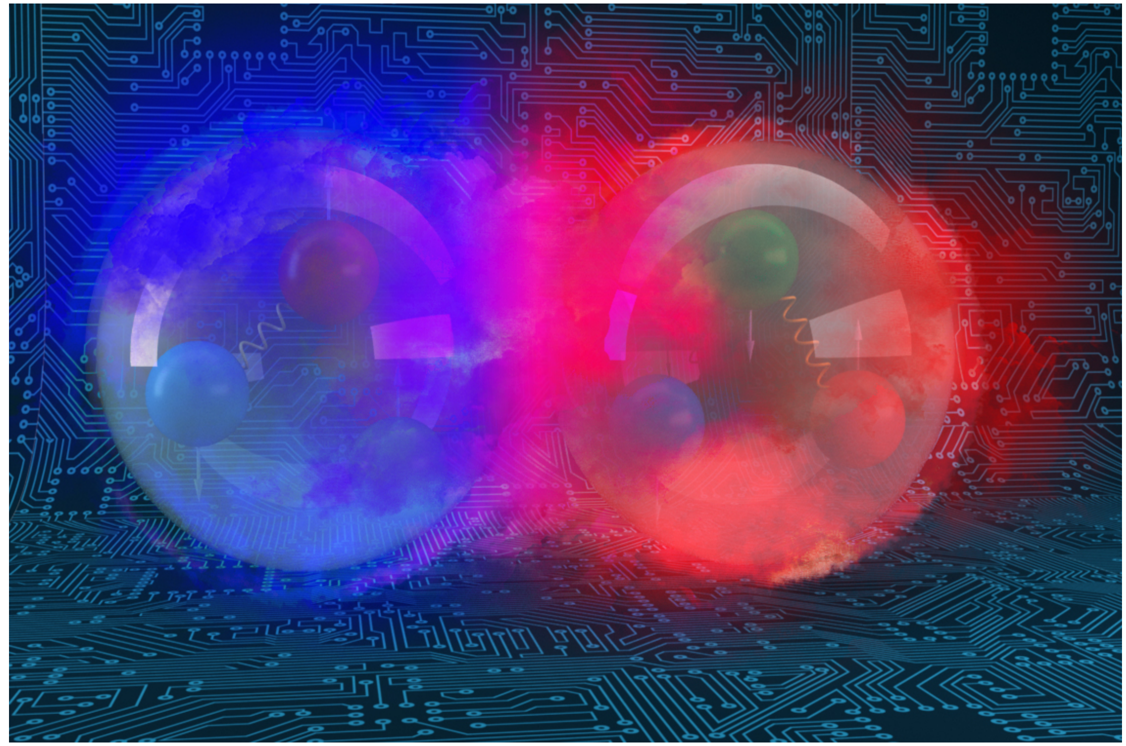
Towards quantum computations of atomic nuclei



Gaute Hagen
Oak Ridge National Laboratory

Journées thématiques IN2P3 - Quantum computing: state of the art and applications

IPN, Orsay, December 2nd 2019

U.S. DEPARTMENT OF ENERGY

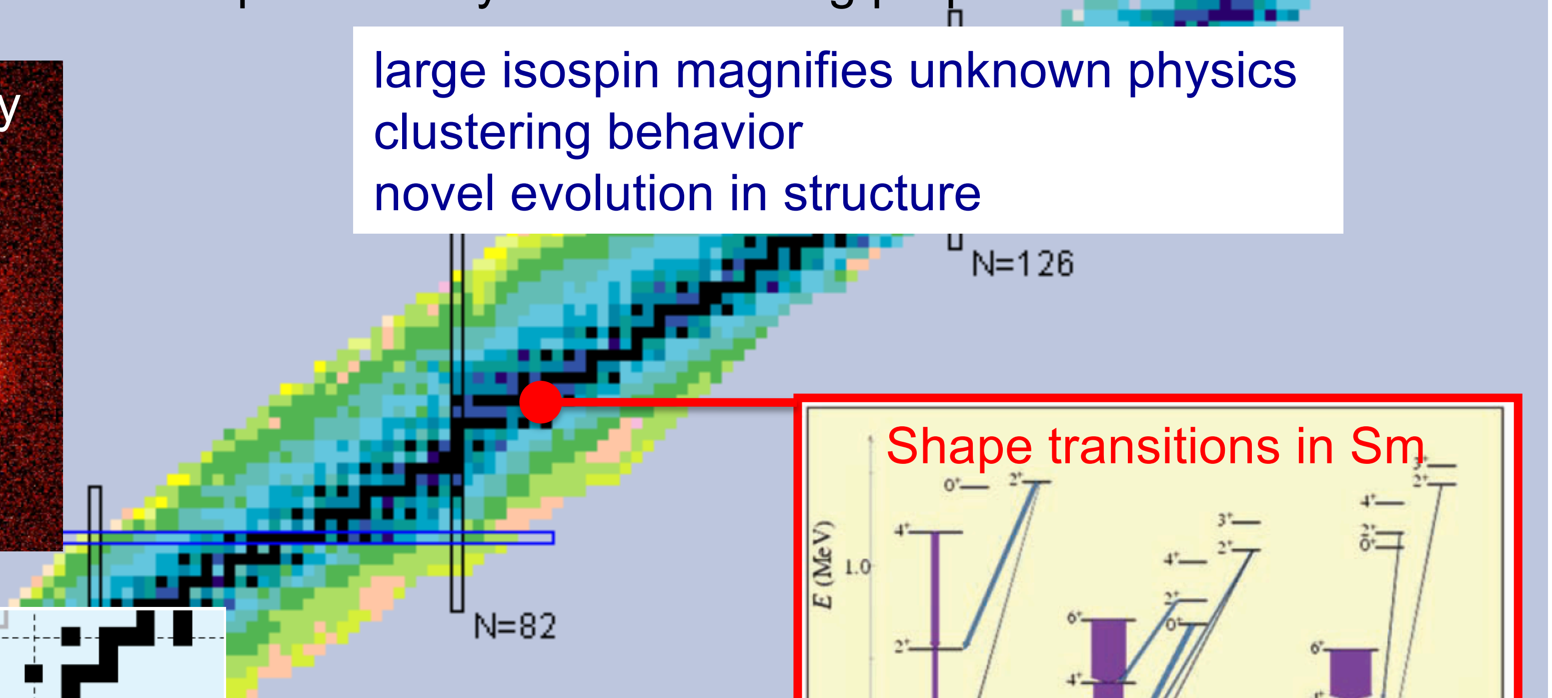
NUCLEI
Nuclear Computational Low-Energy Initiative

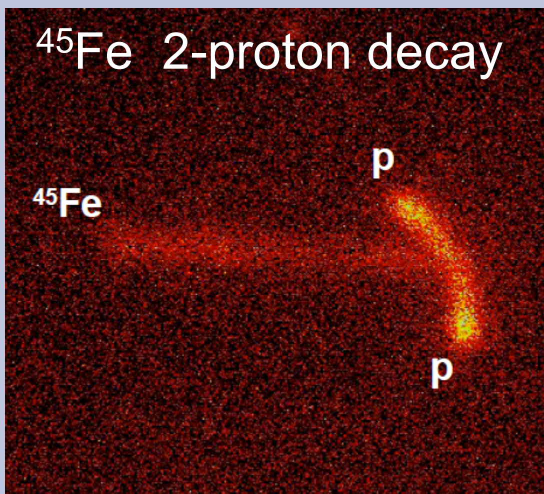
OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

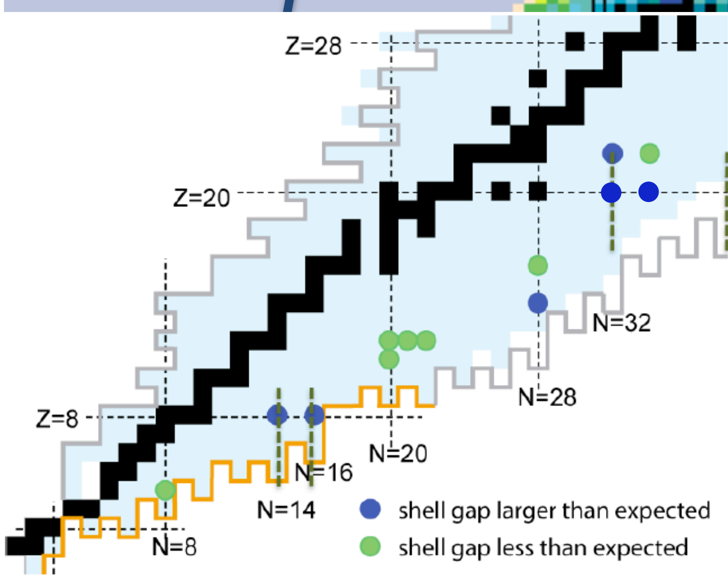
Nuclei across the chart

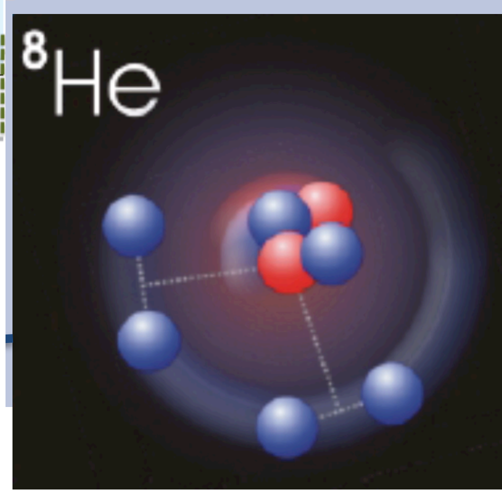
118 chemical elements (94 naturally found on Earth)
288 stable (primordial) isotopes

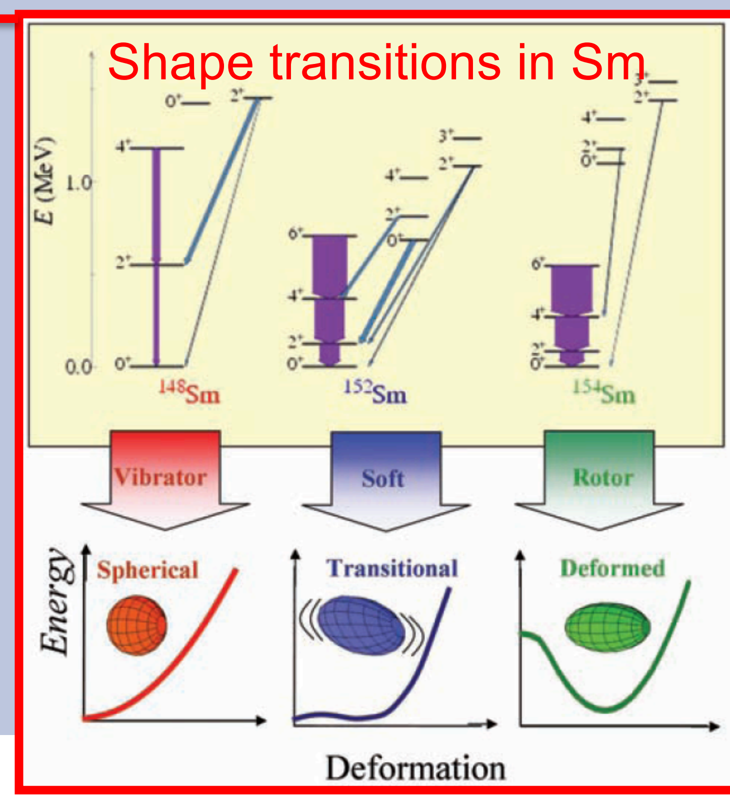
Thousands of short-lived isotopes – many with interesting properties



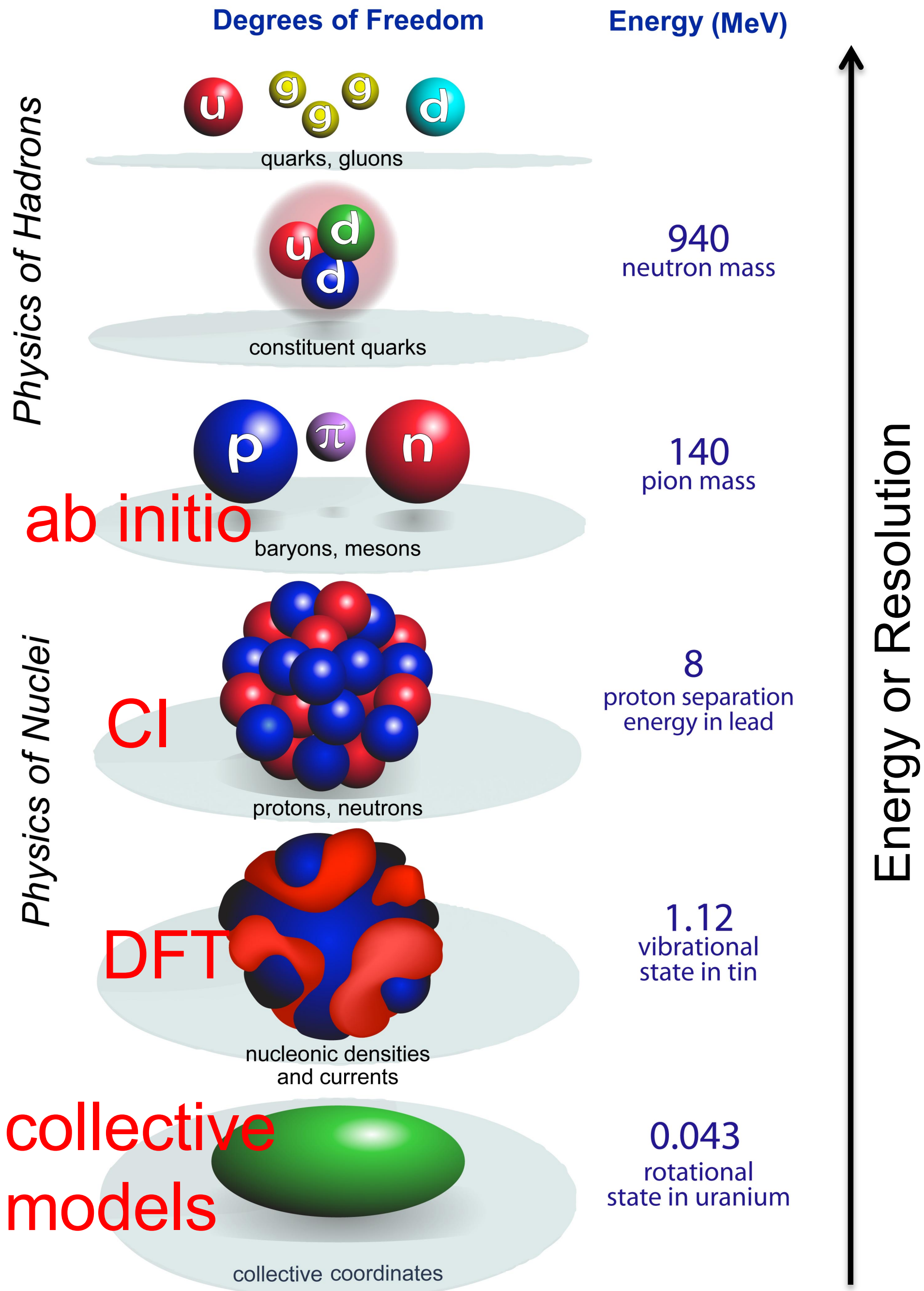








Energy scales and relevant degrees of freedom



Effective theories provide us with model independent approaches to atomic nuclei

Key: Separation of scales

Ab-initio low-energy nuclear physics deals with nucleons (and pions) as dynamical degrees of freedom

Weinberg's third law of Progress in theoretical Physics:

"You may use any degrees of freedom you like to describe a physical system, but if you use the wrong ones, you'll be sorry!"

Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Energy scales and relevant degrees of freedom

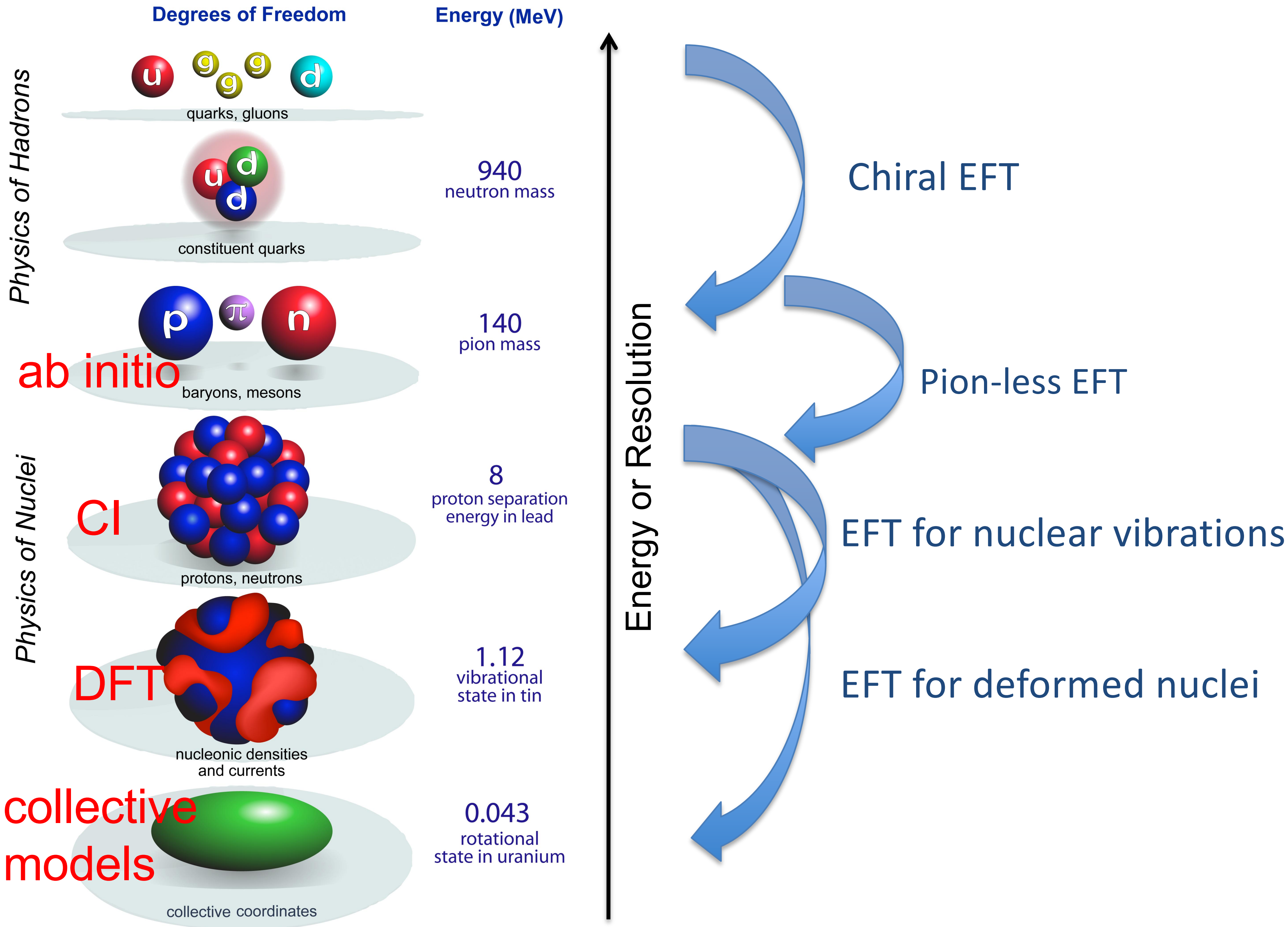


Fig.: Bertsch, Dean, Nazarewicz, SciDAC review (2007)

Trend in realistic ab-initio calculations

- Tremendous progress in recent years because of ideas from EFT and the renormalization group
- Computational methods with polynomial cost (coupled clusters 🙂quantum computing 🤔)
- Ever-increasing computer power?

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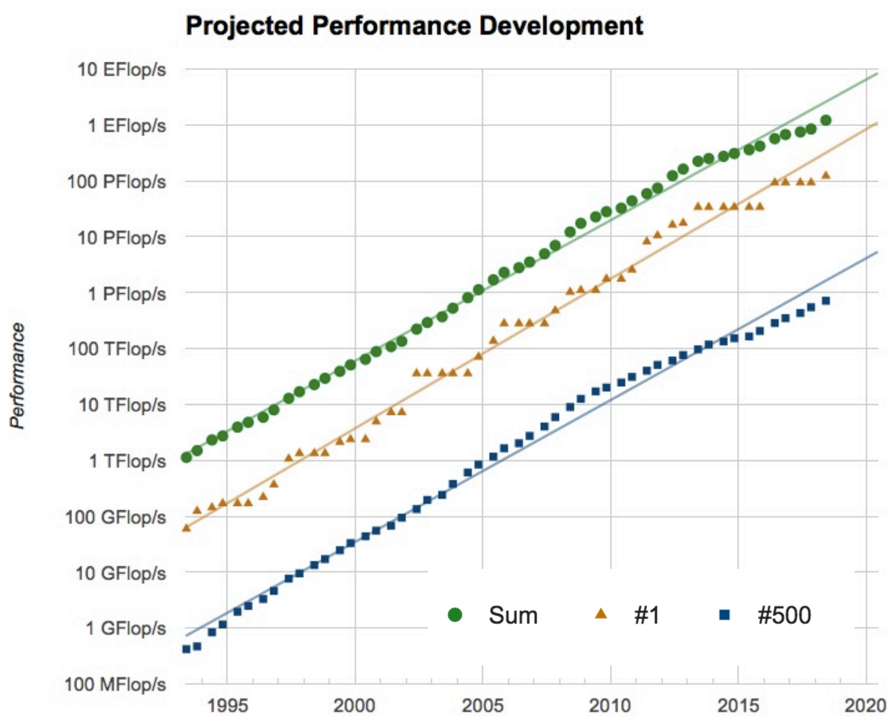
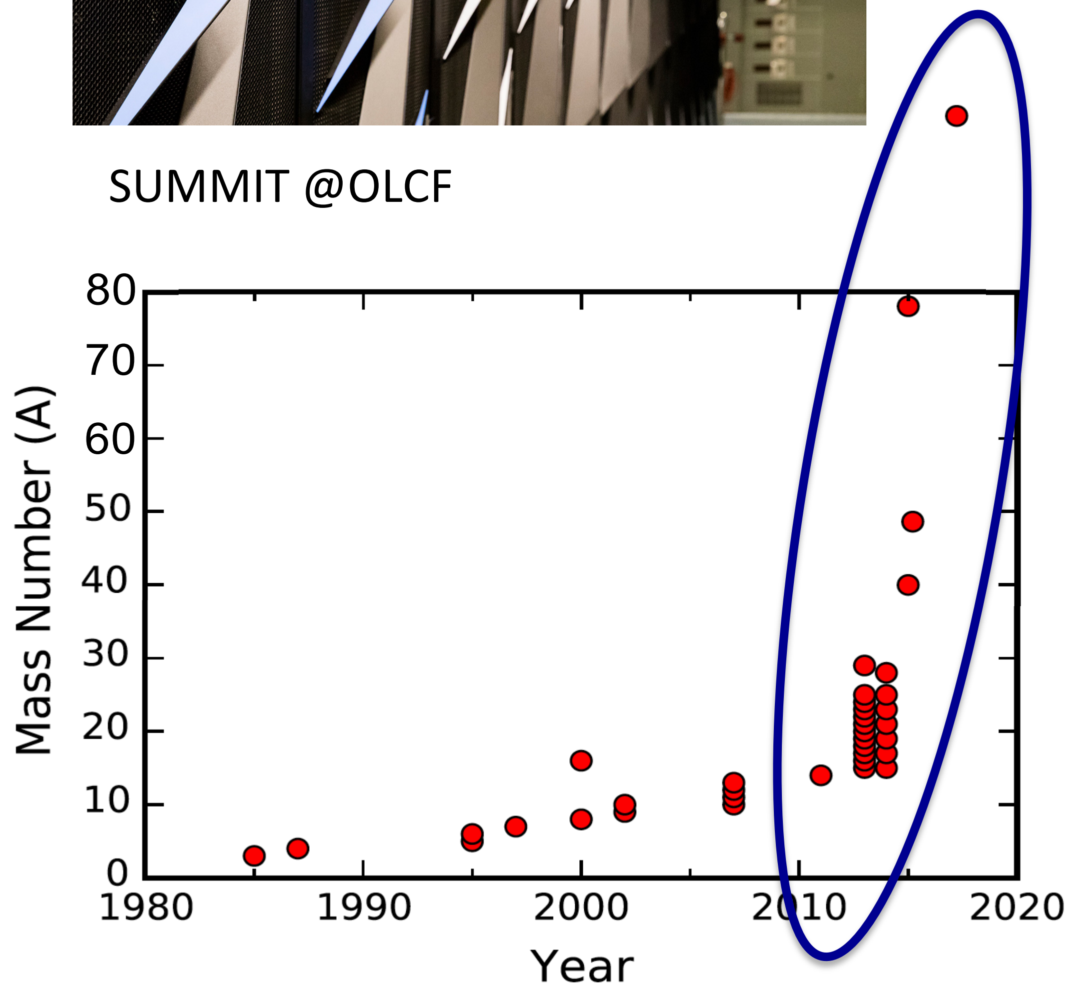
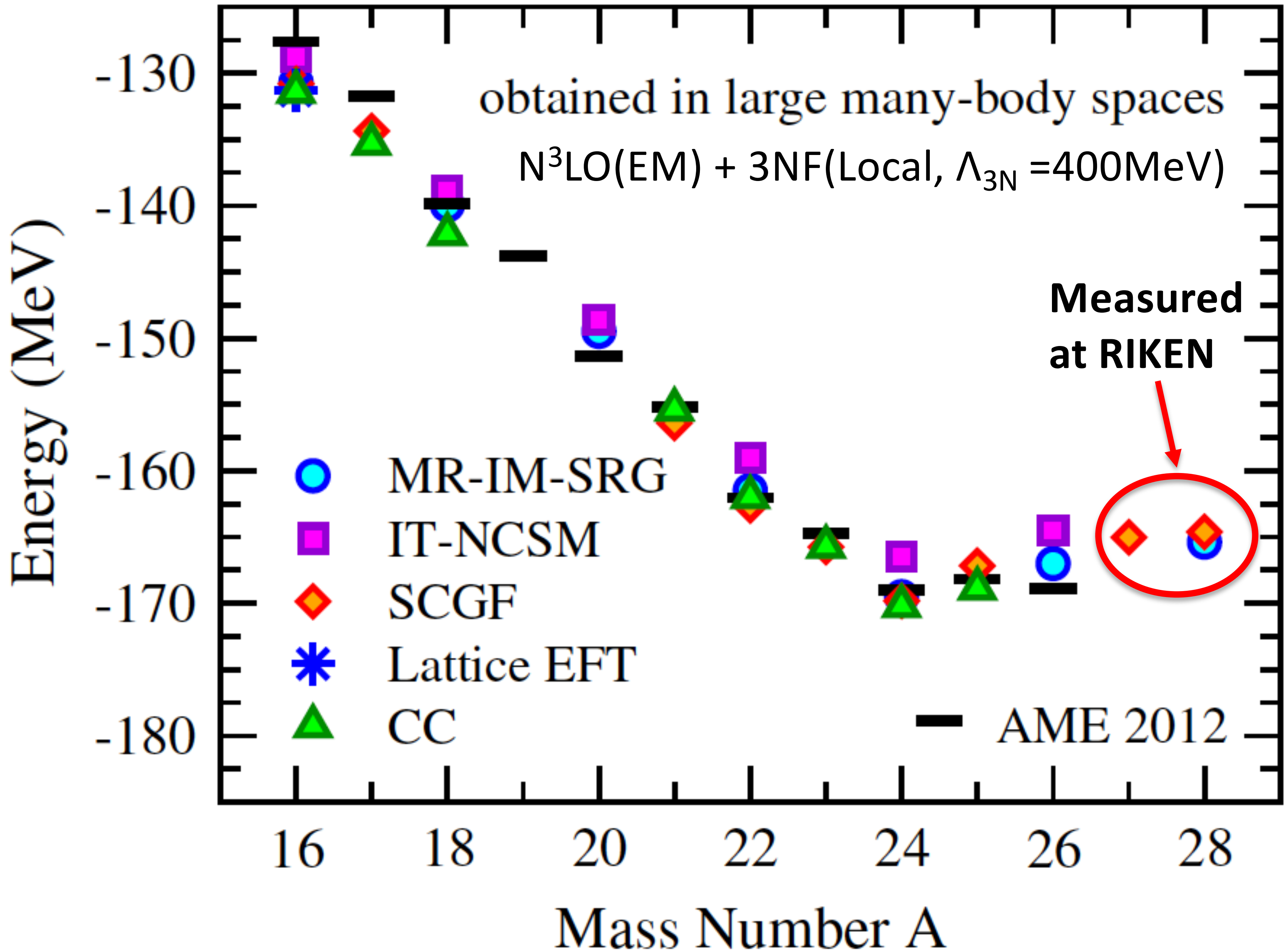
Development with time (top500.org)



