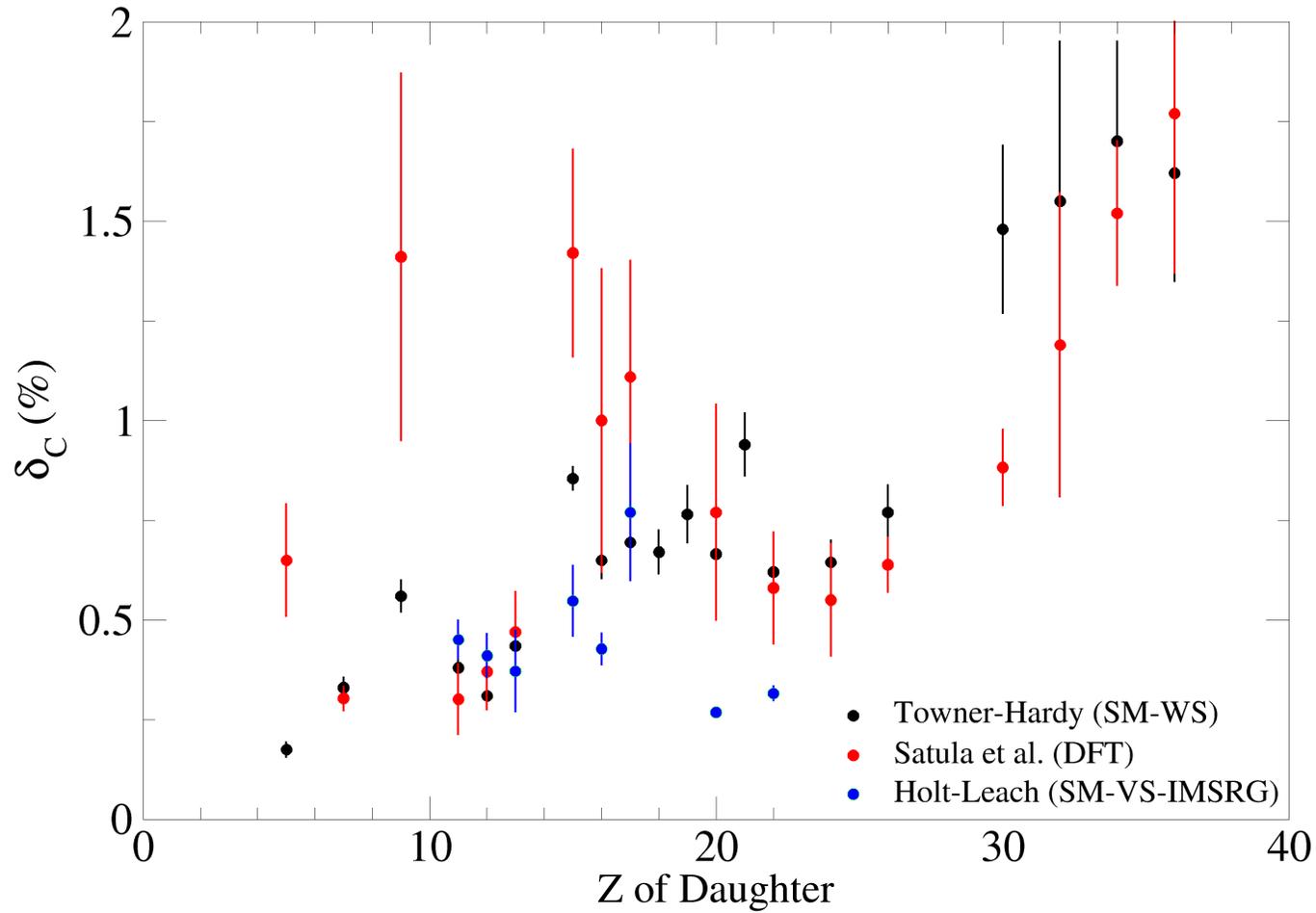
Modest quenching from consistent ab initio wavefunctions and operators



