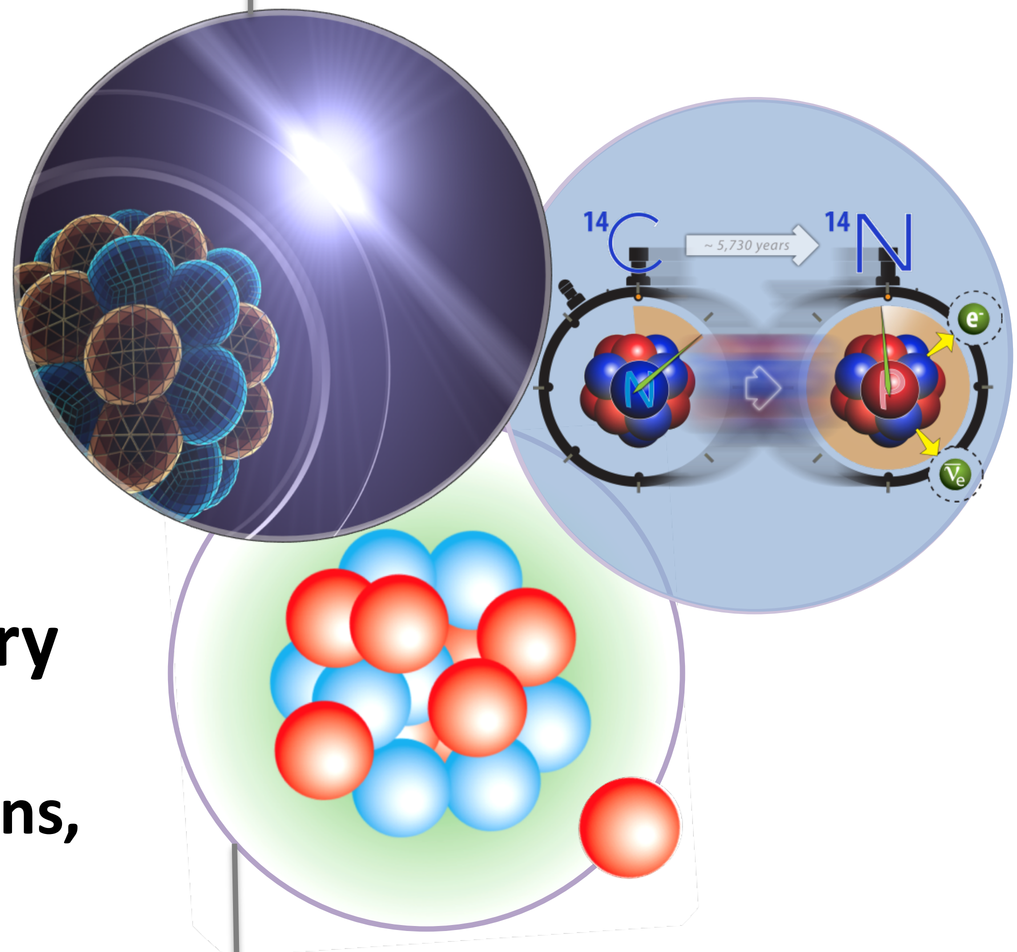
The role of continuum on shell-structure in neutron-rich nuclei

Quantum computation of an atomic nucleus

arXiv:1801.03897



Gaute Hagen
Oak Ridge National Laboratory

Multiparticle resonances in hadrons, nuclei, and ultracold gases

Hirschegg, January 15th, 2018

U.S. DEPARTMENT OF ENERGY

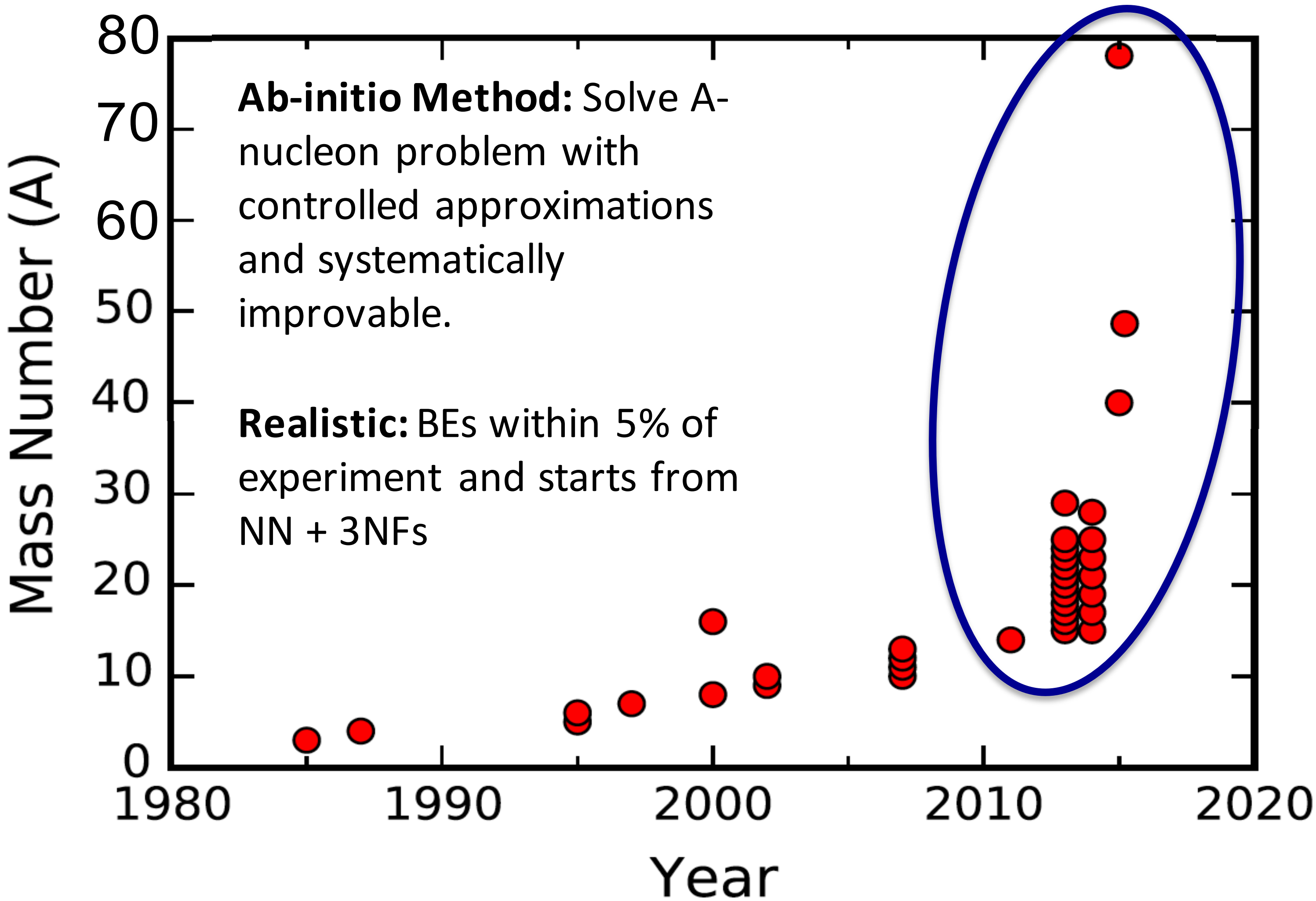
NUCLEI
Nuclear Computational Low-Energy Initiative

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

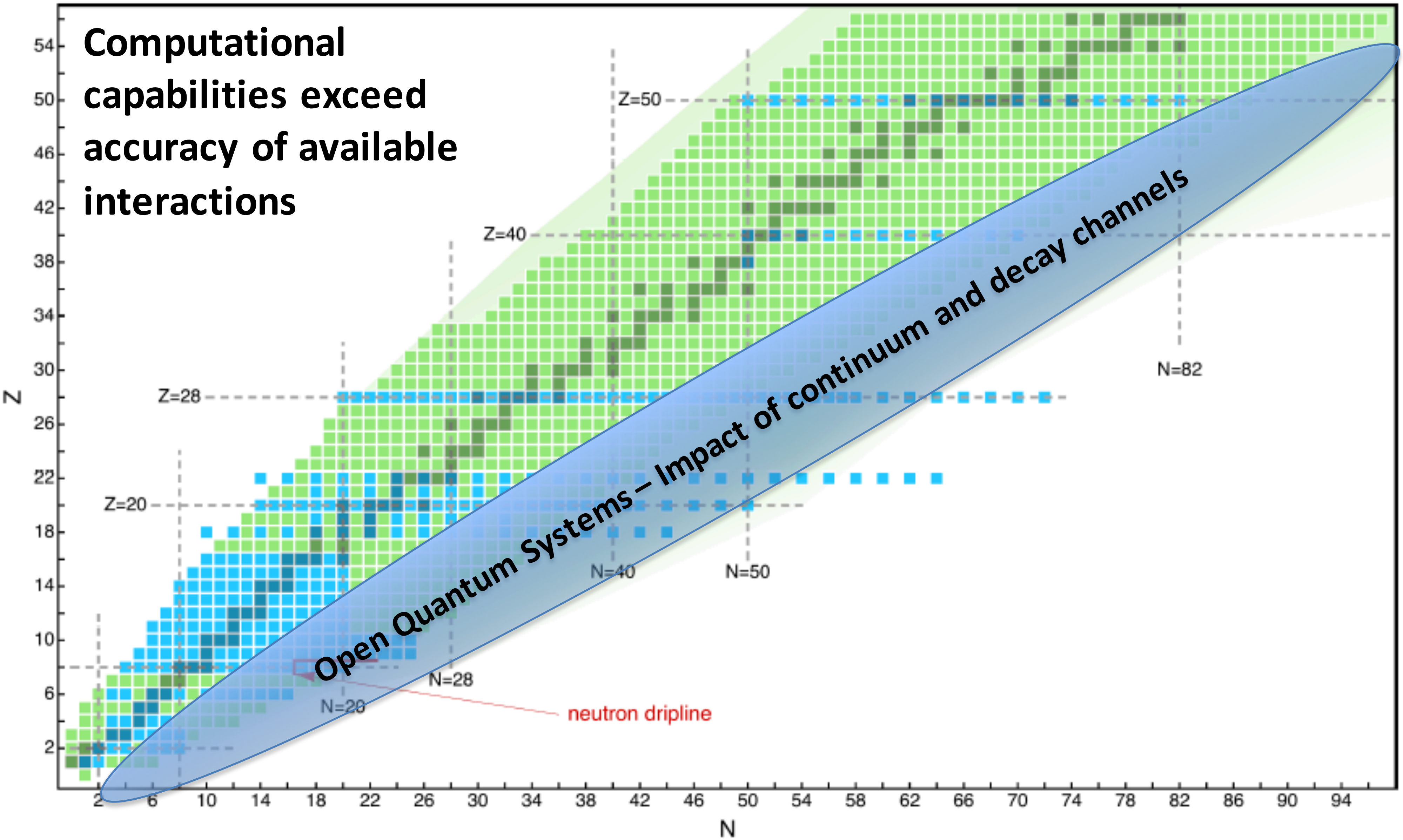
Trend in realistic ab-initio calculations

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

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



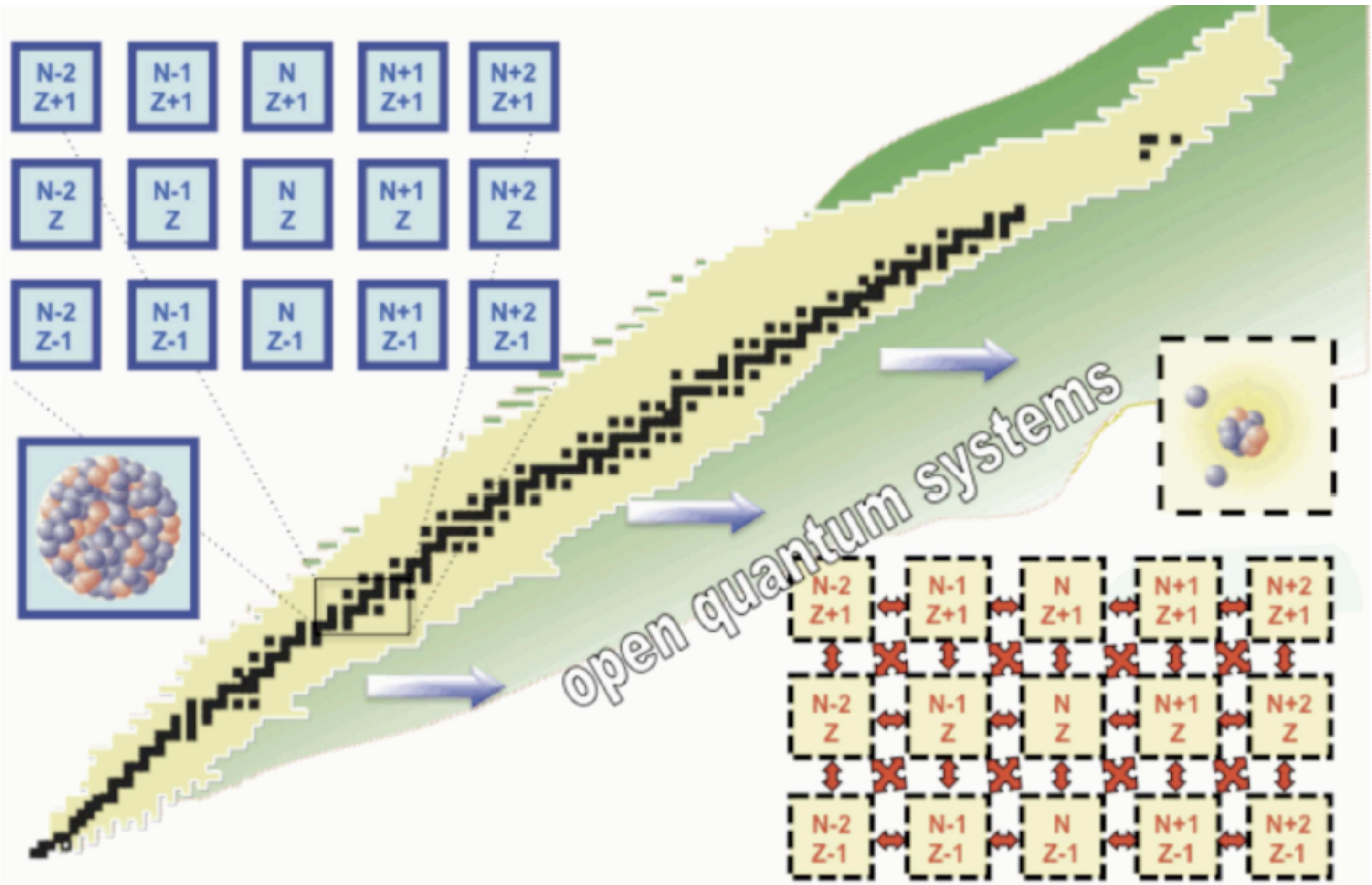
Reach of ab-initio computations of nuclei