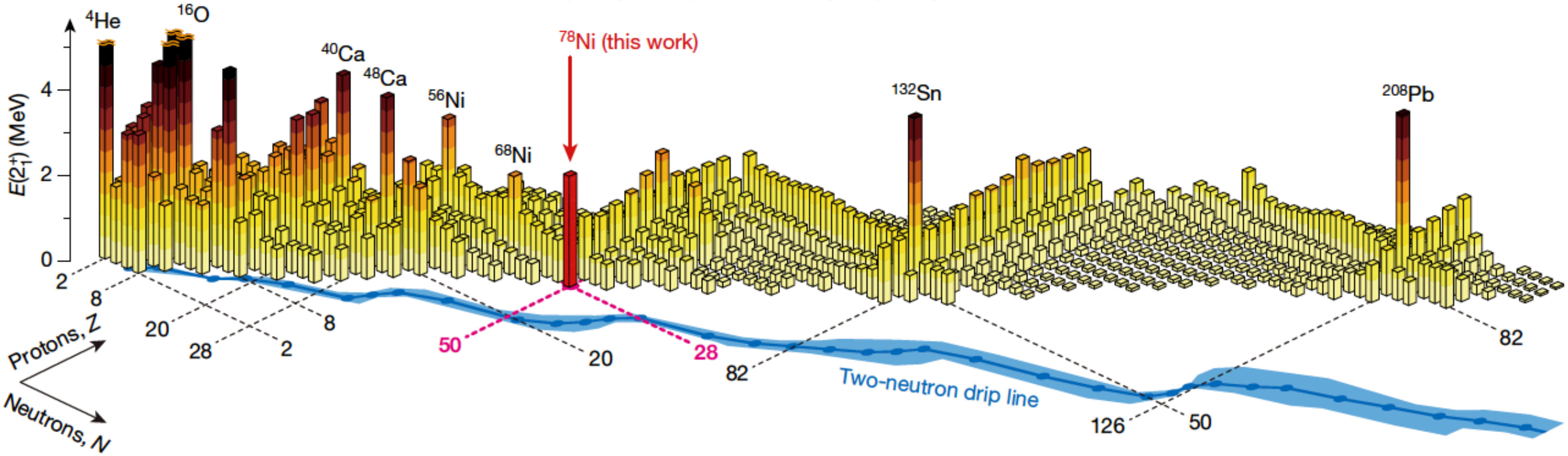


Oxgyen chain with interactions from chiral EFT

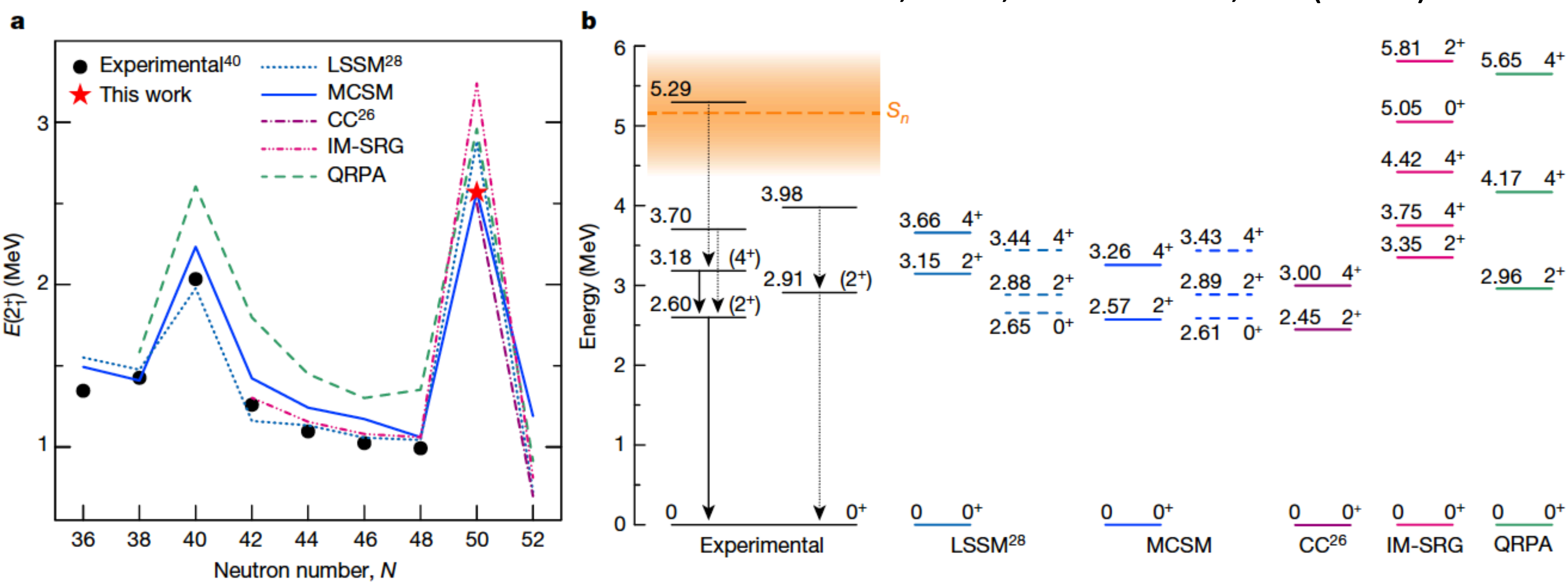


Hebeler, Holt, Menendez, Schwenk, Annu. Rev. Nucl. Part. Sci. 65, 457 (2015)

^{78}Ni – a stronghold against nuclear deformation



R. Taniuchi, et al, Nature **569**, 53 (2019)

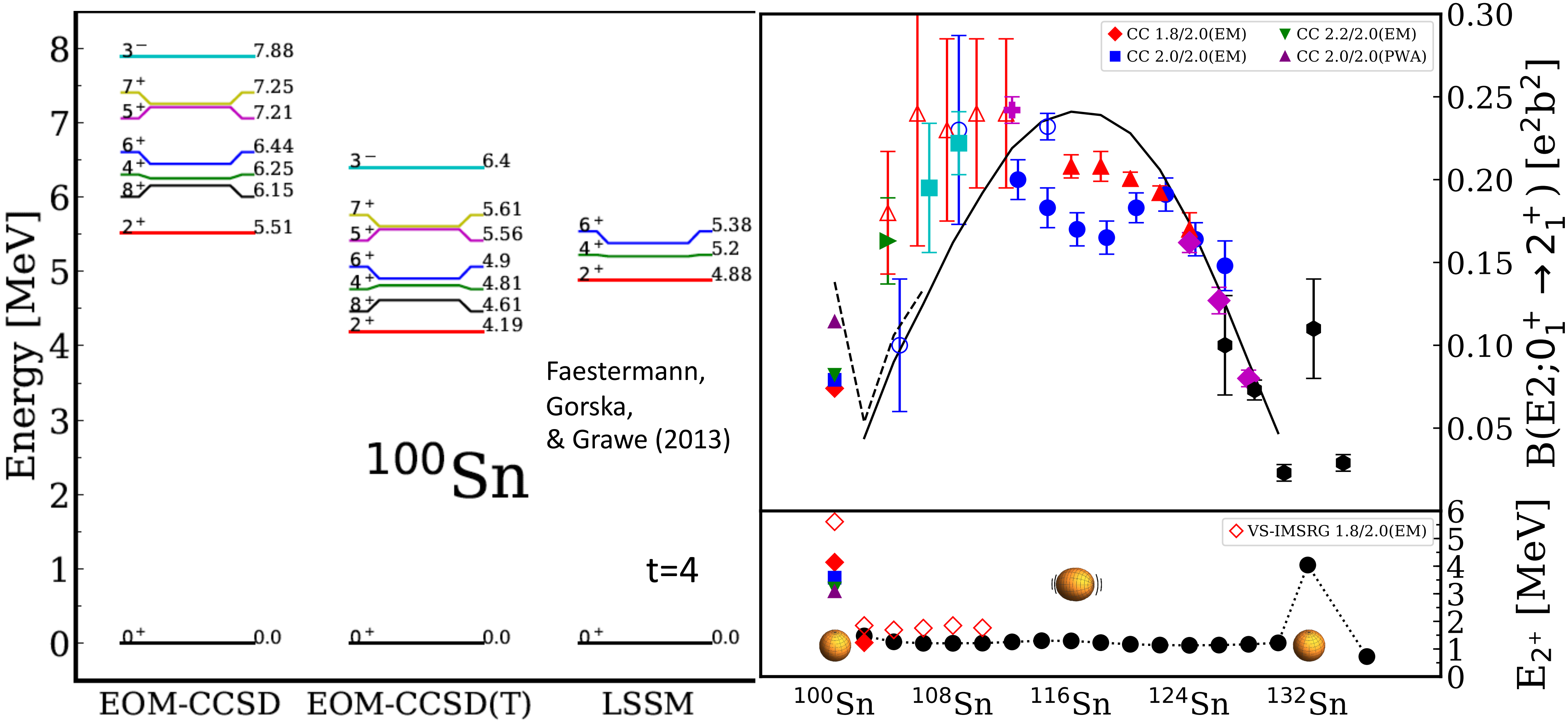


PHYSICAL REVIEW LETTERS **120,** 152503 (2018)

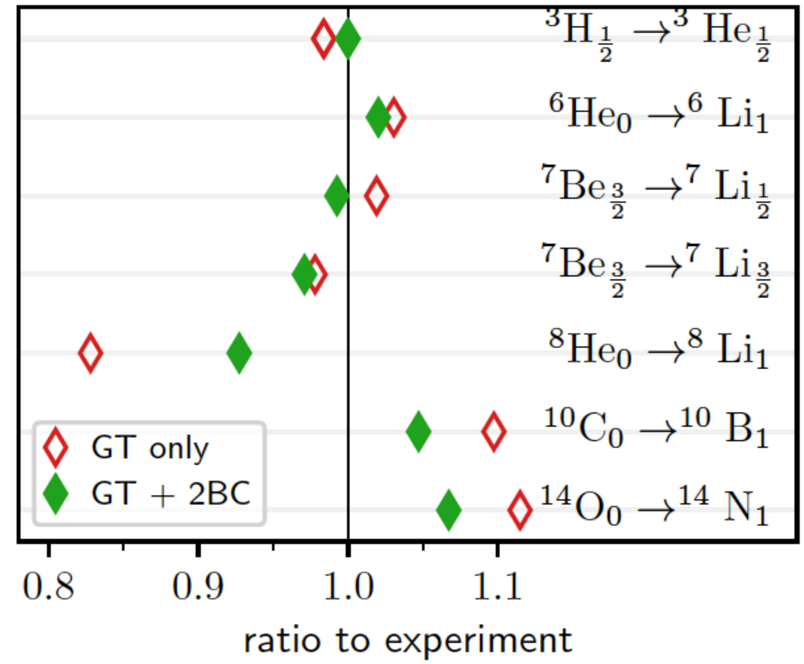
Editors' Suggestion

Structure of the Lightest Tin Isotopes

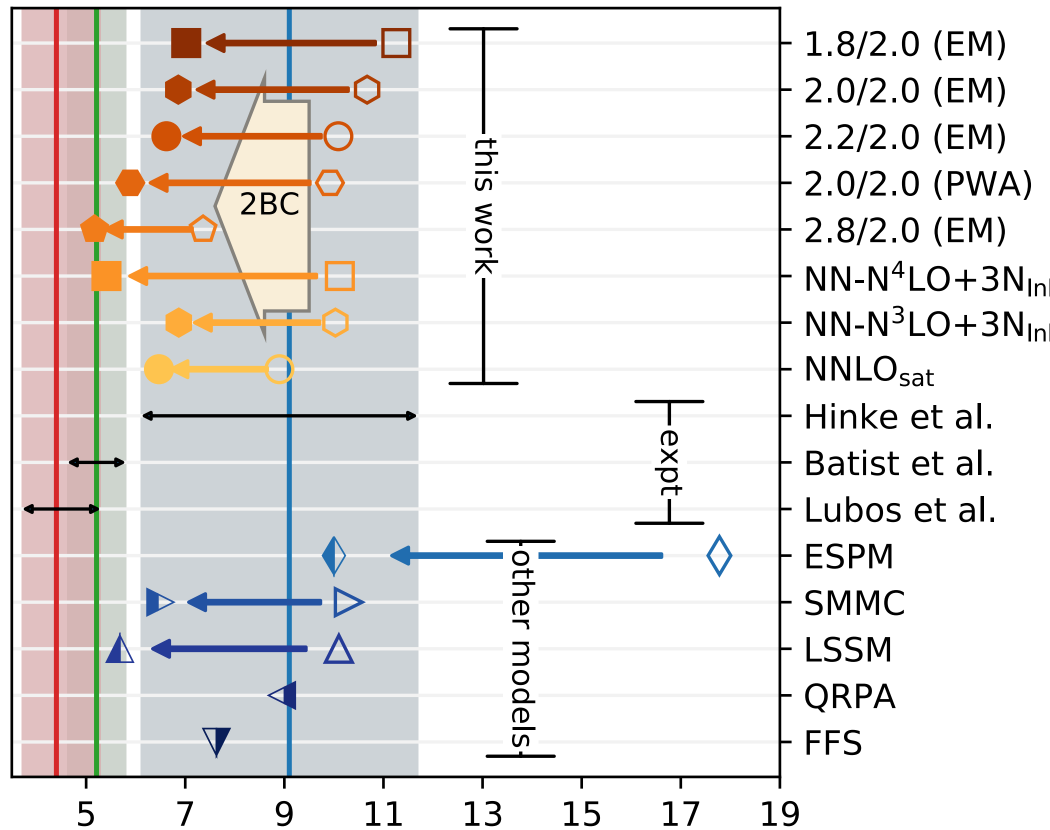
T. D. Morris,[1,2] J. Simonis,[3,4] S. R. Stroberg,[5,6] C. Stumpf,[3] G. Hagen,[2,1] J. D. Holt,[5] G. R. Jansen,[7,2] T. Papenbrock,[1,2] R. Roth,[3] and A. Schwenk[3,4,8]



