Quantum many-body computation on a small quantum computer

Lei Wang (王磊)
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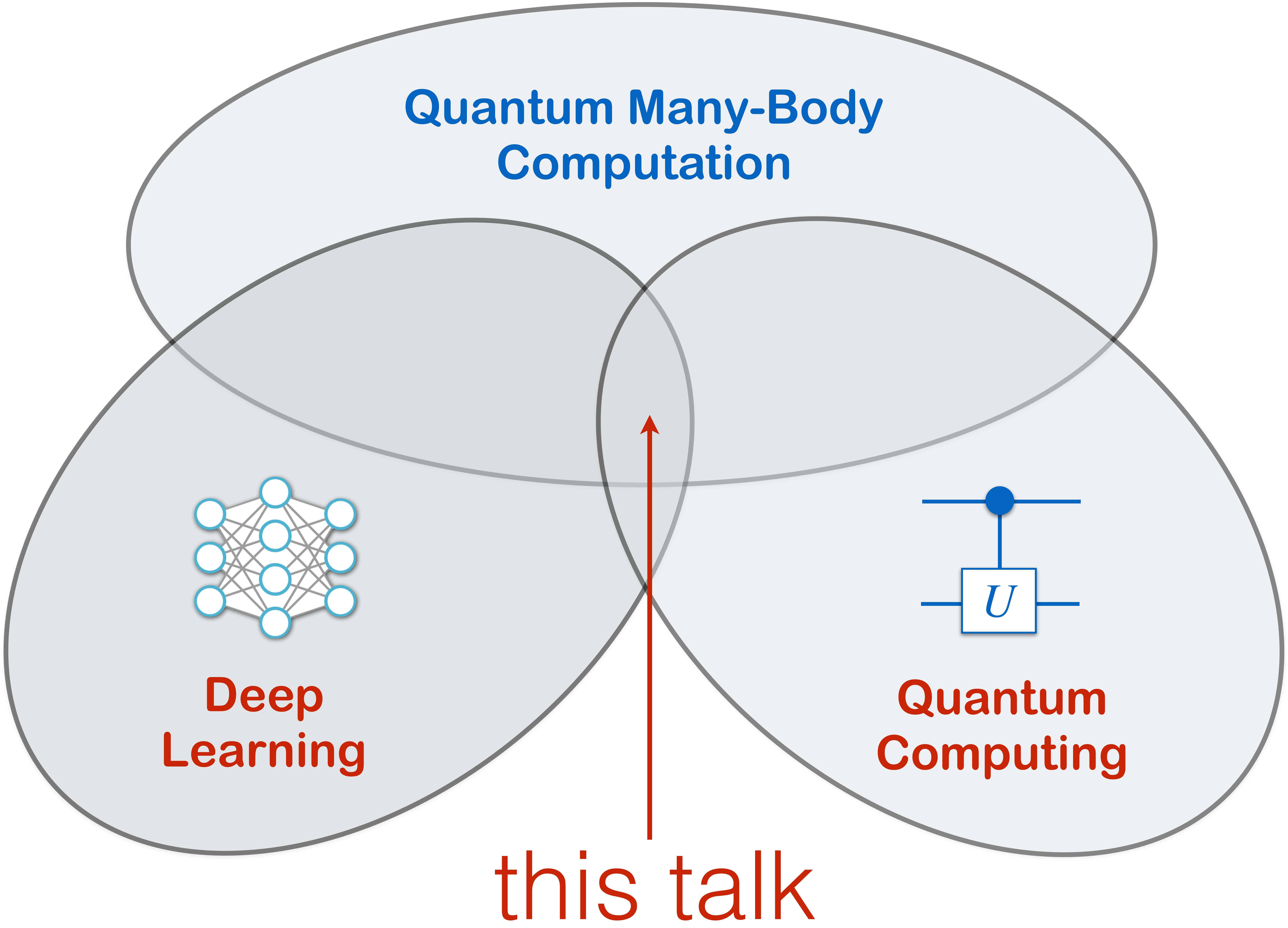
Institute of Physics, CAS



Jin-Guo Liu, Yi-Hong Zhang, Yuan Wan, LW, 1902.02663

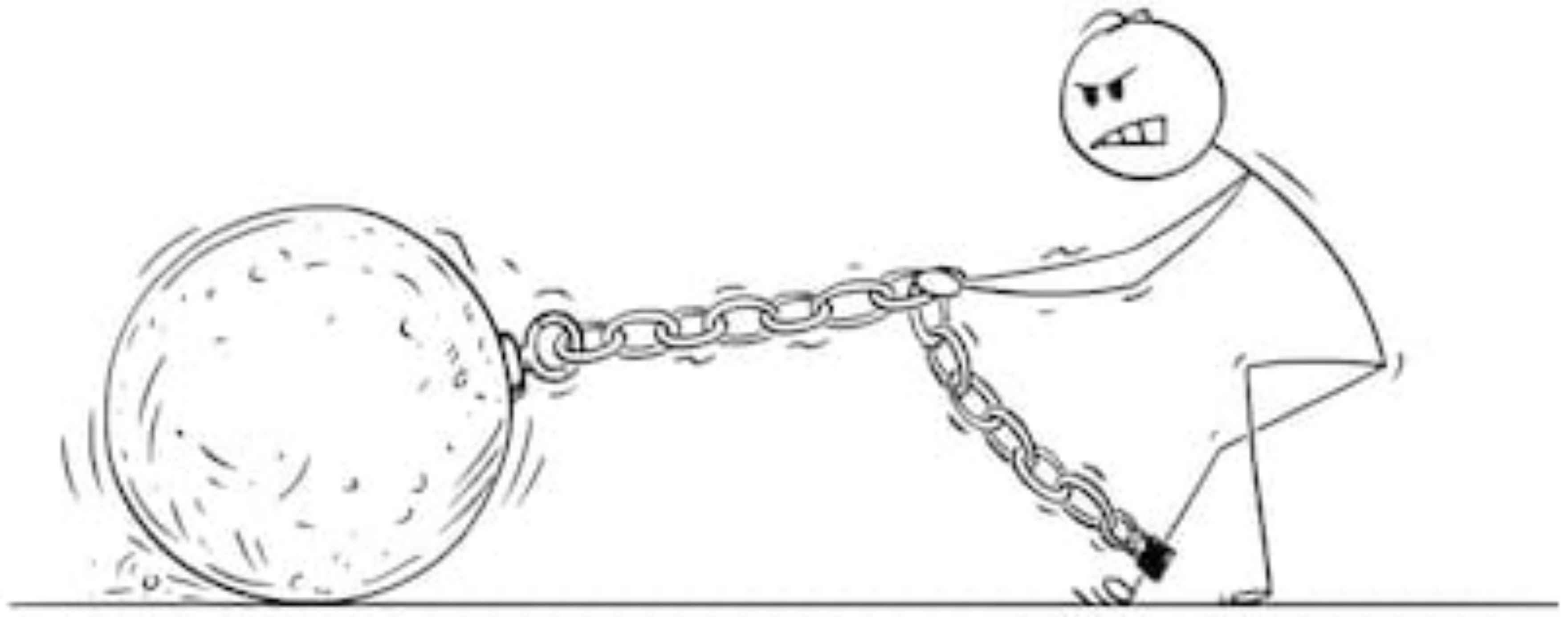
What is the killer app of a <u>near-term</u> quantum computer?

In about next 3 years

Small: $O(10)$-$O(10^3)$ qubits

Shallow: $O(10^2)$-$O(10^4)$ gates

Noisy: no error correction



Factoring ?

4951760154835678088235319297 = 2147483647 x 2305843009213693951

- Shor algorithm needs 4000 qubits with error correction and $O(10^9)$ gates to crack 2048-bits RSA key (Proos and Zalka, quant-ph/0301141)
- BTW, it is not a long-term application either. One can switch to post-quantum cryptography algorithms even now

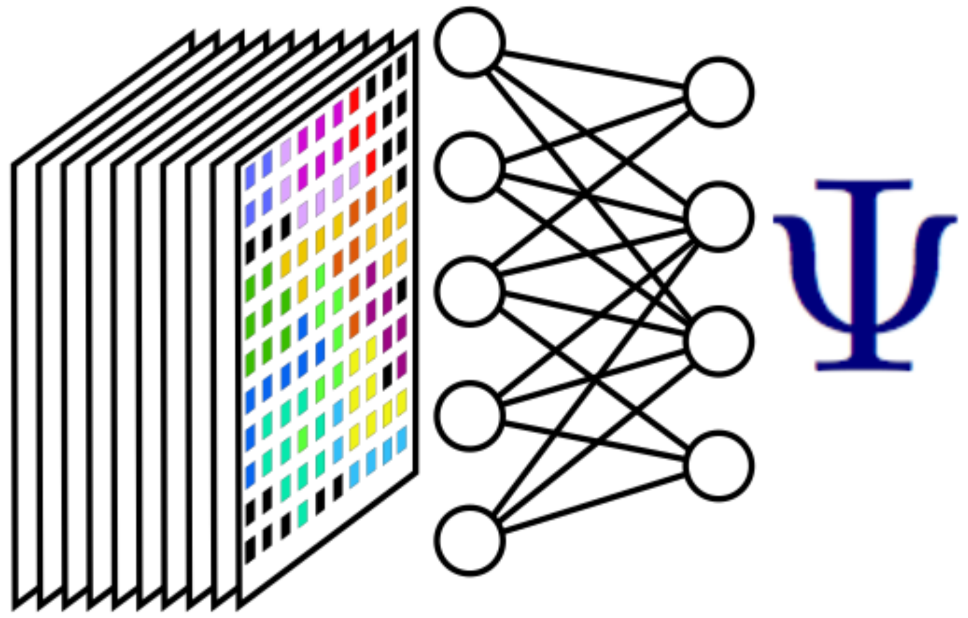
We need a more profitable application

Accelerated linear algebra solver ?

$$A\,|x\rangle = |b\rangle$$

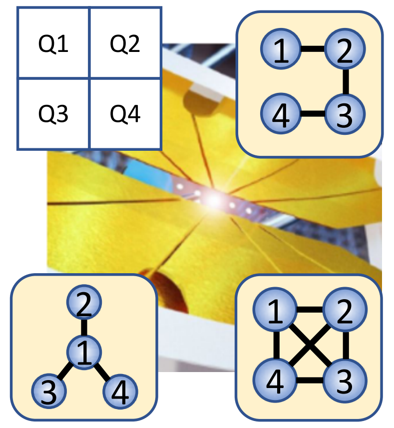
- The “infamous” HHL algorithm with exponential speedup (Harrow et al, PRL ’09)
- Was the core subroutine behind a large wave of quantum machine learning papers
- Requires quantum RAM which we do not know how to build yet. Has several other caveats (Aaronson, Nat. Phys. ’15)
- By far, no clear signature of surpassing (quantum-inspired) classical algorithms (Tang, STOC ’19)

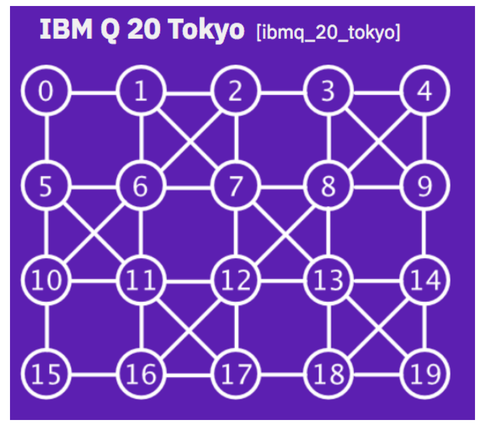
Quantum machine learning ?

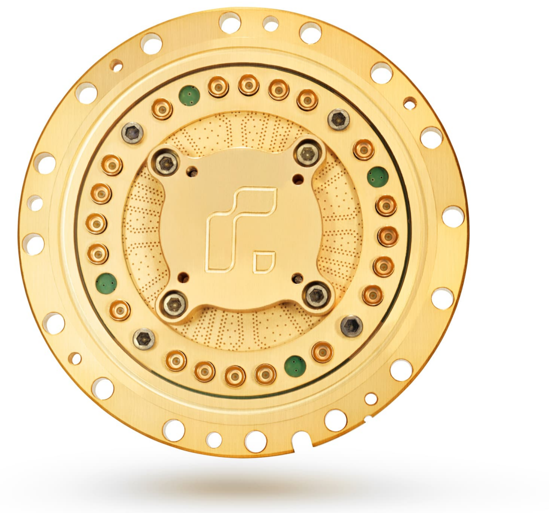


- Extremely overloaded term: HHL—> optimization —> classifier…
- Need to identify the true difficulty of classical machine learning
- Learn, sample and inference of intractable probability distributions
  "Born Machines"

Liu, LW, PRA '18
Cheng, Chen, LW, Entropy '18
Han, Wang, Fan, LW, Zhang, PRX '18







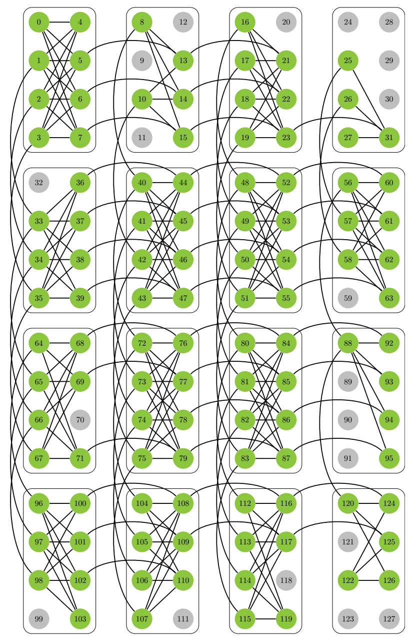
Experiments:

JQI+IonQ+UCL
1801.07686, 1812.08862

Oak Ridge
1811.09905

Regetti
1901.08047, 1904.02214

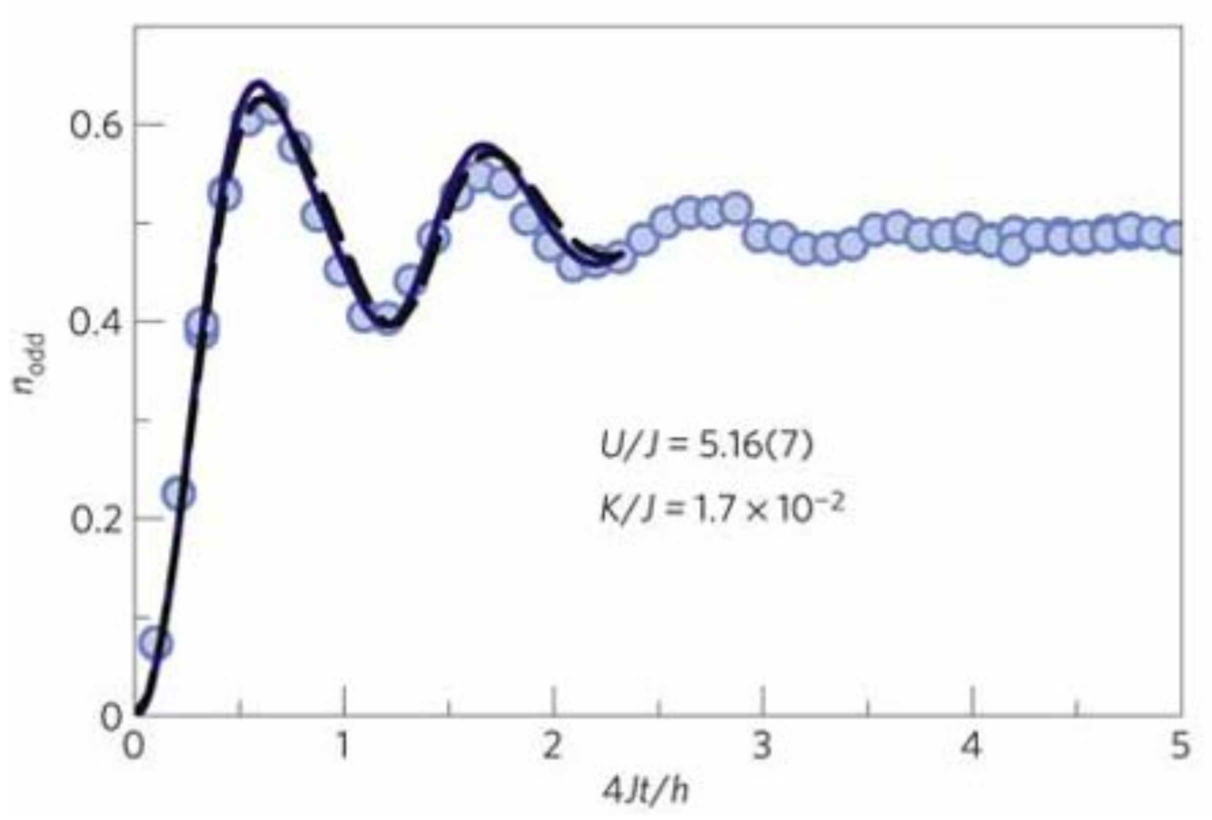
Quantum annealing and optimization ?



- No clear signature of being useful, even with 2000 noisy qubits (Rønnow et al, Science '14)
- Pivoting to a quantum sampling machine (quantum Boltzmann Machine, Amin et al PRX '18). Or, a programmable quantum spin simulator (Harris et al, Science '18, King et al, Nature '18)
- Gate model version: Quantum Approximate Optimization Algorithm (Farhi et al '14) is essentially variational optimization with a quantum circuit probabilistic model

Promising, but still looking for the right optimization problem with $O(10^3)$ variables where quantum really helps

Simulating quantum dynamics ?



Quantum versus classical simulation
Trotzky et al, Nat. Phys. ‘12

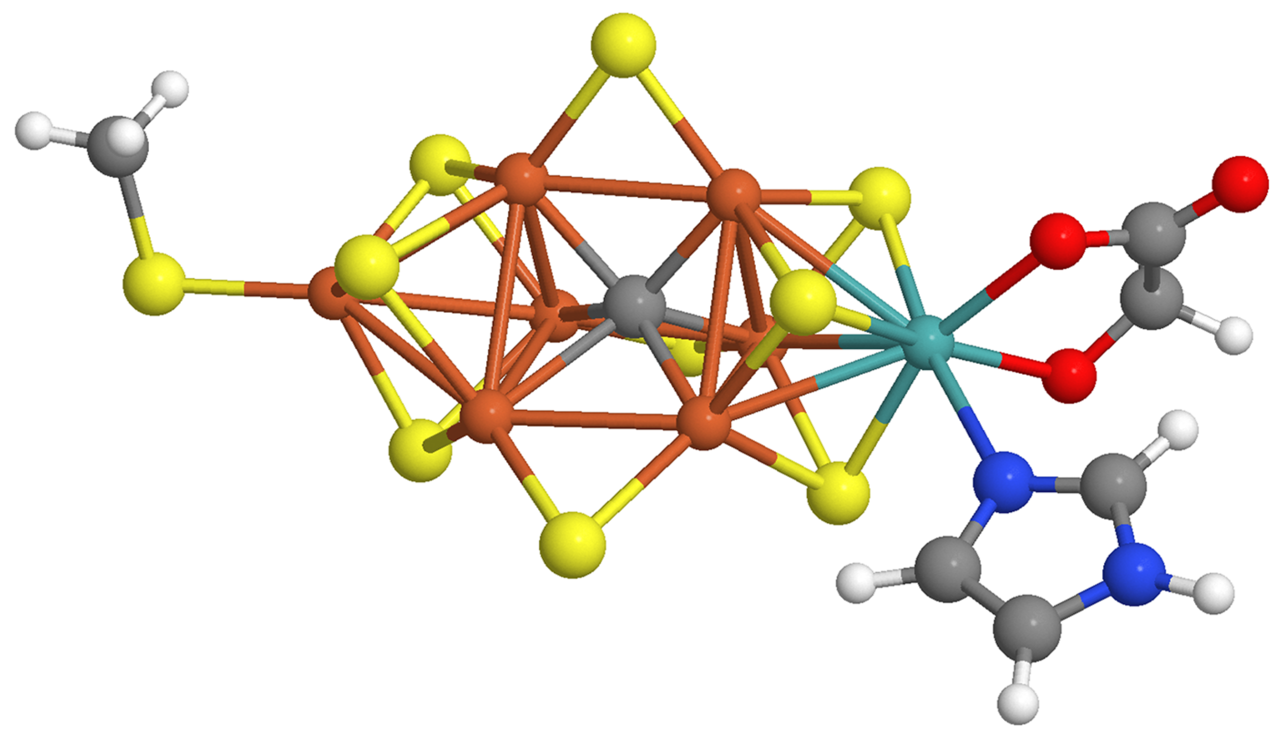
- Closer to Feynman’s original proposal. Native application of quantum computers

- However, no fundamental difference with, say ultracold atoms, quantum simulators

- Again, need to ask useful questions involving O(10)-O(10^3) qubits (thermalization ? quantum chaos ? Kibble-Zurek mechanism ?)

Does not seem to live up to billion $ investment

Quantum chemistry and electronic structures ?



Biological nitrogen fixation
Reiher et al, PNAS '17

- Not as native as dynamics. But can be extremely useful

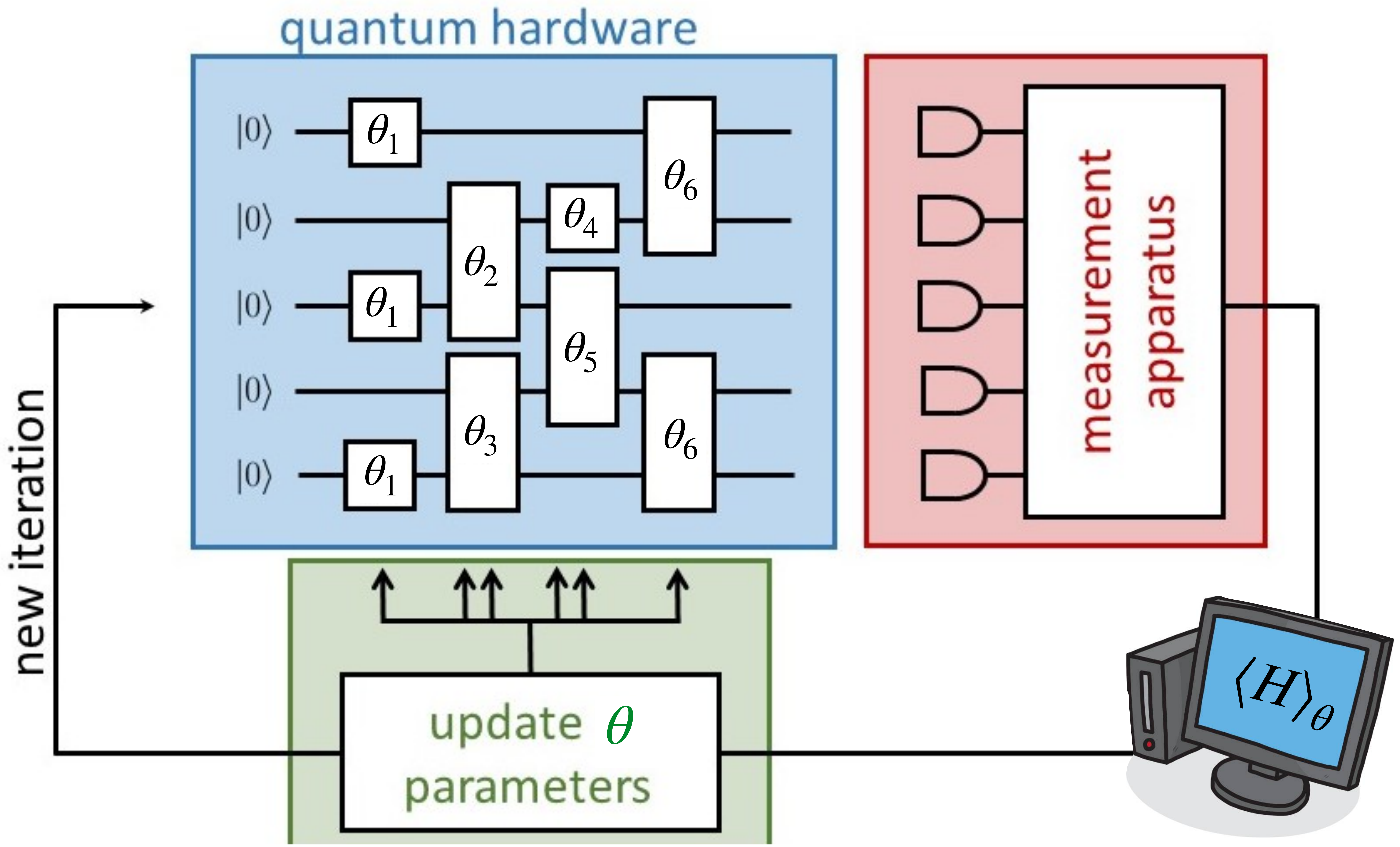
- Quantum phase estimation solves the eigen-problem via unitary time-evolution (Kitaev, '95)