H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

Physics of nuclei at the edges of stability

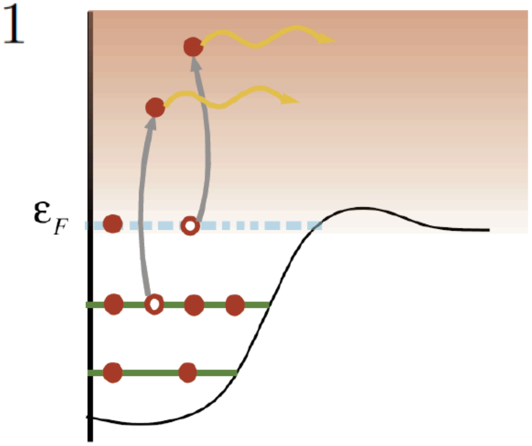
- Three and four neutron resonances – do they exist? (see talks by J. Lynn's and S. Shimoura's)
- At and beyond the neutron dripline, and the role of tetra neutron correlations in 8-He and 28-O (see talk by T. Aumann's)
- **Shell structure towards the dripline**, halo and Borromean structures

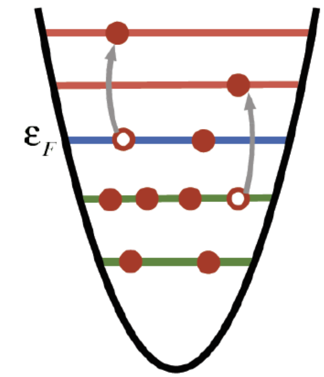


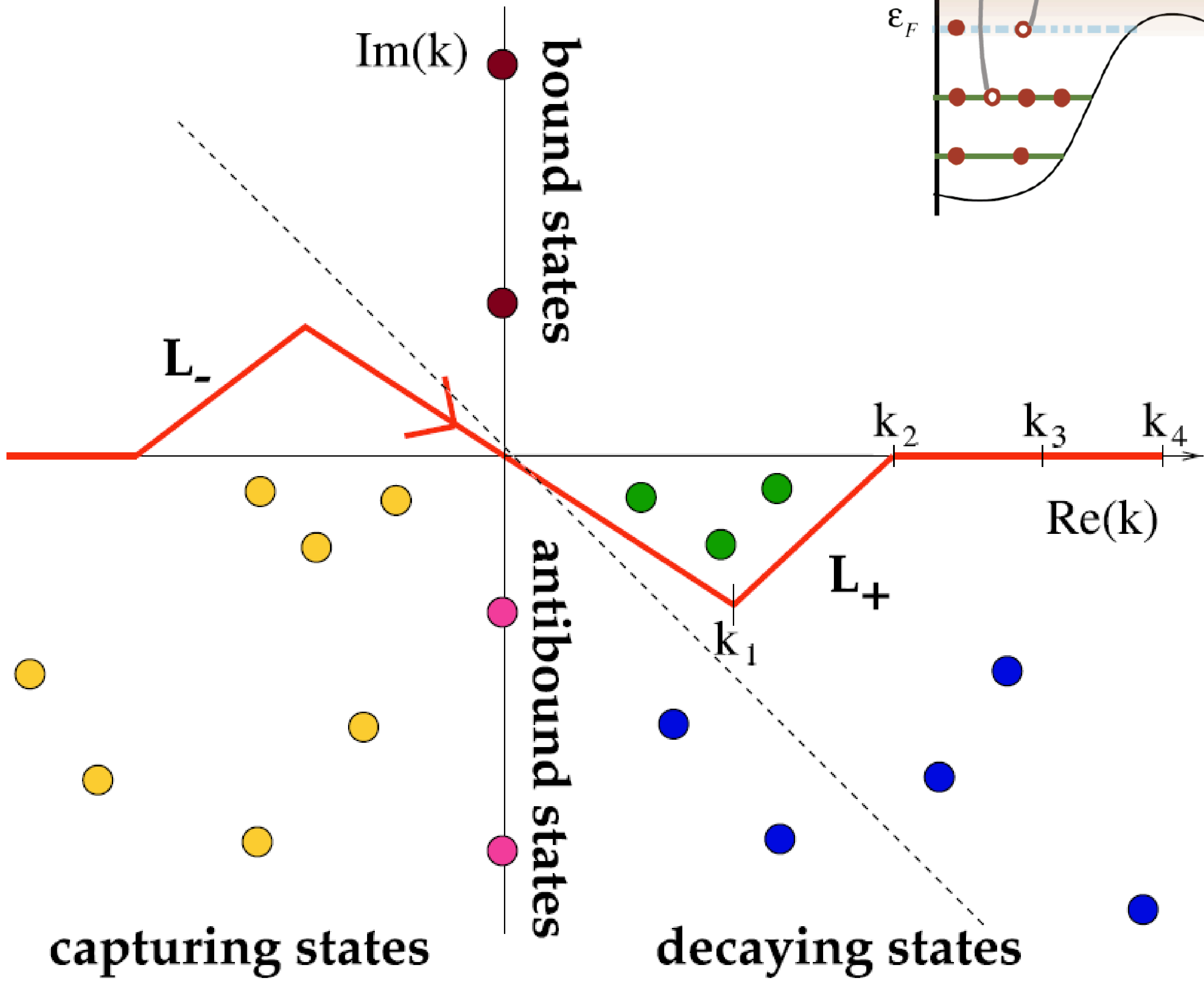
Physics of nuclei at the edges of stability

$$\sum_{n\in(b,d)} |u_n\rangle\langle u_n| + \int_{L^+} |u(k)\rangle\langle u(k)|dk = 1$$

T. Berggren Nucl. Phys. A 109 265 (1968)







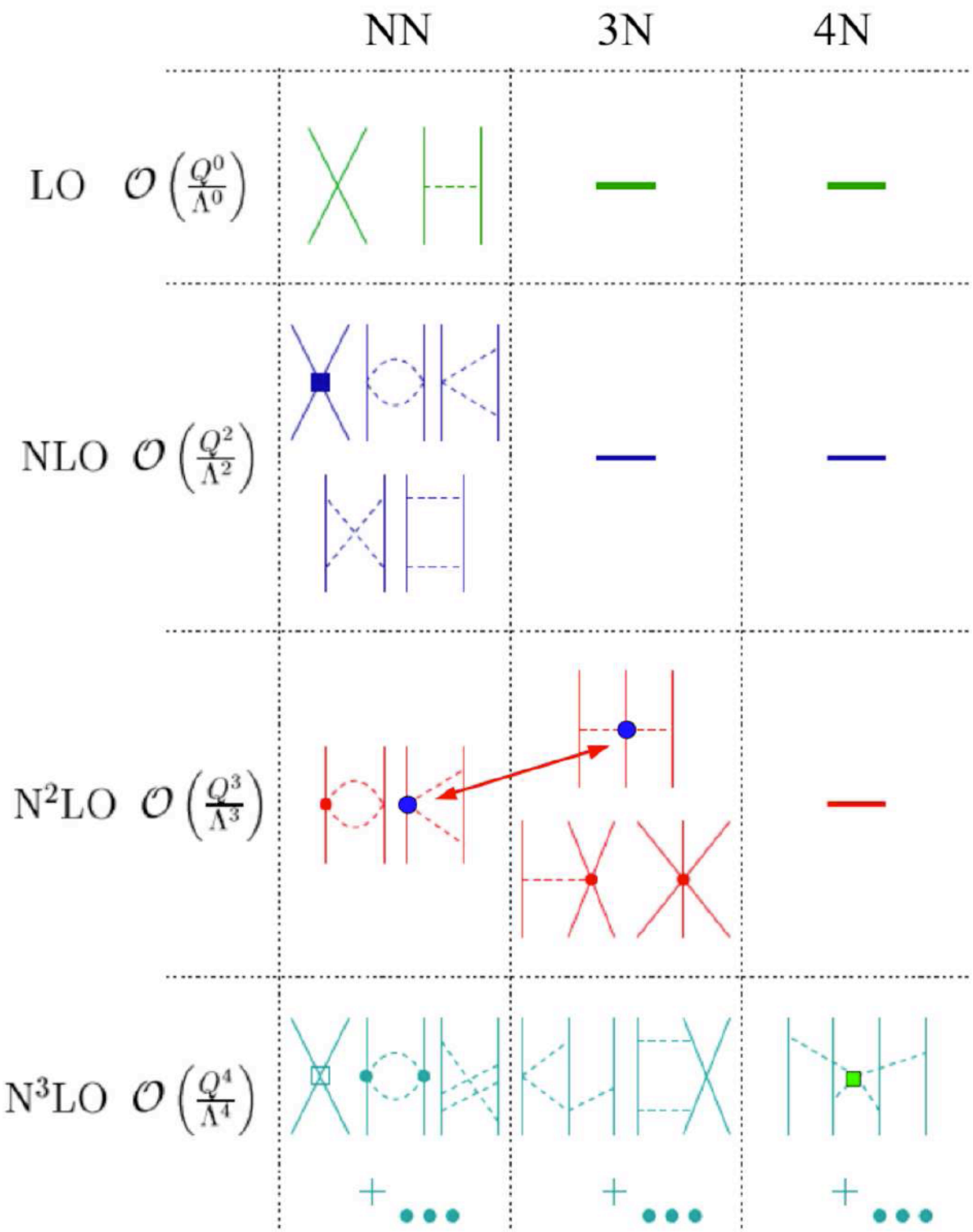
The Berggren completeness treats bound, resonant and scattering states on equal footing.

Has been successfully applied in the shell model in the complex energy plane to light nuclei. For a review see

N. Michel et al J. Phys. G 36, 013101 (2009).

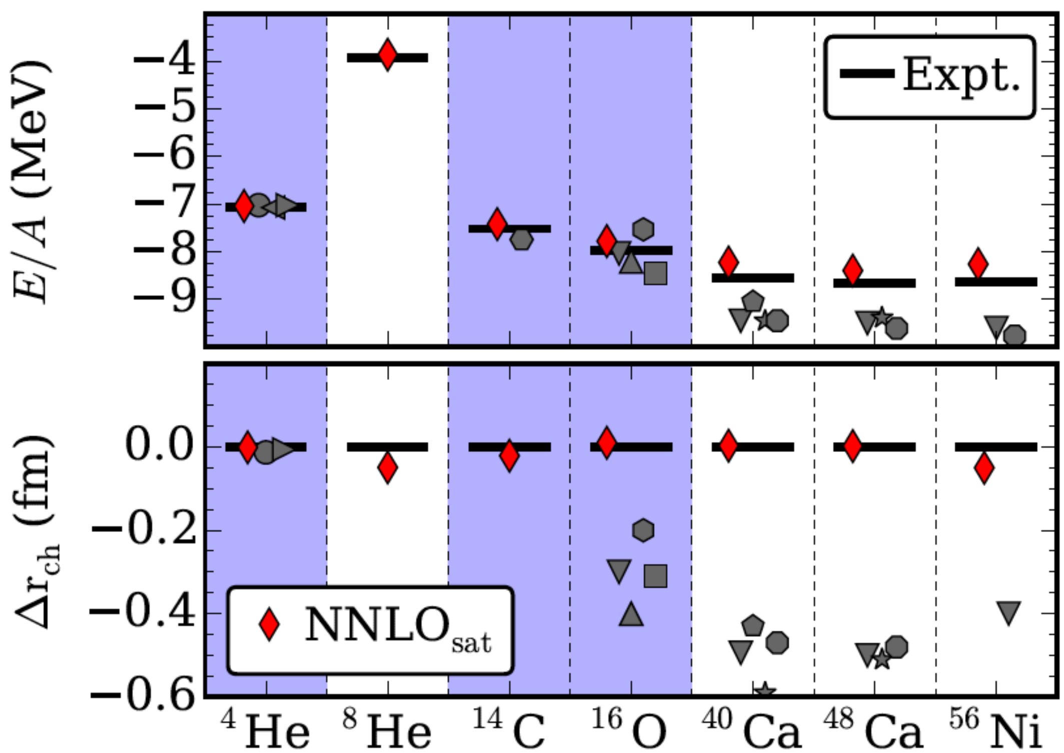
Nuclear forces from chiral effective field theory

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



- Developing higher orders and higher rank (3NF, 4NF) [Epelbaum 2006; Bernard et al 2007; Krebs et al 2012; Hebeler et al 2015; …]
- Propagation of uncertainties on the horizon [Navarro Perez 2014, Carlsson et al 2015]
- Different optimization protocols [Ekström et al 2013, Carlsson et al 2016]
- Improved understanding/handling via SRG [Bogner et al 2003; Bogner et al 2007]
- local / semi-local / non-local formulations [Epelbaum et al 2015, Gezerlis et al 2013/2014]
- Chiral EFT with explicit deltas are being developed and explored (Epelbaum 2008, Piarulli 2014, Ekström 2017)

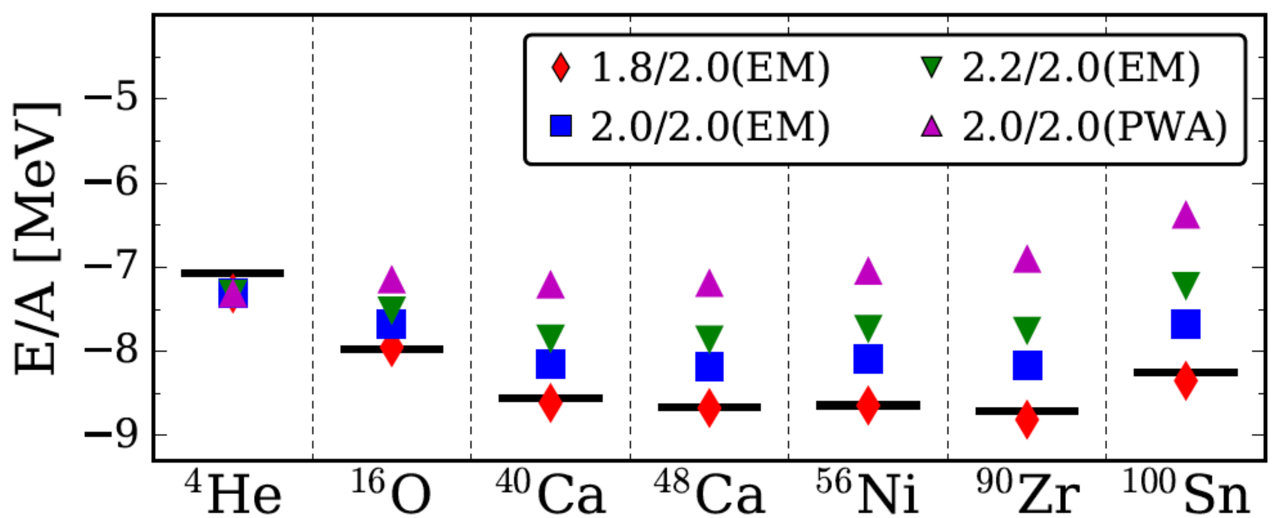
Two remarkable interactions from chiral EFT: $NNLO_{sat}$ & 1.8/2.0 (EM)



