Quantum Computing of the Deuteron

Thomas Papenbrock

THE UNIVERSITY of TENNESSEE UT KNOXVILLE

OAK RIDGE NATIONAL LABORATORY

SciDAC Scientific Discovery through Advanced Computing

Progress in Ab Initio Techniques in Nuclear Physics
TRIUMF, 27-Feb-2018

NUCLEI Nuclear Computational Low-Energy Initiative

Research partly funded by the US Department of Energy

Nuclear Physics & Quantum Computing Collaboration at ORNL

Cloud quantum computing of an atomic nucleus
Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski, arXiv:1801.03897]

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

Classical computing: logical gates

Information is physical (Landauer).

Classical computing uses irreversible gates

0 = False
1 = True

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

Classical gates implement logical operations (AND, OR, etc), and any function can be build from NOR gates alone.

Classical computer: classical gates operate on bits (0, 1).

What is quantum computing?

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

Examples:

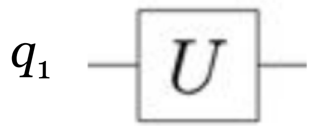
- spin up / spin down
- two polarization states of a photon
- ion in a trap on two levels

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

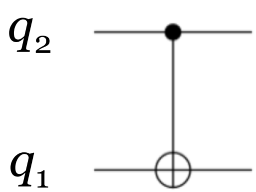
Quantum logical gates

Quantum computing is based on reversible processes (quantum gates perform unitary operations).

Single qubit unitary



Two qubit unitary



$$\begin{array}{cc} & |00\rangle |10\rangle |01\rangle\ |11\rangle \\ \text{CNOT} = & \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \end{array}$$

A set of universal of quantum logical gates can implement any unitary operator.

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).

How are QPUs realized?

- Transmon qubits (two-level system of Josephson junctions coupling an island with 0 or 1 Cooper pairs to a superconducting reservoir) → quantum chips we used for this paper
- Nitrogen vacancy in diamond (“NV diamond”)
- Ion traps
- Photonics
-
-
-

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

Who is doing it? (January 2018)

Company	Type	Technology	Now	Next Goal
Intel	Gate	Superconducting	49	TBD
Google	Gate	Superconducting	22	49
IBM	Gate	Superconducting	50	TBD
Rigetti	Gate	Superconducting	19	TBD
USTC (China)	Gate	Superconducting	10	20
IonQ	Gate	Ion Trap	7	20-50
Silicon Quantum Computing Pty	Gate	Spin	N/A	10
Univ. of Wisconsin	Gate	Neutral Atoms	49	TBD
Harvard/MIT	Quantum Simulator	Rydberg Atoms	51	TBD
Univ. of Maryland / NIST	Quantum Simulator	Ion Trap	53	TBD
D-Wave	Annealing	Superconducting	2048	5000
iARPA QEO Research Program	Annealing	Superconducting	N/A	100
NTT/Univ. of Tokyo/Japan NII	Qtm Neural Network	Photonic	2048	100,000

Many more are building a quantum chip.

Source: QuantumComputingReport.com

Office of Science & Technology Policy

DEPARTMENT OF ENERGY

Department of Energy

APS NEWS

February 2018 (Volume 27, Number 2)

OSTP Emphasizes Quantum Computing

Agency adds quantum information expertise amid calls for a coordinated approach to quantum research

offices. To accelerate development of QIS and apply advances in quantum computing, sensing, and other areas to fundamental research questions, quantum information and materials have been emphasized in the DOE SC Fiscal Year 2018 Budget Request. Recent specific FY 2017 program announcements were also issued for National Laboratory-led

Quantum computing status

There is a lot of excitement due to substantial progress:

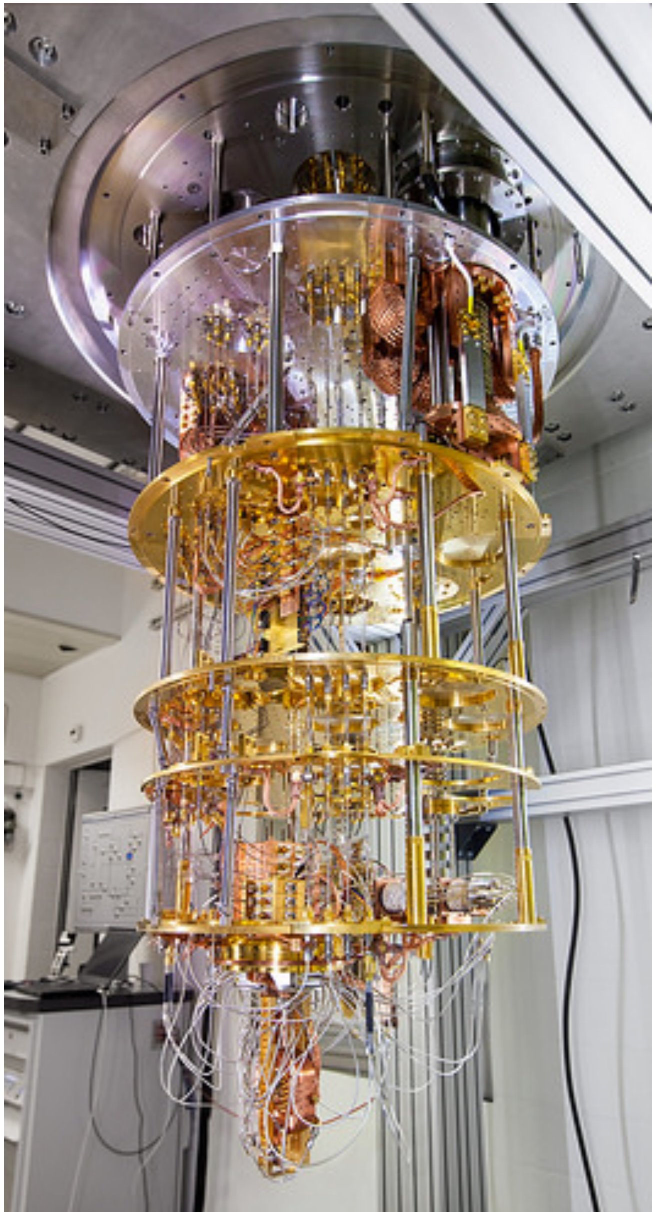
1. Quantum processing units now have ten(s) of qubits.
2. Businesses and science are invested in this.
3. Software is publicly available (OpenFermion, OpenQASM, PyQuil, QISKit, XACC,…).
4. First real-world problems solved: H_2 molecule on two qubits [O'Malley et al., Phys. Rev. X 6, 031007 (2016)]; BeH_2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

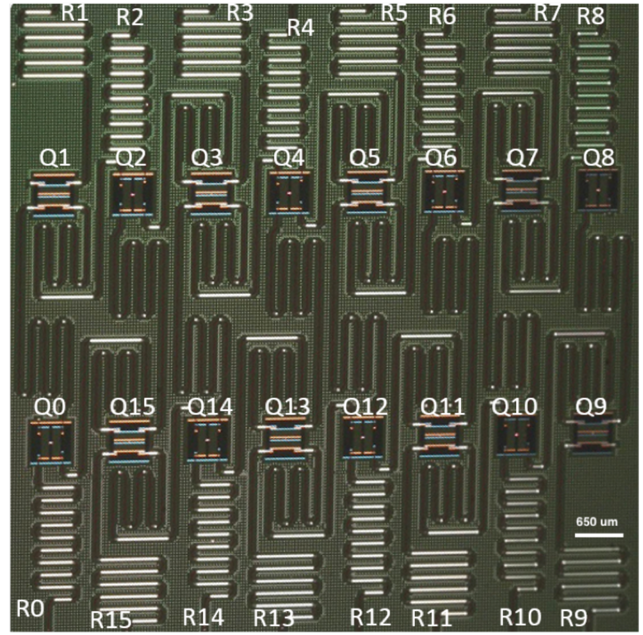
The scientific works were collaborations between theorists and hardware specialists (owners/operators of quantum chips).

