Intro to Quantum Computing / Information

Thomas Papenbrock, The University of Tennessee & Oak Ridge National Laboratory

National Nuclear Physics Summer School

Bloomington, IN, July 15-26, 2024

Work supported by the US Department of Energy

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

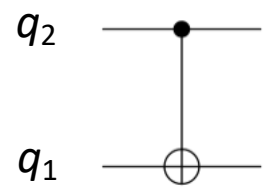
Universality: Any logical functions can be built from a small sets of gates.

Quantum

Qubits |0>, |1>

Reversible unitary operations

$$\begin{bmatrix} e^{i\varphi_1}\cos\theta & e^{i\varphi_2}\sin\theta \\ -e^{-i\varphi_2}\sin\theta & e^{-i\varphi_1}\cos\theta \end{bmatrix}$$



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

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

Single qubit operations

- States on qubit are $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$
- Question: What is the most general state we can make from these basis states?

Single qubit operations

- States on qubit are $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$
- Question: What is the most general state we can make from these basis states?
- Answer: states generated by SU(2) rotations, e.g. by the Wigner matrix $D^{\frac{1}{2}}_{mk}(\alpha, \beta, \gamma)$

$$U(\alpha, \beta, \gamma) = e^{-i\frac{\alpha}{2}\sigma_z} e^{-i\frac{\beta}{2}\sigma_y} e^{-i\frac{\gamma}{2}\sigma_z} = \begin{bmatrix} e^{-i\frac{\alpha}{2}} \cos\frac{\beta}{2} e^{-i\frac{\gamma}{2}} & -e^{-i\frac{\alpha}{2}} \sin\frac{\beta}{2} e^{i\frac{\gamma}{2}} \\ e^{i\frac{\alpha}{2}} \sin\frac{\beta}{2} e^{-i\frac{\gamma}{2}} & e^{i\frac{\alpha}{2}} \cos\frac{\beta}{2} e^{i\frac{\gamma}{2}} \end{bmatrix}$$

Single qubit operations cont'd

- States on qubit are $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$
- Consider Pauli matrices $X \equiv \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $Y \equiv \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, and $Z \equiv \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
- Question: What are the relevant properties of Pauli matrices?
- A1: Pauli matrices are Hermitian
- A2: Pauli matrices are unitary
- A3: All of the above

Single qubit operations cont'd

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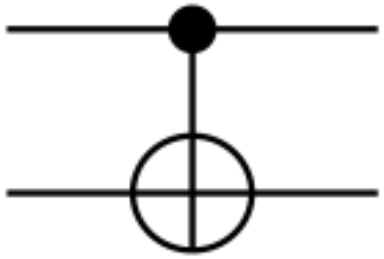
Thus, the Pauli matrices and exponentials $e^{i\theta X}$, $e^{i\theta Y}$, and $e^{i\theta Z}$ are all unitary operators

Two qubit operation: CNOT

Control qubit



Target qubit

Before		After	
Control	Target	Control	Target
$\|0\rangle$	$\|0\rangle$	$\|0\rangle$	$\|0\rangle$
$\|0\rangle$	$\|1\rangle$	$\|0\rangle$	$\|1\rangle$
$\|1\rangle$	$\|0\rangle$	$\|1\rangle$	$\|1\rangle$
$\|1\rangle$	$\|1\rangle$	$\|1\rangle$	$\|0\rangle$

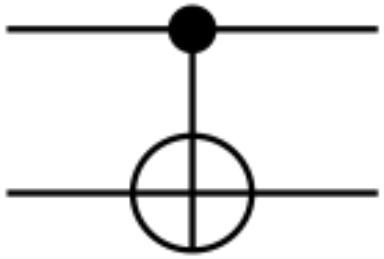
$$\mathrm{CNOT} = e^{i\frac{\pi}{4}(I_1 - Z_1)(I_2 - X_2)} = e^{-i\frac{\pi}{4}(I_1 - Z_1)(I_2 - X_2)}$$

Q: How does the CNOT gate work (look at the table)?

Image credits: wikipedia

Two qubit operation: CNOT

Control qubit



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$\|0\rangle$	$\|0\rangle$	$\|0\rangle$	$\|0\rangle$
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$\|1\rangle$	$\|1\rangle$	$\|1\rangle$	$\|0\rangle$

$$\mathrm{CNOT} = e^{i\frac{\pi}{4}(I_1 - Z_1)(I_2 - X_2)} = e^{-i\frac{\pi}{4}(I_1 - Z_1)(I_2 - X_2)}$$

Q: How does the CNOT gate work (look at the table)?

A: The CNOT gate flips the target qubit if and only if the control qubit is in state $|1\rangle$.

Any unitary operation on N qubits can be realized as a product of single-qubit unitary operations and CNOT operations. The CNOT entangles states of two qubits.

Image credits: wikipedia

Storing and processing information

- Computing frontier: The memory on Frontier's compute nodes can store about 10 Peta Byte $\approx 2^{56}$ bit of information
- Question: How many qubits does one need to store this amount of information?