$NNLO_{sat}$: Accurate radii and BEs

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

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

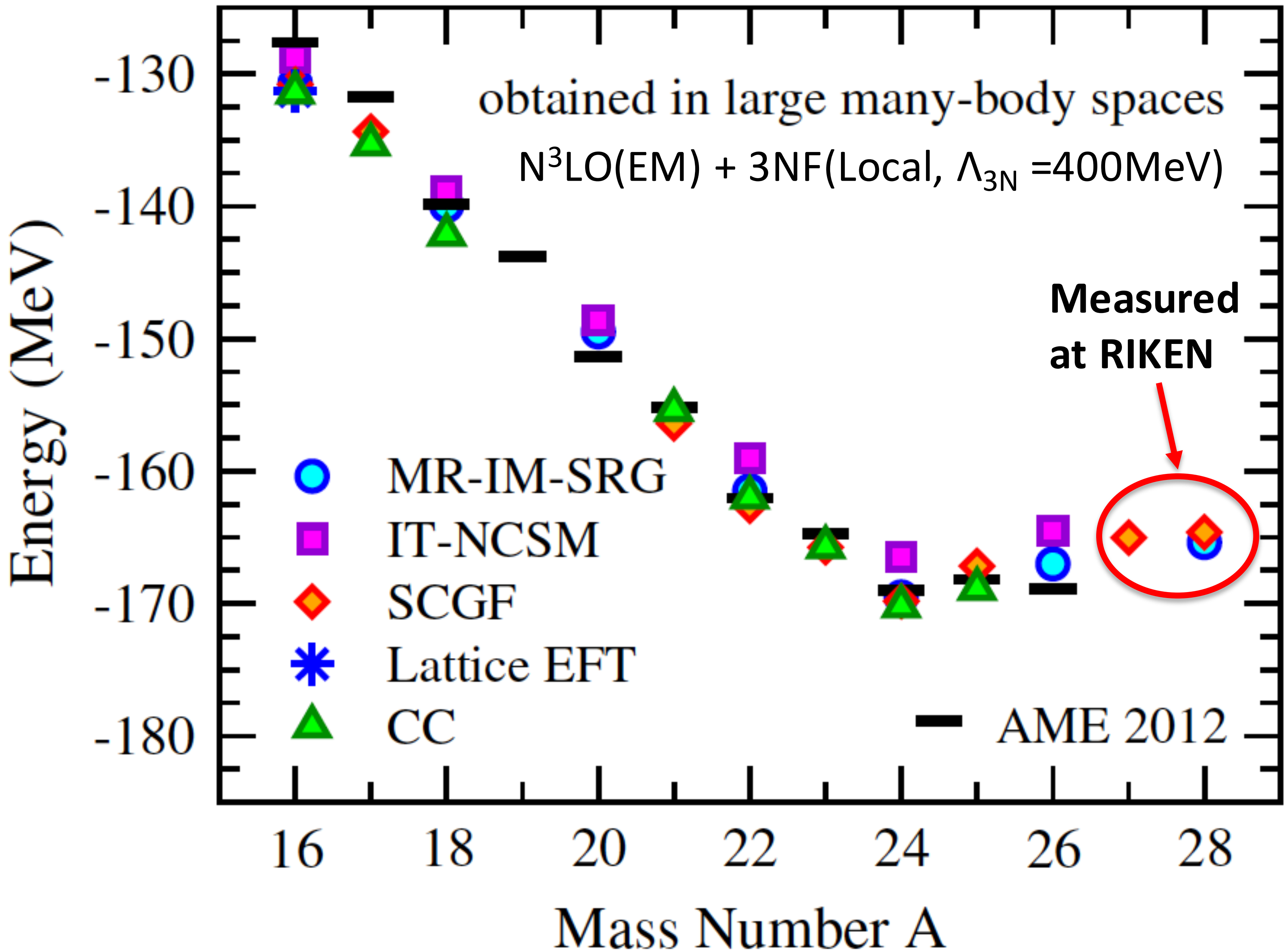


1.8/2.0(EM): Accurate BEs

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

K. Hebeler *et al* PRC (2011).
T. Morris *et al*, arXiv:1709.02786 (2017).

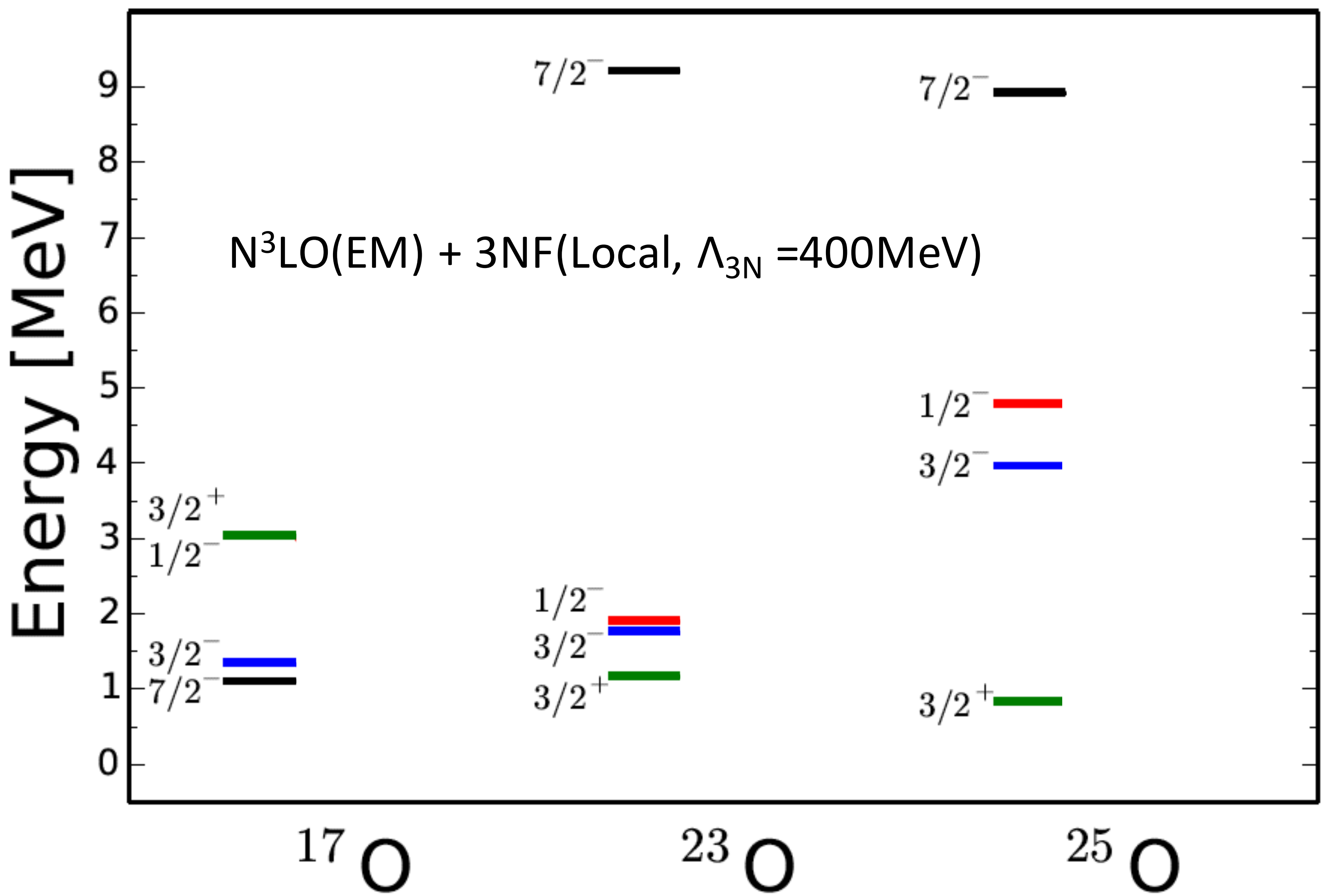
Oxgyen chain with interactions from chiral EFT



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

Role of continuum on unbound states in oxygen isotopes

G. Hagen et al, Phys. Scr. **91**, 063006 (2016).



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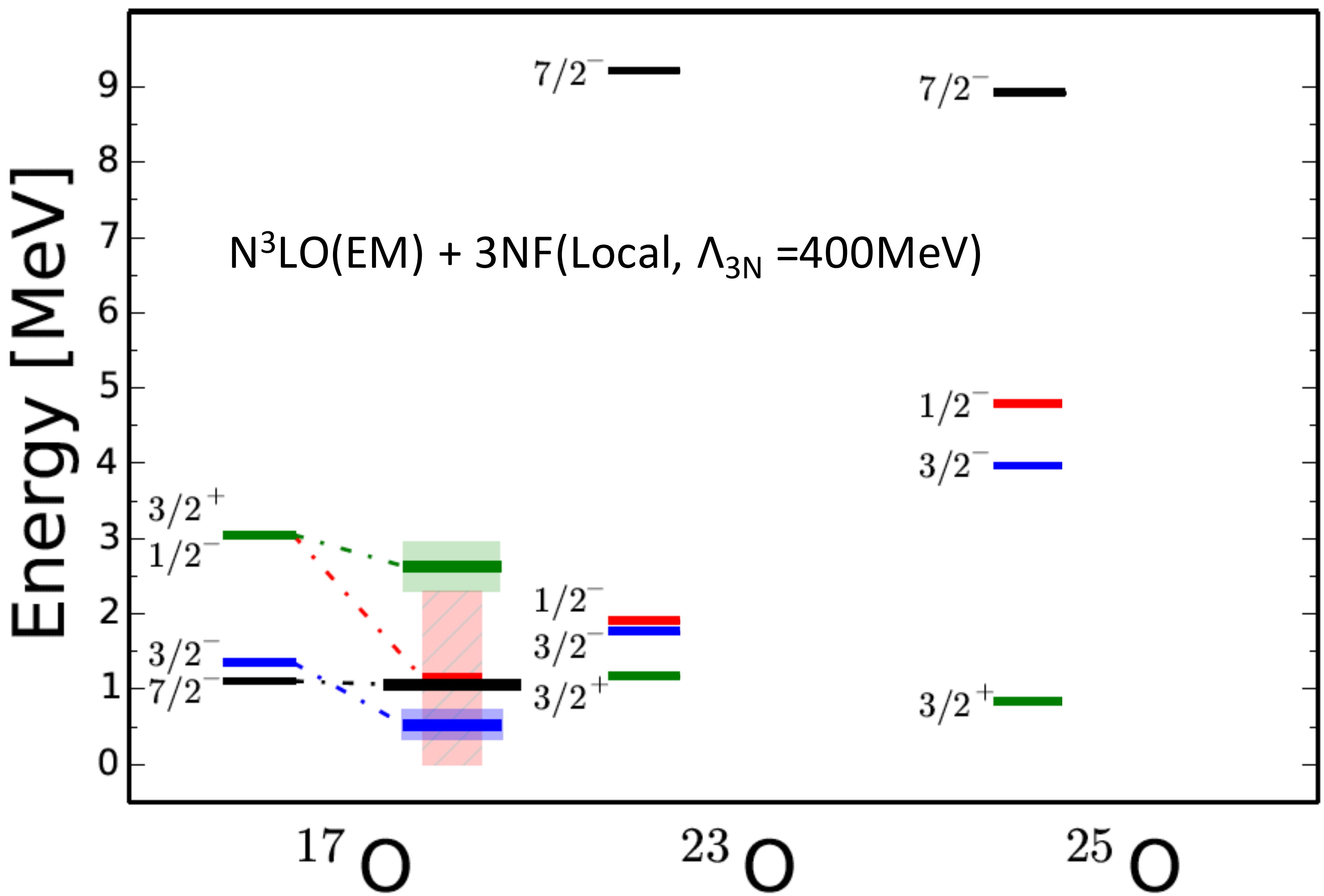

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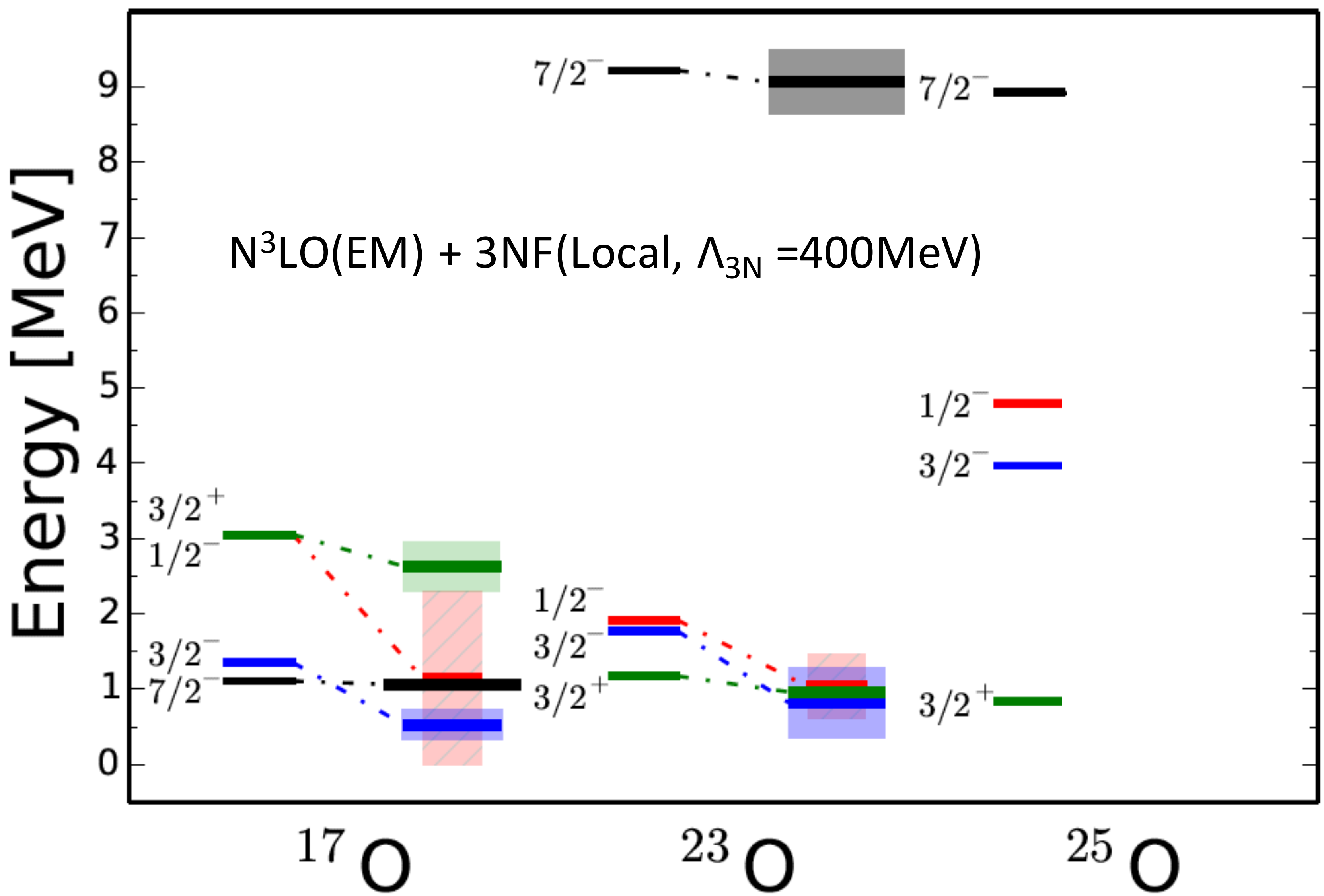