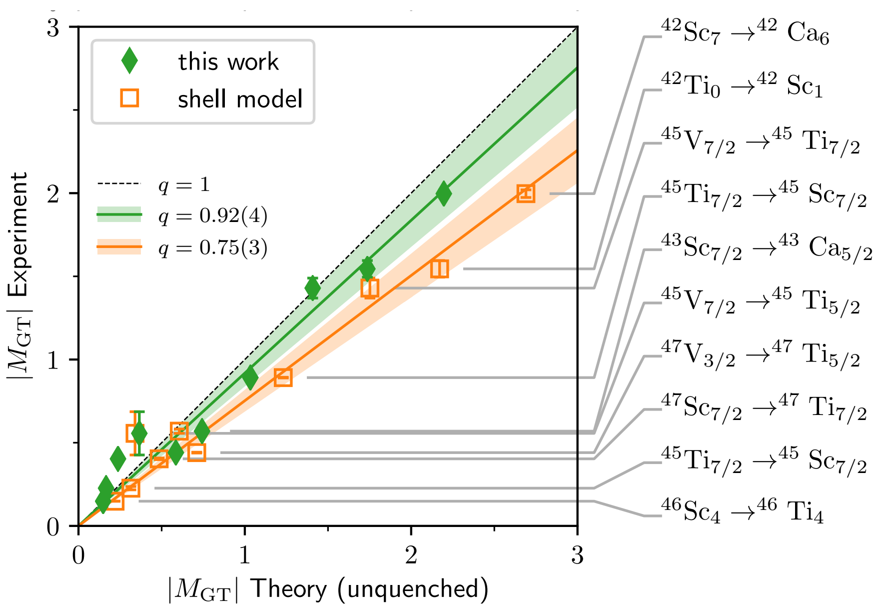
50 year old puzzle of quenched beta decays solved from first principles



See also S. Pastore et al, PRC 97, 022501 (2018).



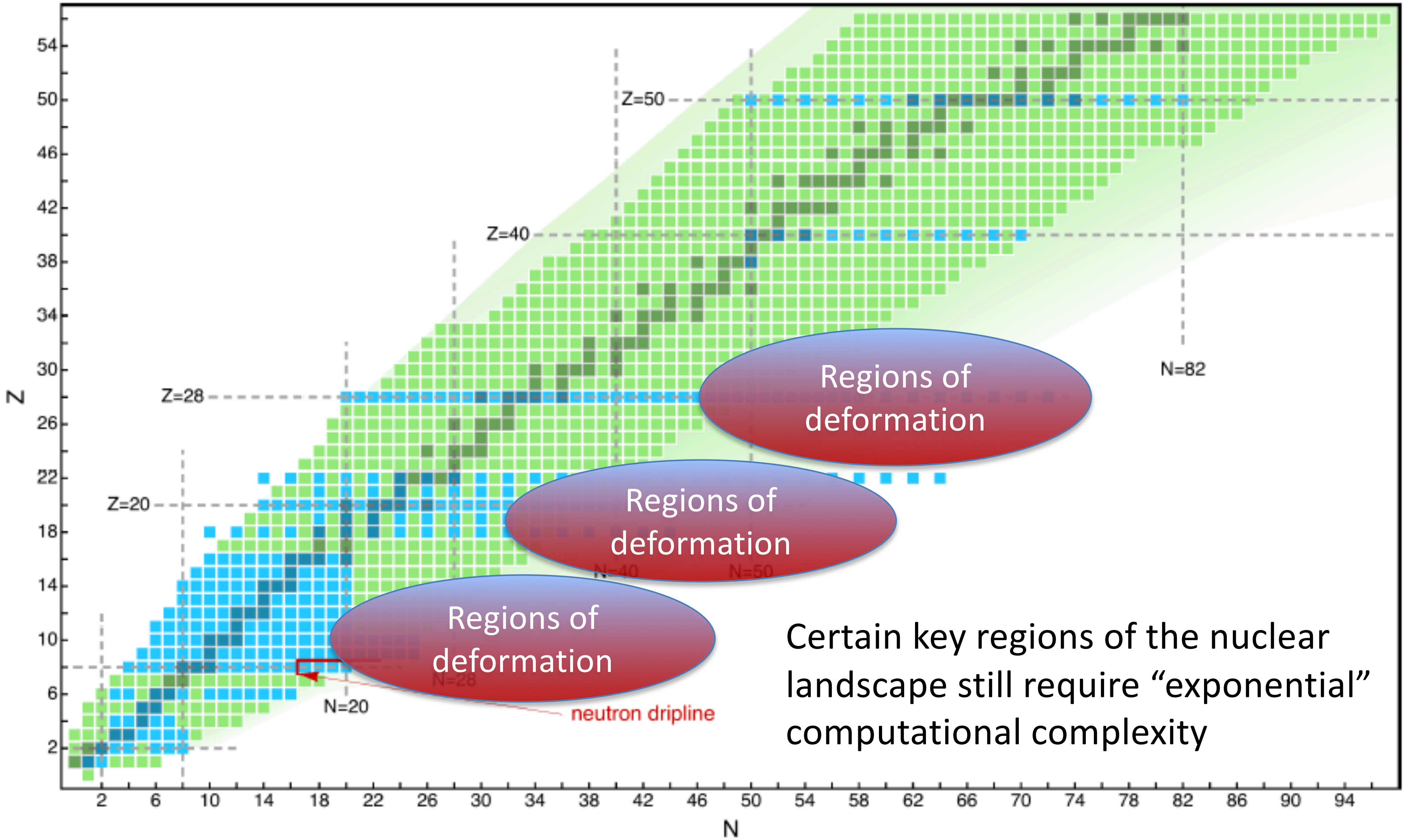
D. Lubos, PRL (2019)



P. Gysbers, et al, Nature Physics 15, 428 (2019)

Strong nuclear correlations and two-body currents solve the beta decay quenching problem

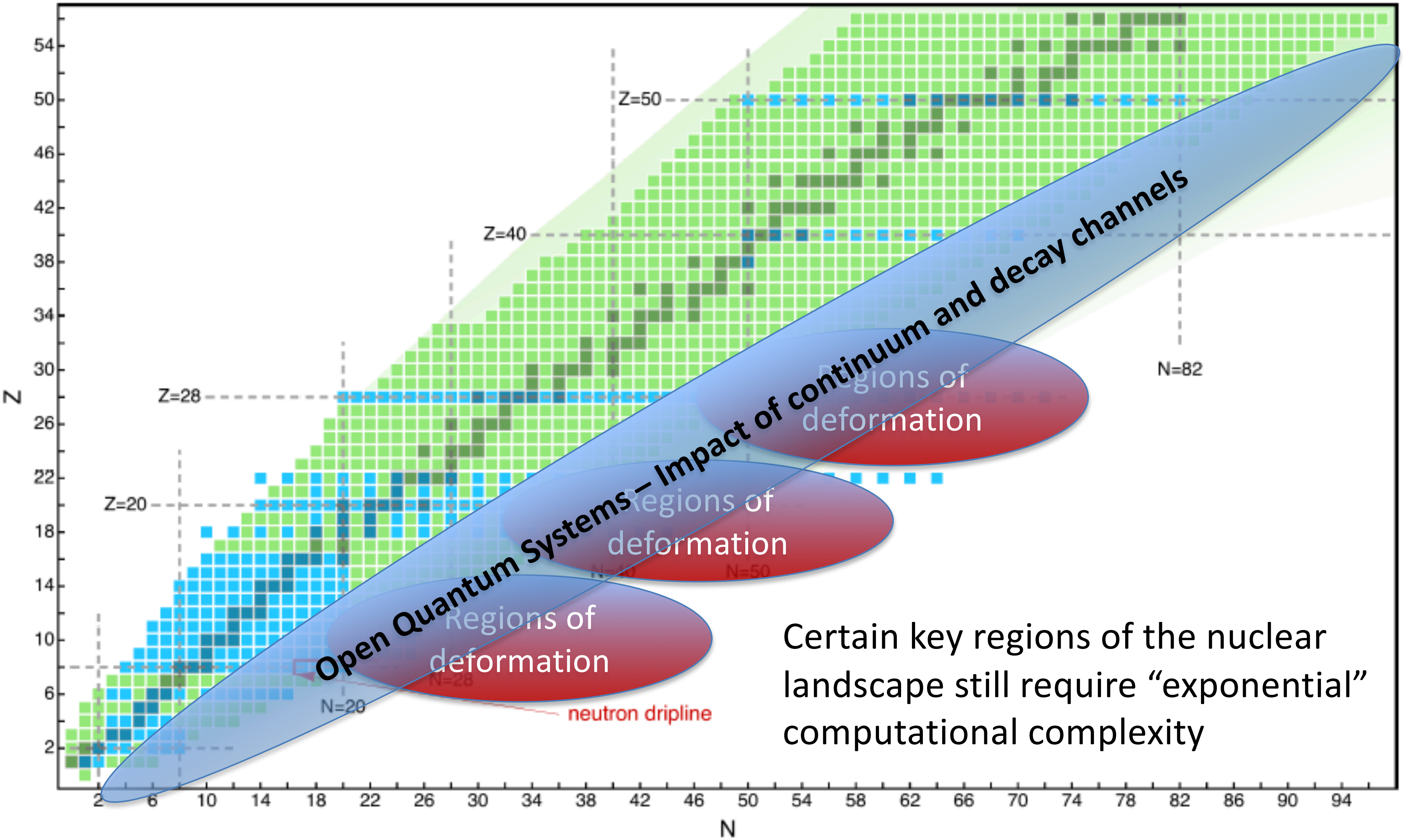
Reach of ab-initio computations of nuclei



Certain key regions of the nuclear landscape still require "exponential" computational complexity

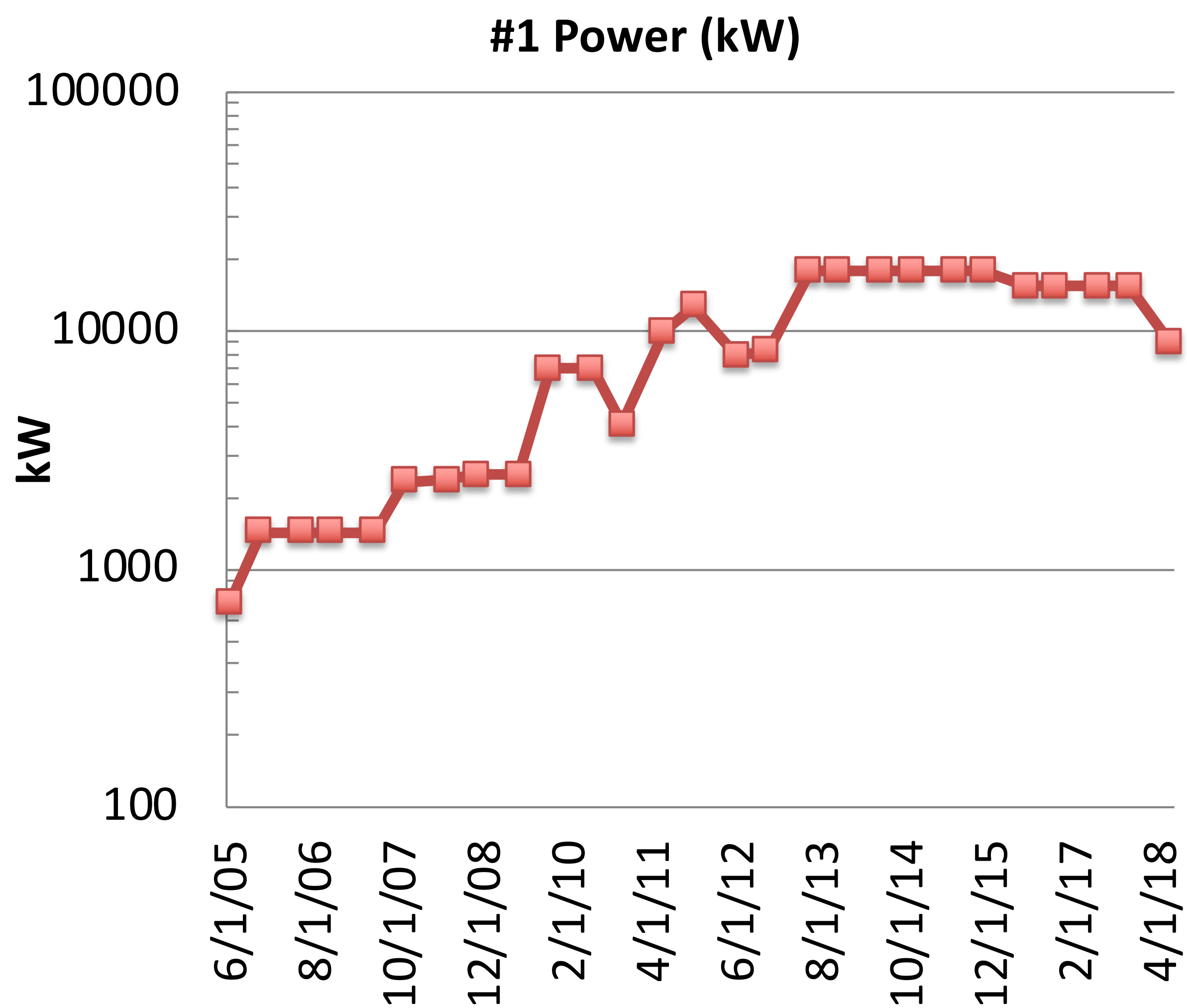
H. Hergert *et al*, Physics Reports 621, 165-222 (2016)