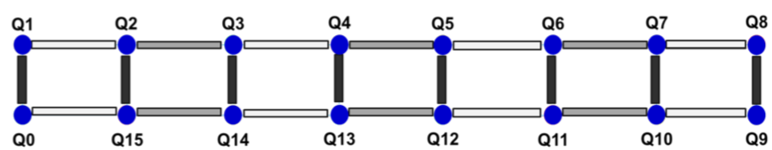
This paper: Cloud access possible; no insider knowledge required!

[Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski, arXiv:1801.03897]

IBM QX5 (16 qubits)



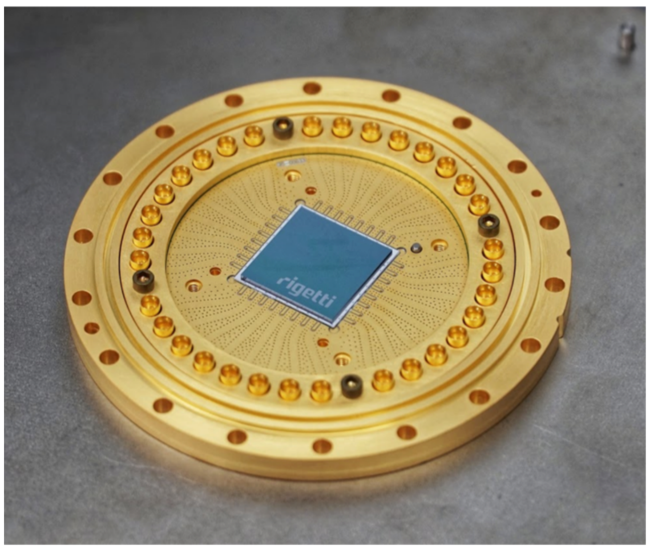


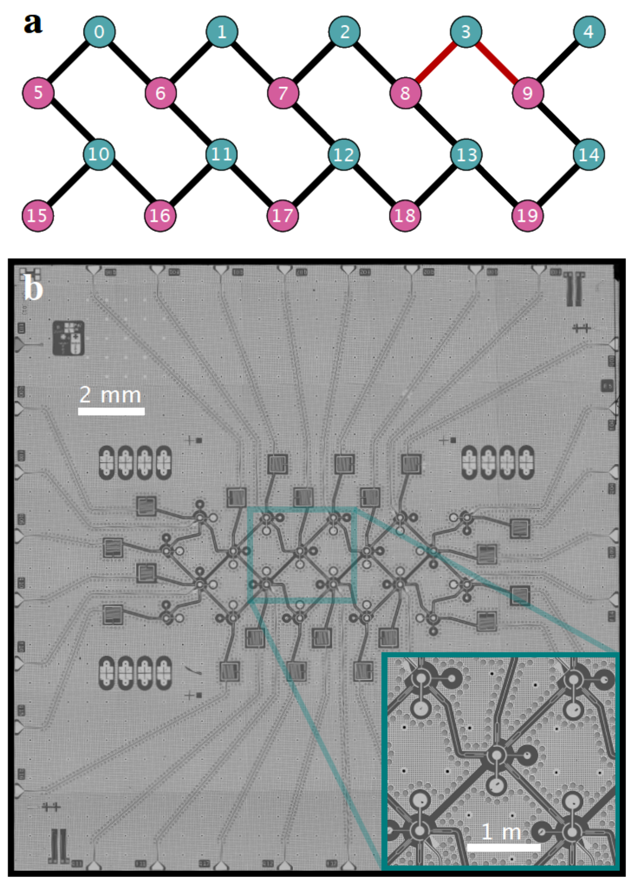


→ IBM Q Experience

Rigetti 19Q (19 qubits)

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

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 existing constraints

1. Gate errors, decoherence → low-depth circuit
2. Limited connectivity of qubits → tailored, simple Hamiltonian
3. Cloud access → only expectation values on QPU
4. Limited fidelity → noise correction

Game plan ("simplest deuteron")

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. (2017)**]; cutoff at about 150 MeV.