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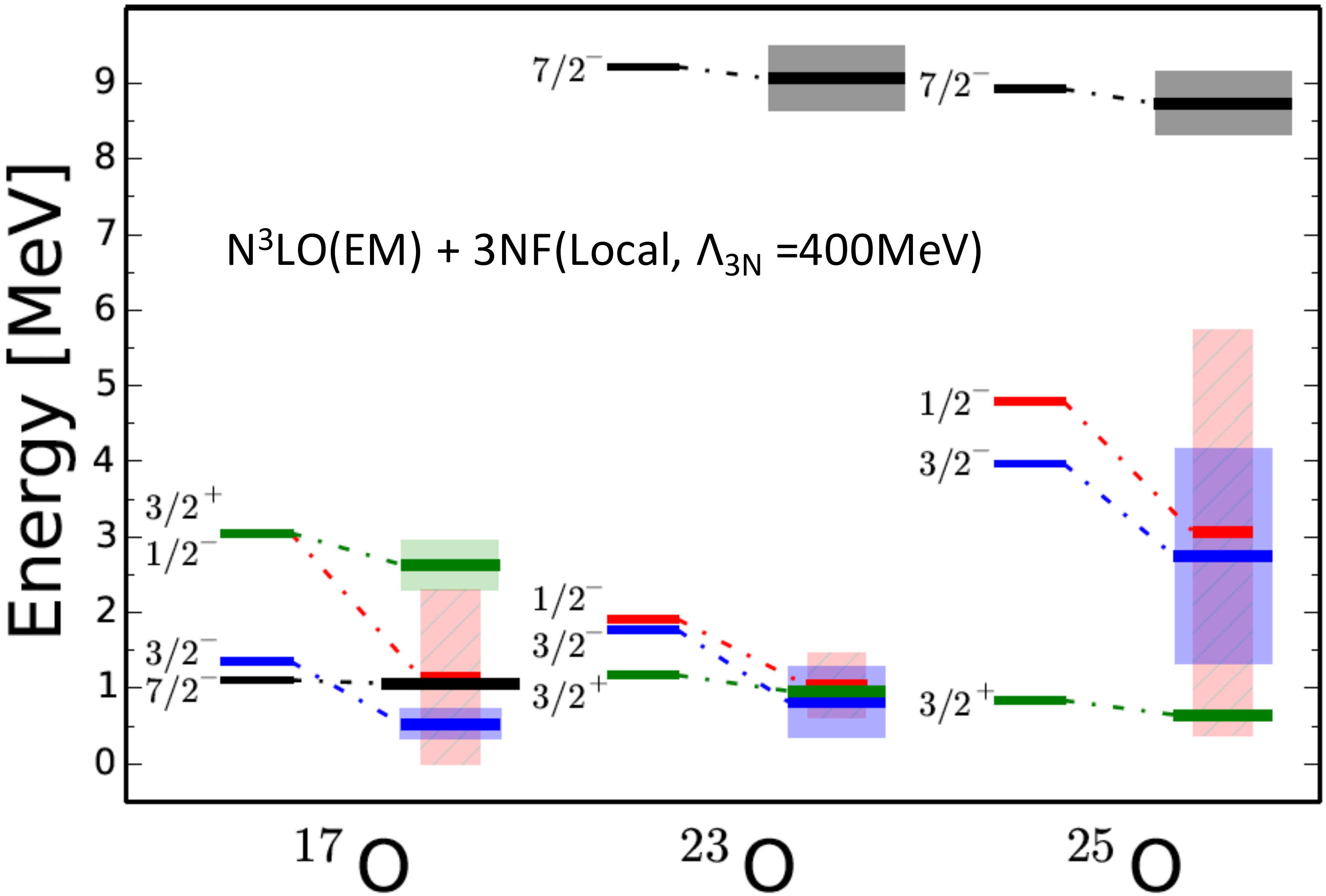
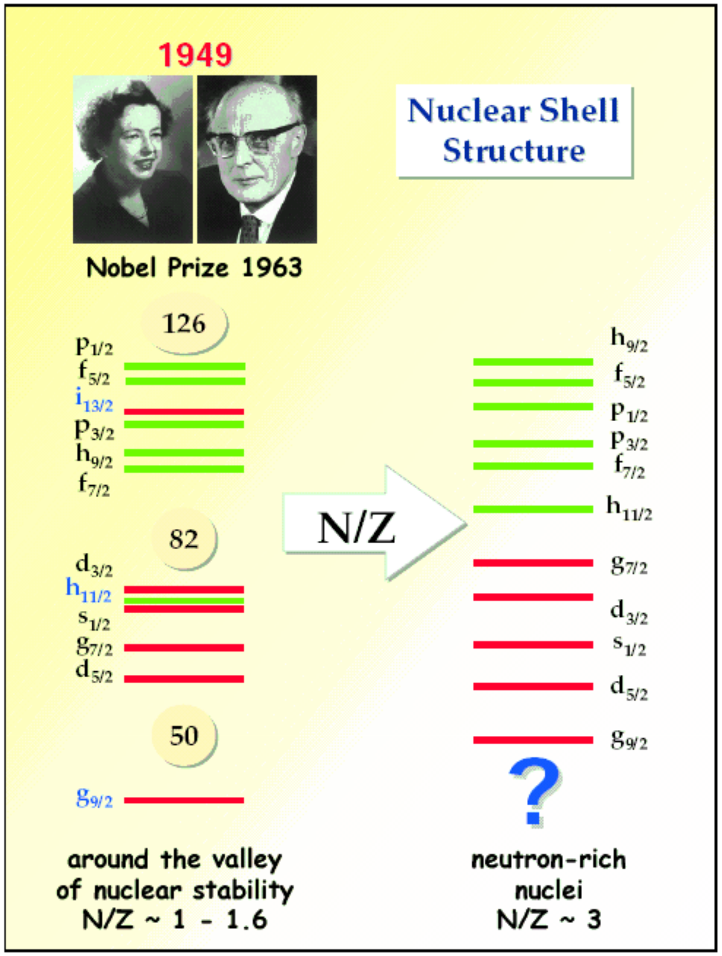
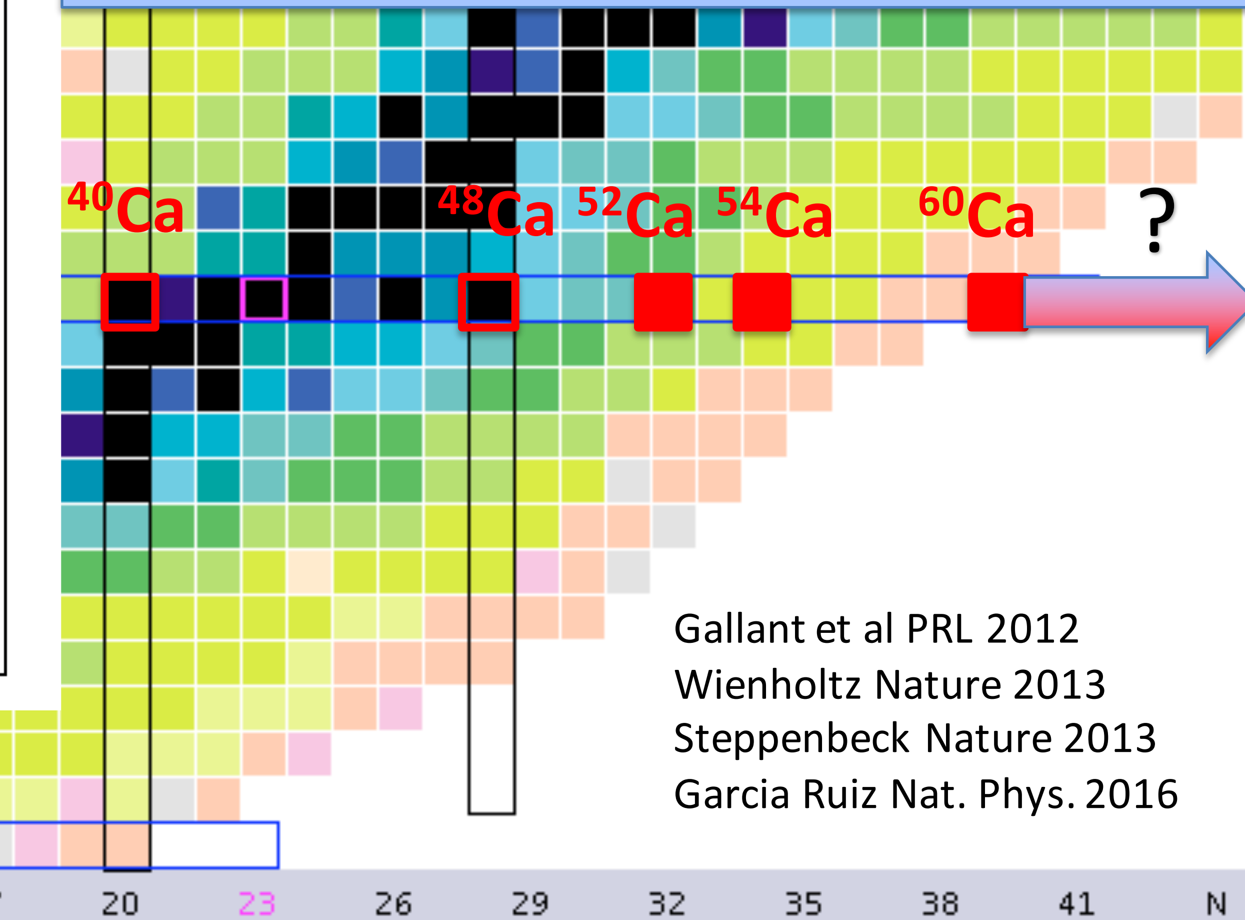


Evolution of shell structure in neutron rich calcium



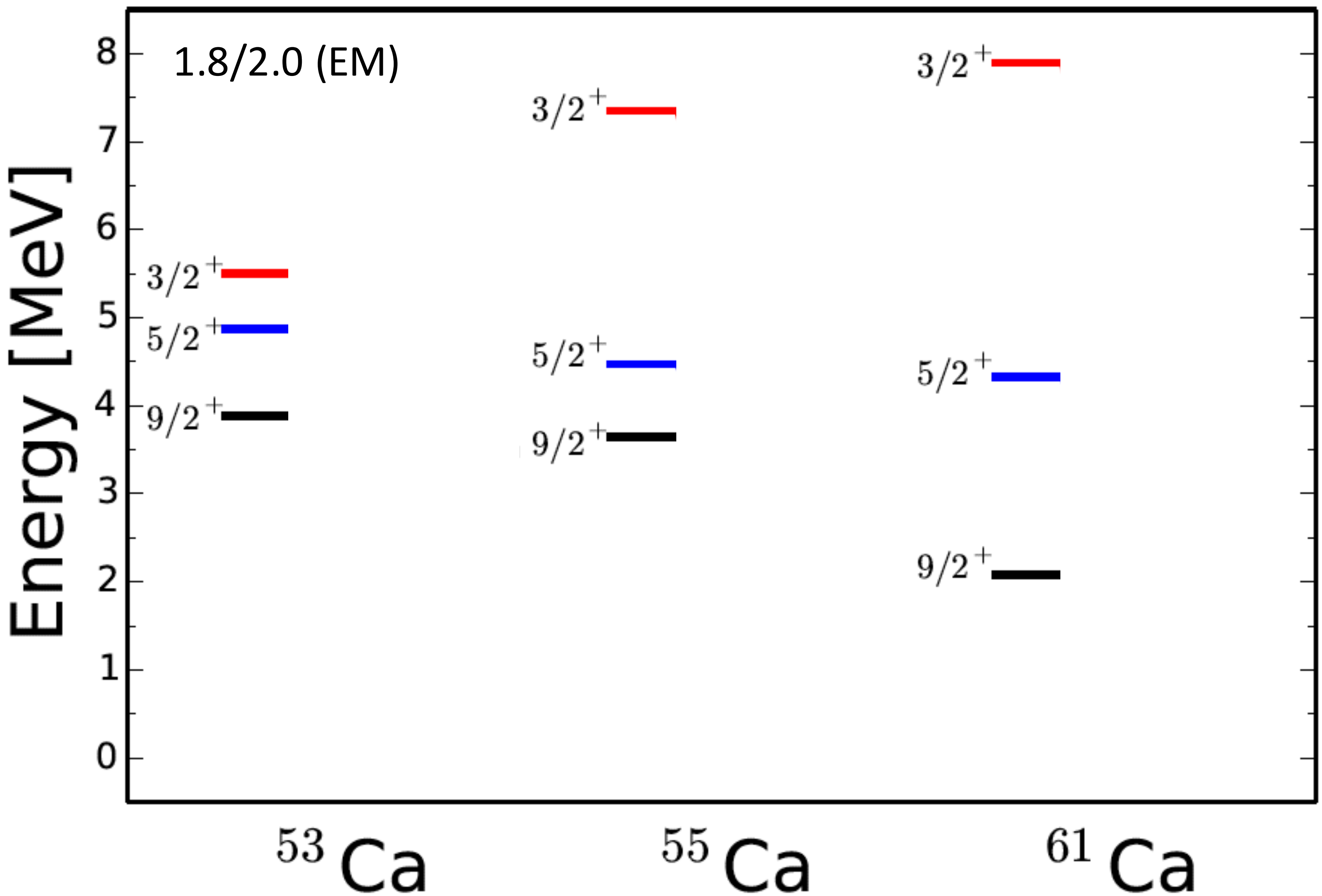
- How do shell closures and magic numbers evolve towards the dripline?
- What are the mechanisms for new shell structure?