Gysbers et al., Nature Phys. (2019)

Further modest quenching from 2BC

Essential for determination of  $V_{ud}$



Standard approach (T/H):

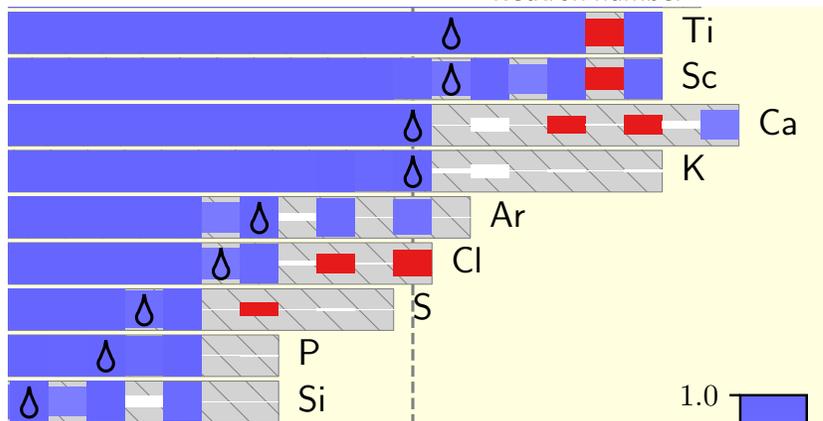
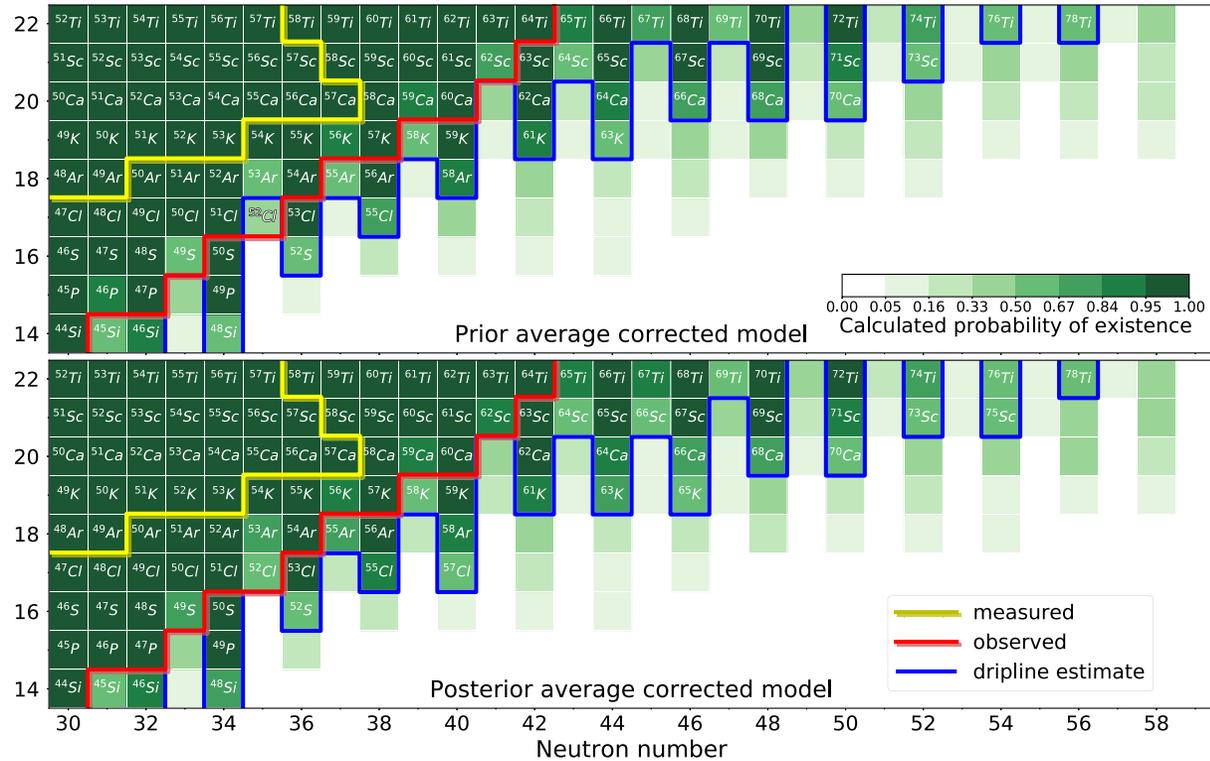
$$\delta_C = \underbrace{\delta_{C1}}_{\text{configuration mixing}} + \underbrace{\delta_{C2}}_{\text{wave function mismatch}}$$