Reach of ab-initio computations of nuclei



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

A big issue: power



Incremental cost of running RHIC: $550k/week

Incremental cost of running Titan: $140k/week

Incremental cost of running Summit: $150k/week

(assume $0.1/kW-h)

SUMMIT @OLCF

June 2005 Tflop/kW = 0.191
June 2018 Tflop/kW = 13.88

72x technology improvement

Quantum computing

Nature isn't classical, dammit, and if you want to make a simulation of nature, you'd better make it quantum mechanical

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

What can quantum computers possibly do well?

Some quantum algorithms outperform their classical counter parts:

- Shor's algorithm: factoring of integers
- Grover's algorithm: inverting a function / searching an unordered list
- Quantum Fourier transform
- Quantum mechanics simulation: N qubits vs. 2^N complex numbers

Hope/expectation: quantum computing could solve problems with polynomial effort that are exponentially hard for classical computers.

Contrasting views:

1. We have classical algorithms that yield approximate ground states for certain Hamiltonians/systems in polynomial time (e.g. DFT, coupled cluster method, IMSRG, SCGF, Monte Carlo methods, …).
2. See Gil Kalai, arXiv:1605.00992 for a pessimistic view.

There is a lot of excitement/hype

NETWORKWORLD
FROM IDG

Home > Security

INSIDER

Quantum computing will break your encryption in a few years

The New York Times

Google Claims a Quantum Breakthrough That Could Change Computing

Forbes

Billionaires Innovation Leadership Money Consumer Industry Lifesty

38,753 views | Feb 24, 2019, 09:11pm

Why Quantum Computing's Time Is Now

Forbes

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The Computer That Could Rule the World

To understand the power of quantum computing, imagine 1,000 Equifax hacks happening at once.

What is quantum computing?

Quantum computing uses qubits, i.e. two-level quantum systems

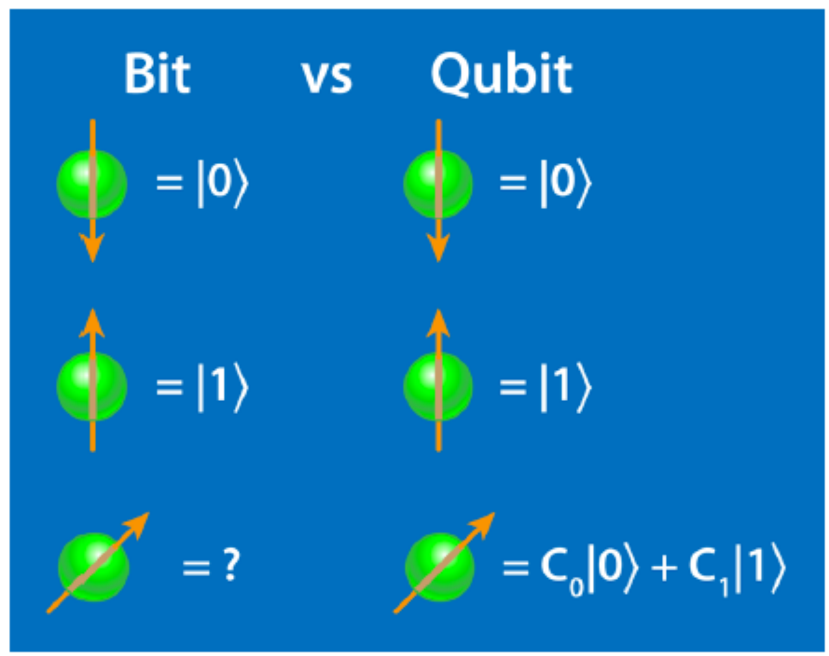
Examples:

- spin up / spin down
- two polarization states of a photon
- ion in a trap of two levels

A qubit can be in a superposition of $|0\rangle$ and $|1\rangle$.

Example from shell-model:
With *N* classical bits they will be in one out of 2^N states while *N* qubits can represent all those states at the same time.

Source: S. Gandofli, Physics Viewpoint, https://physics.aps.org/articles/v11/51



Classical vs Quantum computing

Classical

Bits 0, 1 (False, True)

Irreversible logical operations

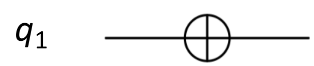
INPUT		OUTPUT
A	B	A OR B
0	0	0
0	1	1
1	0	1
1	1	1

Universality: Any logical functions can be built from a small set of gates.

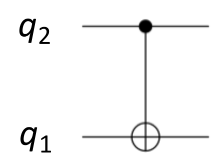
Quantum

Qubits |0>, |1>

Reversible unitary operations



$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$



$$\mathrm{CNOT} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

Universality: Any unitary transformation can be built from a small set of unitary operators/gates.

Quantum circuits

Quantum circuits consist of quantum gate operations on qubits (reversible), followed by measurements / projections (irreversible).

Measurements are irreversible and connect qubits to classical bits

A measurement is irreversible (collapse of the wave function; decoherence due to interaction with a macroscopic environment).

Quantum computation of H_2 molecule using a hybrid quantum/classical algorithm

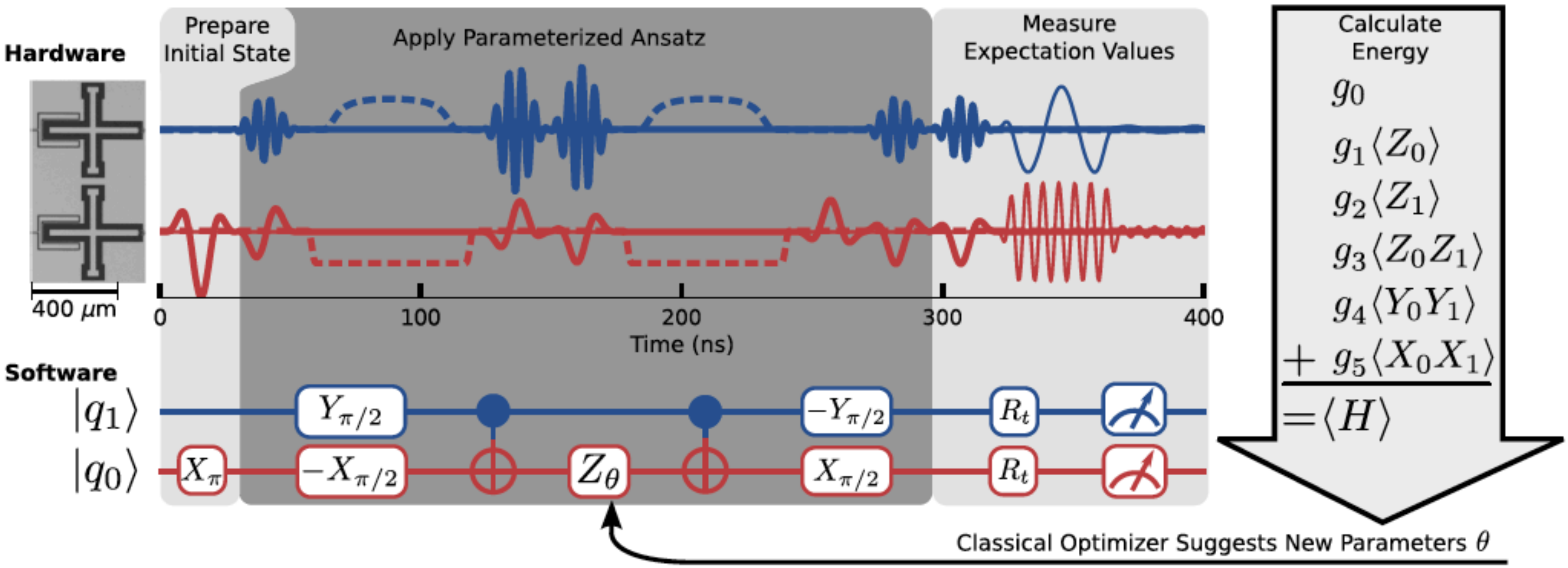
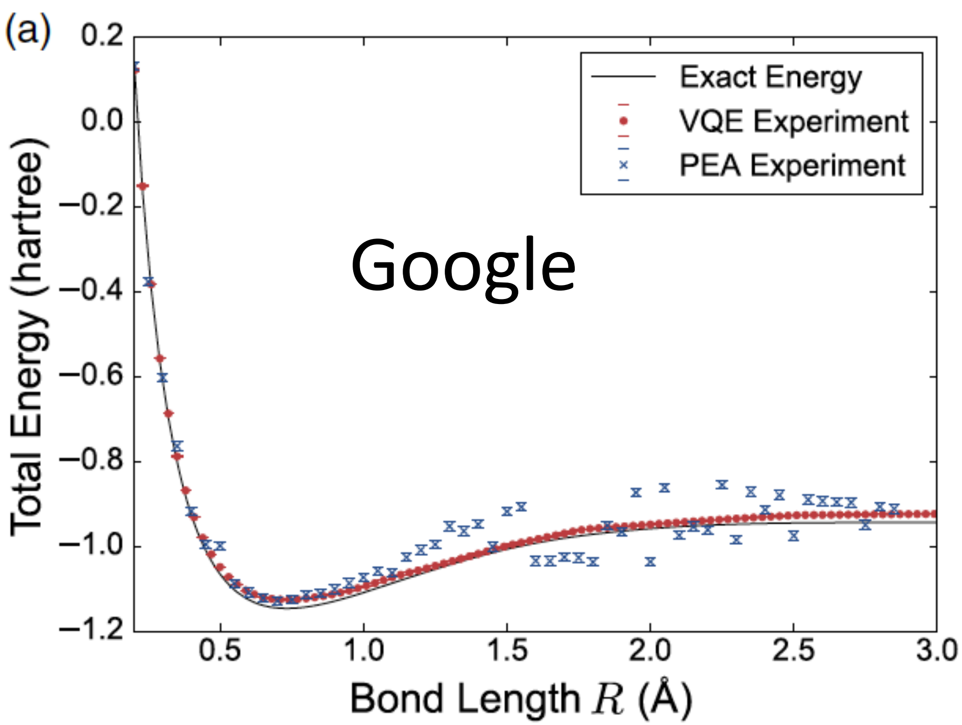


FIG. 1. Hardware and software schematic of the variational quantum eigensolver. (Hardware) micrograph shows two Xmon transmon qubits and microwave pulse sequences to perform single-qubit rotations (thick lines), dc pulses for two-qubit entangling gates (dashed lines), and microwave spectroscopy tones for qubit measurements (thin lines). (Software) quantum circuit diagram shows preparation of the Hartree-Fock state, followed by application of the unitary coupled cluster ansatz in Eq. (3) and efficient partial tomography (R_t) to measure the expectation values in Eq. (1). Finally, the total energy is computed according to Eq. (4) and provided to a classical optimizer which suggests new parameters.