- However, it requires error-correcting qubits with long coherence time

- Hybrid quantum-classical algorithm is more feasible in near-term

Variational Quantum Eigensolver

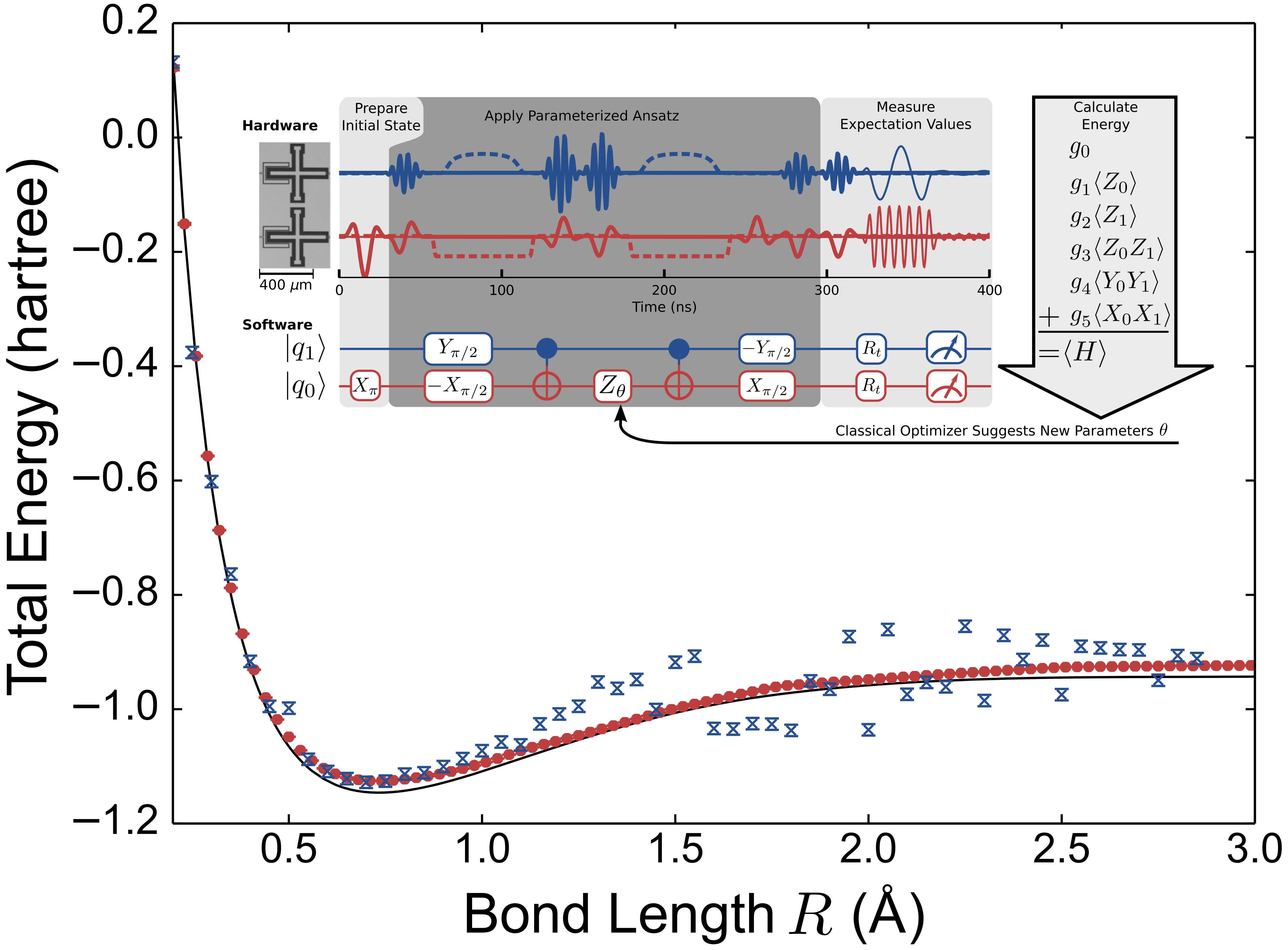
Peruzzo et al, Nat. Comm. ’13



Quantum circuit as a variational ansatz

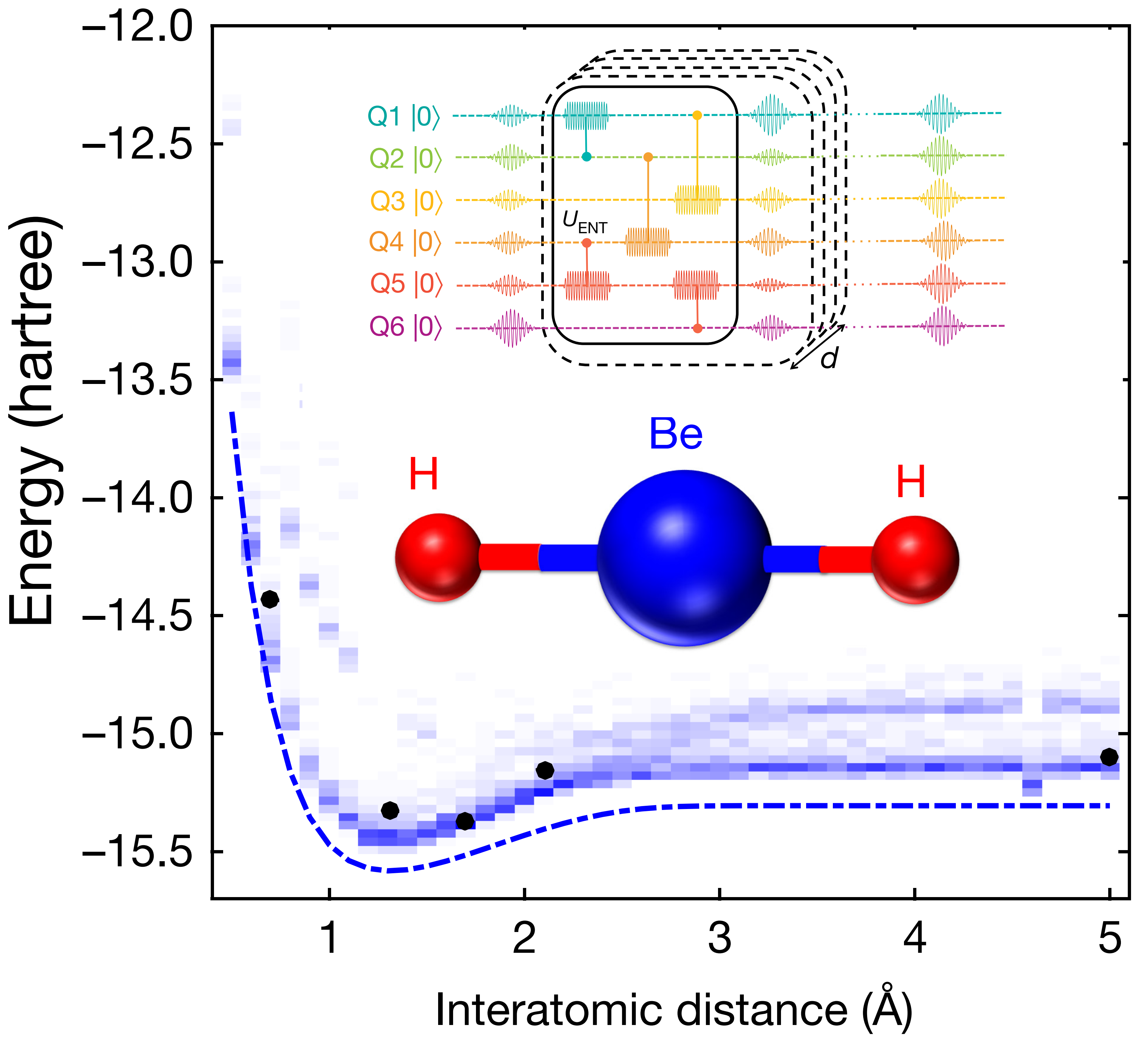
VQE on actual quantum devices

H_2 molecule with 2 qubits



Google PRX '16

BeH_2 molecule with 6 qubits

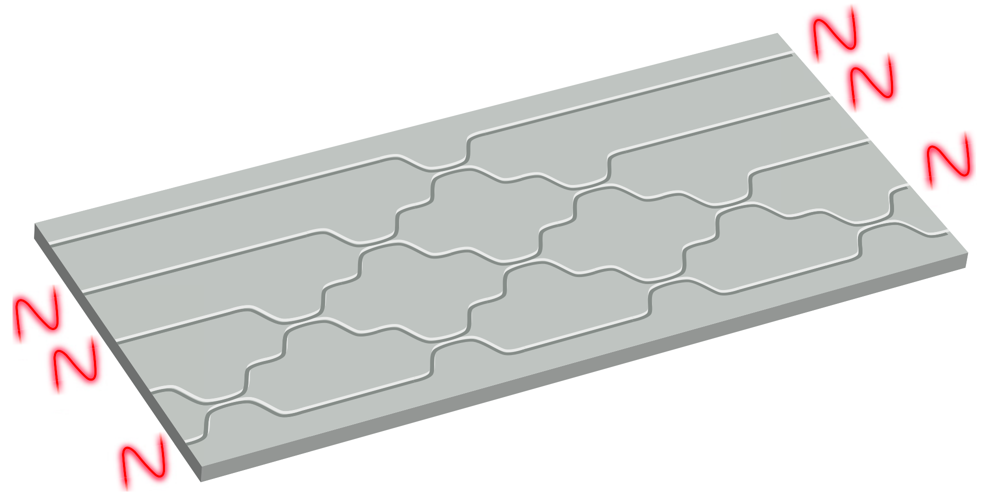


IBM Nature '17

Digression: Two ways of showing quantum advantages

Quantum supremacy **(theoretical computer scientists approach)**

1. Identify some tasks, useful or not (random circuits, boson sampling…)
2. Invent a quantum algorithm
3. Prove there is no classical approach which can match the performance



Harrow et al, Nature ’17

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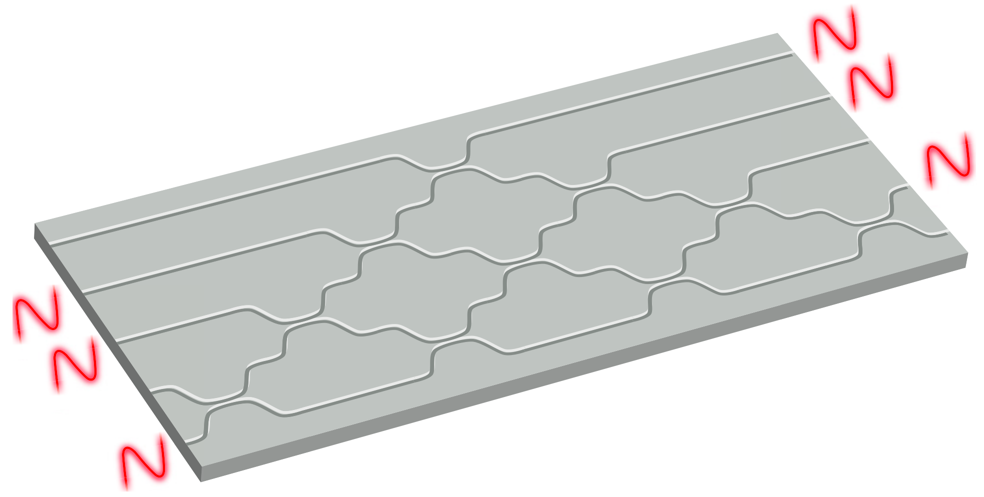
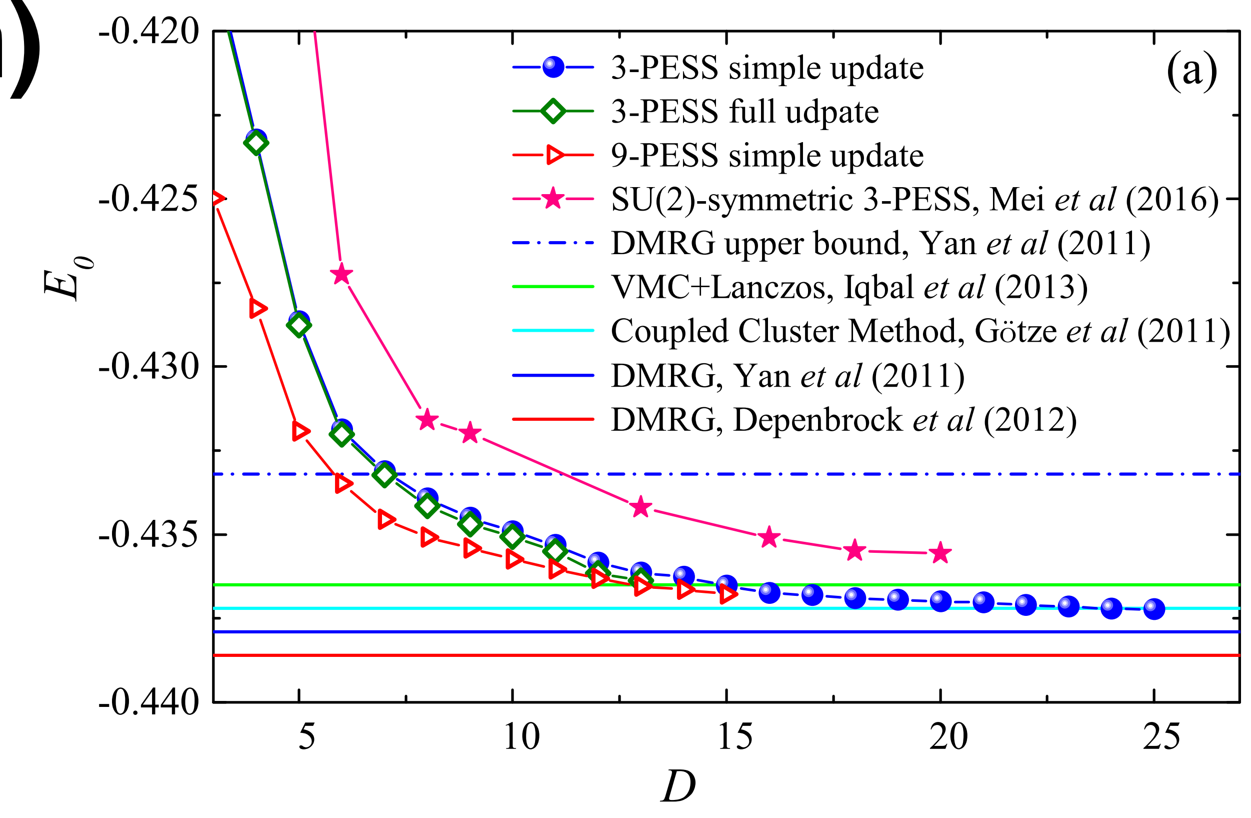


Harrow et al, Nature '17

Quantum variational calculation **(computational physicists approach)**

1. Identify a challenging problem
2. Invent a quantum variational ansatz
3. Try to reach lower variational energy, which is an unambiguous signature of quantum advantage



Frustrated quantum magnets
Hai-Jun Liao et al, PRL'17

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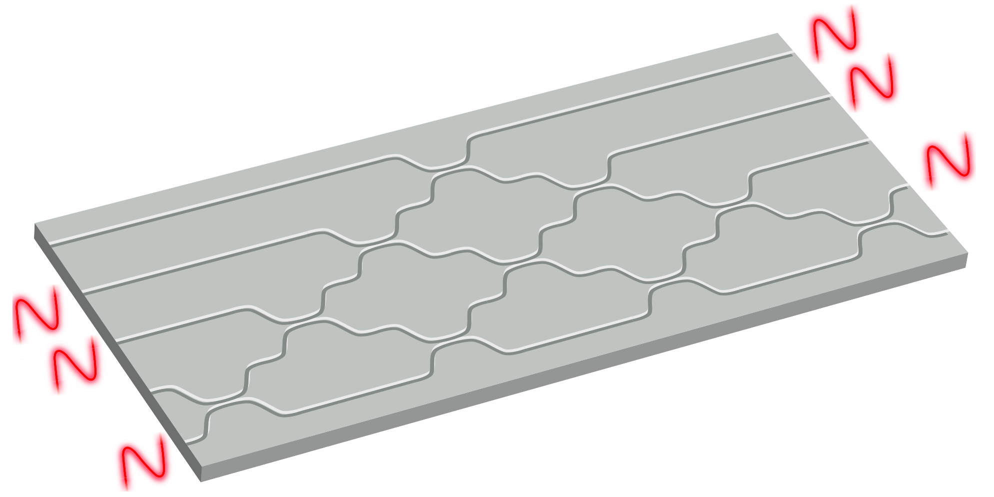