Gallant et al PRL 2012
Wienholtz Nature 2013
Steppenbeck Nature 2013
Garcia Ruiz Nat. Phys. 2016

Role of continuum on unbound states in neutron rich calcium

G. Hagen et al, Phys. Scr. **91**, 063006 (2016).



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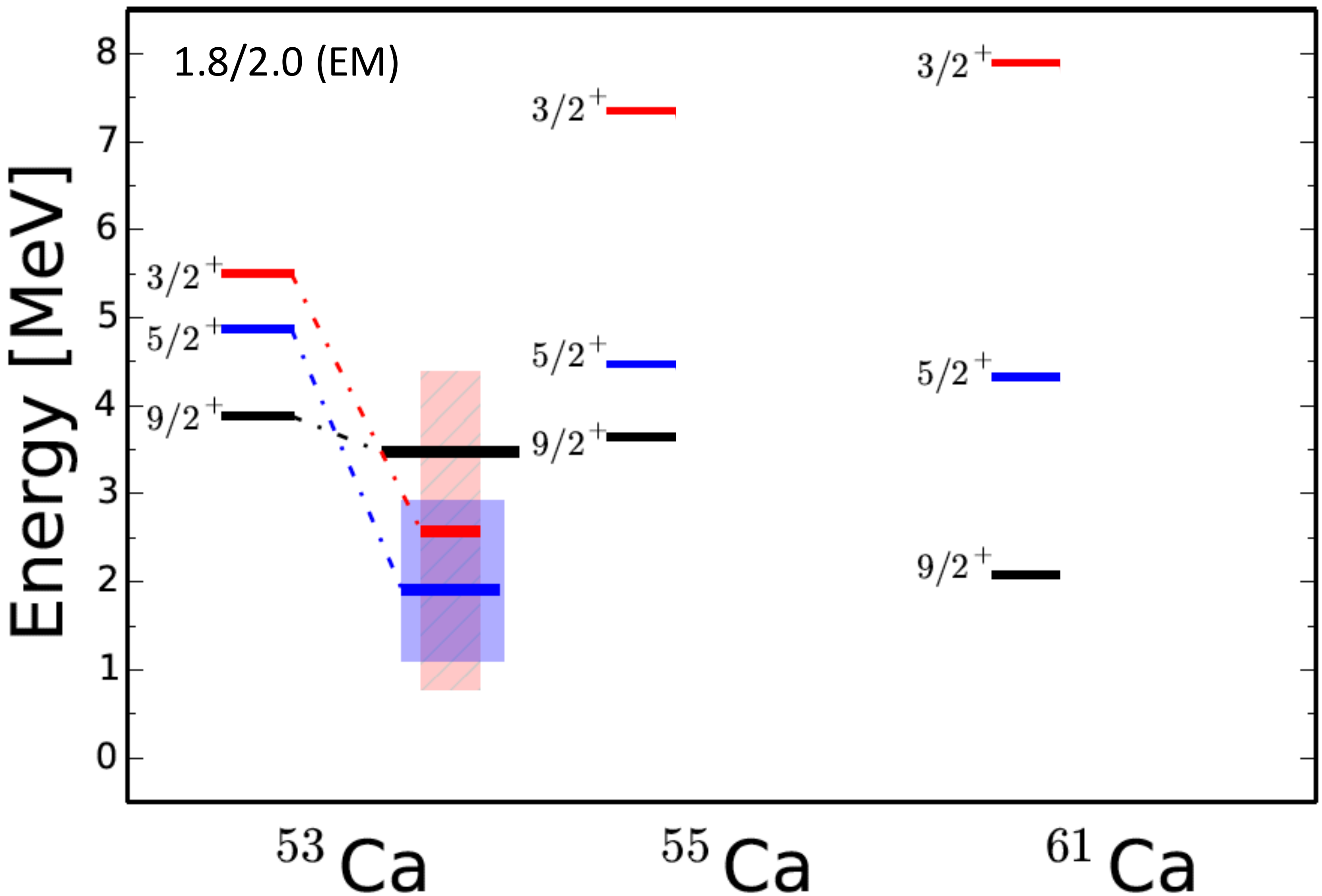

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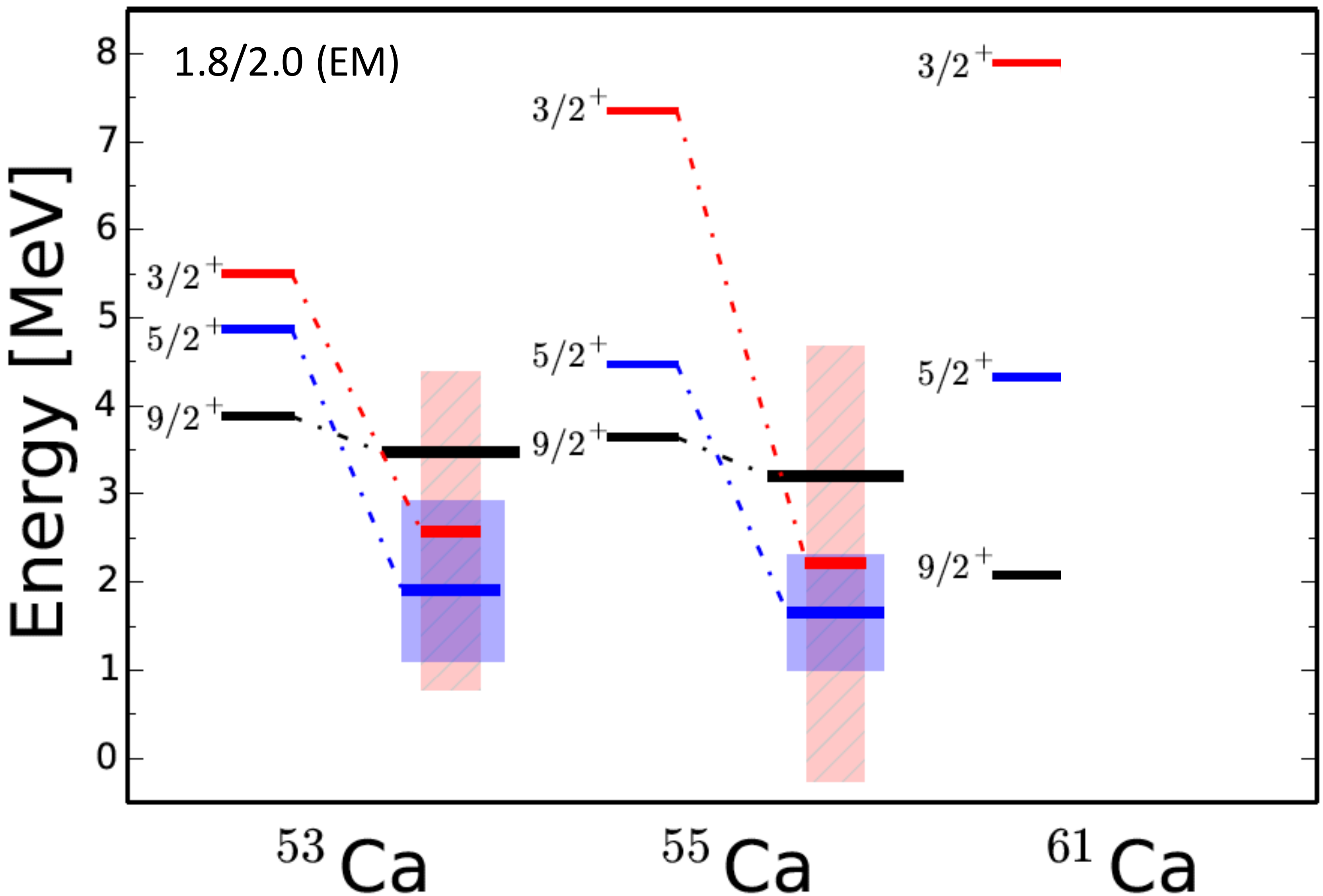

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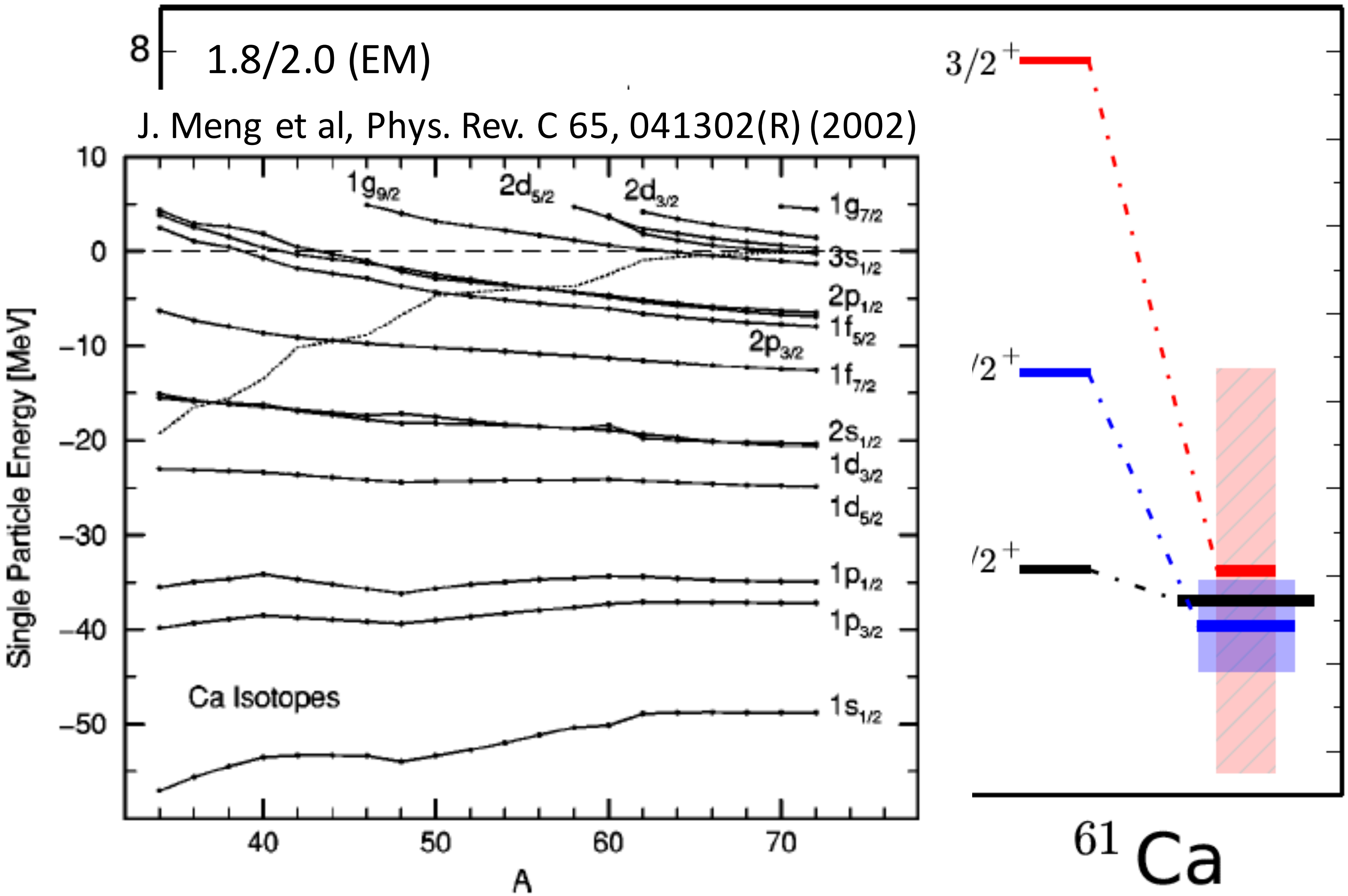
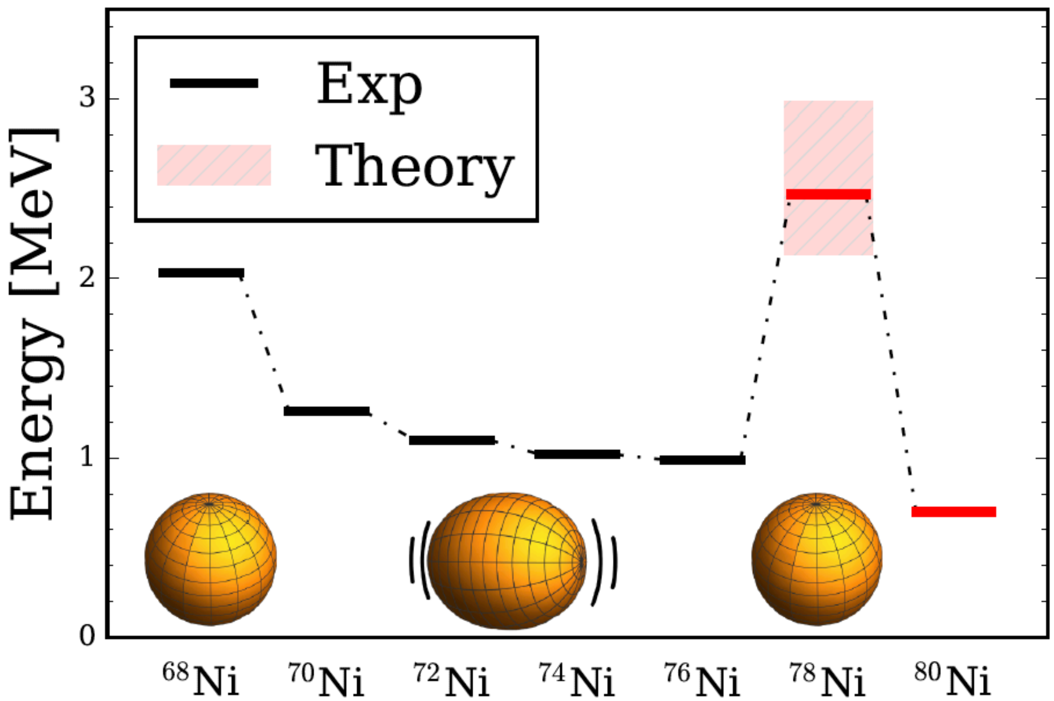


Structure of ^{78}Ni from first principles

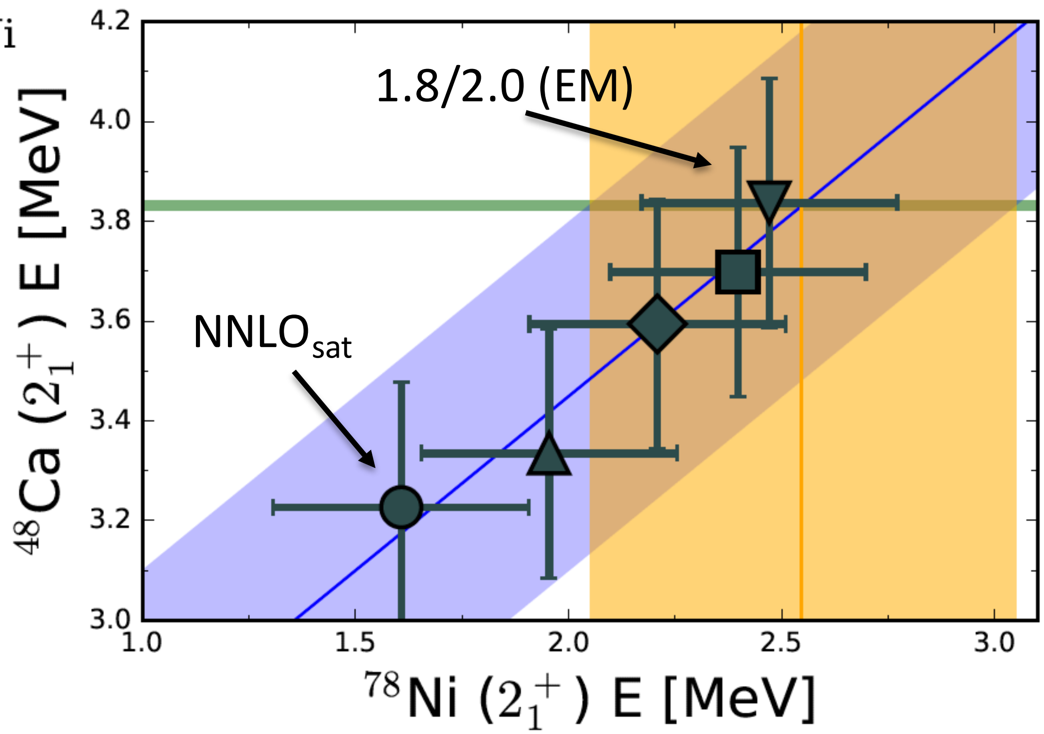


A high 2$^+$ energy in ^{78}Ni indicates that this nucleus is doubly magic

Consistent with recent shell-model studies
F. Nowacki *et al.,* PRL 117, 272501 (2016)