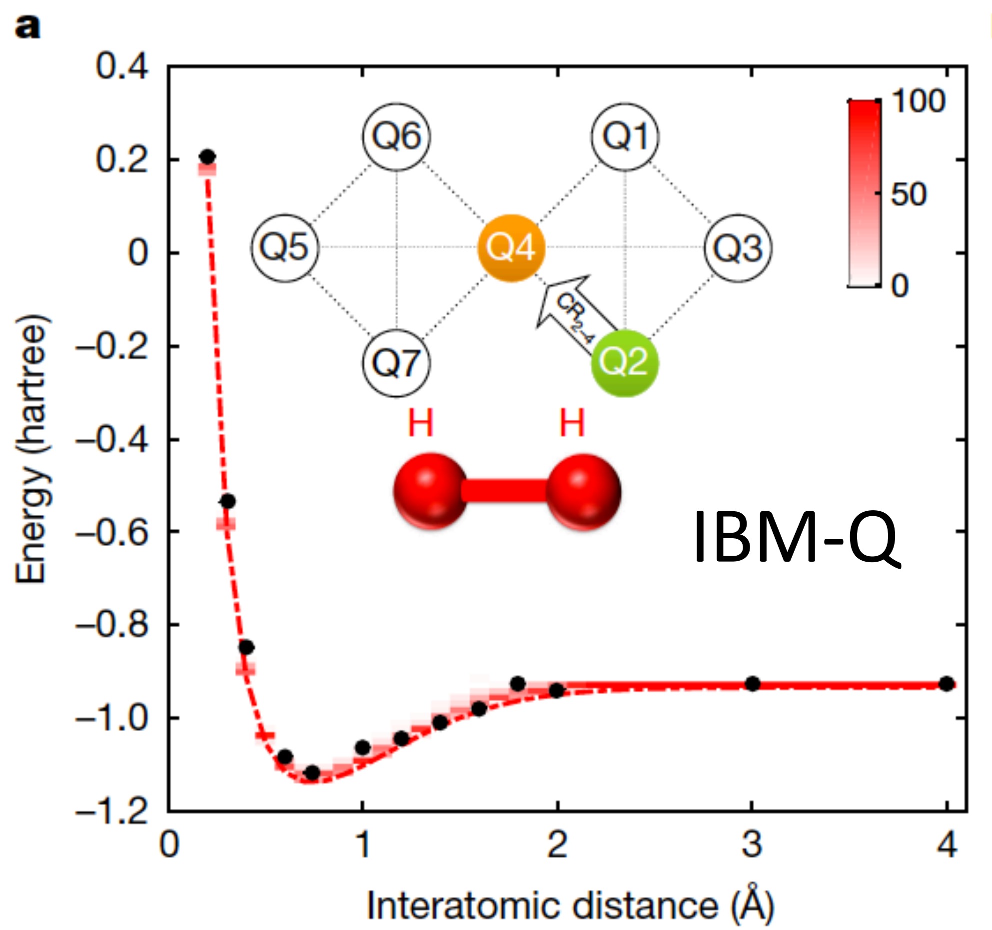
$$H = g_0 \mathbb{1} + g_1 Z_0 + g_2 Z_1 + g_3 Z_0 Z_1 + g_4 Y_0 Y_1 + g_5 X_0 X_1$$

Quantum computation of H_2 molecule using a hybrid quantum/classical algorithm

O'Malley et al. Phys. Rev. X 6, 031007 (2016)



Kandala et al., Nature 549, 242-246 (2017)



Kandala et al used 10^5 measurements on the IBM-Q for the BeH_2 molecule. The Hamiltonian consisted of more than hundred Pauli terms

Quantum computing

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

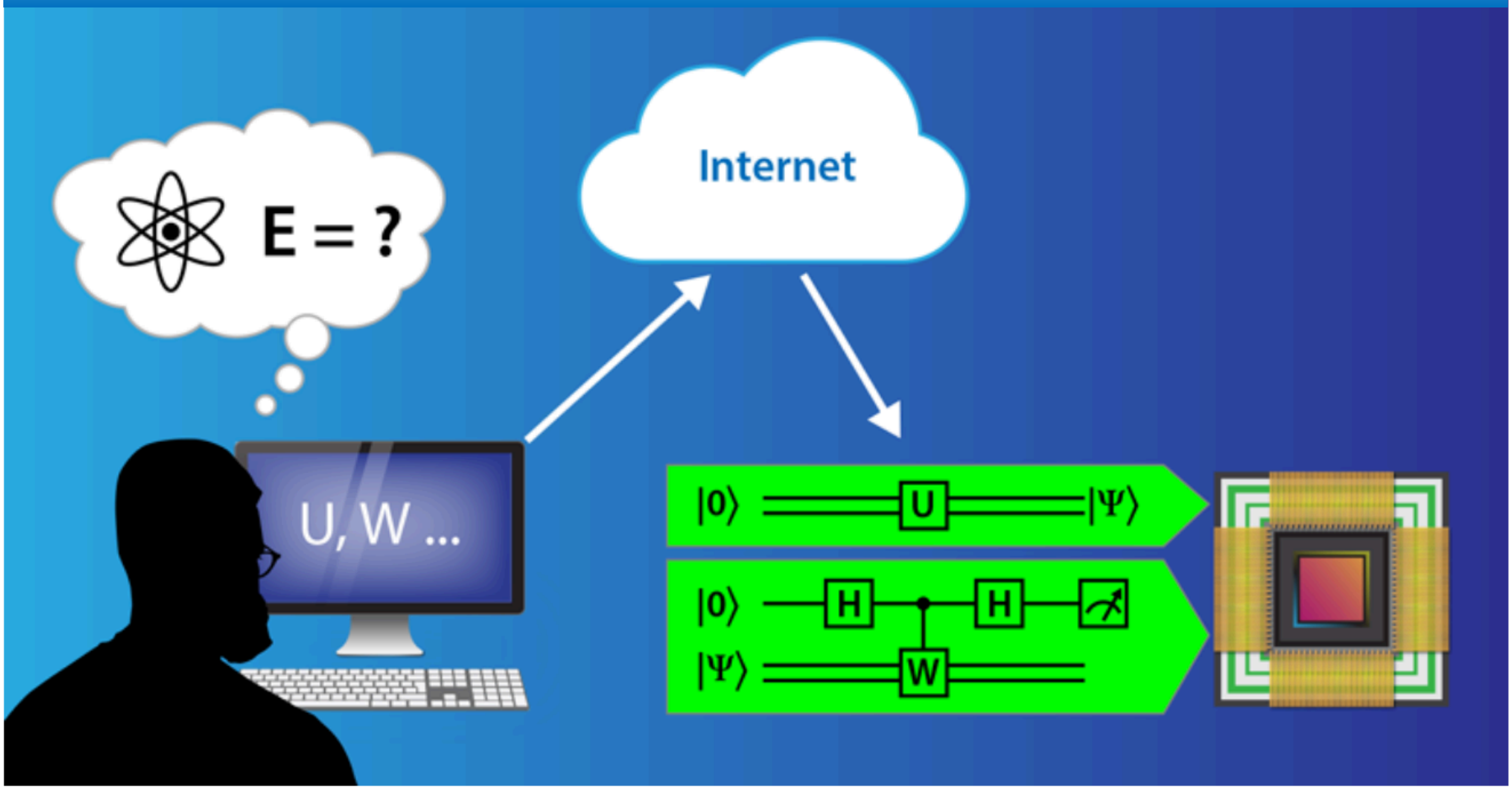
1. Quantum processing units now have ten(s) of qubits
2. Businesses are driving this: Google, IBM, Microsoft, Rigetti, D-Wave, …
3. Software is publicly available (PyQuil, XACC, OpenQASM, OpenFermion)
4. First real-world problems solved: H_2 molecule on two qubits [O'Malley et al., Phys. Rev. X 6, 031007 (2016)]; BeH_2 on six qubits [Kandala et al., Nature 549, 242 (2017)]; …

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

Now also lots of activity in nuclear physics: E. Dumitrescu et al, PRL (2019), D. Kaplan, N. Klco, A. Roggero, arXiv (2017), S. Beane et al, PRL (2019), N. Klco and M. J. Savage PRA (2019), N. Klco, et al, PRA (2018), A. Roggero and J. Carlson, arXiv (2018), Hsuan-Hao Lu, N. Klco et al PRA (2019)

Cloud access to quantum computers/simulators

Now: Cloud access possible; no insider knowledge required!
[Dumitrescu, McCaskey, Hagen, Jansen, Morris, Papenbrock, Pooser, Dean, Lougovski, Phys. Rev. Lett. **120**, 210501 (2018)]



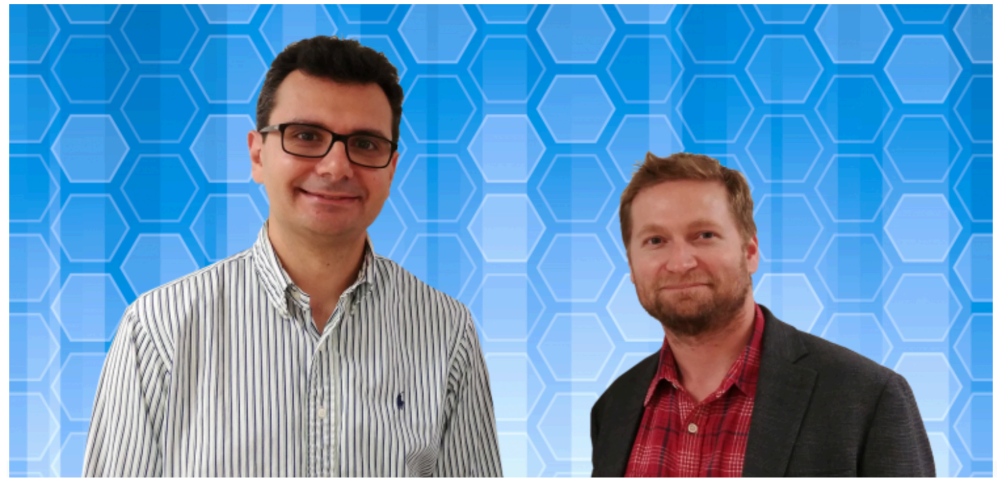
Source: S. Gandofli, Physics Viewpoint,
https://physics.aps.org/articles/v11/51

Nuclear Physics & Quantum Computing Collaboration at ORNL

Two ORNL-led research teams receive $10.5 million to advance quantum computing for scientific applications (ORNL news, October 2017)

Eugene Dumitrescu

Alex McCaskey



Pavel Lougovski

Raphael Pooser

PHYSICAL REVIEW LETTERS **120,** 210501 (2018)

Editors' Suggestion Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

[1]*Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
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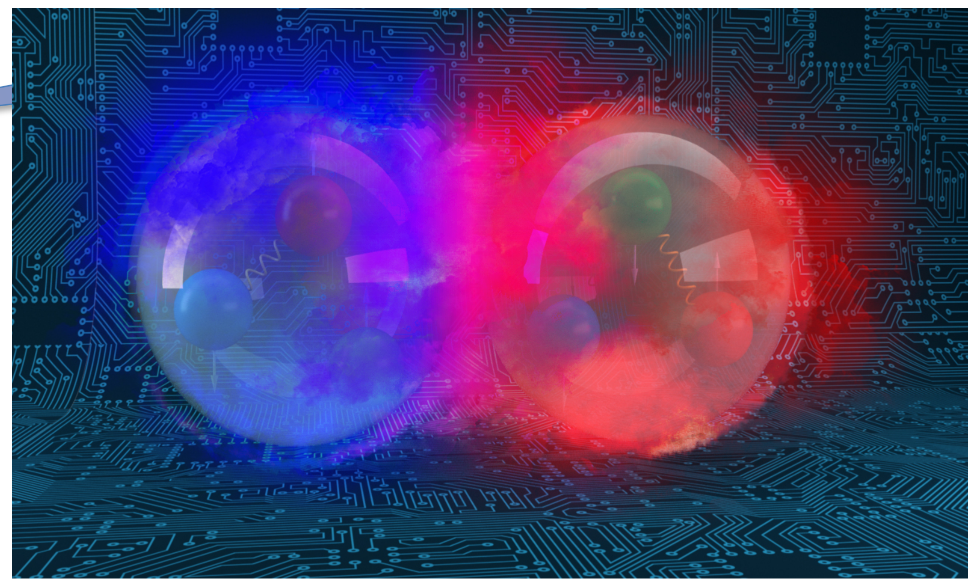
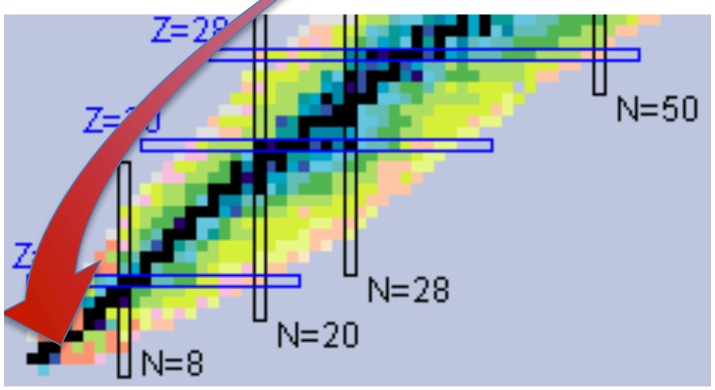
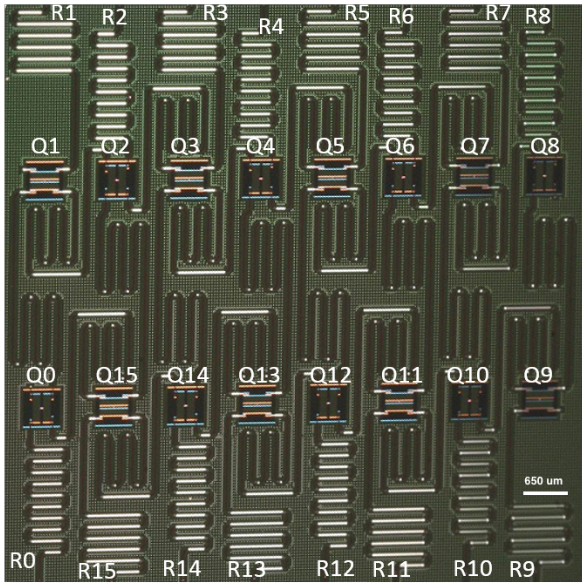
(Received 12 January 2018; published 23 May 2018)