Ab initio approach

$$|M_F|^2 = |M_F^0|^2 (1 - \delta_C)$$

$$\delta_C = \left\{ H_{pp}(s) \neq H_{nn}(s) \neq H_{pn}(s) \right\} + \left\{ \tau(s) = U(s)\tau U^\dagger(s) \right\} + \left\{ \langle \phi_p^{\text{HF}} | \tau | \phi_n^{\text{HF}} \rangle \neq 1 \right\}$$

Recent DFT analysis from Si-Ti based on Bayesian machine learning



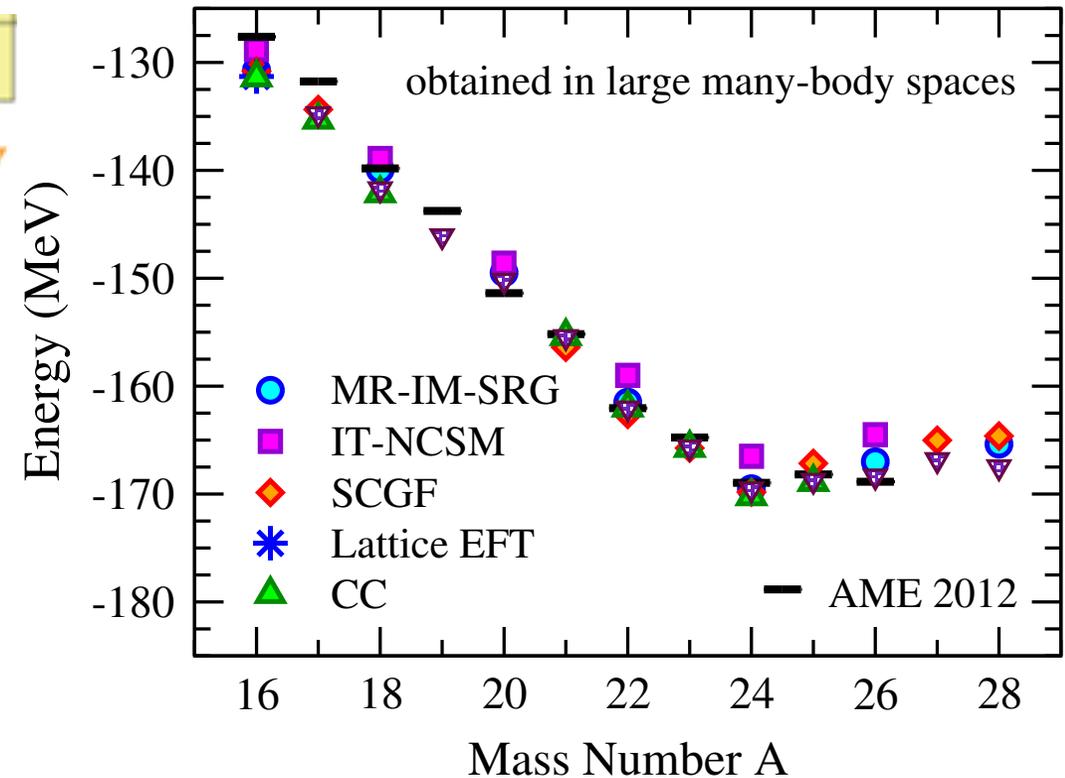