Storing and processing information

- Computing frontier: The memory on Frontier's compute nodes can store about 10 Peta Byte $\approx 2^{56}$ bit of information
- Answer: 56 error corrected qubits

  Thus it seems that quantum computers could revolutionize storage and processing of information

… drum roll

Quantum ~~Supremacy~~

Article

Quantum supremacy using a programmable superconducting processor

https://doi.org/10.1038/s41586-019-1666-5

Received: 22 July 2019

Accepted: 20 September 2019

Published online: 23 October 2019

Frank Arute[1], Kunal Arya[1], Ryan Babbush[1], Dave Bacon[1], Joseph C. Bardin[1,2], Rami Barends[1], Rupak Biswas[3], Sergio Boixo[1], Fernando G. S. L. Brandao[1,4], David A. Buell[1], Brian Burkett[1], Yu Chen[1], Zijun Chen[1], Ben Chiaro[5], Roberto Collins[1], William Courtney[1], Andrew Dunsworth[1], Edward Farhi[1], Brooks Foxen[1,5], Austin Fowler[1], Craig Gidney[1], Marissa Giustina[1], Rob Graff[1], Keith Guerin[1], Steve Habegger[1], Matthew P. Harrigan[1], Michael J. Hartmann[1,6], Alan Ho[1], Markus Hoffmann[1], Trent Huang[1], Travis S. Humble[7], Sergei V. Isakov[1], Evan Jeffrey[1], Zhang Jiang[1], Dvir Kafri[1], Kostyantyn Kechedzhi[1], Julian Kelly[1], Paul V. Klimov[1], Sergey Knysh[1], Alexander Korotkov[1,8], Fedor Kostritsa[1], David Landhuis[1], Mike Lindmark[1], Erik Lucero[1], Dmitry Lyakh[9], Salvatore Mandrà[3,10], Jarrod R. McClean[1], Matthew McEwen[5], Anthony Megrant[1], Xiao Mi[1], Kristel Michielsen[11,12], Masoud Mohseni[1], Josh Mutus[1], Ofer Naaman[1], Matthew Neeley[1], Charles Neill[1], Murphy Yuezhen Niu[1], Eric Ostby[1], Andre Petukhov[1], John C. Platt[1], Chris Quintana[1], Eleanor G. Rieffel[3], Pedram Roushan[1], Nicholas C. Rubin[1], Daniel Sank[1], Kevin J. Satzinger[1], Vadim Smelyanskiy[1], Kevin J. Sung[1,13], Matthew D. Trevithick[1], Amit Vainsencher[1], Benjamin Villalonga[1,14], Theodore White[1], Z. Jamie Yao[1], Ping Yeh[1], Adam Zalcman[1], Hartmut Neven[1] & John M. Martinis[1,5]*

Google claim: 10,000 years on Summit

IBM: 2.5 days on Summit (October 2019)

Quantum ~~Advantage~~

nature communications

arXiv:2208.02199

Article

https://doi.org/10.1038/s41467-023-37587-6

Evaluating the evidence for exponential quantum advantage in ground-state quantum chemistry

Received: 31 January 2023

Accepted: 22 March 2023

Published online: 07 April 2023

Check for updates

Seunghoon Lee[1], Joonho Lee[2], Huanchen Zhai[1], Yu Tong[3], Alexander M. Dalzell[4], Ashutosh Kumar[5,6], Phillip Helms[1], Johnnie Gray[1], Zhi-Hao Cui[1], Wenyuan Liu[1], Michael Kastoryano[4,7], Ryan Babbush[8], John Preskill[4,9], David R. Reichman[2], Earl T. Campbell[10], Edward F. Valeev[5], Lin Lin[3,11] & Garnet Kin-Lic Chan[1]

Due to intense interest in the potential applications of quantum computing, it is critical to understand the basis for potential exponential quantum advantage in quantum chemistry. Here we gather the evidence for this case in the most common task in quantum chemistry, namely, ground-state energy estimation, for generic chemical problems where heuristic quantum state preparation might be assumed to be efficient. The availability of exponential quantum advantage then centers on whether features of the physical problem that enable efficient heuristic quantum state preparation also enable efficient solution by classical heuristics. Through numerical studies of quantum state preparation and empirical complexity analysis (including the error scaling) of classical heuristics, in both ab initio and model Hamiltonian settings, we conclude that evidence for such an exponential advantage across chemical space has yet to be found. While quantum computers may still prove useful for ground-state quantum chemistry through polynomial speedups, it may be prudent to assume exponential speedups are not generically available for this problem.

"While quantum computers ***may*** still ***prove useful*** for ground-state quantum chemistry through polynomial speedups, it may be prudent to assume exponential speedups are not generically available for this problem."

Quantum chemistry: coupled-cluster methods scale polynomially. Will be hard to beat.