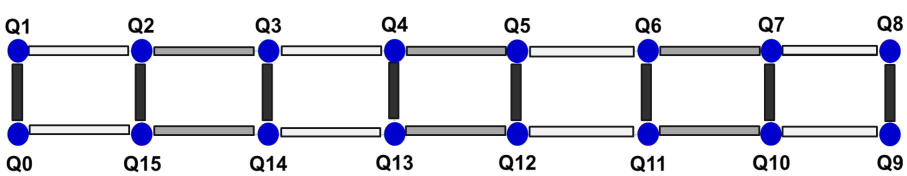
Quantum computing 101: the deuteron



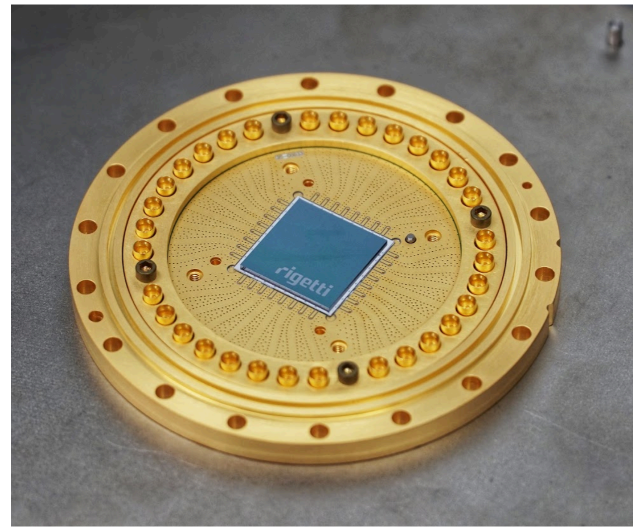


Superconducting qubits “transmons”
IBM QX5 and Rigetti 19Q

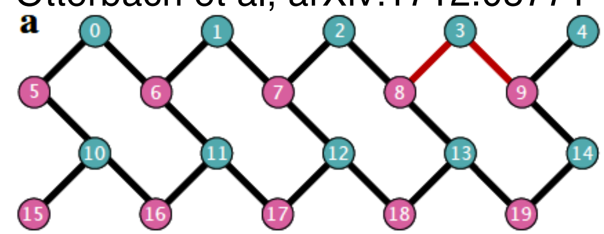




→ IBM Q Experience



Otterbach et al, arXiv:1712.05771



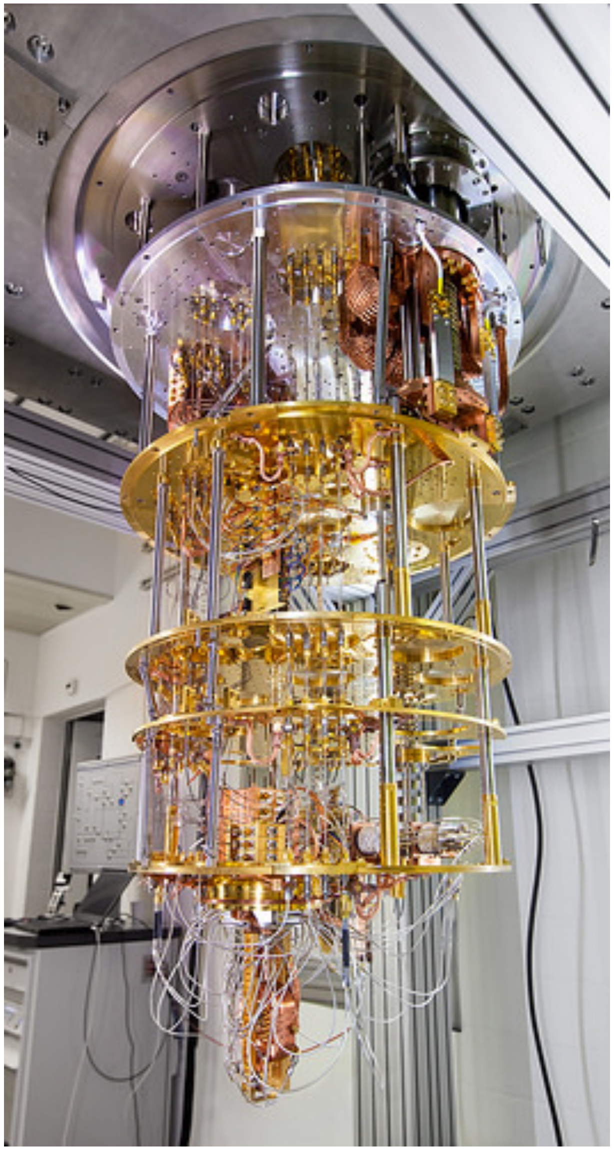
→ Rigetti Forest

Qubit fidelities

	1-Qubit Gate Fidelity			2-Qubit Gate Fidelity			Read Out Fidelity		
Computer	Min	Max	Ave	Min	Max	Ave	Min	Max	Ave
IBM QX2	99.71%	99.88%	99.79%	94.22%	97.12%	95.33%	92.20%	98.20%	96.24%
IBM QX4	99.83%	99.96%	99.88%	95.11%	98.39%	97.11%	94.80%	97.10%	95.60%
IBM QX5	99.59%	99.87%	99.77%	91.98%	97.29%	95.70%	88.53%	96.66%	93.32%
IBM QS1_1	96.93%	99.92%	99.48%	82.28%	98.87%	95.68%	69.05%	93.55%	83.95%
Rigetti 19Q	94.96%	99.42%	98.63%	79.00%	93.60%	87.50%	84.00%	97.00%	93.30%

Sources: QuantumComputingReport.com; Rigetti.com

Mitigating exisiting constraints



IBM QX5, 16 qubits

- Limited connectivity between qubits → tailored simple Hamiltonian
- Gate errors and decoherence → Low depth quantum circuits
- Intermittent cloud access in a scheduled environment must be taken into account
- Limited fidelity → noise correction

John Preskill, “Quantum Computing in the NISQ era and beyond”, Quantum 2, 79 (2018) -- arXiv:1801.00862

Game plan

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of $^3S_1$ partial wave [à la Binder et al. (2016); **Aaina Bansal et al. (2018)**]; cutoff at about 150 MeV.

$$H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^\dagger a_n \qquad \langle n'|V|n\rangle = V_0 \delta_n^0 \delta_n^{n'}$$

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

For example the $N = 2$ Hamiltonian is given by:

$$H_2 = \begin{bmatrix} -1.677 & 2.339 \\ 2.339 & 22.242 \end{bmatrix}$$

Easily diagonalized on a piece of paper.

Game plan

2. Map single-particle states |n⟩ onto qubits using |0⟩ = |↑⟩ and |1⟩ = |↓⟩. This is an analog of the Jordan-Wigner transform.

$$a_p^\dagger \leftrightarrow \sigma_-^{(p)} \equiv \frac{1}{2}(X_p - iY_p) \qquad a_p \leftrightarrow \sigma_+^{(p)} \equiv \frac{1}{2}(X_p + iY_p)$$

$$H_2 = \begin{bmatrix} -1.677 & 2.339 \\ 2.339 & 22.242 \end{bmatrix} =$$

$$5.9067I + 0.21729Z_0 - 0.125Z_1 - 2.143(X_0X_1 + Y_0Y_1)$$

3. Solve H_1, H_2 (and H_3) and extrapolate to infinite space using harmonic oscillator variant of Lüscher's formula [More, Furnstahl, Papenbrock (2013)]

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

Variational wave function

Wave functions on two qubits

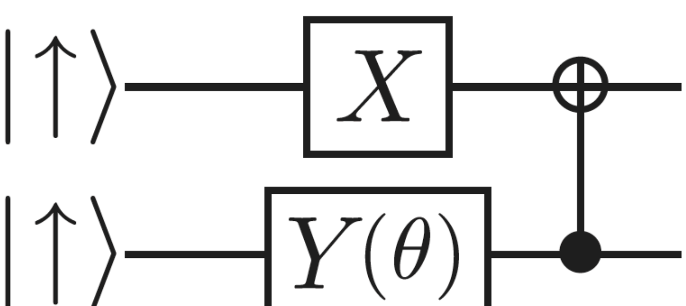
$U(\theta)|\downarrow\uparrow\rangle$ $$U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)}$$

Wave functions on three qubits

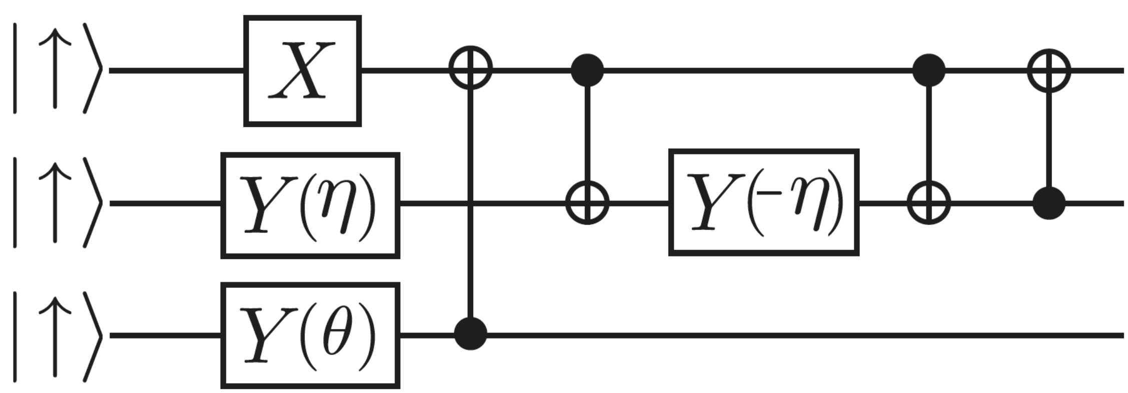
$U(\eta,\theta)|\downarrow\uparrow\uparrow\rangle$ $$U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right) + \theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$$

Minimize number of two-qubit CNOT operations to mitigate low two-qubit fidelities (construct a "low-depth circuit")

$U(\theta)$

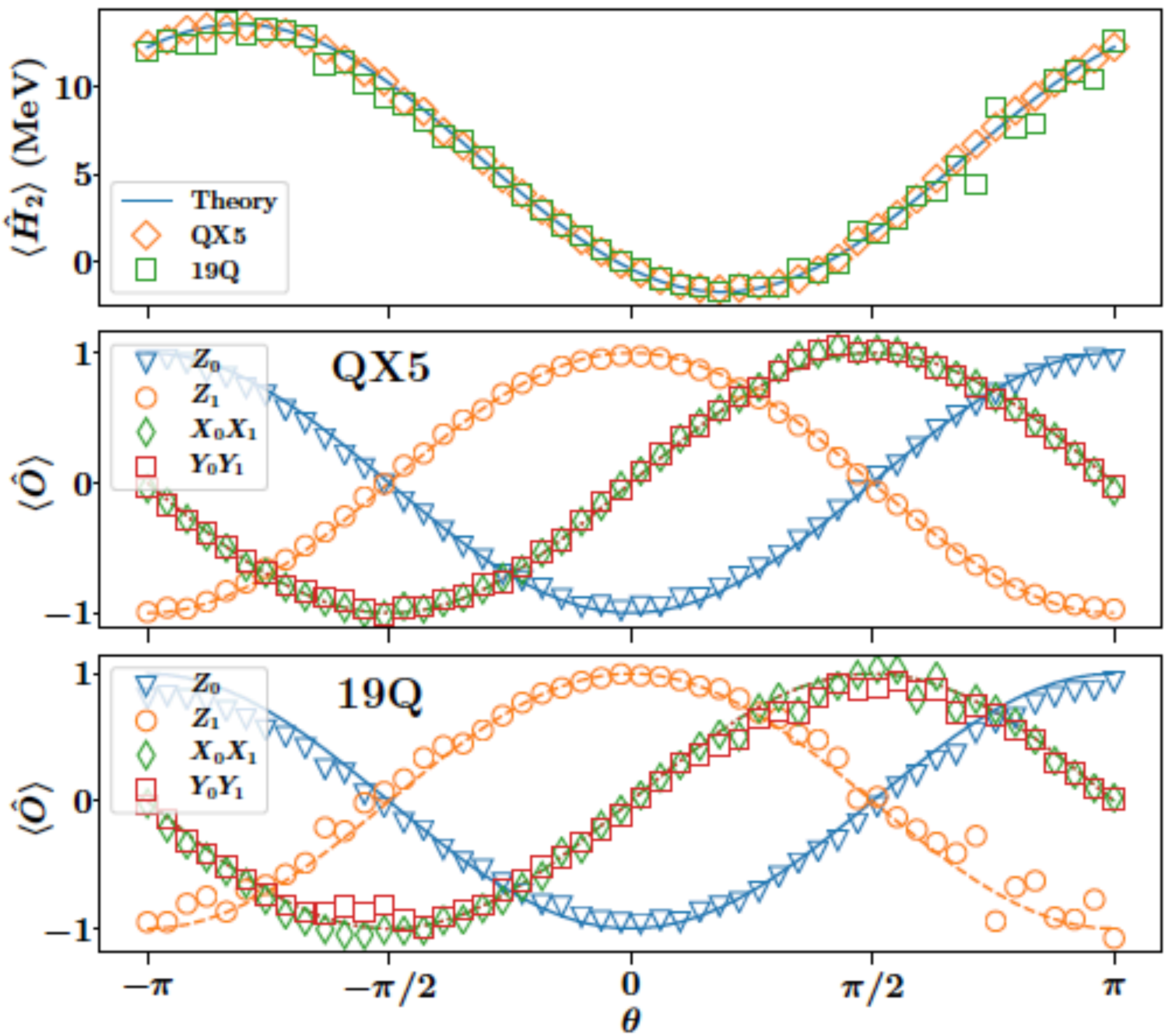


$U(\eta,\theta)$



Hamiltonian on two qubits

$$H_2 = 5.906709 I + 0.218291 Z_0 - 6.125 Z_1 - 2.143304 \left(X_0 X_1 + Y_0 Y_1 \right)$$