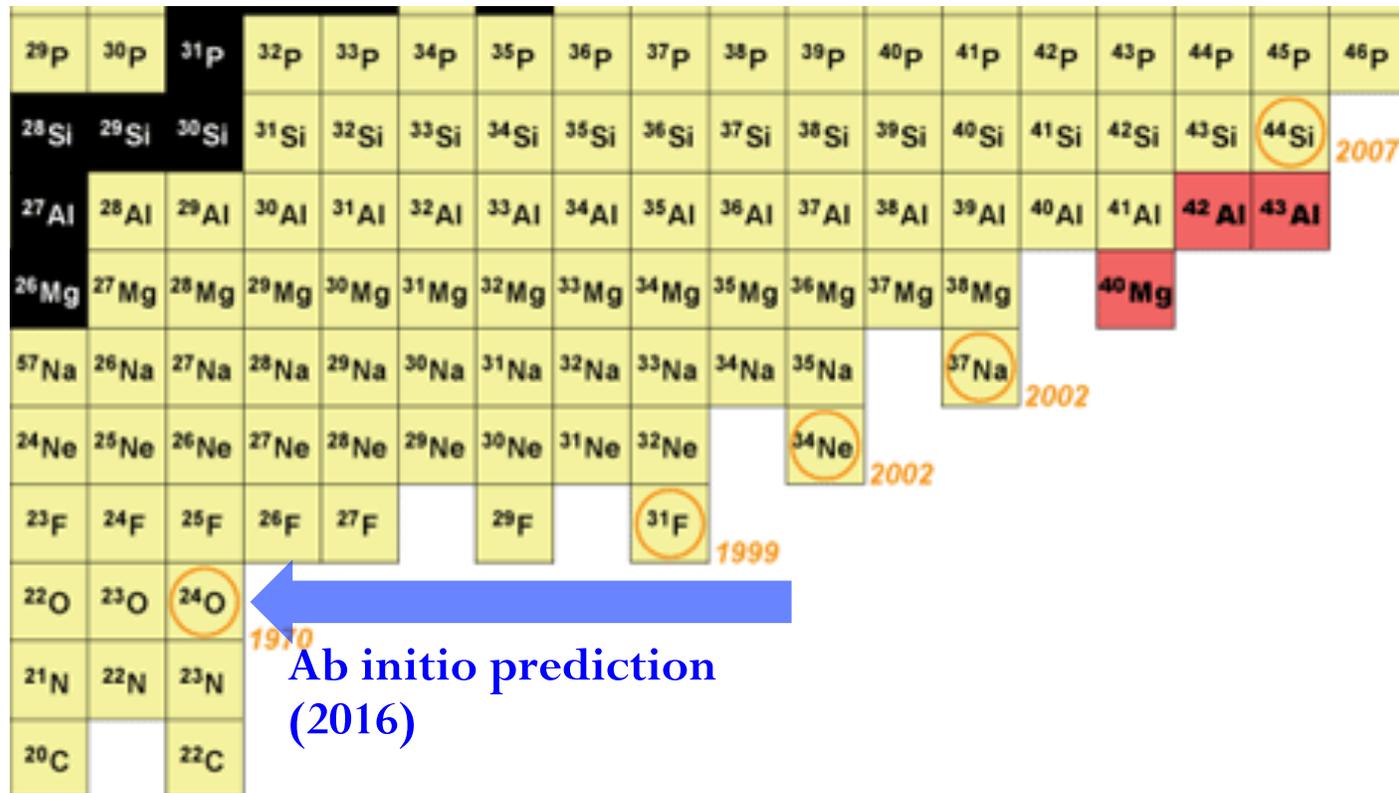
**Largely consistent prediction of drip line**

## Where (and what) is the nuclear dripline?

Limits defined as last isotope with positive neutron separation energy

- Nucleons “drip” out of nucleus

Neutron dripline experimentally established to  $Z=8$



Same result from same input NN+3N forces

Already well beyond where fit to data!