Quantum Utility

Quantum computers will probably be around in the future

1. Let us find out how they could be used in nuclear (structure) theory
2. Let us find out how ideas from quantum information might be useful in nuclear theory

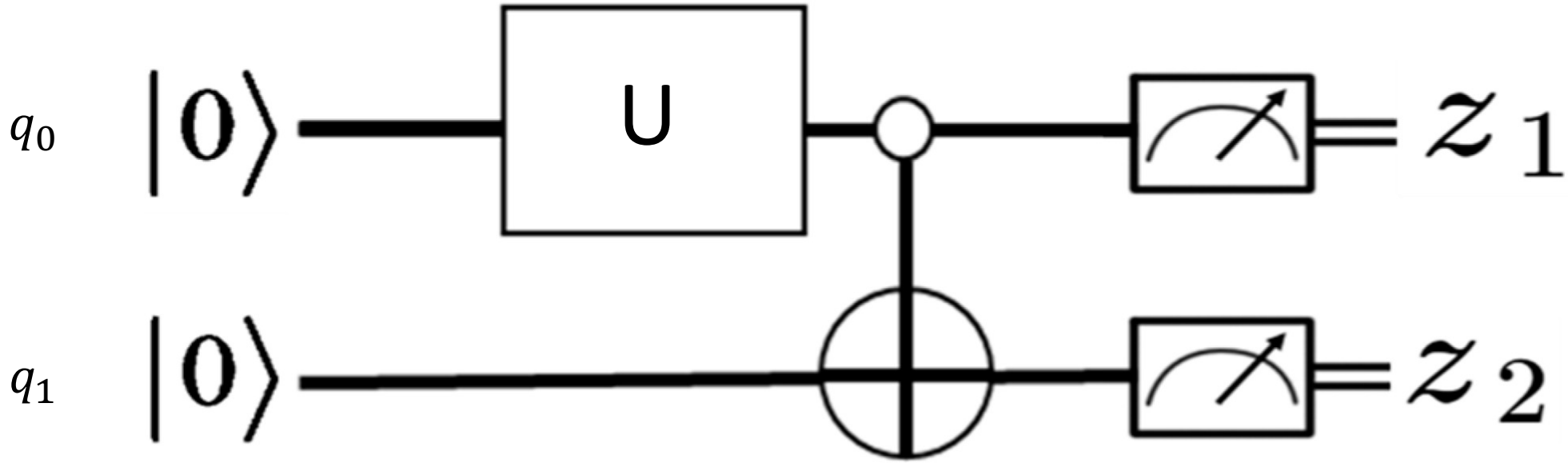
Quantum computing summary

- Only unitary transformations are allowed
  - these are reversible
  - No information is lost
- Measurements (i.e. projections of states onto the computational basis states $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$) at the end of a computation are irreversible
- So quantum computing means:
  - transform a sequence of unitary operations on qubits
  - make a measurement at the end

Quantum Circuits

Single-qubit unitary U acts on q_0.

Measurements on each qubit yields results $z_{1,2}$.



Qubits are initially in $|0\rangle$

Two-qubit unitary CNOT acts on q_0 and q_1.
Creates entangled quantum states.

time

Image credit:
https://dojo.qulacs.org/en/qp_main/notebooks/1.4_quantum_circuit_diagram.html

Mapping fermions to qubits

- States on qubit q are $|\uparrow\rangle_q = |0\rangle_q$ and $|\downarrow\rangle_q = |1\rangle_q$
- Reminds us of fermion states $|1\rangle_q = \hat{a}_q^+ |0\rangle_q$
- Note: lowering the spin of state $|0\rangle$ generates the "occupied" state $|1\rangle$, thus spin lowering and fermion creation are related (and spin raising and fermion annihilation)

Mapping of operators

- Spin raising / lowering operator $\sigma_{\pm} = \frac{1}{2}\left(\sigma_x \pm i\sigma_y\right) = \begin{cases} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \end{cases}$
- Notation: $\left(\sigma_x^{(q)} \pm i\sigma_y^{(q)}\right) \equiv X_q \pm iY_q$
- Thus, we have $\frac{1}{2}(X_q - iY_q)|0\rangle = |1\rangle$ and $\frac{1}{2}(X_q + iY_q)|1\rangle = |0\rangle$
- Question: How do we implement $\hat{a}_q^+$ using spin operators?

  Hint: need $\left\{\hat{a}_p\,, \hat{a}_q^+\right\} = \delta_{pq}$ and $\left\{\hat{a}_p^+\,, \hat{a}_q^+\right\} = 0$

Mapping of operators

- Spin raising / lowering operator $\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y) = \begin{cases} \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \\ \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \end{cases}$
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- Thus, we have $\frac{1}{2}(X_q - iY_q)|0\rangle = |1\rangle$ and $\frac{1}{2}(X_q + iY_q)|1\rangle = |0\rangle$
- Answer: $\hat{a}_q^+ = \frac{1}{2}\prod_{n=0}^{q-1}(-Z_n)\,(X_q - iY_q)$

  Thus the convention is $\hat{a}_0^+\hat{a}_1^+ \cdots \hat{a}_{k-1}^+|0\rangle = |1,1,\cdots,1\rangle$. $q = 0, 1, \cdots, k-1$
- Note the cost of this Jordan-Wigner mapping is $O(N)$ for N qubits; Bravyi-Kitaev mapping has cost $O(\log N)$

Quantum computing naturally relates to fermions

- Bosons are harder (unlike in classical computing): need many (strictly: infinitely many) qubits for a single boson.
- Question: How many qubits do we need to compute a system of A fermions on n single-particle states?
- A1: n qubits
- A2: $\log_2 \binom{n}{A}$ qubits
- A3: both answers are correct and can lead to useful solutions