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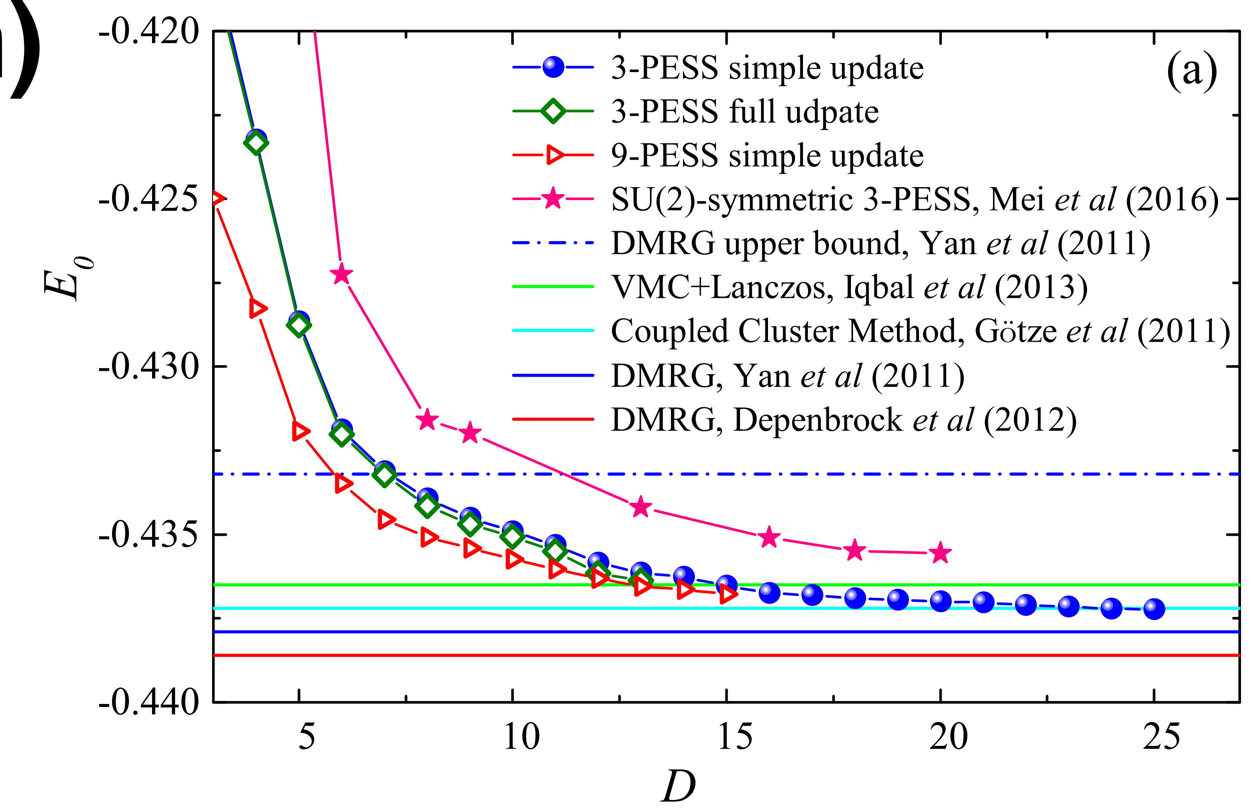
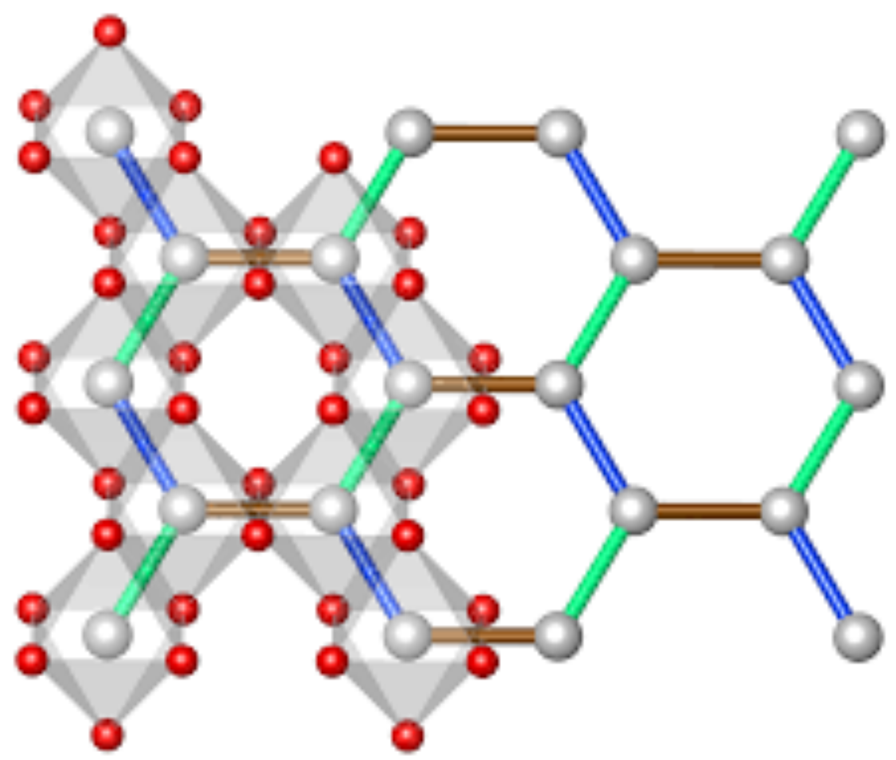


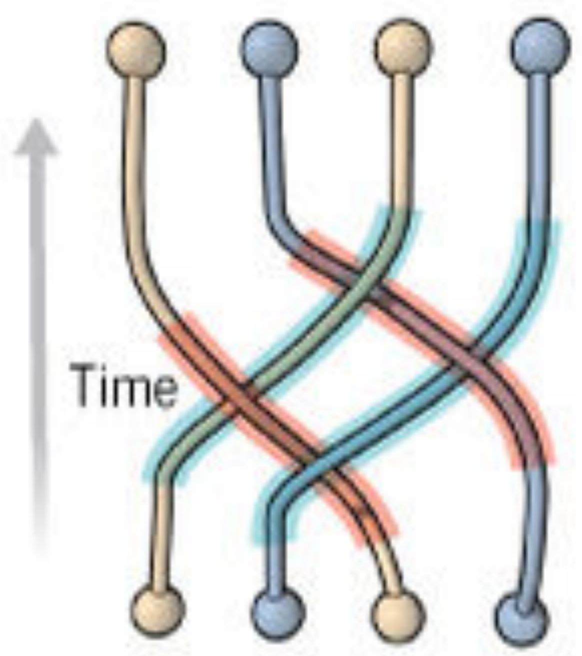
Frustrated quantum magnets
Hai-Jun Liao et al, PRL'17

We will see this in quantum magnets before quantum chemistry

1. $O(N^4)$ Hamiltonian terms
2. Overhead in mapping fermions to quantum spins
3. Chemists care more about excitations than we do

Bonus: a positive feedback loop





Quantum spin models
e.g. Kitaev materials

Better quantum computer
with fault tolerant qubits

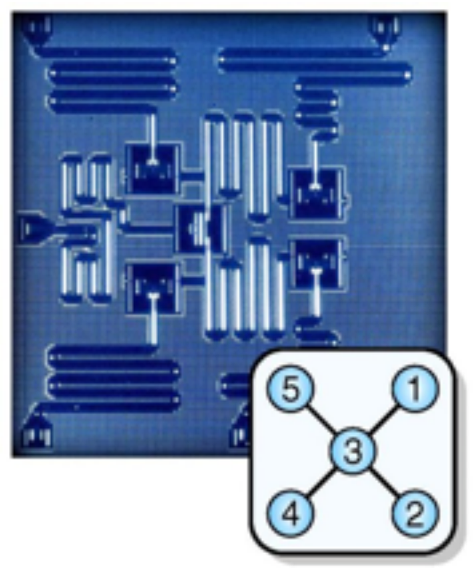
Studying quantum magnets with quantum computer helps building a better quantum computer

However, there is a HUGE GAP in the qubit number

What we want to solve

What current technology offers

to infinity and beyond

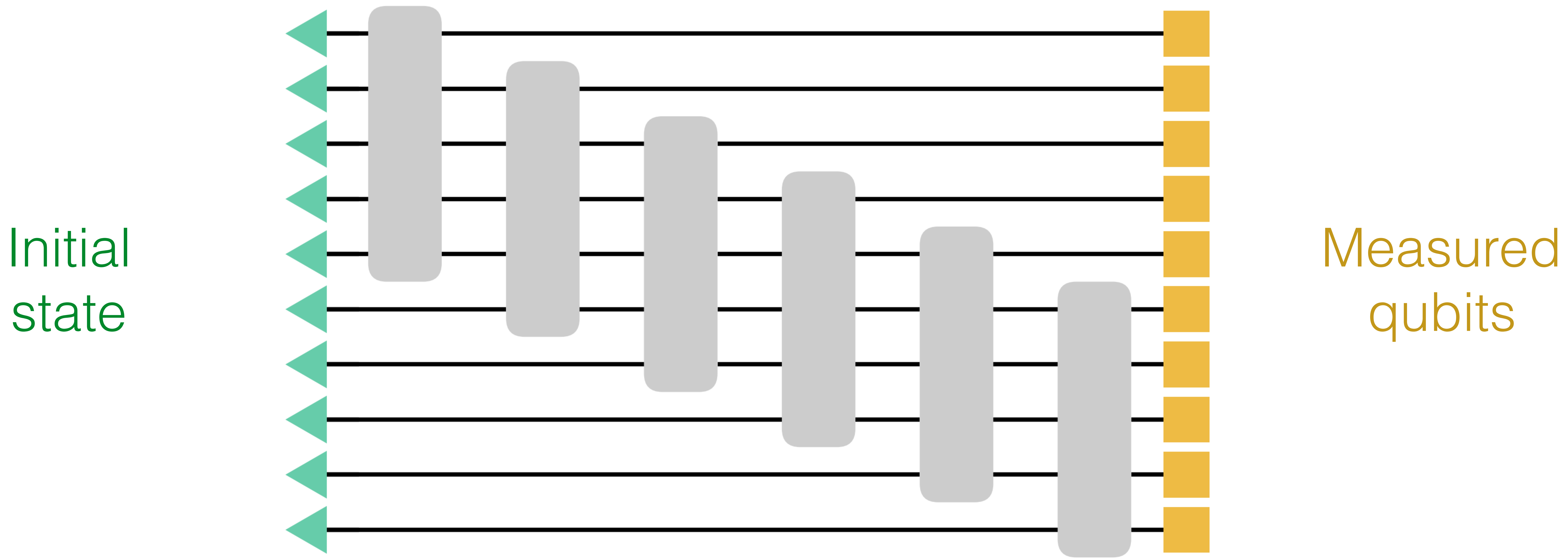


a handful of qubits

Variational quantum eigensolver with fewer qubits

Jin-Guo Liu, Yi-Hong Zhang, Yuan Wan, LW, 1902.02663

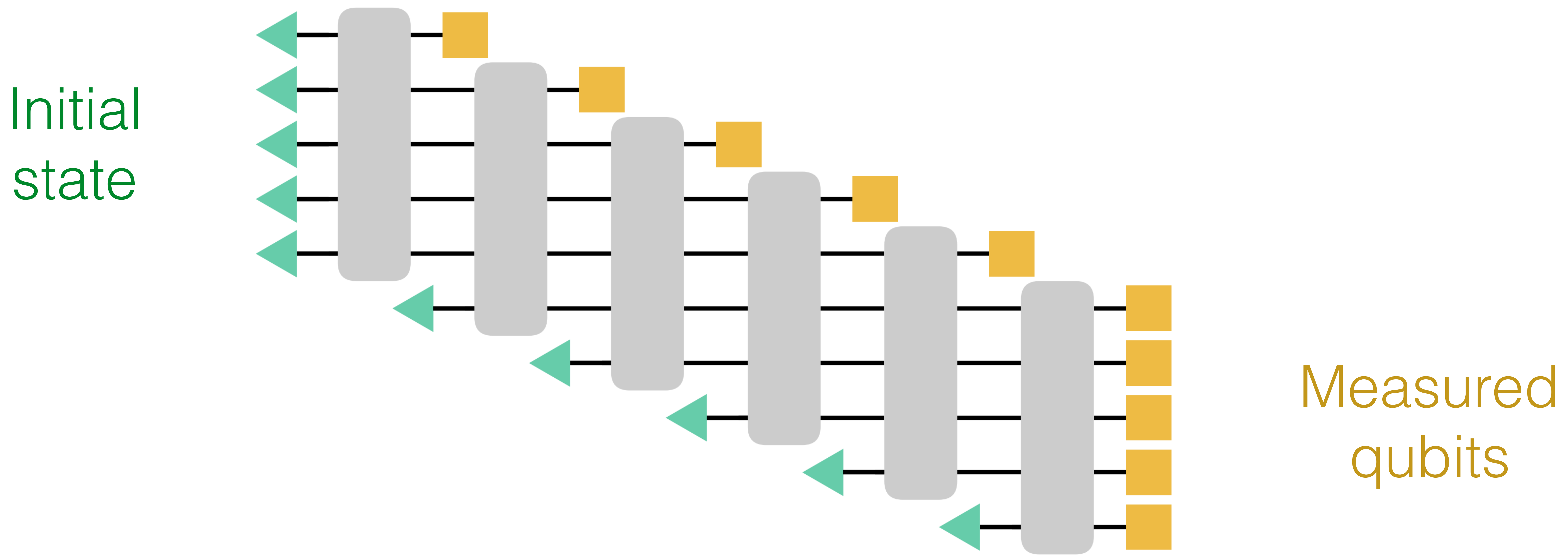
A qubit efficient variational circuit



Huggins, Patel, Whaley, Stoudenmire, 1803.11537
see also Cramer et al, Nat. Comm. '10

Tensor network inspired quantum circuit architecture

A qubit efficient variational circuit



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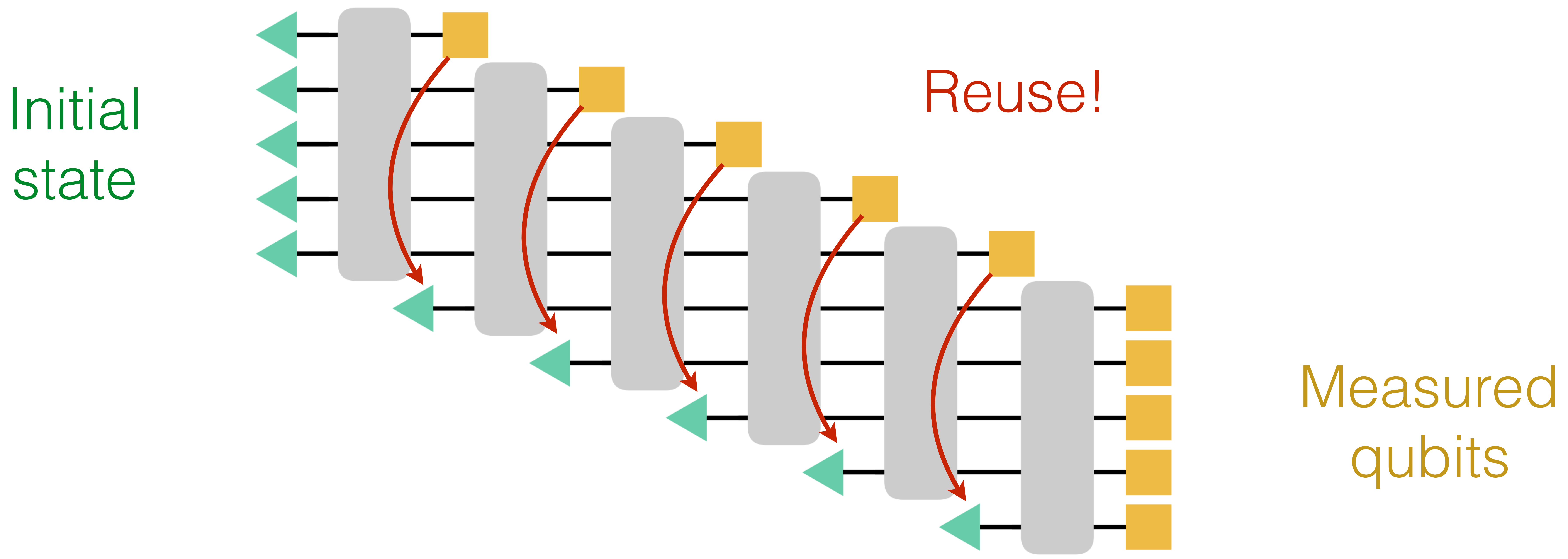