Explicitly construct unitary transformation from sequence of rotations

$$U = e^\Omega = e^{\eta_n} \dots e^{\eta_1} \quad \eta = \frac{1}{2} \arctan \left( \frac{2H_{\text{od}}}{\Delta} \right) - \text{h.c.}$$

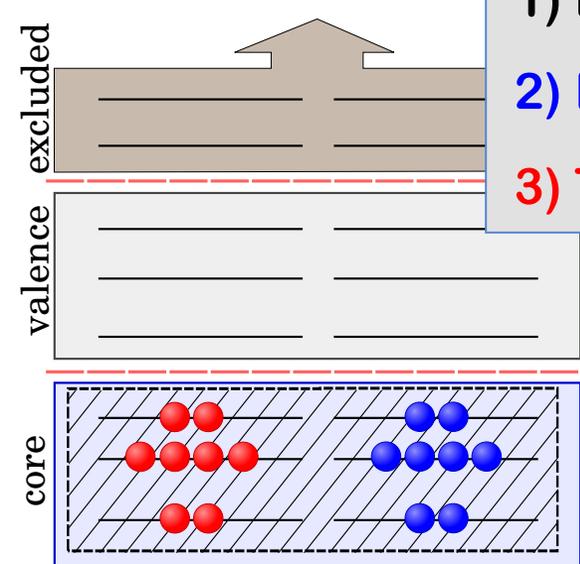
$$\tilde{H} = e^\Omega H e^{-\Omega} = H + [\Omega, H] + \frac{1}{2} [\Omega, [\Omega, H]] + \dots$$

$$\tilde{\mathcal{O}} = e^\Omega \mathcal{O} e^{-\Omega}$$

### Potential sources of error

- 1) Deficiencies in nuclear forces / neglected EW currents
- 2) Incomplete convergence in basis ✓ (N,Z < 50)
- 3) Truncations in many-body operators?

, Bogner, Schwenk, PRC 2012  
 Pzuchowski, Bogner, PRC 2015



$$|\Phi_0\rangle = |^{16}\text{O}\rangle$$

decouple

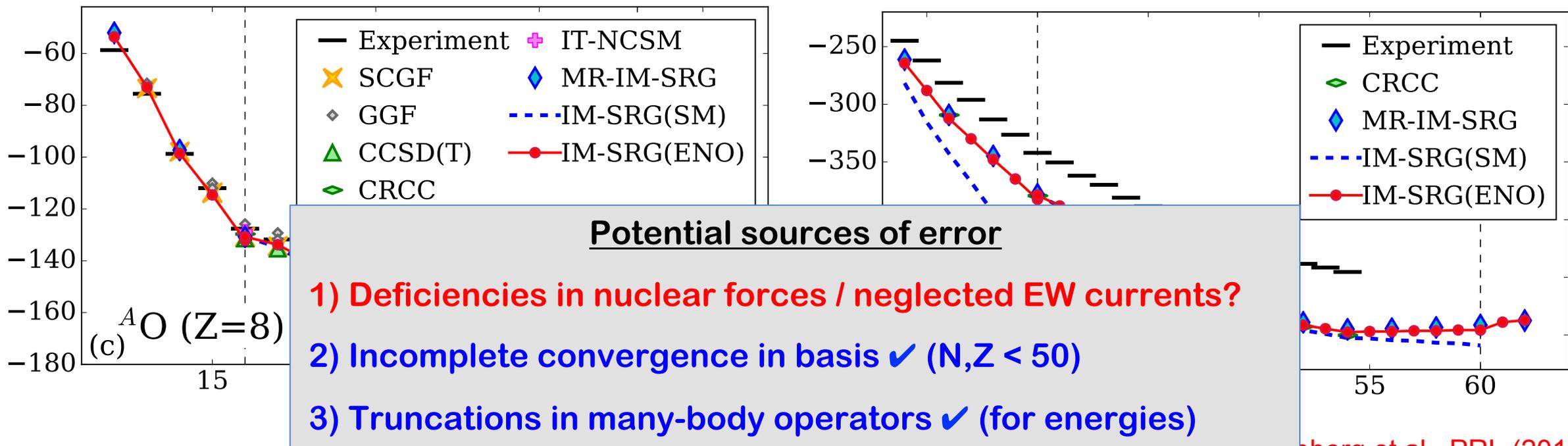
$$\langle \tilde{\Psi}_n | P \tilde{H} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | H | \Psi_i \rangle$$