A1: n qubits

- This is probably most natural: direct translation from Hamiltonians to qubits, and spin-raising/lowering operators
- "Second quantization" is the tool
- Frontiers in computational nuclear structure:
  - Ab initio calculations use up to $n \approx 4000$ single-particle states
  - Shell model (exact diagonalization): pf($g_{9/2}$) shell $n \approx 40 - 50$ single-particle states
- OpenFermion python package
  https://github.com/quantumlib/OpenFermion
  arXiv:1710.07629

A2: $\log_2 \binom{n}{A}$ qubits

- Tremendous reduction in resource demands
- But:
  - complicated mapping from many-body states to qubit states
  - number of matrix elements of the A-body Hamiltonian matrix scales exponentially with A
- Potentially attractive for Noisy Intermediate Scale Quantum (NISQ) computing [NISQ: Preskill, arXiv:1801.00862]
- Example: [Di Matteo, McCoy, Gysbers, Miyagi, Woloshyn, Navratil, Phys. Rev. A 103, 042405 (2021), arXiv:2008.05012]

Let's work through an example

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*
[2]*Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[3]*Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[4]*Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA*
[5]*National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

(Received 12 January 2018; published 23 May 2018)

We report a quantum simulation of the deuteron binding energy on quantum processors accessed via cloud servers. We use a Hamiltonian from pionless effective field theory at leading order. We design a low-depth version of the unitary coupled-cluster ansatz, use the variational quantum eigensolver algorithm, and compute the binding energy to within a few percent. Our work is the first step towards scalable nuclear structure computations on a quantum processor via the cloud, and it sheds light on how to map scientific computing applications onto nascent quantum devices.

Example: “simplest deuteron” via quantum computing

1. Hamiltonian from pionless EFT at leading order; fit to deuteron binding energy; constructed in harmonic-oscillator basis of ${}^3S_1$ partial wave; cutoff at about 150 MeV.

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

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

2. Map single-particle radial harmonic-oscillator states $|n\rangle$, n=0, 1, 2, … onto qubits. This is an analog of the Jordan-Wigner transform. Quantum computing convention: $|\uparrow\rangle = |0\rangle$ and $|\downarrow\rangle = |1\rangle$

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

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)]

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

Example: “simplest deuteron” via quantum computing

What is the deuteron?

Q: Particle content?

Q: Spin = ? Isospin = ?

Q: State decomposed into partial waves as ?

Example: “simplest deuteron” via quantum computing

What is the deuteron?

Q: Bound state of a neutron and a proton

Q: Spin = ? Isospin = ?

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Example: “simplest deuteron” via quantum computing

What is the deuteron?

Q: Bound state of a neutron and a proton

Q: Spin = 1, Isospin = 0

Q: State decomposed into partial waves as ?

Example: “simplest deuteron” via quantum computing

What is the deuteron?

Q: Bound state of a neutron and a proton

Q: Spin = 1, Isospin = 0

Q: $|\psi\rangle = \cos\eta\,(|L=0\rangle\times|S=1\rangle)^{(J=1)} + \sin\eta\,(|L=2\rangle\times|S=1\rangle)^{(J=1)}$

The d-wave admixture is small. So, we will model the s-wave only (and suppress the trivial spin-isospin state).

This approximation is also consistent with pionless effective field theory at leading order.

Q: $H = T + V$. What is the potential?

Example: “simplest deuteron” via quantum computing

What is the deuteron?

Q: Bound state of a neutron and a proton

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The d-wave admixture is small. So, we will model the s-wave only (and suppress the trivial spin-isospin state).

This approximation is also consistent with pionless effective field theory at leading order.

Q: $H = T + V$. What is the potential?

A: $V = V_0\delta_a^{(3)}(r)$ where V_0 is a low-energy constant and a a finite range (inverse cutoff)

We will use spherical harmonic oscillator states as a basis, only need the radial quantum number $n = 0,1,2,\ldots$ and we have states $|n\rangle$.

Example: “simplest deuteron” via quantum computing

Hamiltonian constructed in harmonic-oscillator basis of $^3S_1$ partial wave:

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

$$\langle n'|T|n\rangle = \frac{\hbar\omega}{2}\Big[(2n+3/2)\delta^{n'}_n - \sqrt{n(n+1/2)}\delta^{n'+1}_n - \sqrt{(n+1)(n+3/2)}\delta^{n'-1}_n\Big],$$

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

$\hbar\omega = 7$ MeV corresponds to a momentum cutoff of about 150 MeV

$V_0 = -5.68658111$ MeV yields the deuteron ground-state energy -2.22 MeV in large model spaces (many basis states)

Mapping quantum states onto qubits

Q: How do we do map the basis states $|n\rangle$ with $n = 0,1,2, \dots, N-1$ onto qubits?

A1:

A2:

Mapping quantum states onto qubits

Q: How do we do map the basis states $|n\rangle$ with $n = 0,1,2, \dots, N-1$ onto qubits?