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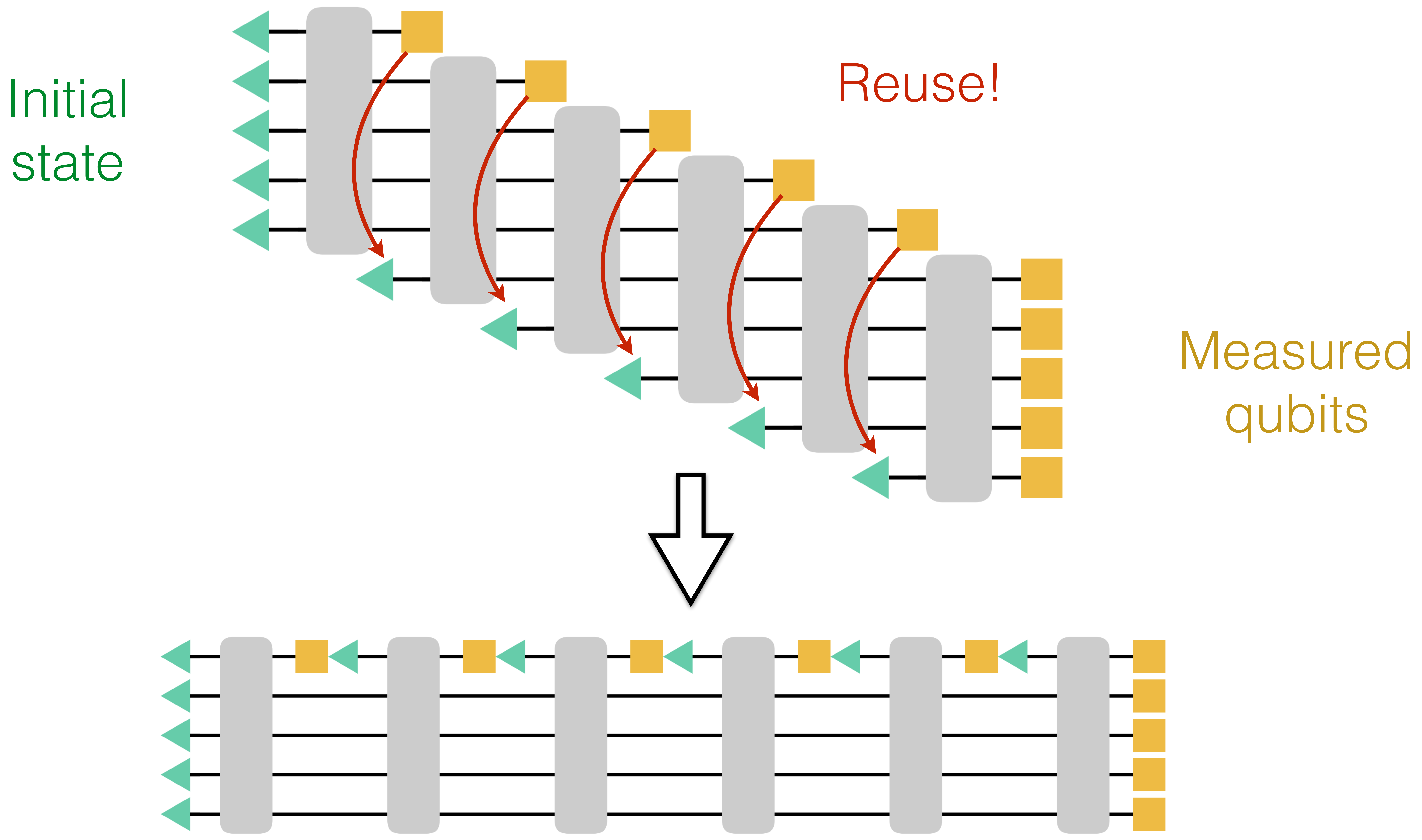
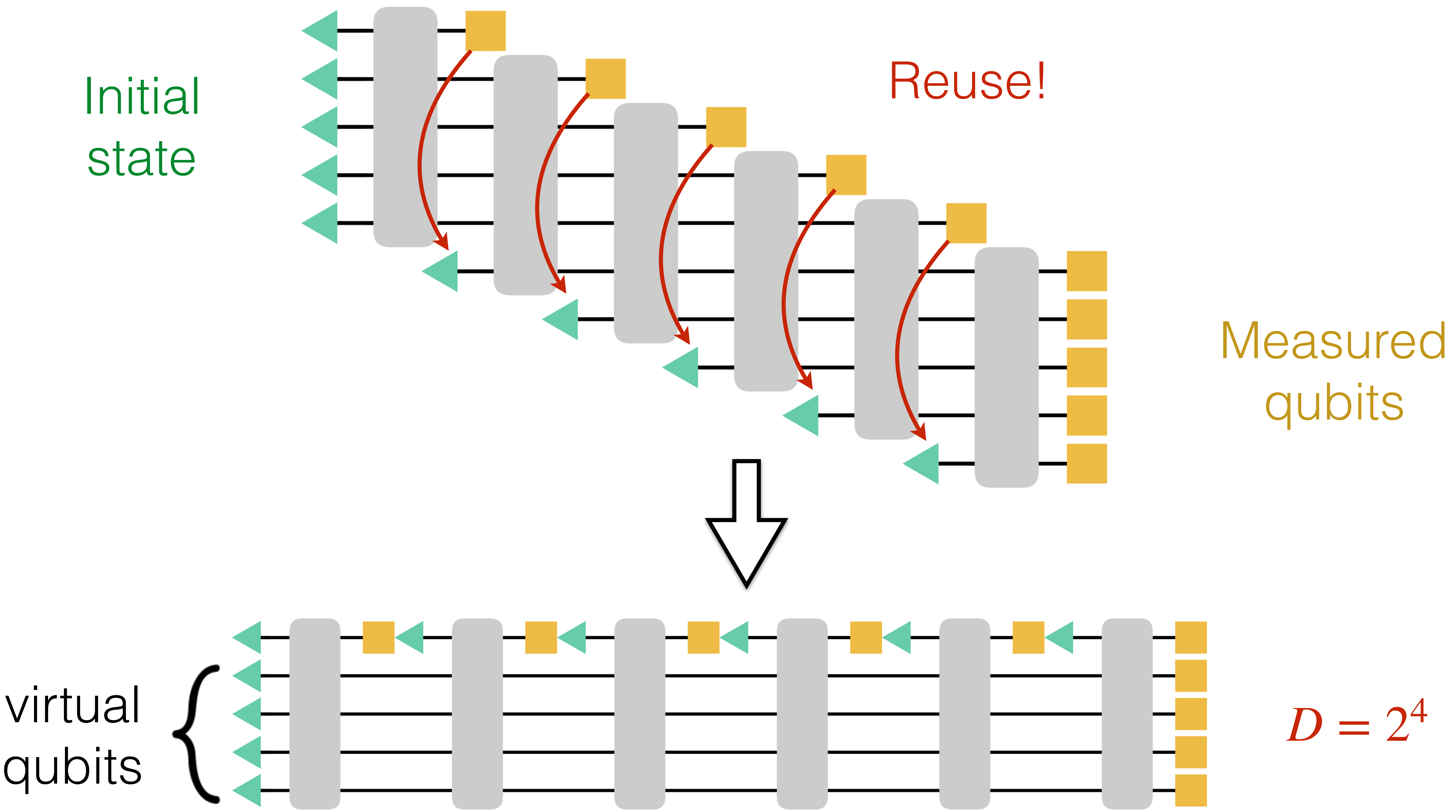


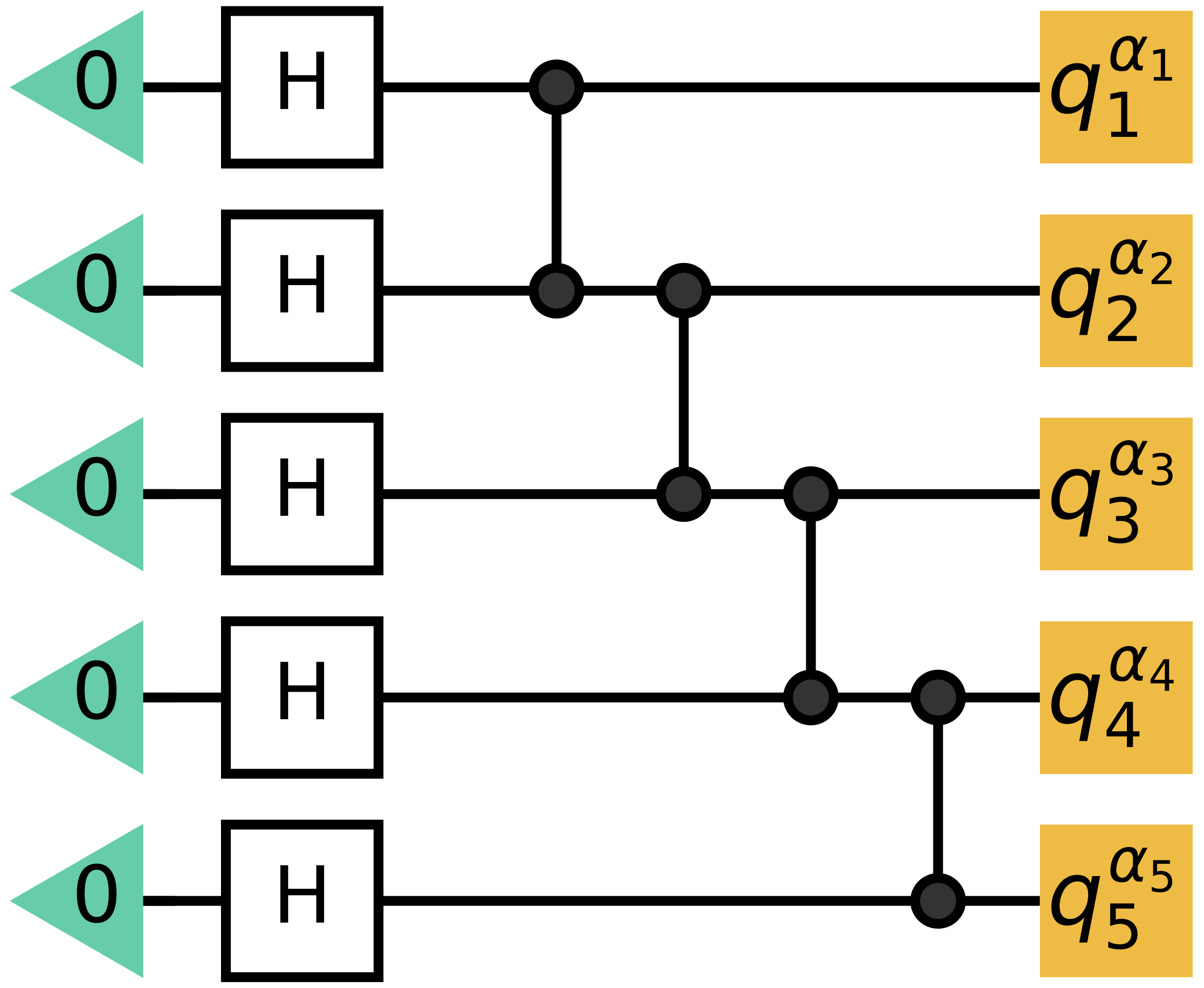
Matrix Product State with exponentially large bond dimensions

A qubit efficient variational circuit



Matrix Product State with exponentially large bond dimensions

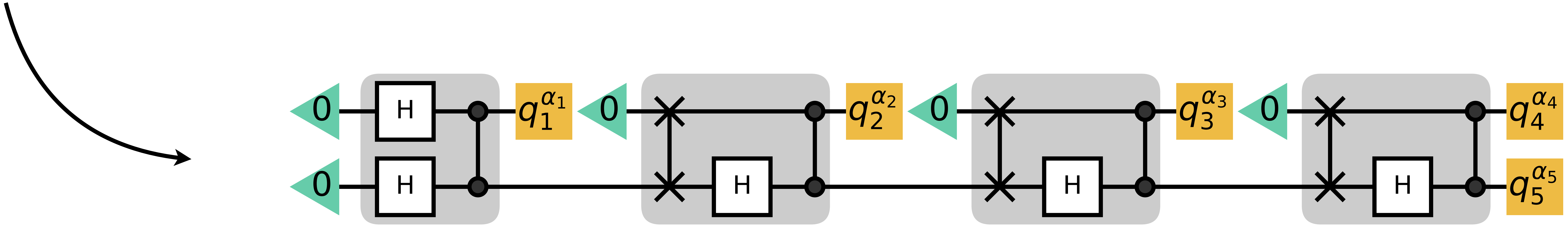
A concrete example



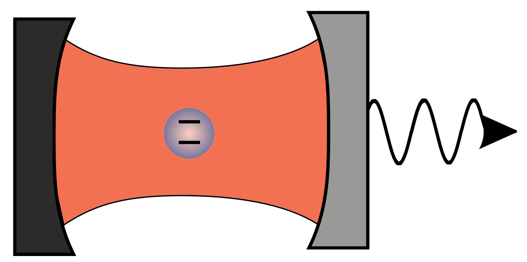
Prepare a 5-qubit cluster state using only 2 qubits