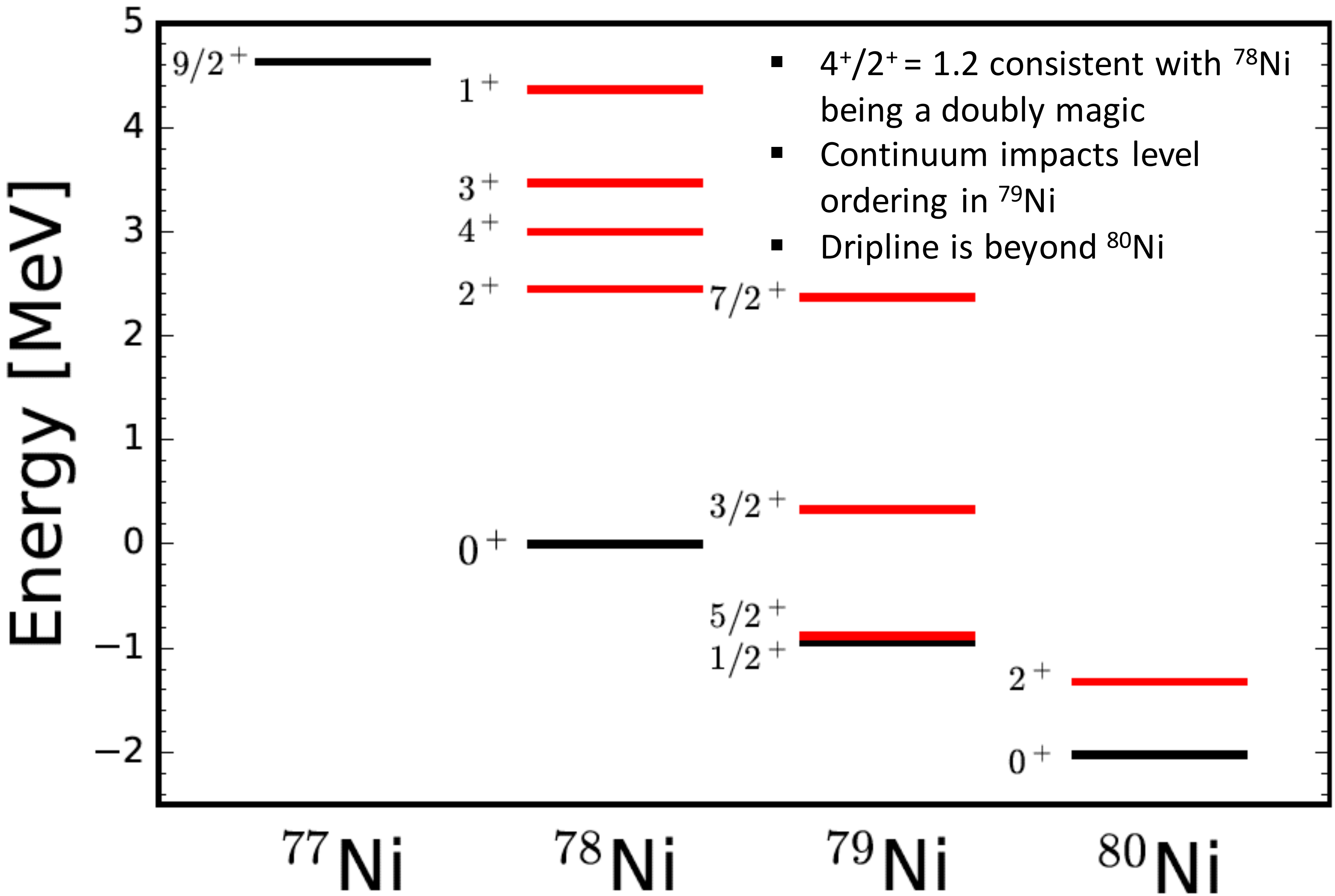
A measurement of this state has been made at RIBF, R. Taniuchi *et al.*, in preparation

- From an observed correlation we predict the 2$^+$ excited state in ^{78}Ni using the experimental data for the 2$^+$ state in ^{48}Ca
- Similar correlations have been observed in other nuclei, e.g. Tjon line in light nuclei



G. Hagen, G. R. Jansen, and T. Papenbrock
Phys. Rev. Lett. **117**, 172501 (2016)

Excited states in ^{78}Ni and its neighbors



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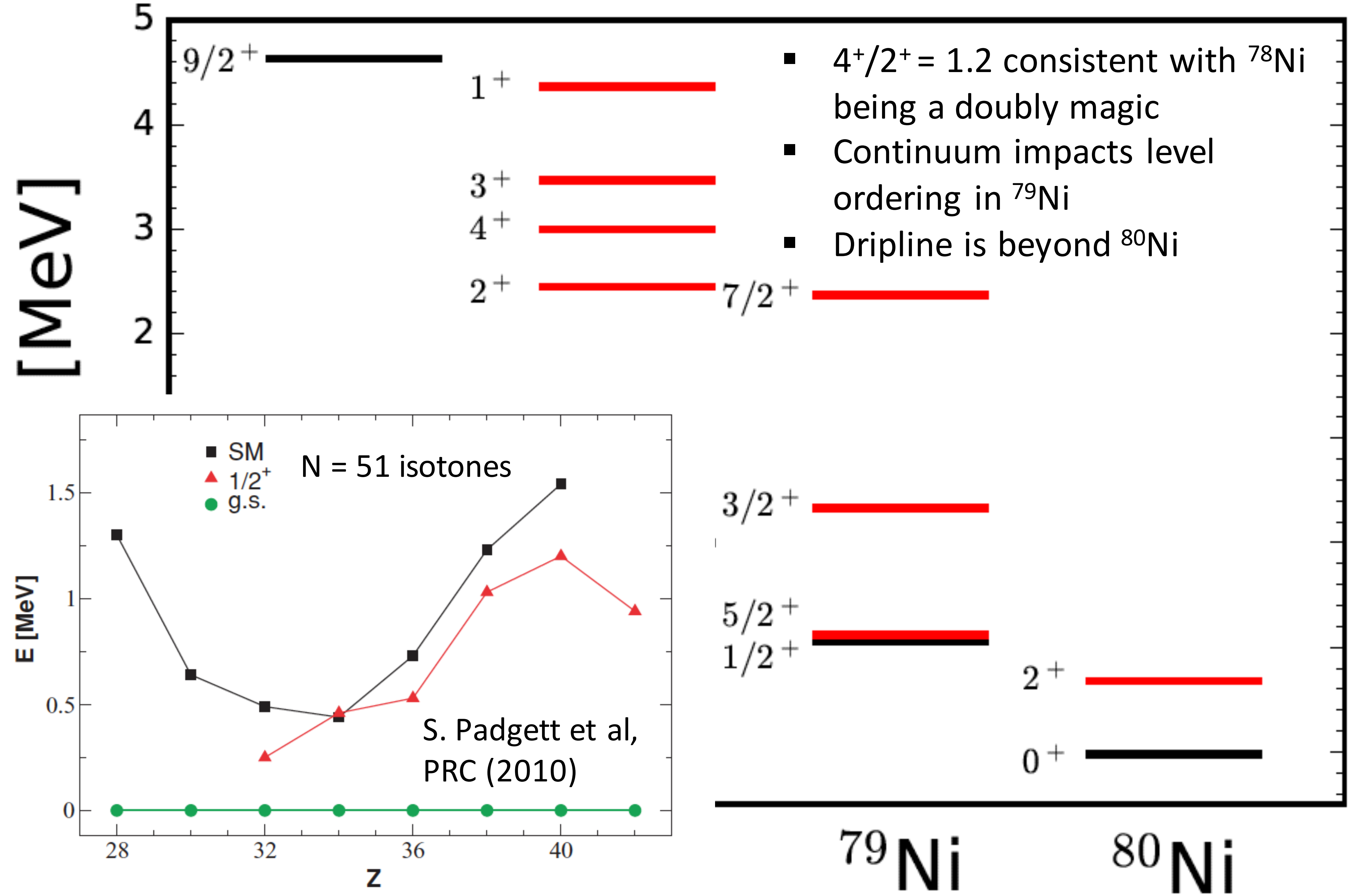

- $4^+/2^+ = 1.2$ consistent with ^{78}Ni being a doubly magic
- Continuum impacts level ordering in ^{79}Ni
- Dripline is beyond ^{80}Ni

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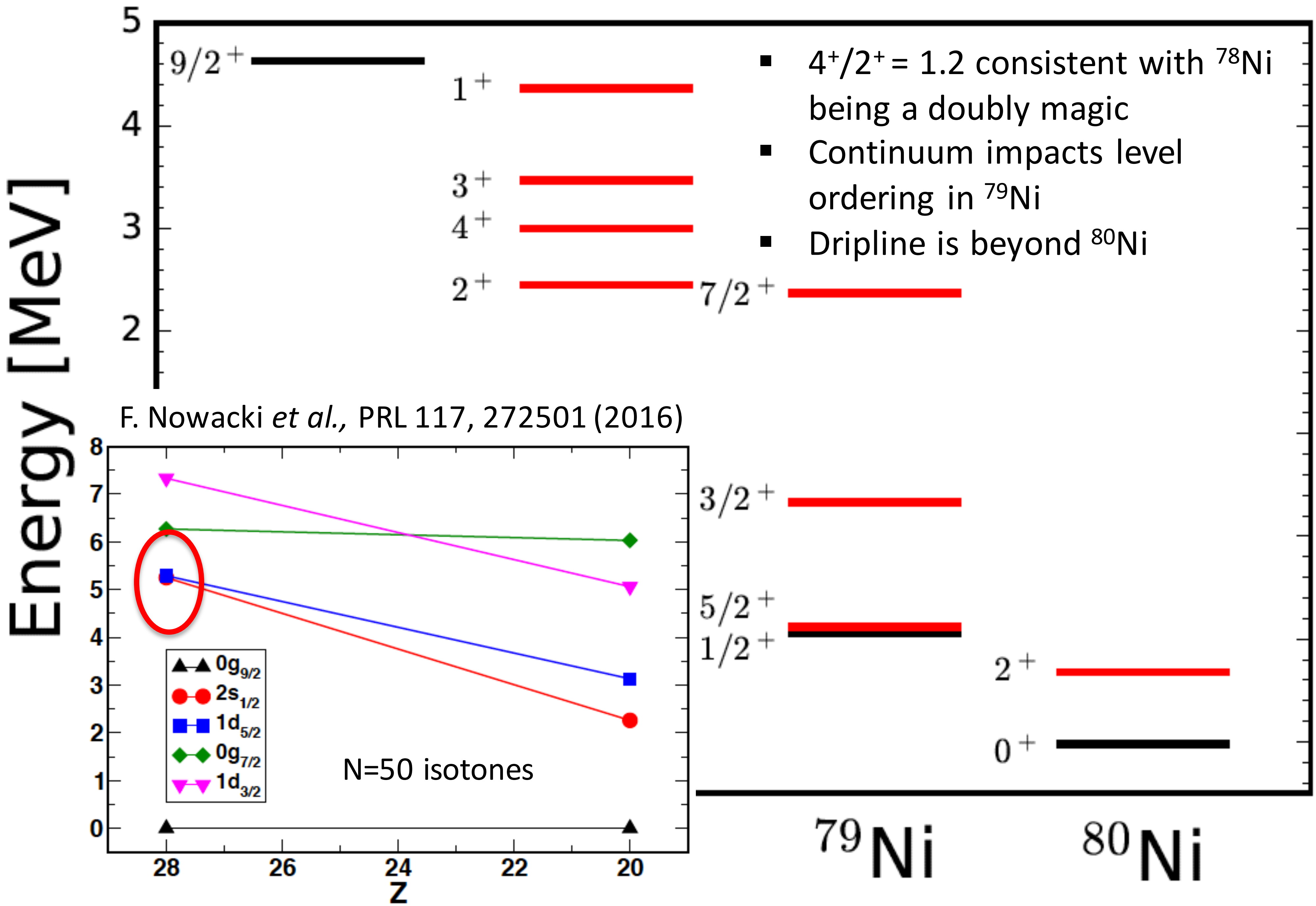
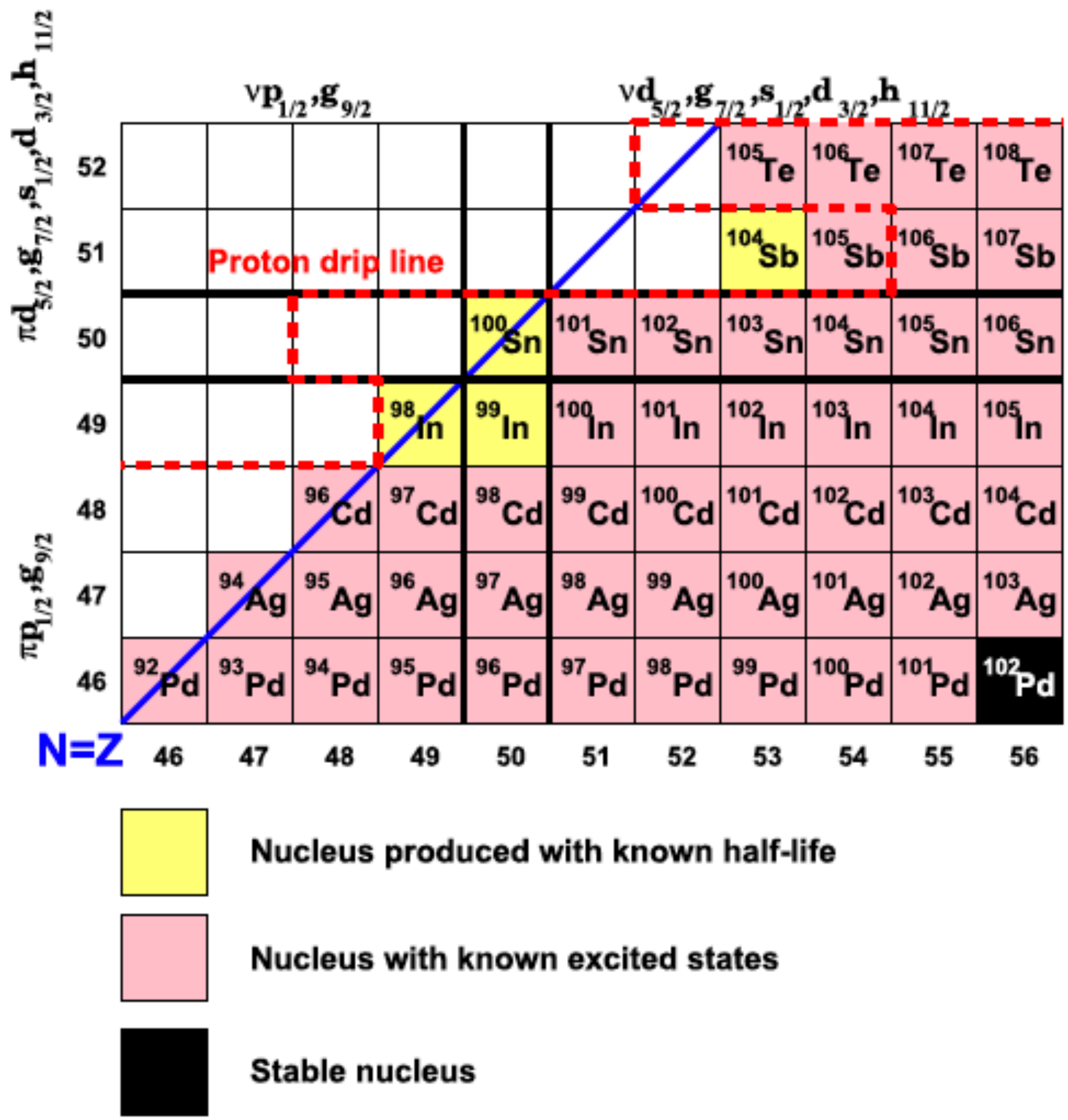