A1: binary mapping: $|n = 0\rangle = |0000 \dots 0\rangle$, $|n = 1\rangle = |1000 \dots 0\rangle$,
$|n = 2\rangle = |0100 \dots 0\rangle$ etc. Then K qubits can hold 2^K states.

A2:

Mapping quantum states onto qubits

Q: How do we do map the basis states $|n\rangle$ with $n = 0,1,2, \dots, N-1$ onto qubits?

A1: binary mapping: $|n = 0\rangle = |0000 \dots 0\rangle$, $|n = 1\rangle = |1000 \dots 0\rangle$,
$|n = 2\rangle = |0100 \dots 0\rangle$ etc. Then K qubits can hold 2^K states.

A2: "Second quantization" mapping $|n = 0\rangle = |1000 \dots 0\rangle$, $|n = 1\rangle = |0100 \dots 0\rangle$,
$|n = 2\rangle = |0010 \dots 0\rangle$ etc. Then K qubits can hold K states.

We will take A2. (Choice by taste, not substance) $H_N = \sum_{n,n'=0}^{N-1} \langle n'|(T+V)|n\rangle a_{n'}^{\dagger} a_n$

We will limit ourselves to two qubits.

How to prepare the ground state?

Q: Given basis state $|n\rangle$ with $n = 0,1$ what is the most general state?

A:

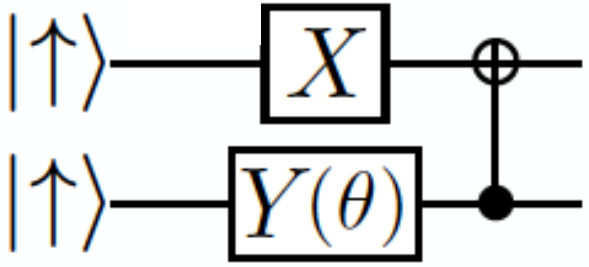
How to prepare the ground state?

Q: Given basis state $|n\rangle$ with $n = 0,1$ what is the most general state?

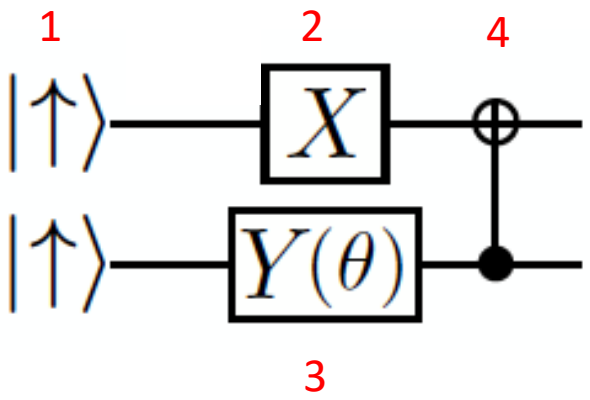
A: $\cos\theta\,|n=0\rangle + \sin\theta\,|n=1\rangle$

Q: Why is this sufficient? Why not a full SU(2) transformation with three angles?

This is the circuit we used to achieve this:



State-preparation circuit on two qubits



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

$$Y(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

CNOT: flips the target qubit if and only if the control qubit is in state $|1\rangle = |\downarrow\rangle$

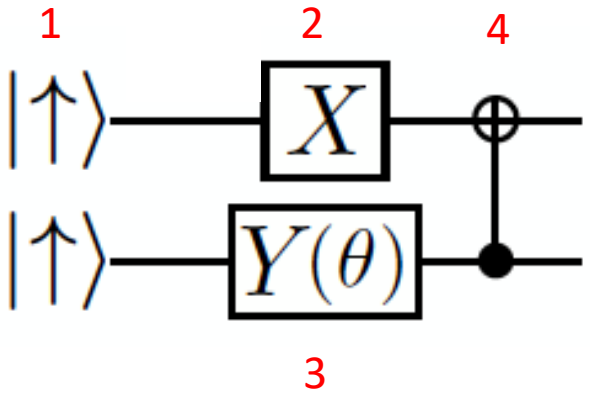
Q1: What is the state of the system after 1 ?

Q2: What is the state of the system after 2 ?

Q3: What is the state of the system after 3 ?

Q4: What is the state of the system after 4 ?

State-preparation circuit on two qubits



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CNOT: flips the target qubit if and only if the control qubit is in state $|1\rangle = |\downarrow\rangle$

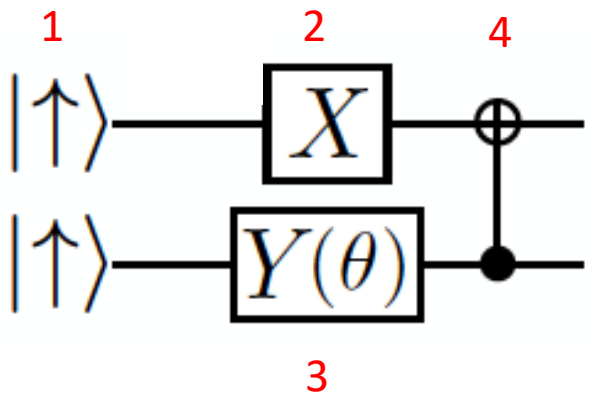
A1: $|\uparrow\rangle|\uparrow\rangle = |\uparrow\uparrow\rangle$. This is the vacuum: no deuteron.