Any measurement outcome is identical on these two circuits

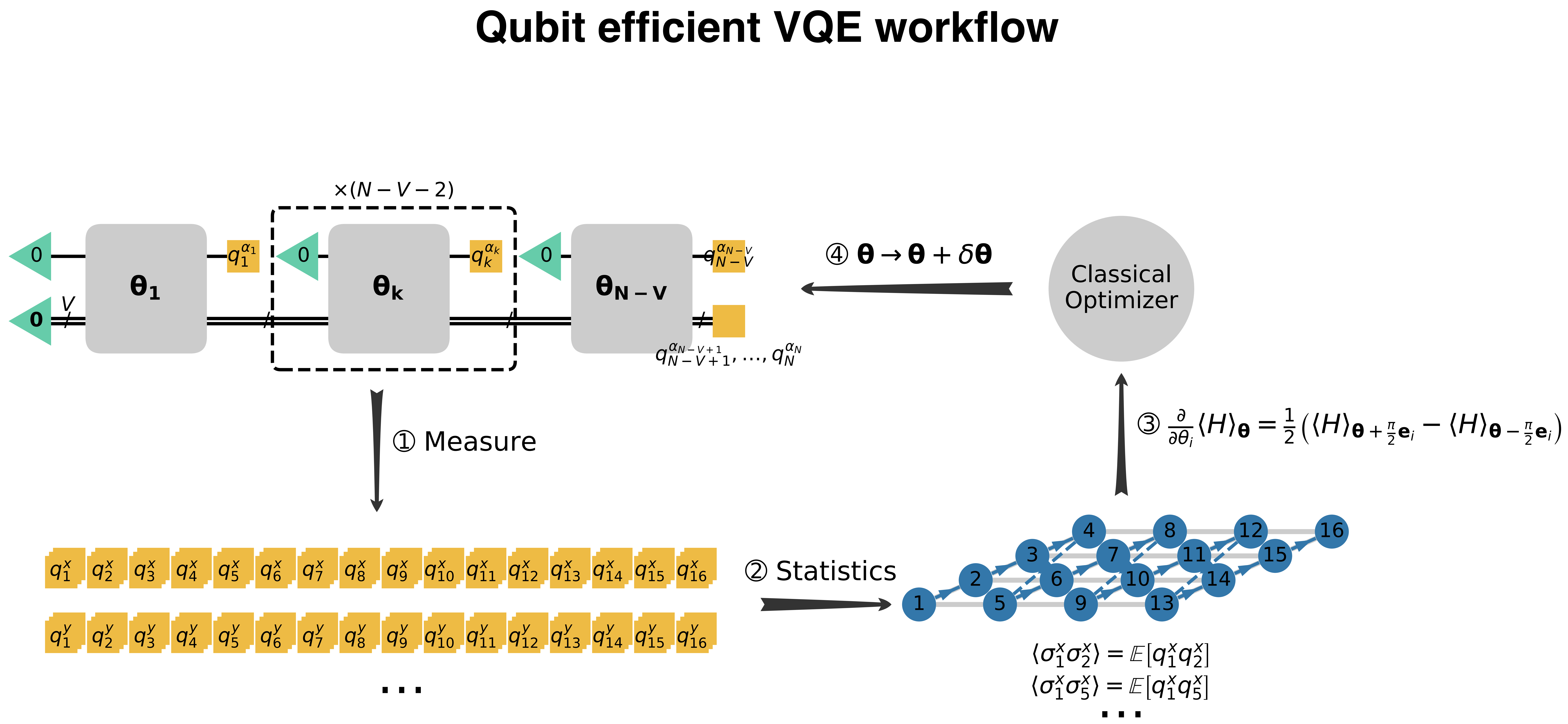
Key fact: the target state has low quantum entanglement



Cavity QED produces continuous MPS of photons

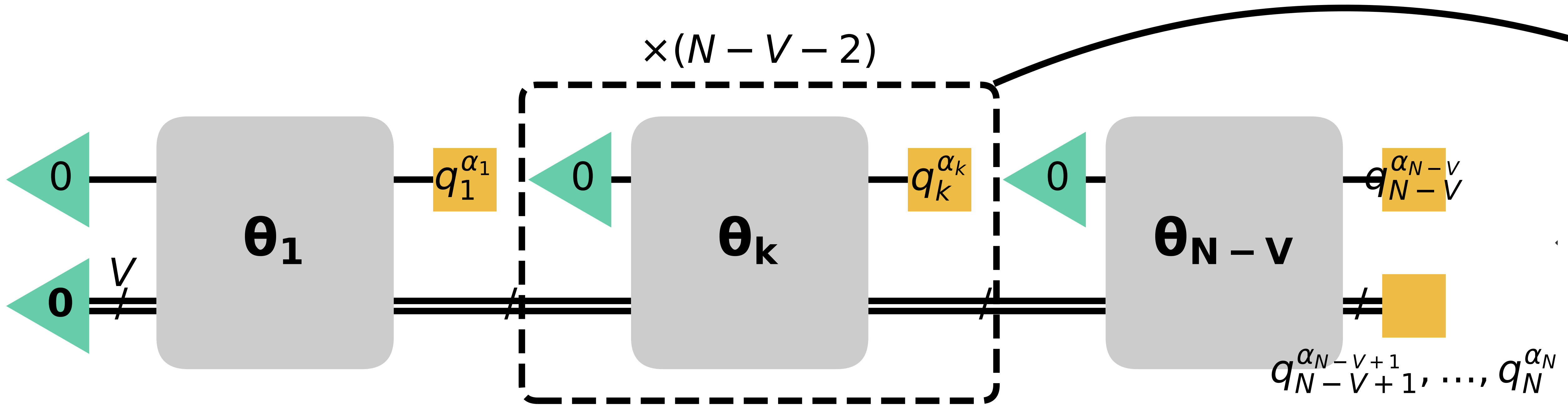


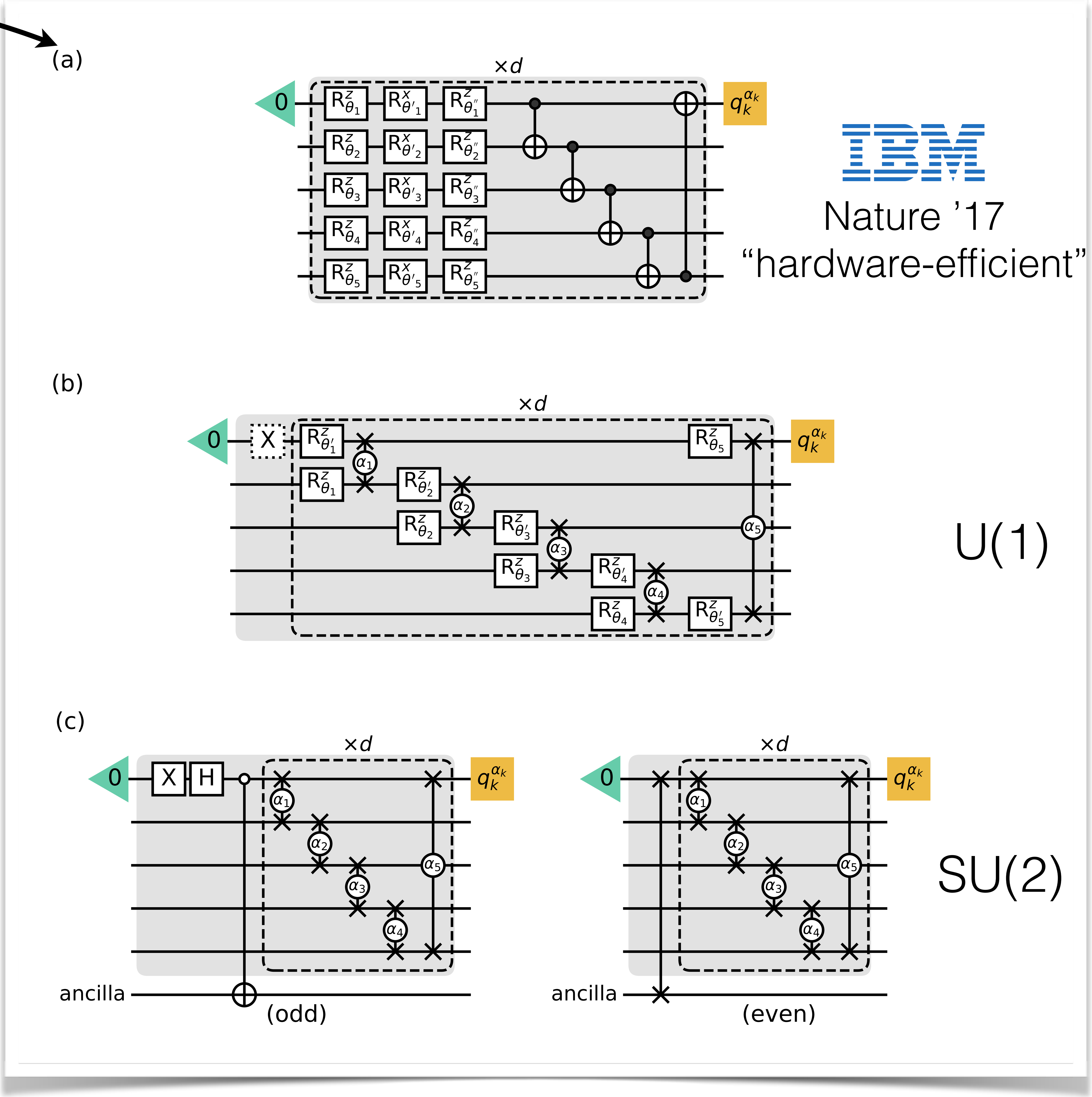
Barrett et al, PRL ’13, Eichler et al, PRX ‘15



Qubit efficient VQE workflow
×(N − V − 2)
0
0
0
0
V
θ1
θk
θN − V
$q_1^{\alpha_1}$
$q_k^{\alpha_k}$
$q_{N-V}^{\alpha_{N-V}}$
$q_{N-V+1}^{\alpha_{N-V+1}}, \ldots, q_N^{\alpha_N}$
④ $\boldsymbol{\theta} \to \boldsymbol{\theta} + \delta\boldsymbol{\theta}$
Classical Optimizer
① Measure
③ $\frac{\partial}{\partial\theta_i}\langle H\rangle_{\boldsymbol{\theta}} = \frac{1}{2}\left(\langle H\rangle_{\boldsymbol{\theta}+\frac{\pi}{2}\mathbf{e}_i} - \langle H\rangle_{\boldsymbol{\theta}-\frac{\pi}{2}\mathbf{e}_i}\right)$
q_1^x q_2^x q_3^x q_4^x q_5^x q_6^x q_7^x q_8^x q_9^x q_{10}^x q_{11}^x q_{12}^x q_{13}^x q_{14}^x q_{15}^x q_{16}^x
q_1^y q_2^y q_3^y q_4^y q_5^y q_6^y q_7^y q_8^y q_9^y q_{10}^y q_{11}^y q_{12}^y q_{13}^y q_{14}^y q_{15}^y q_{16}^y
...
② Statistics
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
$\langle\sigma_1^x\sigma_2^x\rangle = \mathbb{E}[q_1^x q_2^x]$
$\langle\sigma_1^x\sigma_5^x\rangle = \mathbb{E}[q_1^x q_5^x]$
...

Quantum circuit variational ansatz

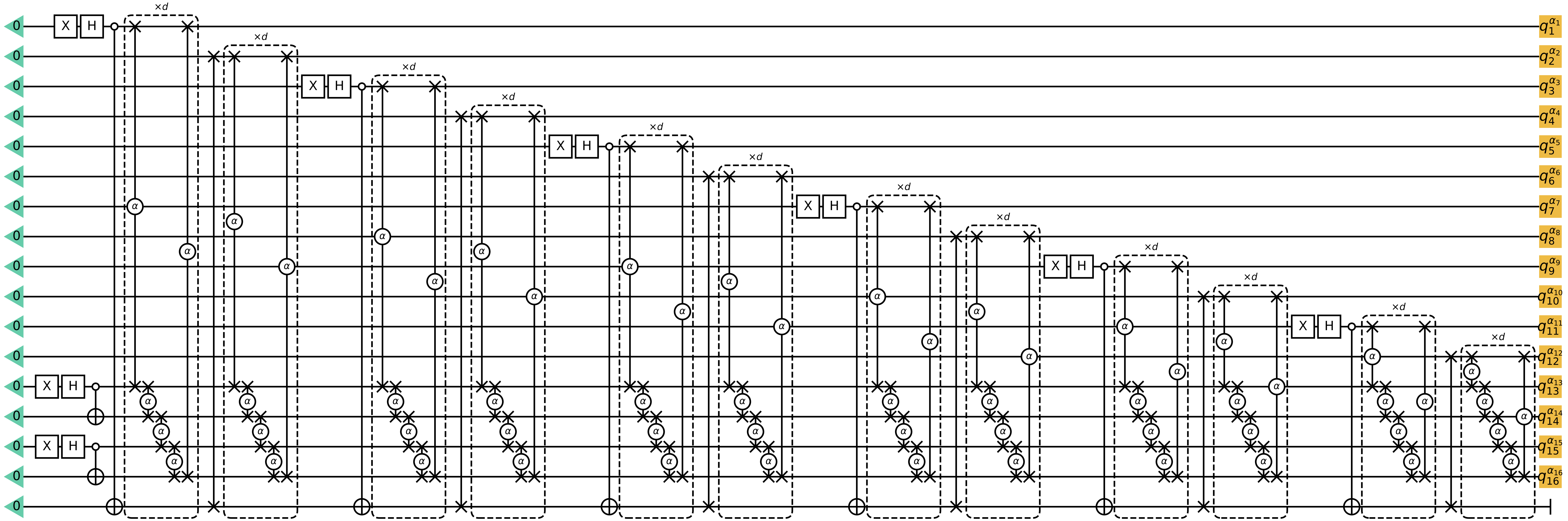




- Variational ansatz given by circuit architecture design
- Imposing physical U(1) and SU(2) symmetries is straightforward
- A variational family of resonating-valanced-bond states (Liang et al '88) which is hard to sample classically