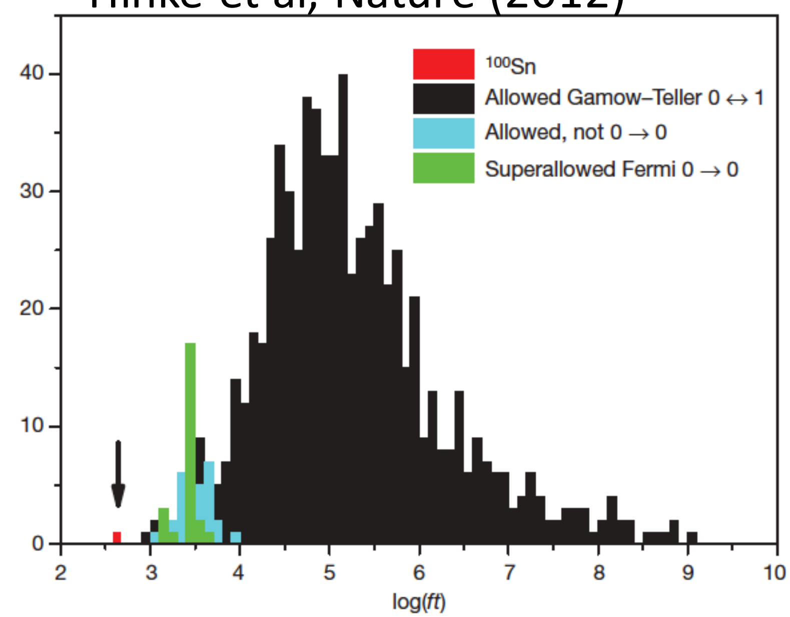
F. Nowacki *et al.*, PRL 117, 272501 (2016)

^{100}Sn – a nucleus of superlatives

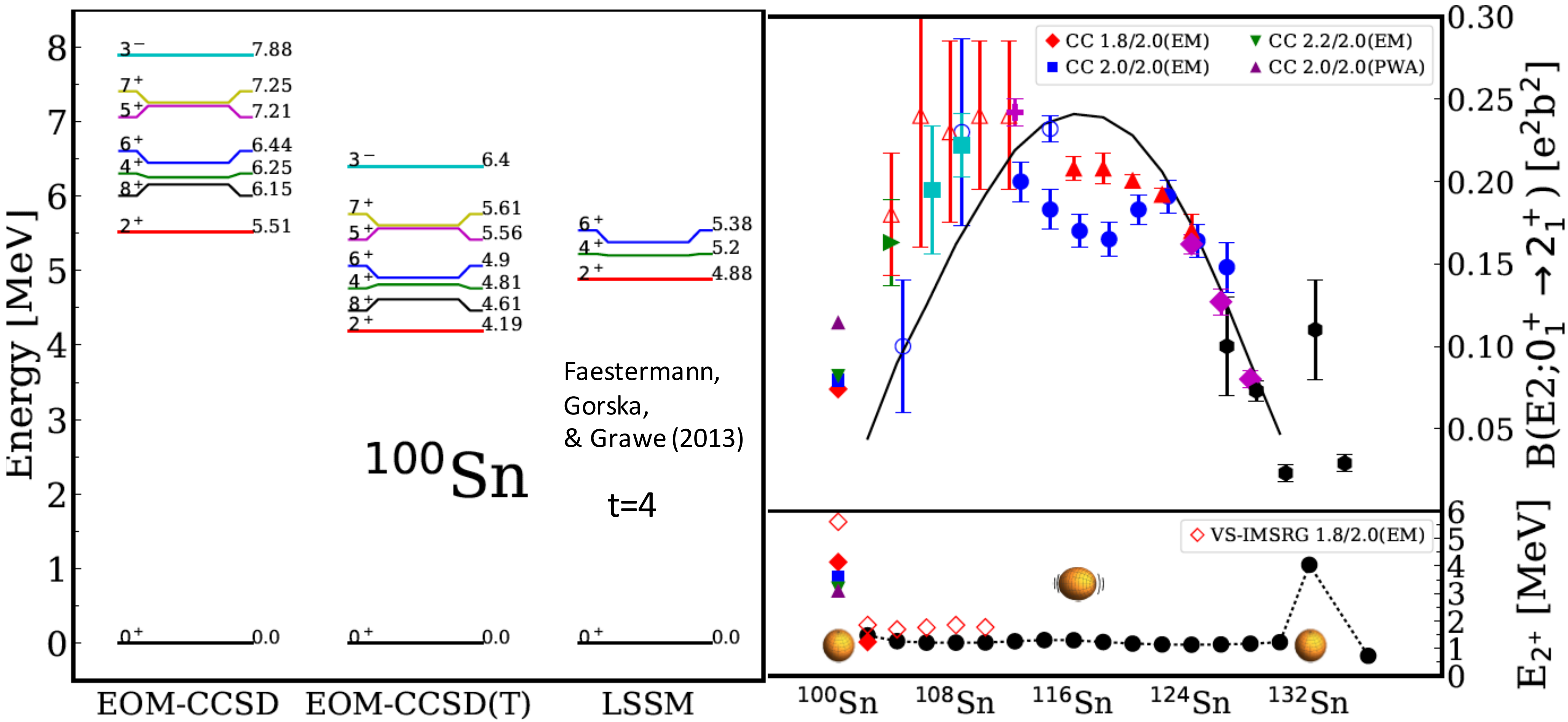


- Heaviest self-conjugate doubly magic nucleus
- Largest known strength in allowed nuclear β-decay
- In the closest proximity to the proton dripline

Hinke et al, Nature (2012)

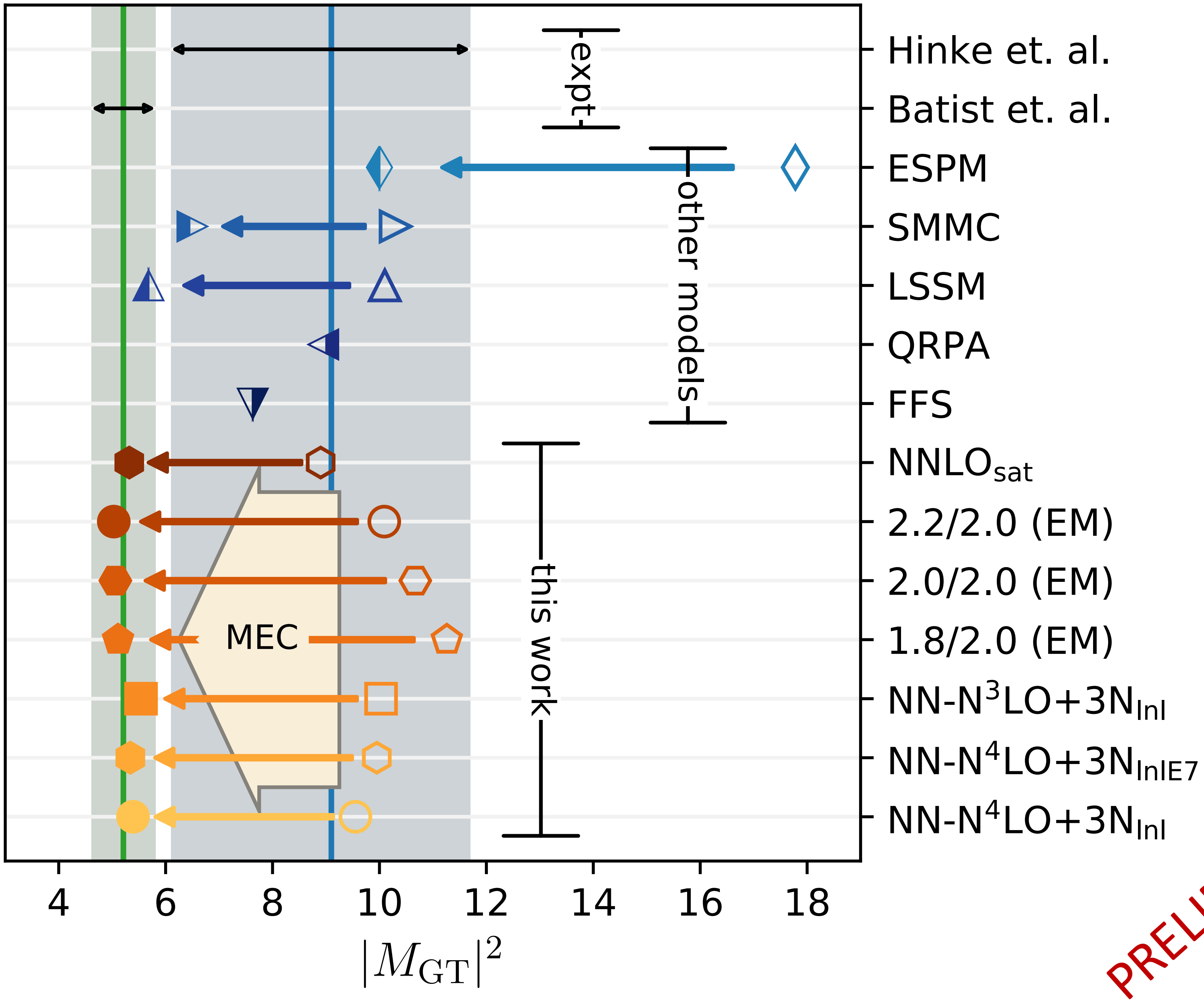


Structure of the ligthest tin isotopes



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

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



PRELIMINARY

Quantum computing

1. The quantum many-body problem is one the key challenges in physics
2. Exponential growth of Hilbert space in wave function based methods and sign problem in Monte-Carlo methods.
3. Quantum computers promise to reduce computational complexity from exponential to polynomial cost
4. A quantum computer with about 100 error corrected qubits could potentially revolutionize nuclear shell-model calculations

Quantum computing

There is a lot of excitement in this field due to substantial progress

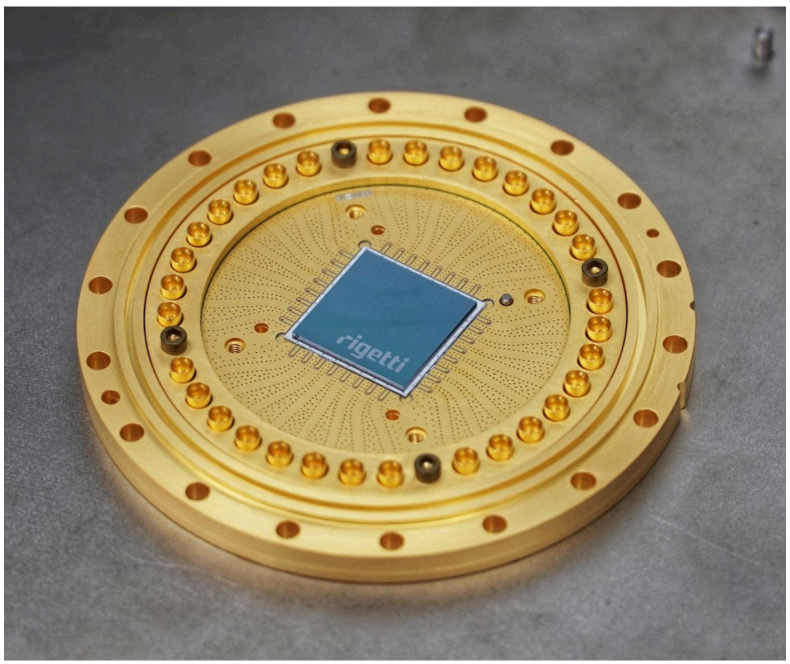
1. Quantum processing units now have ten(s) of qubits
2. Businesses are driving this: Google, IBM, Microsoft, Rigetti, D-Wave, …
3. Software is publicly available (PyQuil, XACC, OpenQASM, OpenFermion)
4. First real-world problems solved on 2 to 6 qubits [O'Malley et al. Phys. Rev. X 6, 031007 (2016); Kalandar et al., Nature 549, 242(246 (2017)]

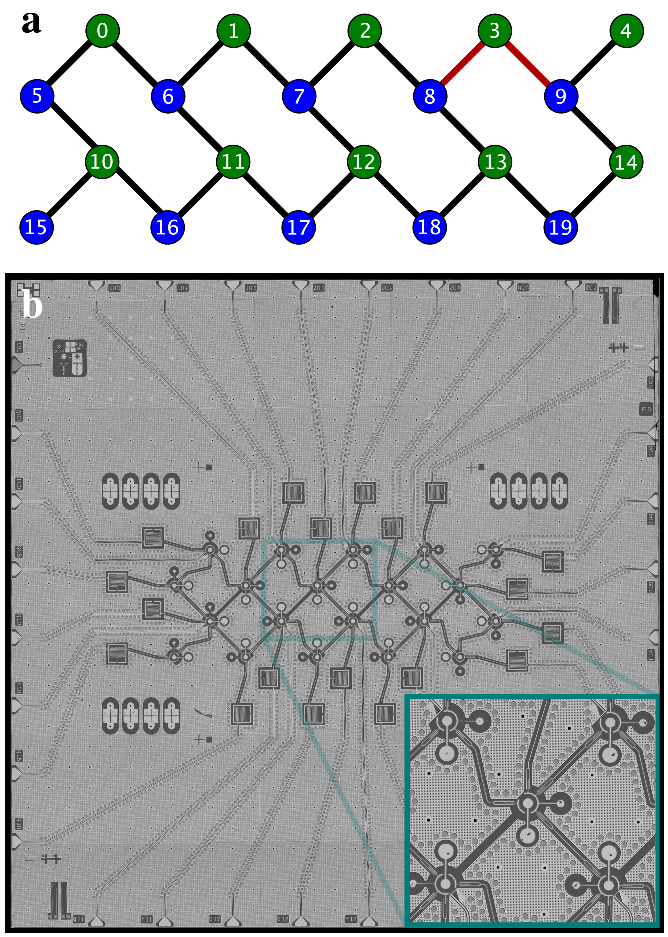
The scientific works were collaborations between theorists and hardware specialists (owners/operators of quantum chips)

Now: Cloud access possible; no insider knowledge required!
[Dumitrescu, McCaskey, Hagen, Jansen, Morris, Papenbrock, Pooser, Dean, Lougovski, arXiv:1801.03897]