Q2: What is the state of the system after 2 ?

Q3: What is the state of the system after 3 ?

Q4: What is the state of the system after 4 ?

State-preparation circuit on two qubits



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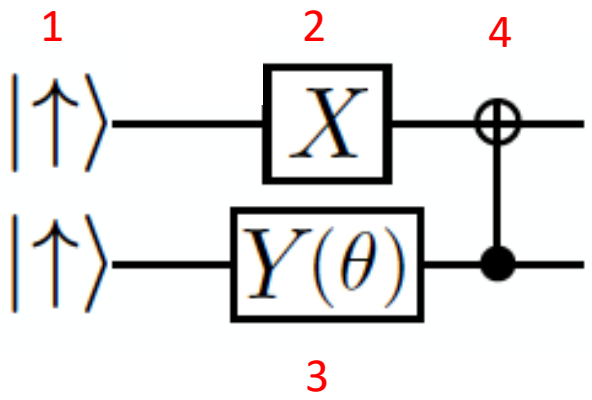
A1: $|\uparrow\rangle|\uparrow\rangle = |\uparrow\uparrow\rangle$. This is the vacuum: no deuteron.

A2: $|\downarrow\rangle|\uparrow\rangle = |\downarrow\uparrow\rangle$. Now we have a deuteron in the state $|n = 0\rangle$.

Q3: What is the state of the system after 3 ?

Q4: What is the state of the system after 4 ?

State-preparation circuit on two qubits



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

$$Y(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

CNOT: flips the target qubit if and only if the control qubit is in state $|1\rangle = |\downarrow\rangle$

A1: $|\uparrow\rangle|\uparrow\rangle = |\uparrow\uparrow\rangle$. This is the vacuum: no deuteron.

A2: $|\downarrow\rangle|\uparrow\rangle = |\downarrow\uparrow\rangle$. Now we have a deuteron in the state $|n = 0\rangle$.

Q3: $|\downarrow\rangle(|\uparrow\rangle\cos\theta + |\downarrow\rangle\sin\theta)$. This is a superposition of one and two deuterons.

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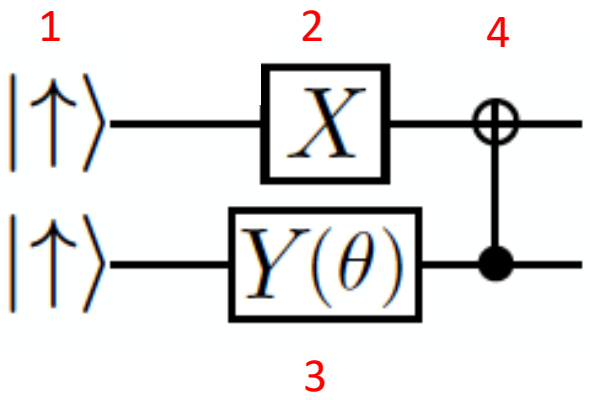

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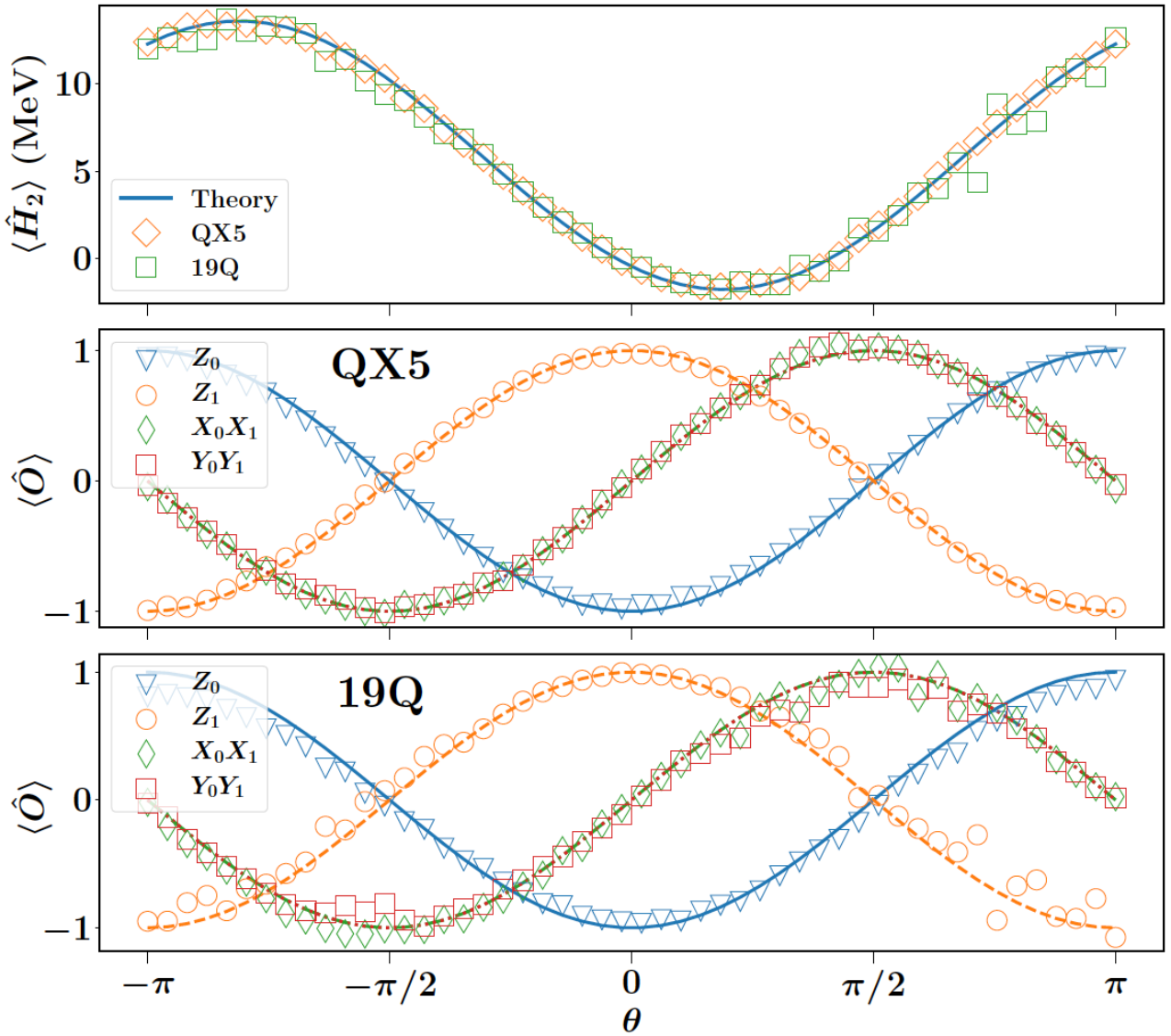
Q4: $|\downarrow\rangle|\uparrow\rangle\cos\theta + |\uparrow\rangle|\downarrow\rangle\sin\theta$. This is a deuteron in $|\mathrm{n} = 0\rangle\cos\theta + |\mathrm{n} = 1\rangle\sin\theta$.