The RVB quantum circuit in the expanded view

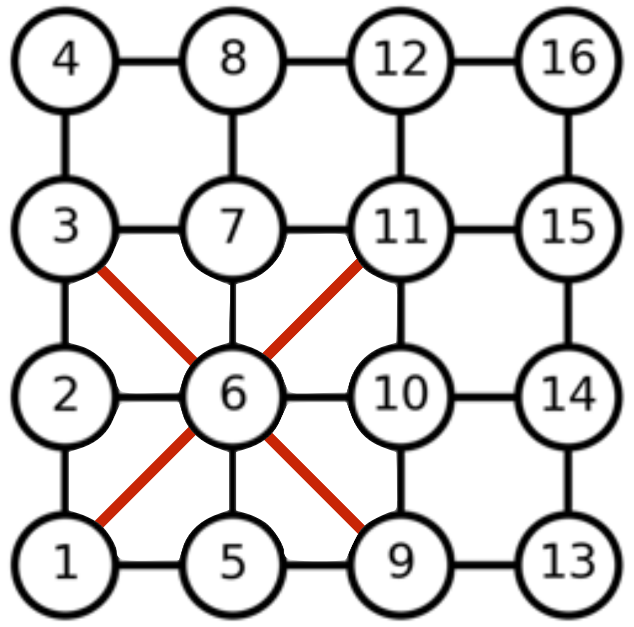
There are 17 qubits in this circuit

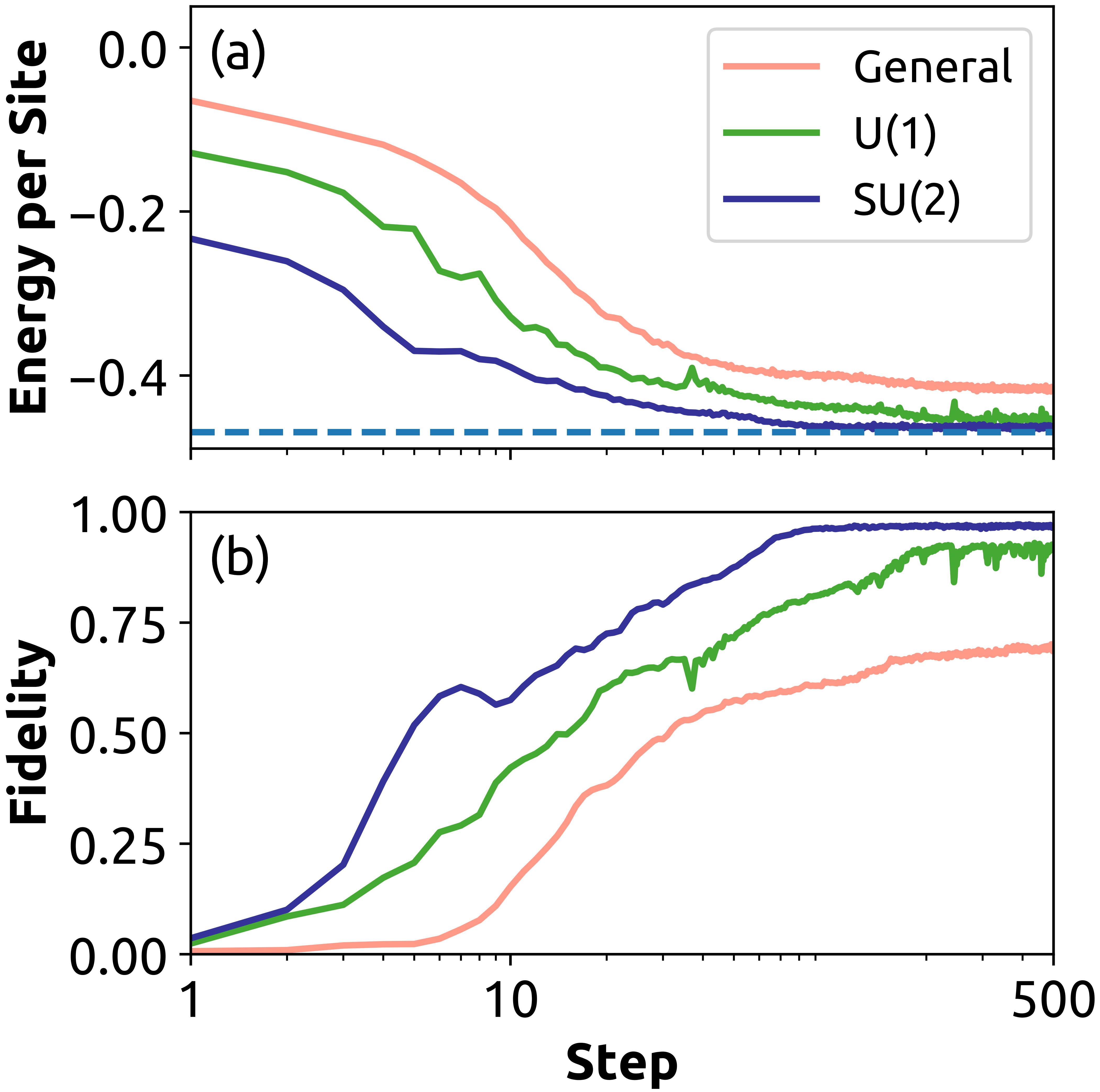


One can actually perform the experiment with 6 qubits
The ansatz is an MPS with bond dimension 2^5

Simulation results

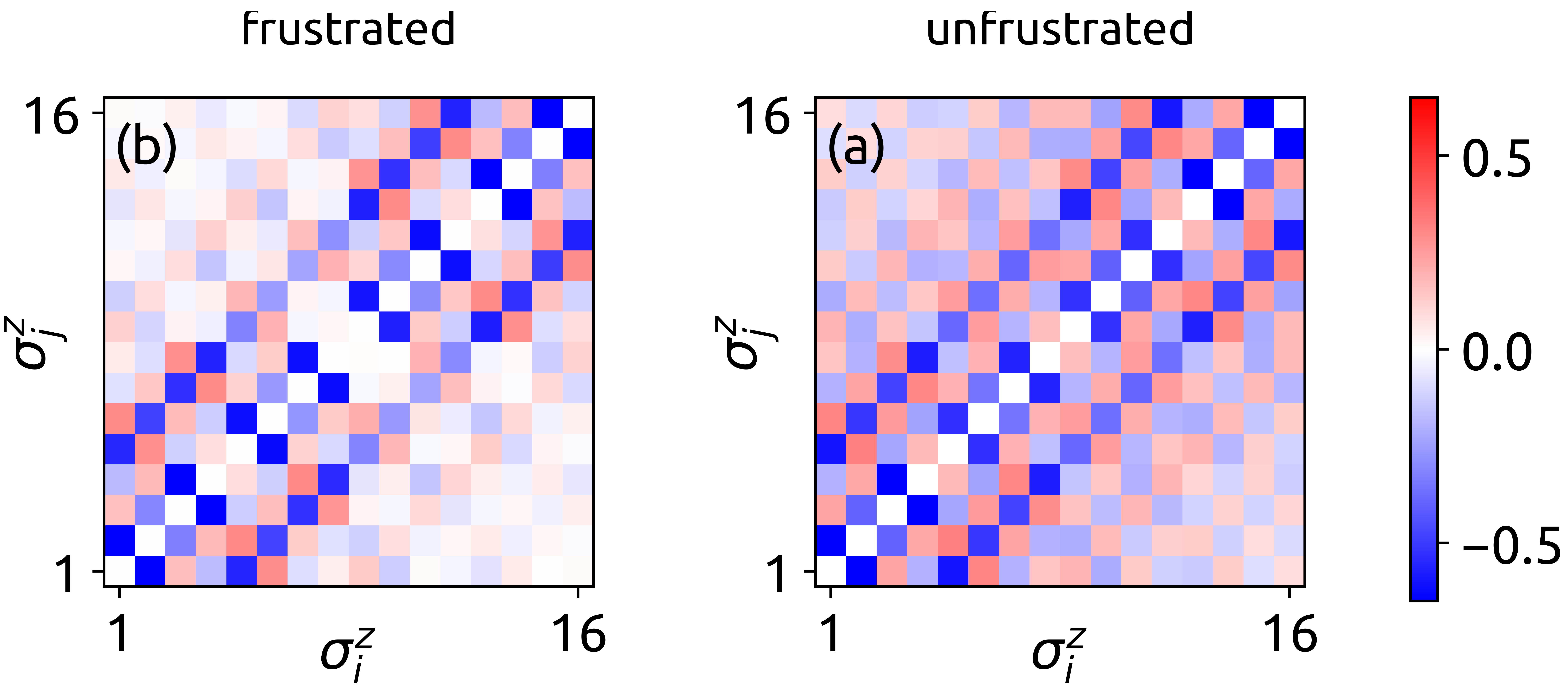
$$H = \frac{1}{4}\left(\sum_{\langle i,j\rangle} \vec{\sigma}_i\vec{\sigma}_j + J_2 \sum_{\langle\!\langle i,j\rangle\!\rangle} \vec{\sigma}_i\vec{\sigma}_j\right)$$





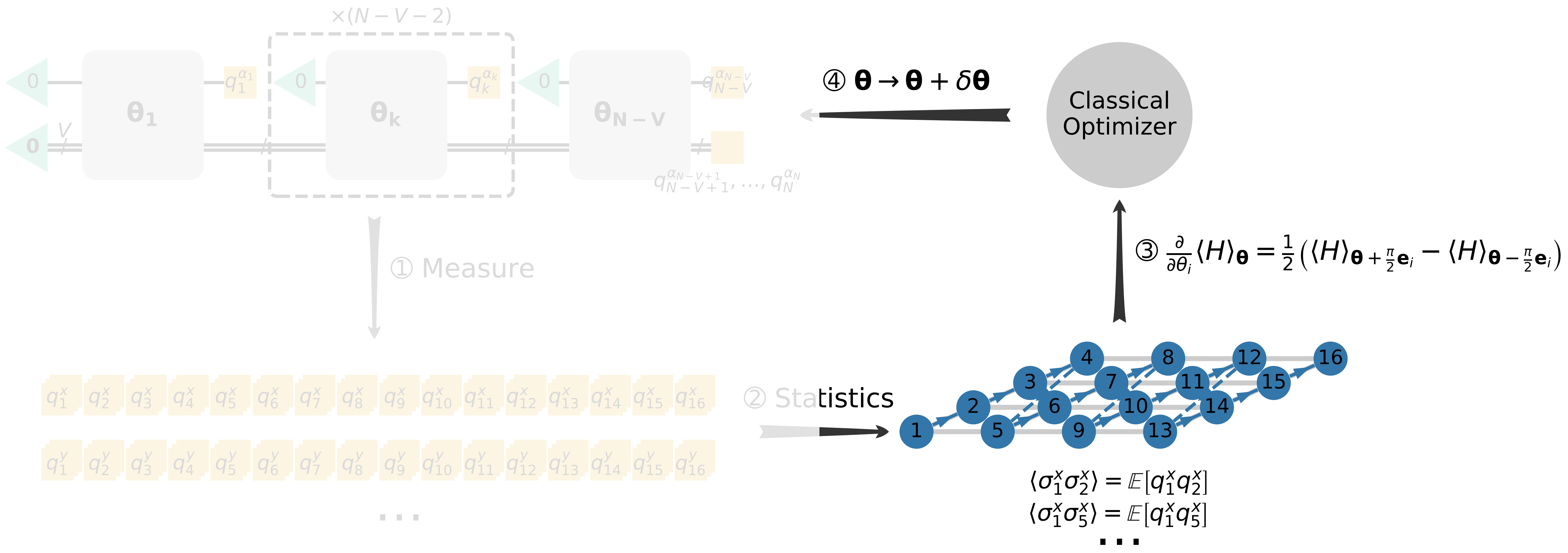
97% ground state fidelity for 4x4 frustrated Heisenberg model with only 6 qubits

Spin-spin correlations $\langle \sigma_i^z \sigma_j^z \rangle$



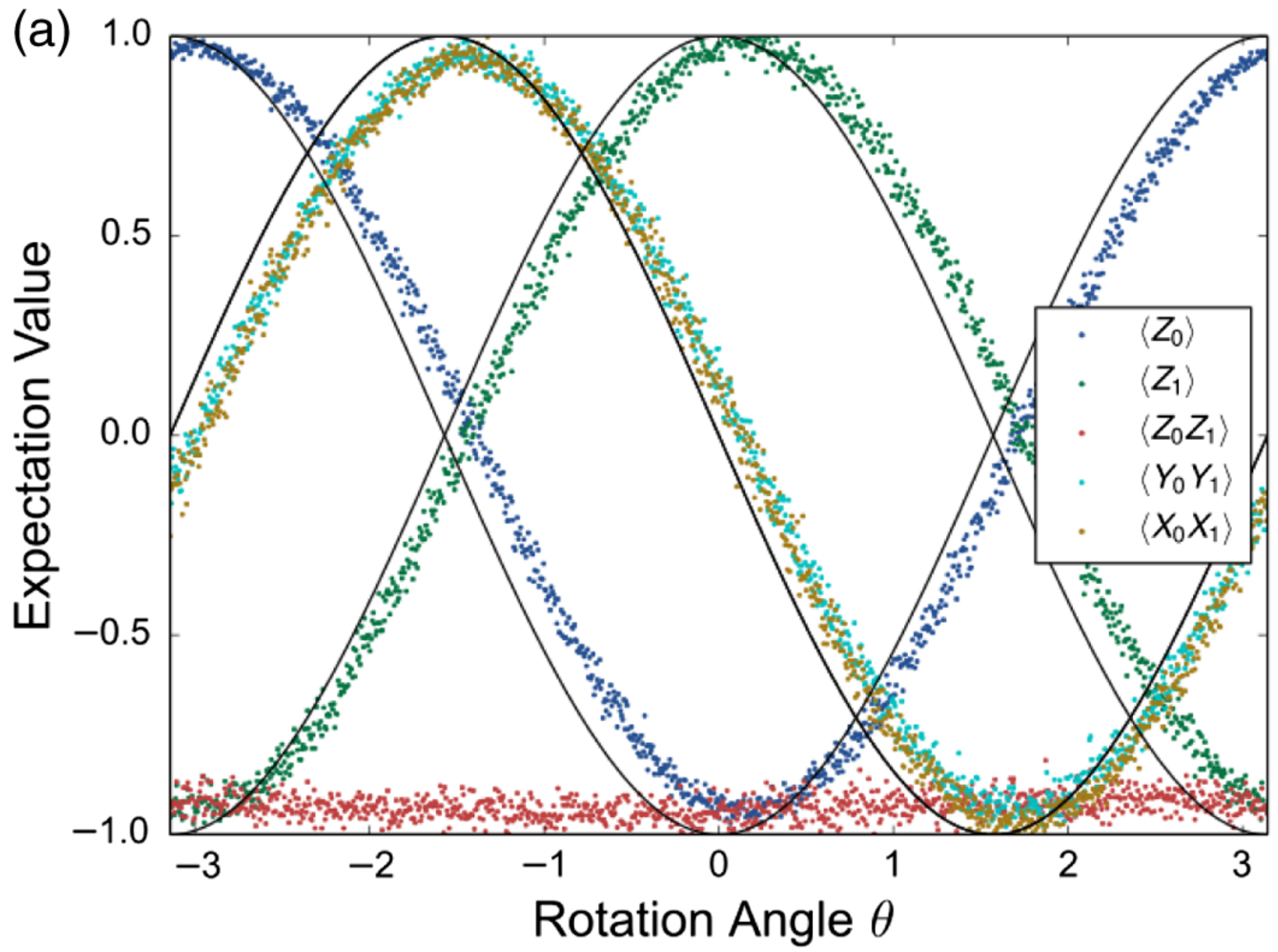
Read out the physics of a 4x4=16 quantum spins using only 6 qubits

How to optimize the quantum circuit?