Rigetti 19Q

Superconducting qubits

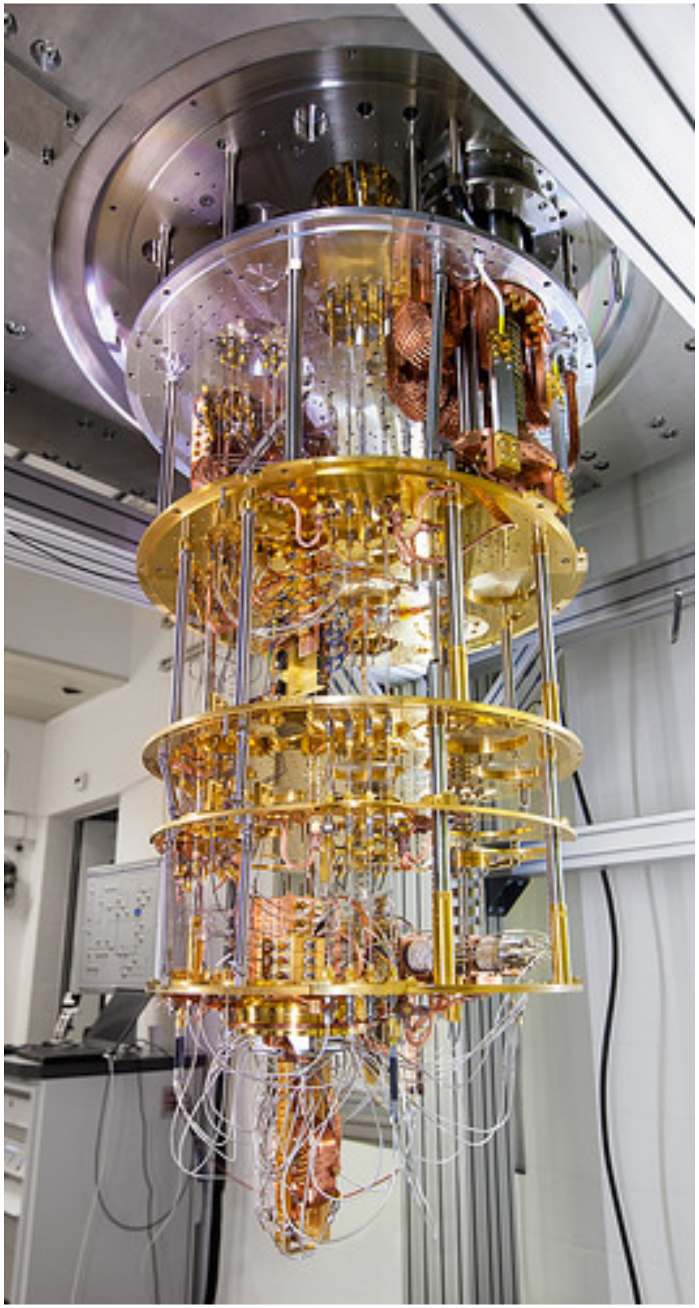


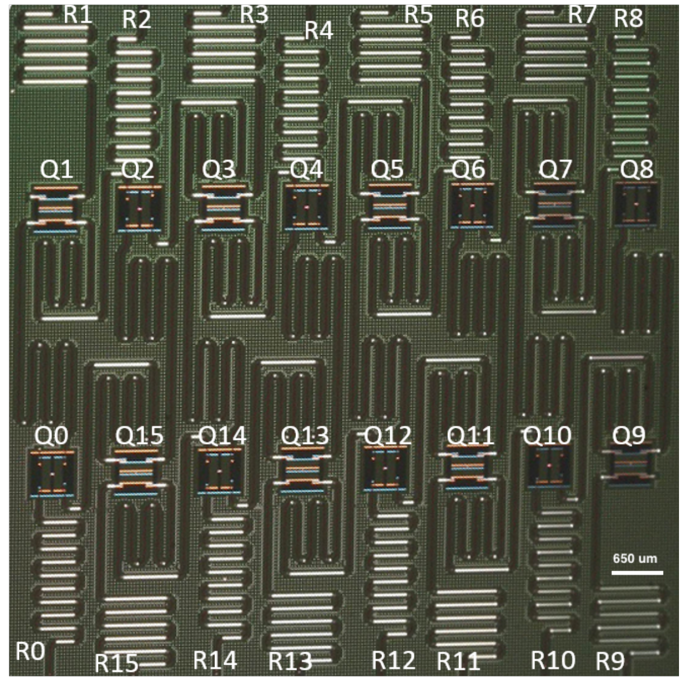


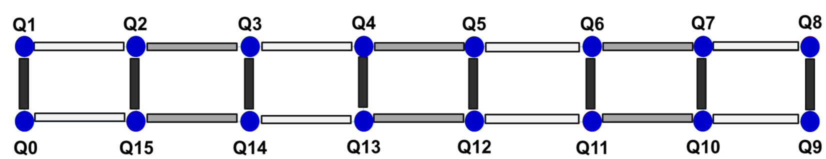
Connectivity of Rigetti 19Q.
a, *Chip schematic showing tunable transmons (green circles) capacitively coupled to fixed-frequency transmons (blue circles).*
b, *Optical chip image. Note that some couplers have been dropped to produce a lattice with three-fold, rather than four-fold connectivity.*

Otterbach et al, arXiv:1712.05771

IBM QX5 (16 qubits)







→ IBM Q Experience

Current limitations/challenges

- Faced with limited connectivity between qubits on a quantum chip
- Limited to low depth (the number of sequential gates) of quantum circuits due to decoherence
- Limited number of measurements via the cloud
- Intermittent cloud access in a scheduled environment must be taken into account

Game plan

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis; [à la Binder et al. (2016)]

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a^\dagger_{n'} a_n \qquad \langle n'|V|n\rangle = V_0 \delta^0_n \delta^{n'}_n$$

$$V_0 = -5.68658111 \text{ MeV}$$

2. Map single-particle states |n> onto qubits; (Analog of Jordan-Wigner transform)

$$a^\dagger_p \leftrightarrow \sigma^{(p)}_- \equiv \frac{1}{2}(X_p - iY_p)$$
$$a_p \leftrightarrow \sigma^{(p)}_+ \equiv \frac{1}{2}(X_p + iY_p)$$

3. Solve H_1, H_2 (and H_3), and extrapolate to infinite space [Furnstahl, More, Papenbrock (2014)]

$$E_N = -\frac{\hbar^2 k^2}{2m}\left(1 - 2\frac{\gamma^2}{k} e^{-2kL} - 4\frac{\gamma^4 L}{k} e^{-4kL}\right) + \frac{\hbar^2 k \gamma^2}{m}\left(1 - \frac{\gamma^2}{k} - \frac{\gamma^4}{4k^2} + 2w_2 k \gamma^4\right) e^{-4kL}$$

Variational wave function

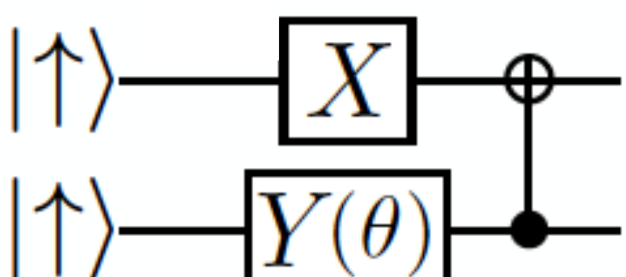
Generate unitary transformation for two and three qubit case

$$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0 Y_1 - X_1 Y_0)}$$

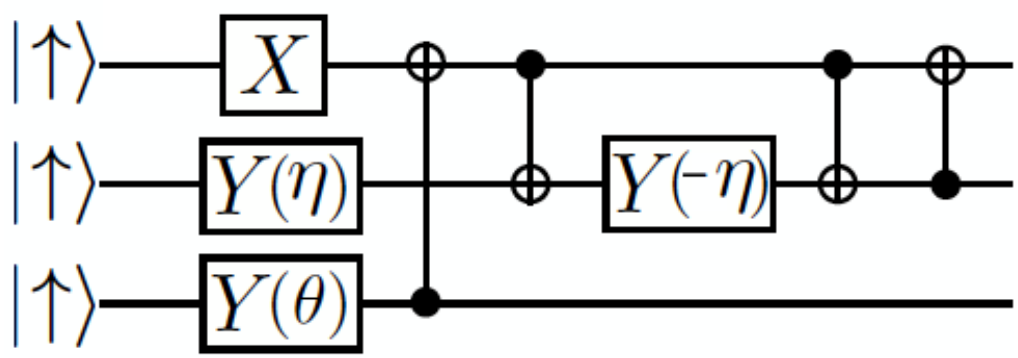
$$U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)+\theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

Minimize number of two-qubit CNOT (controlled not) operations to minimize noise ("low-depth circuit")

$U(\theta)$

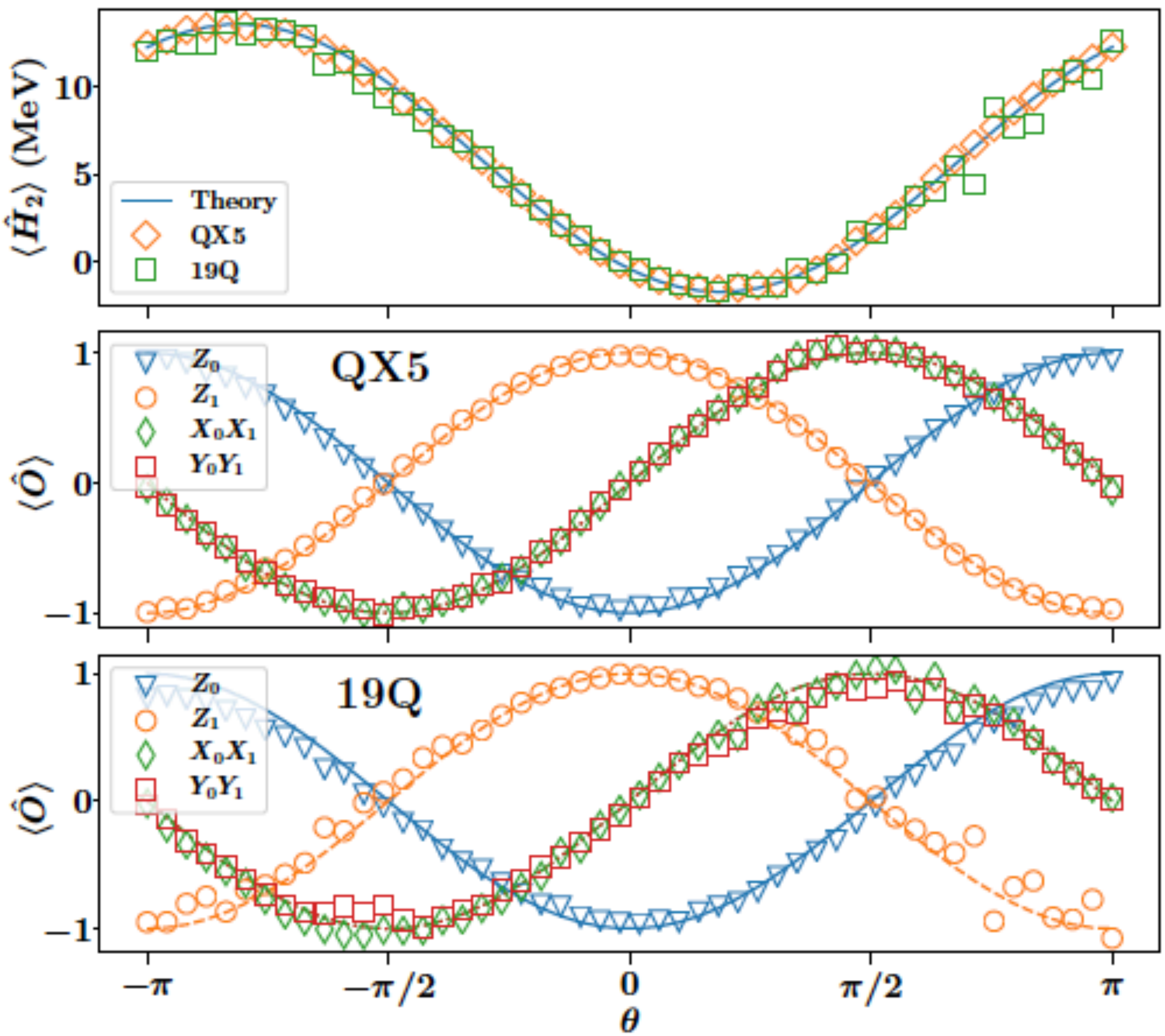


$U(\eta,\theta)$



Hamiltonian on two qubits

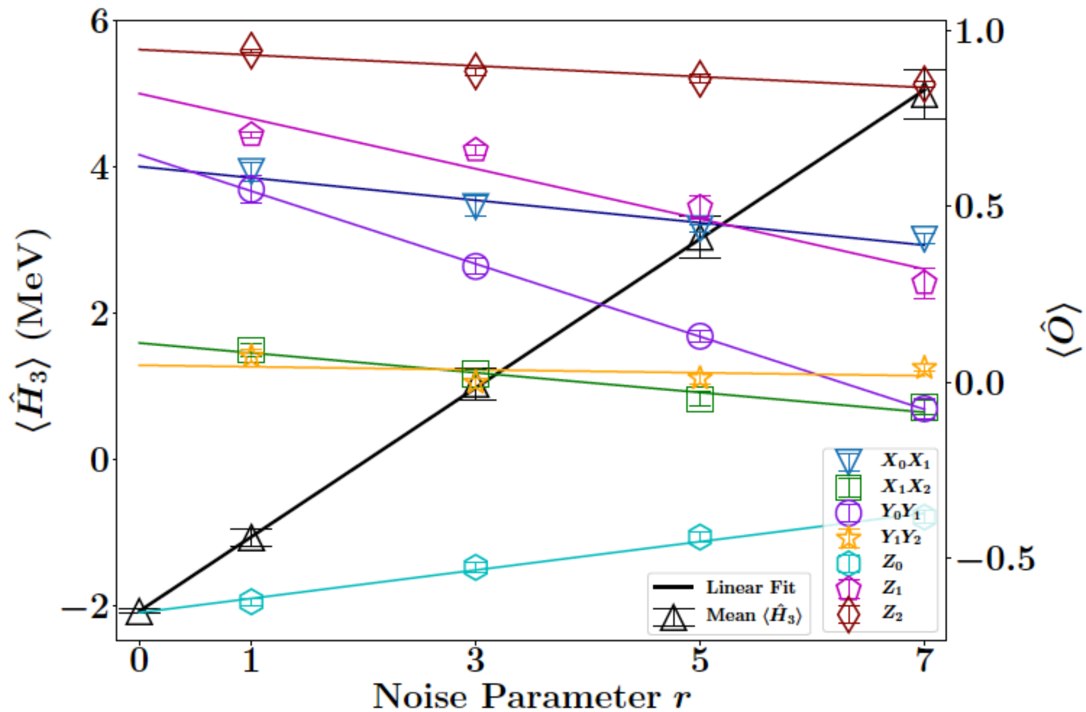
$$H_2 = 5.906709I + 0.218291Z_0 - 6.125Z_1 - 2.143304\left(X_0X_1 + Y_0Y_1\right)$$



To manage noise we performed 8,192 (10,000) measurements on QX5 (19Q)

Final results

Three qubits have more noise. Insert r pairs of CNOT (unity operators) to extrapolate to r=0



E from exact diagonalization				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	-1.749	-2.39	-2.19	
3	-2.046	-2.33	-2.20	-2.21
E from quantum computing				
N	E_N	$\mathcal{O}(e^{-2kL})$	$\mathcal{O}(kLe^{-4kL})$	$\mathcal{O}(e^{-4kL})$
2	$-1.74(3)$	$-2.38(4)$	$-2.18(3)$	
3	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

Final results of deuteron energies from a qunatum computer cpmpared to exact results, E_∞=-2.22 MeV

Summary

- Continuum impact the neutron dripline and the evolution of shell structure in neutron rich nuclei.
- Structure and decay of ^{100}Sn from first principles
- First step towards scalable nuclear structure calculations on a quantum processors accessed via the cloud
- Cloud quantum computation of atomic nuclei now possible

Collaborators

@ ORNL / UTK: D. J. Dean, G. R. Jansen, **E. Dimistrescu**, P. Lougovski, A. J. McCaskey, **T. Morris**, T. Papenbrock, R. C. Pooser

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

@ MSU/ U Oslo: M. Hjorth-Jensen

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

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

@ LLNL: K. Wendt, Sofia Quaglioni