$$\langle \tilde{\Psi}_n | P \tilde{M}_{0\nu} P | \tilde{\Psi}_n \rangle \approx \langle \Psi_i | M_{0\nu} | \Psi_i \rangle$$

$\langle P   H   P \rangle$	$\langle P   H   Q \rangle \rightarrow 0$
$\langle Q   H   P \rangle \rightarrow 0$	$\langle Q   H   Q \rangle$

**Careful benchmarking essential!**

**New approach accesses *\*all\** nuclei:** agrees to 1% with large-space methods



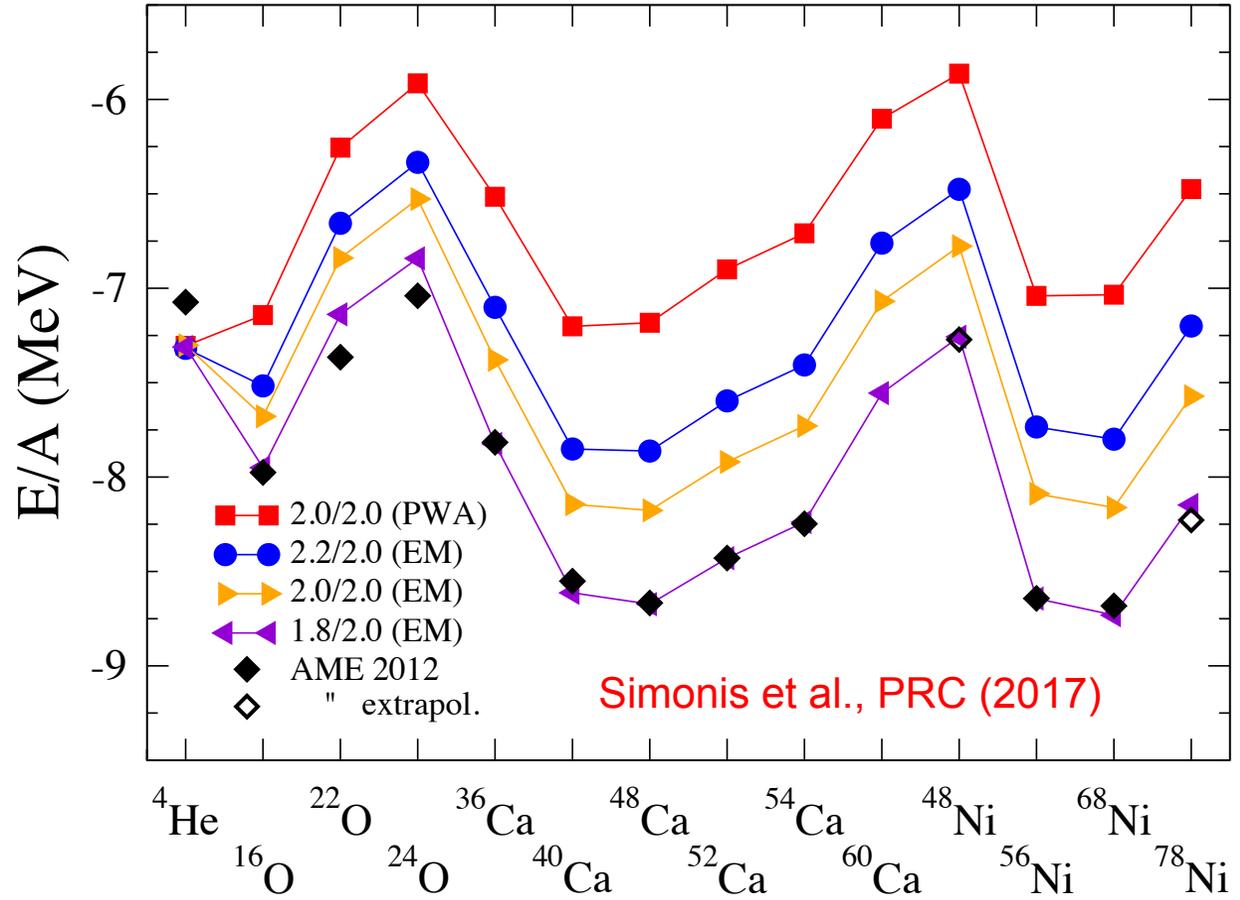
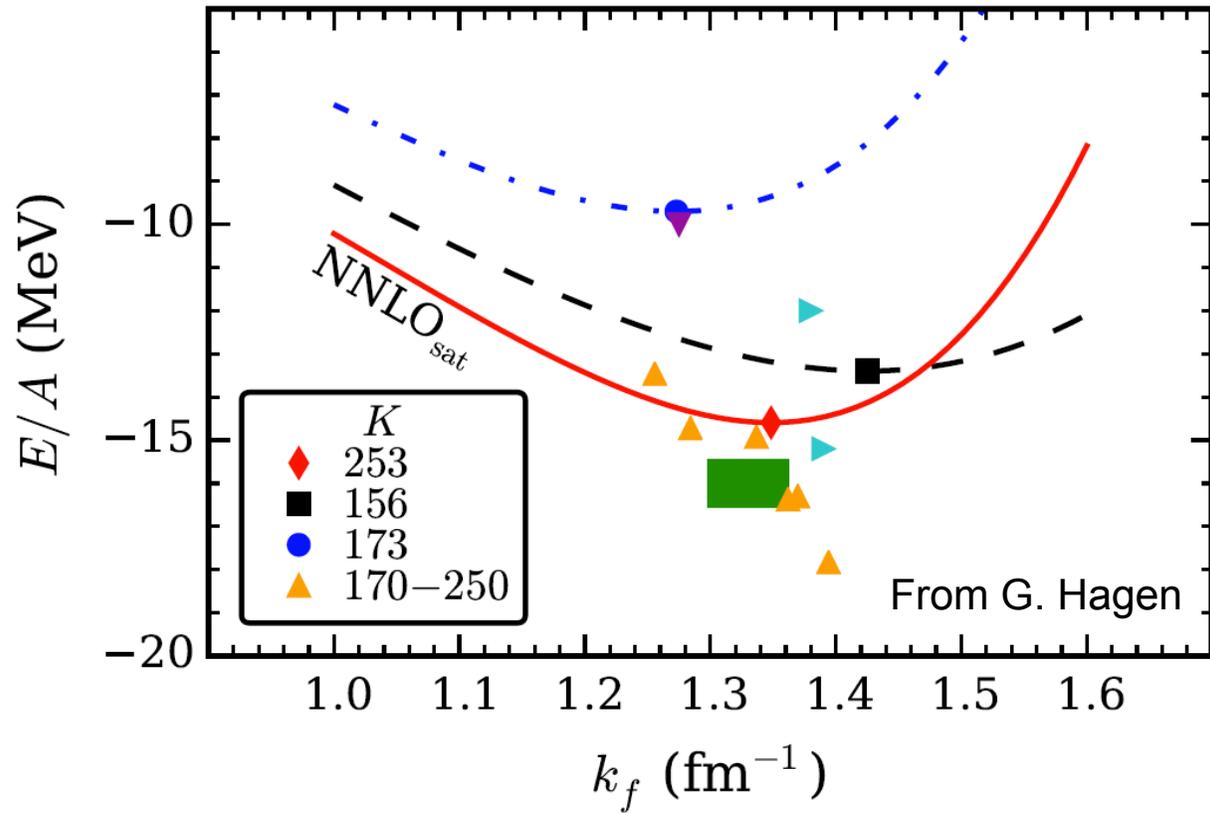
Stroberg et al., PRL (2017)