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]

Measure expectation values of individual Pauli terms to measure energy on quantum chip.

Expectation values on QPU. 8129 measurements (“shots”) taken for each product of Pauli terms. Minimization on CPU.

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A1: Duh, the result of a measurement is $\langle\psi|H_2|\psi\rangle$.

A2: Wait, this is actually QM: The result is any eigenvalue E_n of H_2 and the probability is given by the overlap $|\langle\psi|\phi_n\rangle|^2$ where $|\phi_n\rangle$ is the (unknown) exact eigenstate of E_n. We need to make many measurements to get the expectation value (and a single measurement gives us an eigenvalue E_n).

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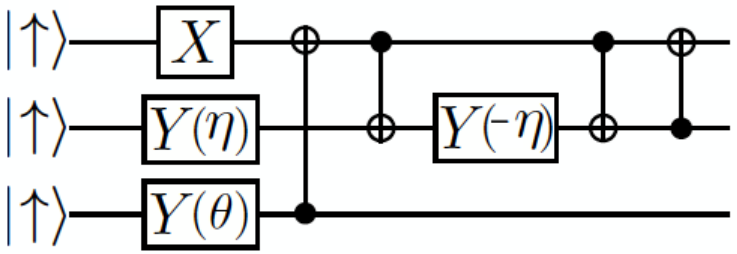
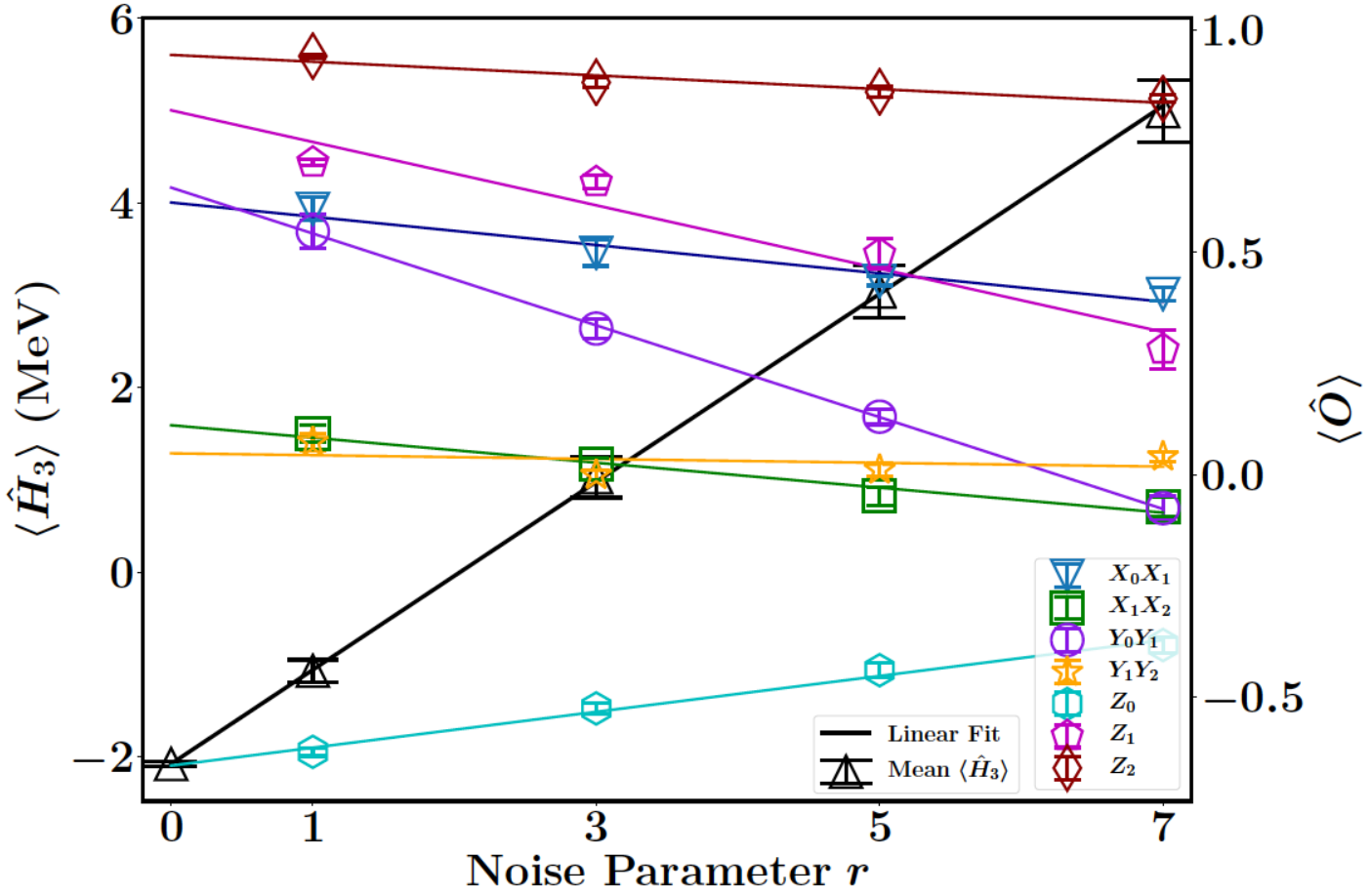
A3. Wait, this is even more complicated! We can only measure the expectation values of products of Pauli terms that make up the Hamiltonian. Each measurement is a stochastic result. One then multiplies the measurement of each product of Pauli terms with the coefficient that appears in the Hamiltonian and sums up all expectation values to get the result.

Three qubits

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





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

Final results

Deuteron ground-state energies from quantum computing compared to the exact $E_\infty = -2.22$ 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, PRL **120**, 210501 (2018)]

Snapshot

- Many researchers have explored how to compute ground and excited states on quantum computers