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

$$\langle n'|V|n\rangle = V_0 \delta^0_n \delta^{n'}_n$$

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

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

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

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

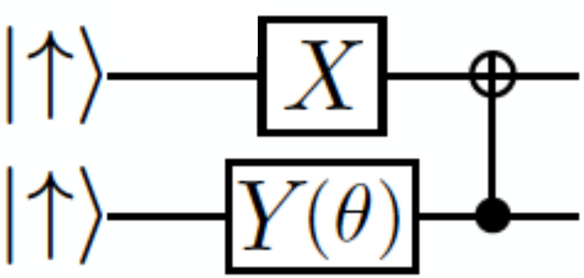
$U(\theta)|\downarrow\uparrow\rangle$ $\quad\quad$ $U(\theta) \equiv e^{\theta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right)} = e^{i\frac{\theta}{2}(X_0Y_1 - X_1Y_0)}$

Wave functions on three qubits

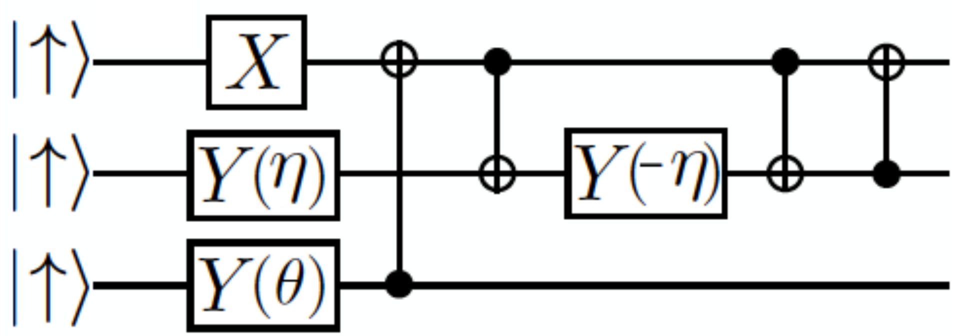
$U(\eta,\theta)|\downarrow\uparrow\uparrow\rangle$ $\quad\quad$ $U(\eta,\theta) \equiv e^{\eta\left(a_0^\dagger a_1 - a_1^\dagger a_0\right) + \theta\left(a_0^\dagger a_2 - a_2^\dagger a_0\right)}$