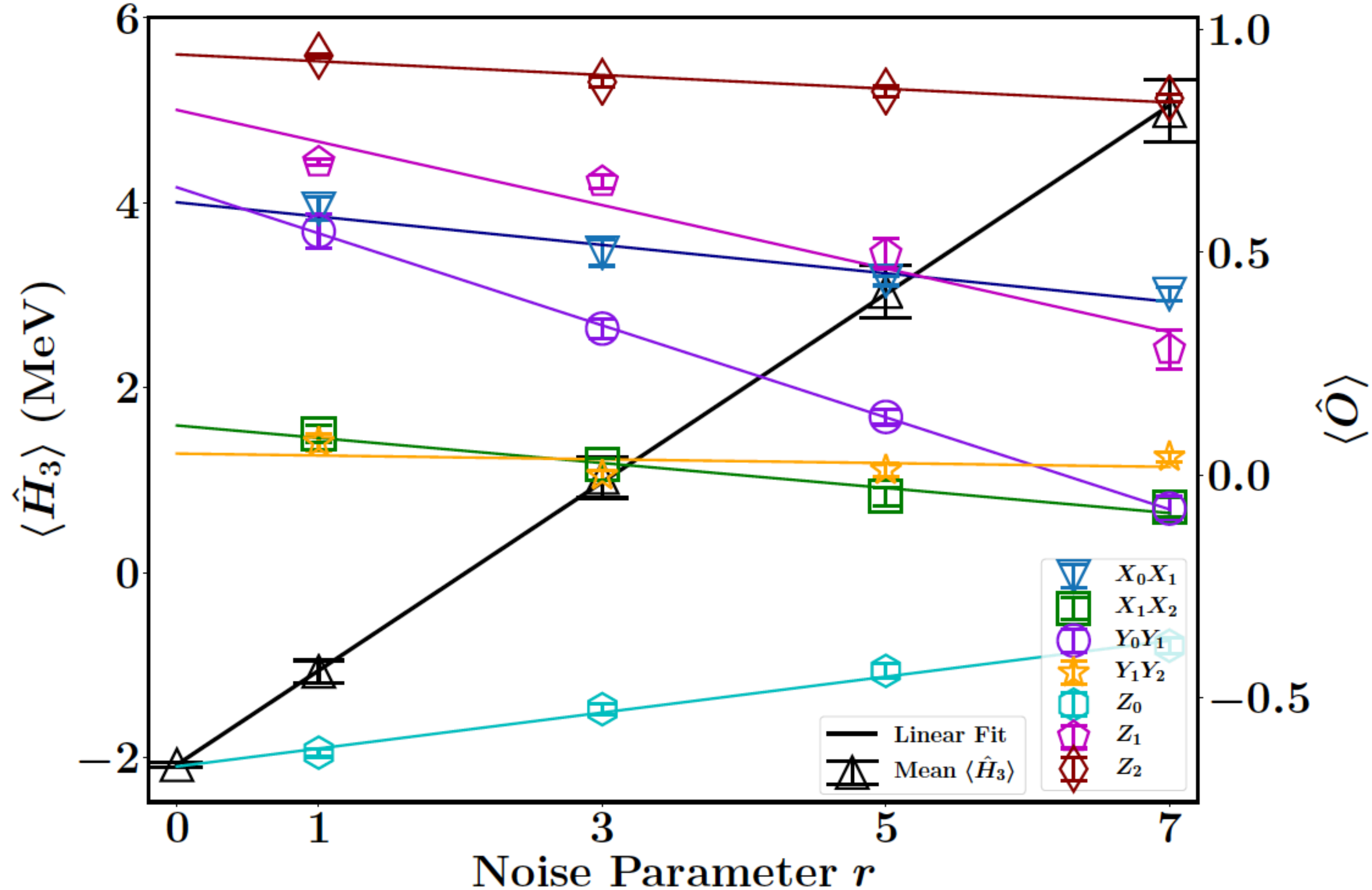
Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Expectation values on QPU. Minimization on CPU.

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

Three qubits

$$H_3 = H_2 + 9.625(I - Z_2) - 3.913119\,(X_1X_2 + Y_1Y_2)$$



Three qubits have more noise. Insert pairs of CNOT (unity operators) to extrapolate to *r*=0. [See, e.g., Ying Li & S. C. Benjamin 2017]

Final results

Deuteron ground-state energies from a quantum computer compared to the exact result, E_∞=-2.22 MeV.

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	$-2.08(3)$	$-2.35(2)$	$-2.21(3)$	$-2.28(3)$

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

PHYSICAL REVIEW LETTERS **120,** 210501 (2018)

Editors' Suggestion   Featured in Physics

Cloud Quantum Computing of an Atomic Nucleus

E. F. Dumitrescu,[1] A. J. McCaskey,[2] G. Hagen,[3,4] G. R. Jansen,[5,3] T. D. Morris,[4,3] T. Papenbrock,[4,3,*] R. C. Pooser,[1,4] D. J. Dean,[3] and P. Lougovski[1,†]

MIT Technology Review

The Best of the Physics arXiv (week ending January 20, 2018

This week's most thought-provoking papers from the Physics arXiv.

by Emerging Technology from the arXiv   January 20, 2018

A roundup of the most interesting papers from the arXiv:

Cloud Quantum Computing of an Atomic Nucleus

Black Holes as Brains: Neural Networks with Area Law Entropy

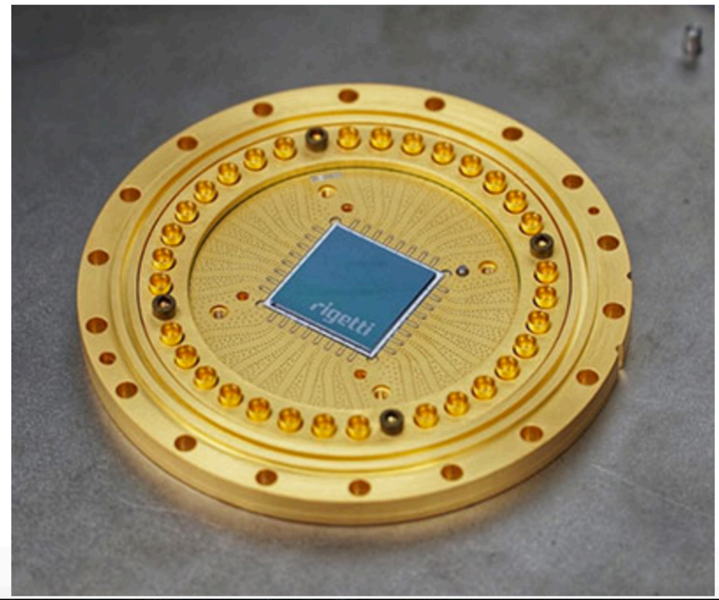
The Dynamical Structure of Political Corruption Networks

Measuring the Complexity of Consciousness

Scale-Free Networks are Rare

Cloud quantum computing calculates nuclear binding energy

Jan 29, 2018



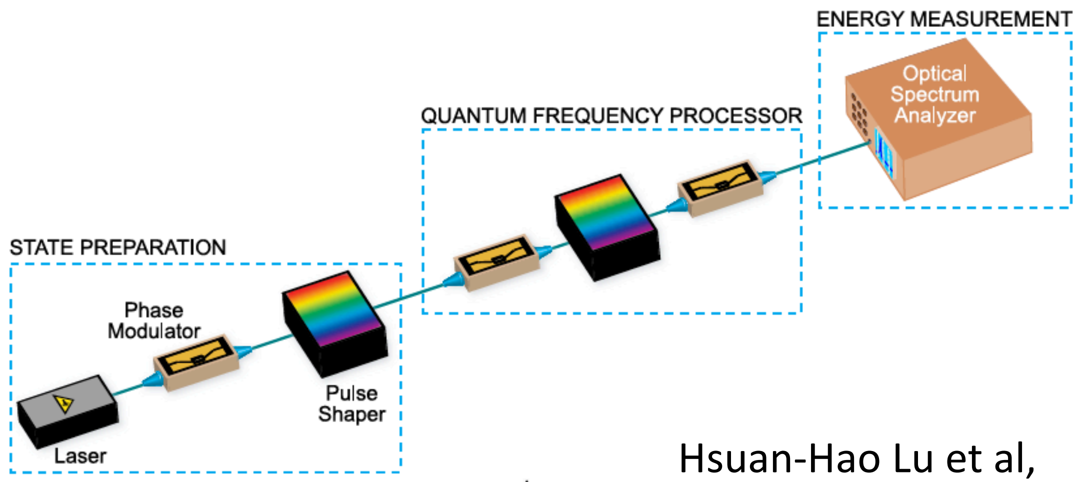
Cloud based quantum computing used to calculate nuclear binding energy

February 2, 2018 by Bob Yirka, Phys.org report

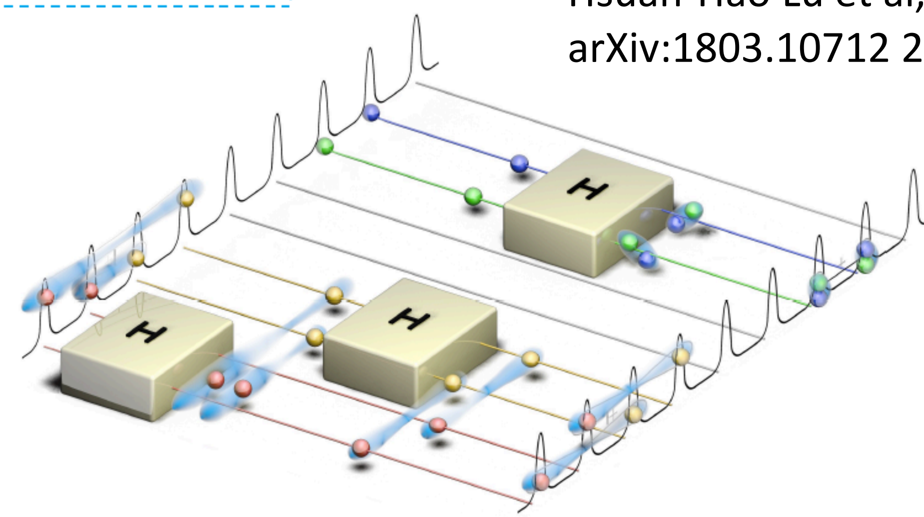
Simulations of atomic nuclei on a quantum frequency processor

Use an all-optical quantum frequency processor (QFP), to compute the ground-state energies of the light nuclei with a record-high 68-dimensional Hilbert space

- Encode qubits into narrow frequency bins
- Prepare quantum state by using a pulse shaper
- Use QFP to mix adjacent frequency bins
- Measure the density matrix and calculate expectation value



Hsuan-Hao Lu et al, arXiv:1803.10712 2018)

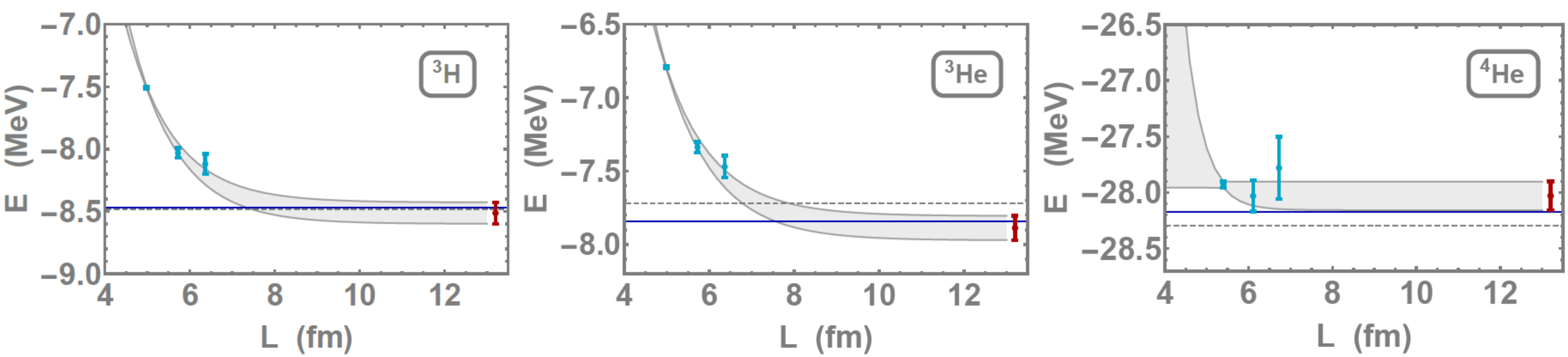


Hsuan-Hao Lu, Natalie Klco, Joseph M. Lukens, Titus D. Morris, et al, Phys. Rev. A 100, 012320 (2019)

Simulating atomic nuclei on a QFP

$N_{\max}$	Quantum frequency processor ^{3}H	^{3}He	^{4}He	Exact diagonalization ^{3}H	^{3}He	^{4}He
2	−7.508(8)	−6.794(7)	−27.93(3)	−7.513	−6.800	−27.947
4	−8.031(40)	−7.338(37)	−28.03(14)	−8.060	−7.366	−28.106
6	−8.120(81)	−7.470(75)	−27.78(28)	−8.275	−7.600	−28.148
N_A	—	—	—	−8.482	−7.830	−28.165
∞	−8.51(9)	−7.89(8)	−28.04(14)	−8.47	−7.84	−28.17
Exp.	−8.482	−7.718	−28.296	−8.482	−7.718	−28.296

Matrix dimensions: d(A=3) = 5,15, 34 & d(A=4) = 5,20, 64



Hsuan-Hao Lu, Natalie Klco, Joseph M. Lukens, Titus D. Morris, et al, Phys. Rev. A 100, 012320 (2019)

Summary

- Tremendous progress in first principles computations of nuclei using classical computers
- 50 year old puzzle of quenched beta decays solved from first principles
- Quantum computing has gained lots of excitement in the field
- Performed first quantum computation of an atomic nucleus
- Photonic based quantum simulations of subatomic physics
- Noisy Intermediate-Scale Quantum (NISQ) technology will be available in the near future

Collaborators

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

+ collaborators at Chalmers, IonQ/UMD, MSU, Purdue, and UW