  - Variational quantum eigensolver (VQE)
    - Needs efficient ansatz for variational wave function, e.g, via unitary coupled cluster method
  - Phase estimation
    - More expensive than VQE; not as popular on NISQ machines
- Symmetry projection seems a natural candidate for quantum computing.
  - Q: Why?
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- Dynamics seems a natural candidate for quantum computing
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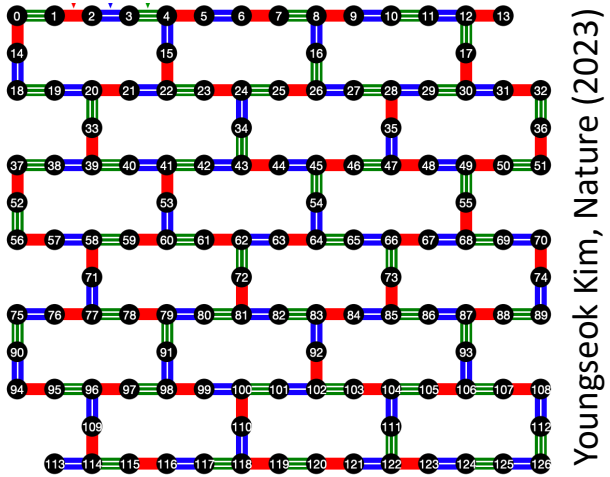
- Symmetry projection seems a natural candidate for quantum computing.
  - Q: Why?
  - A: symmetry projection uses unitary operators such as $e^{-i\theta J_y}$
- Dynamics seems a natural candidate for quantum computing
  - Q: Why?
  - A: time evolution operator e^{-itH} is unitary (and hard to to classically)

Challenges in the NISQ era

1. Qubits are noisy:
   - On the one hand, one wants to keep a fragile quantum system isolated.
   - On the other hand, one wants to manipulate the system from the outside
2. Not all qubits are physically connected to all others; no 3D layouts for transmons
   - Entangling distant qubits requires many intermediate steps



Youngseok Kim, Nature (2023)

IBM 127 qubit quantum chip

3. How to optimize quantum circuits?
4. How do you verify a result that you cannot simulate of any classical computer?

Summary

- Exciting possibilities exploring and advancing quantum computing in nuclear physics
  - Dynamics, neutrino oscillations, …
- Hardware is advancing rapidly but no logical/error-corrected qubits yet
- Demand for AI/ML and QC/QI workforce