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

$U(\theta)$

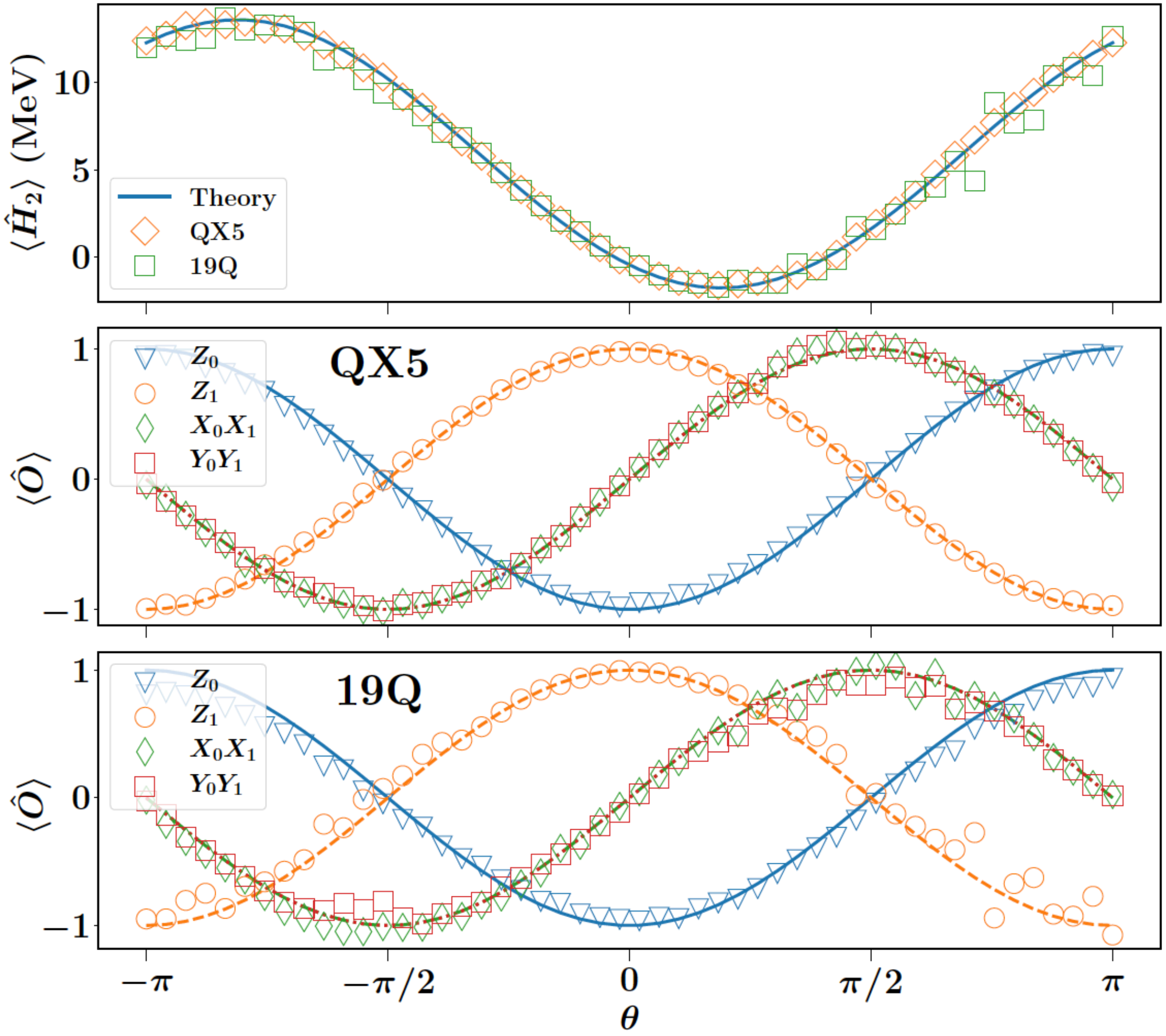


$U(\eta,\theta)$



Hamiltonian expectation value on two qubits

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

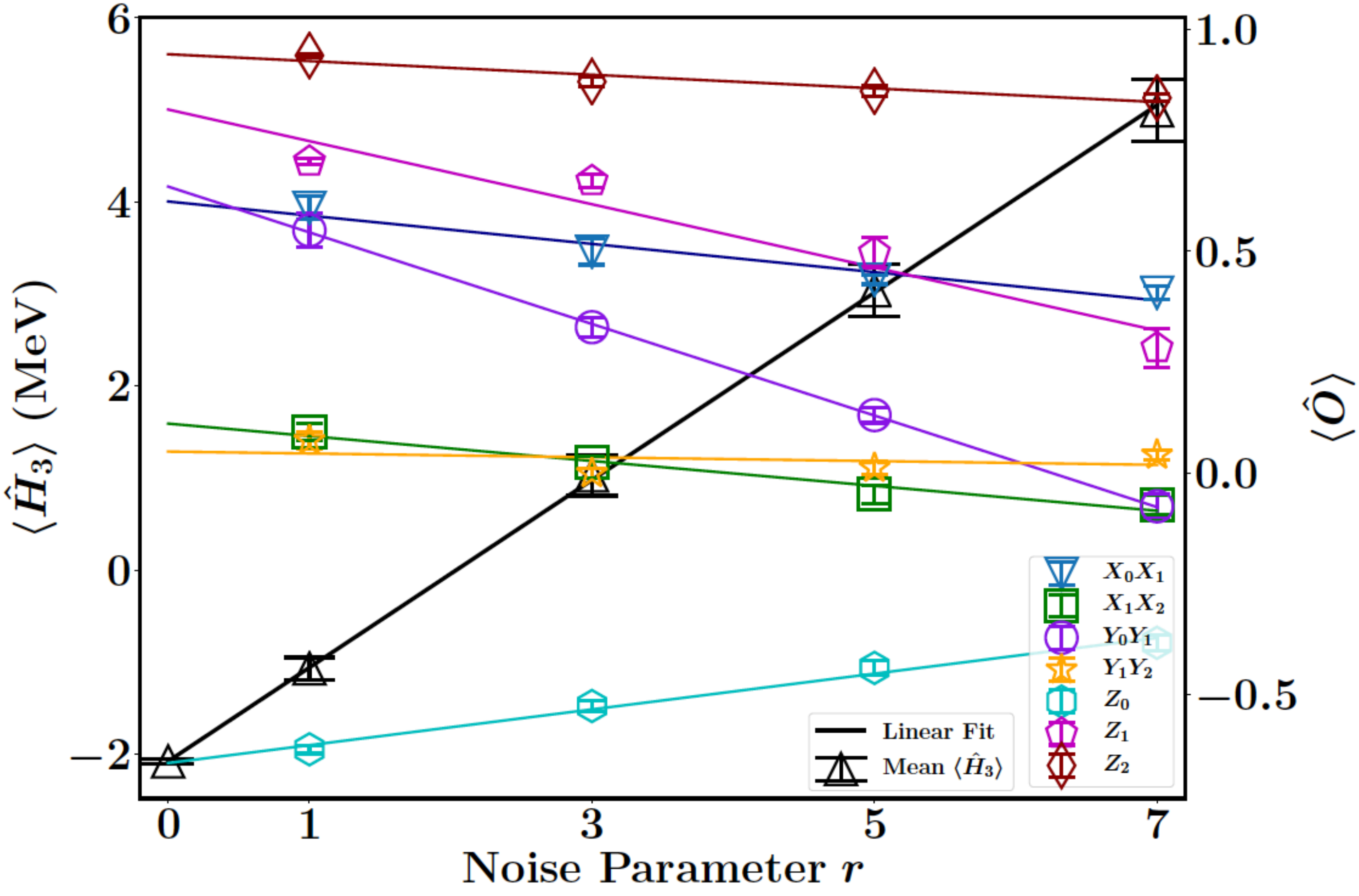


Quantum-classical hybrid algorithm VQE [Peruzzo et al. 2014; McClean et al 2016]:

Expectation values on QPU.
Minimization on CPU.

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

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

[Dumitrescu, McCaskey, Hagen, Jansen, Morris, TP, Pooser, Dean, Lougovski, arXiv:1801.03897]

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