Agreement with *experiment* deteriorates for heavy chains (due to input Hamiltonian)

Significant gain in applicability with little/no sacrifice in accuracy; **Any operator can be calculated**

**Low computational cost:** ~1 node-day/nucleus

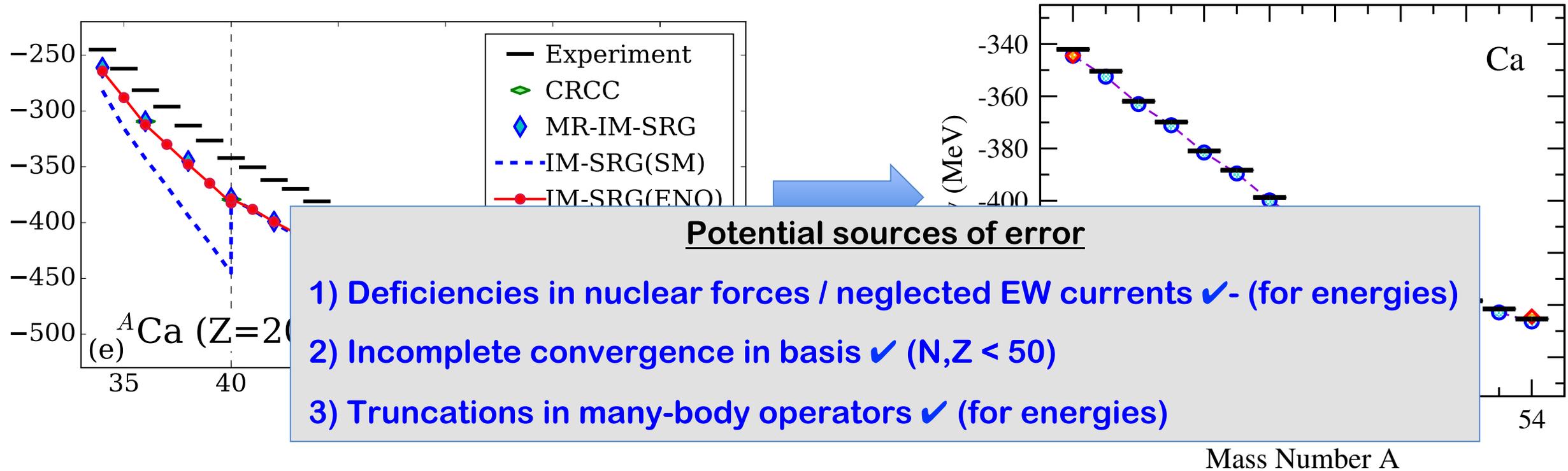
## NN+3N force with good reproduction of ground-state energies



1.8/2.0 (EM) reproduces ground-state energies through  $^{78}\text{Ni}$

Slight underbinding for neutron-rich oxygen

Dramatic improvement with respect to experimental data



Opens possibility for reliable ab initio predictions across the nuclear chart!

Accesses **all** properties of **all** nuclei:

- Ground states, excited states, charge radii, electroweak transitions...
- Test nuclear forces across range of nuclei