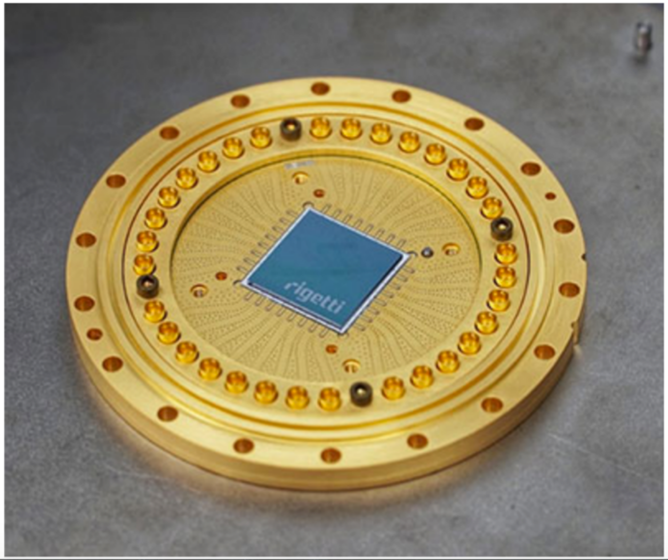
News archive

2018
- February 2018
- January 2018

2017
2016
2015
2014
2013
2012
2011
2010
2009
2008
2007
2006
2005
2004
2003
2002
2001

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

Summary

- Quantum computers have started to solve realistic problems, e.g. in quantum chemistry and nuclear physics.
- Still far away from solving quantum mechanics for systems that cannot be solved on a classical computer.

- We computed the deuteron, with a Hamiltonian from pion-less EFT, on quantum chips using two and three qubits.
- This required us to use a simple Hamiltonian, efficient wave function preparations, low-depth circuits, and noise extrapolation.