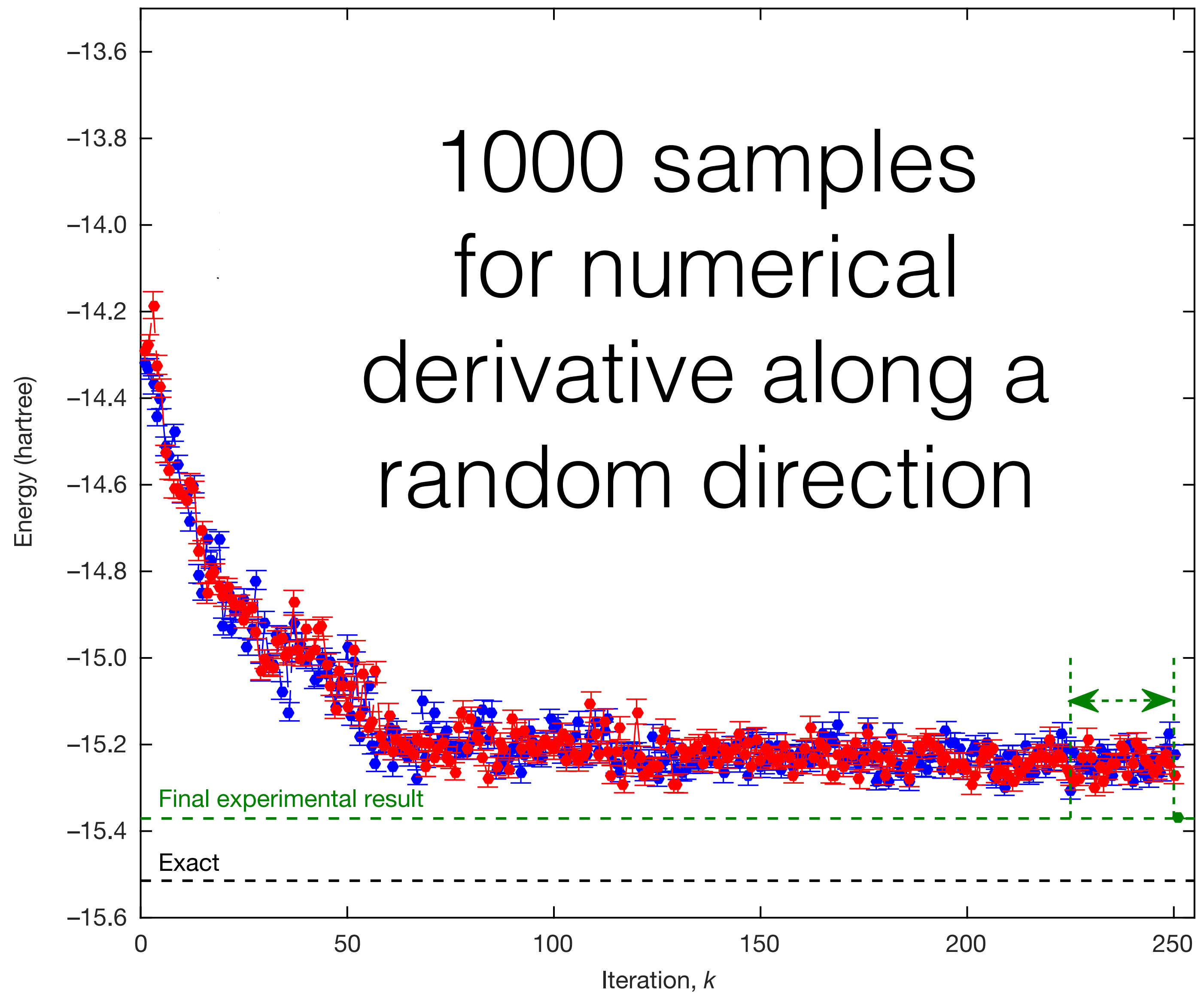
How did they optimize the quantum circuit ?

Google PRX '16



Scan 1000 values of the single variational parameter

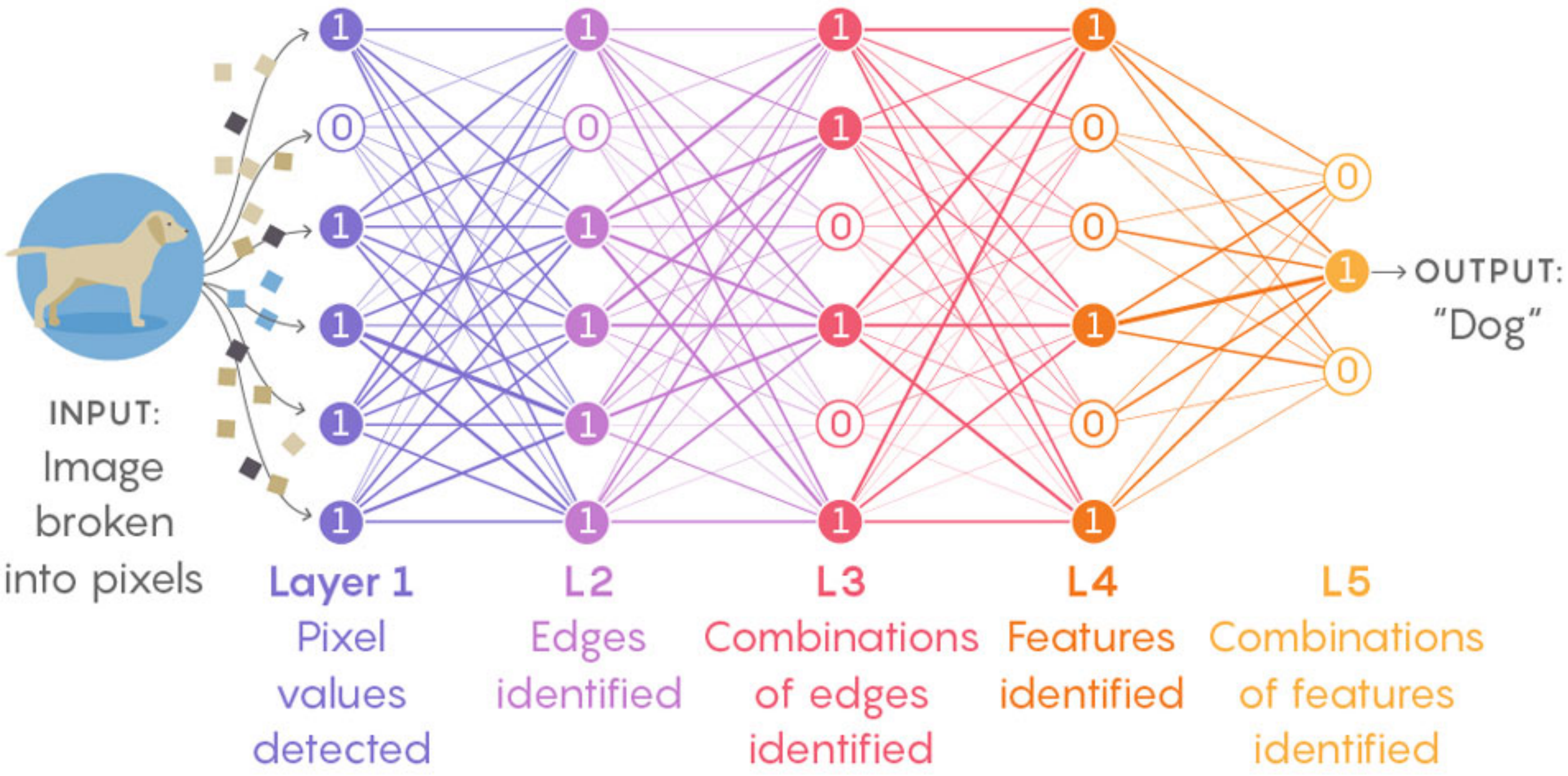
IBM Nature '17



Stochastic gradient descend with random perturbation

These optimization schemes do not scale to higher dimensions

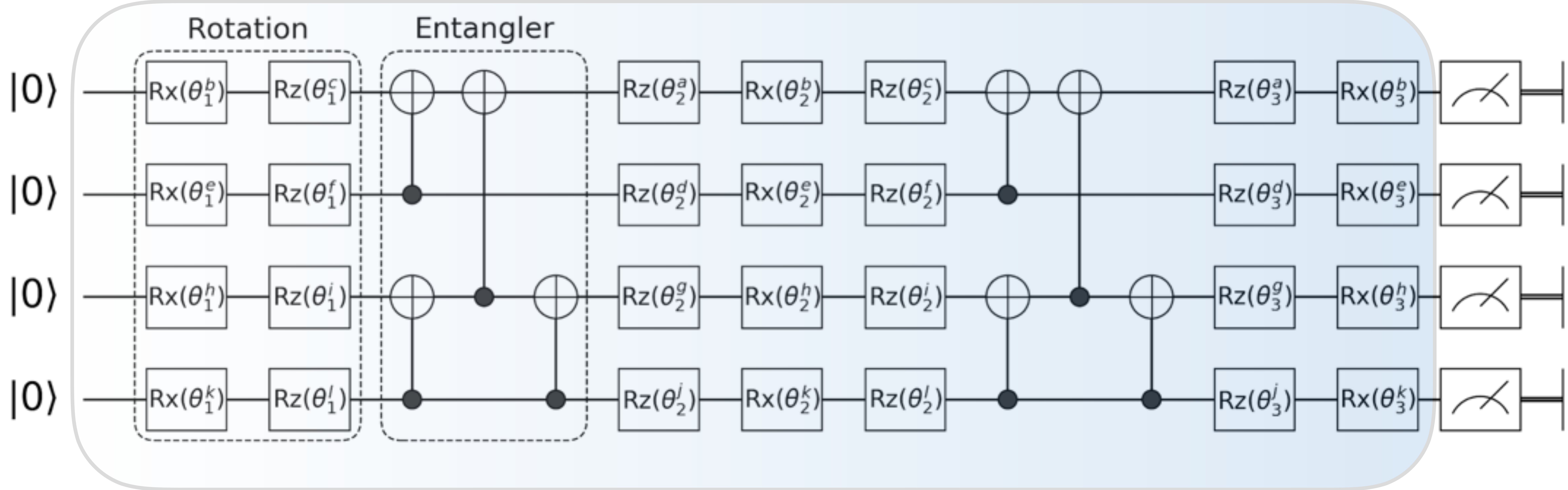
The lesson from deep learning



Scales to >1 billion parameters

Differentiable programing is the engine of deep learning
So it will be for variational quantum circuit optimization

Differentiable quantum circuits



Parametrized gate of the form

$$e^{-\frac{i\theta}{2}\Sigma} \text{ with } \Sigma^2 = 1$$

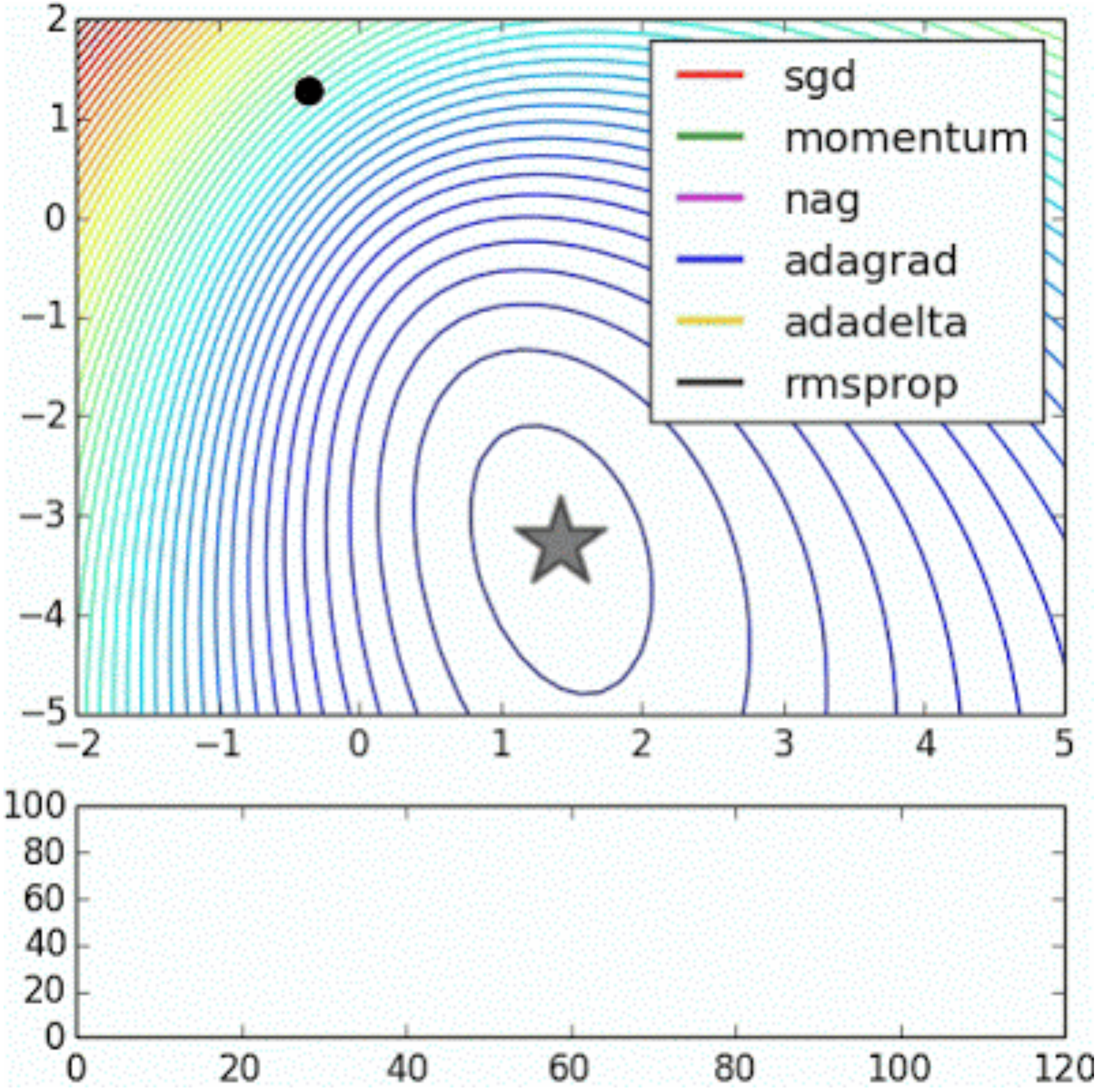
eg, X, Y, Z, CNOT, SWAP…

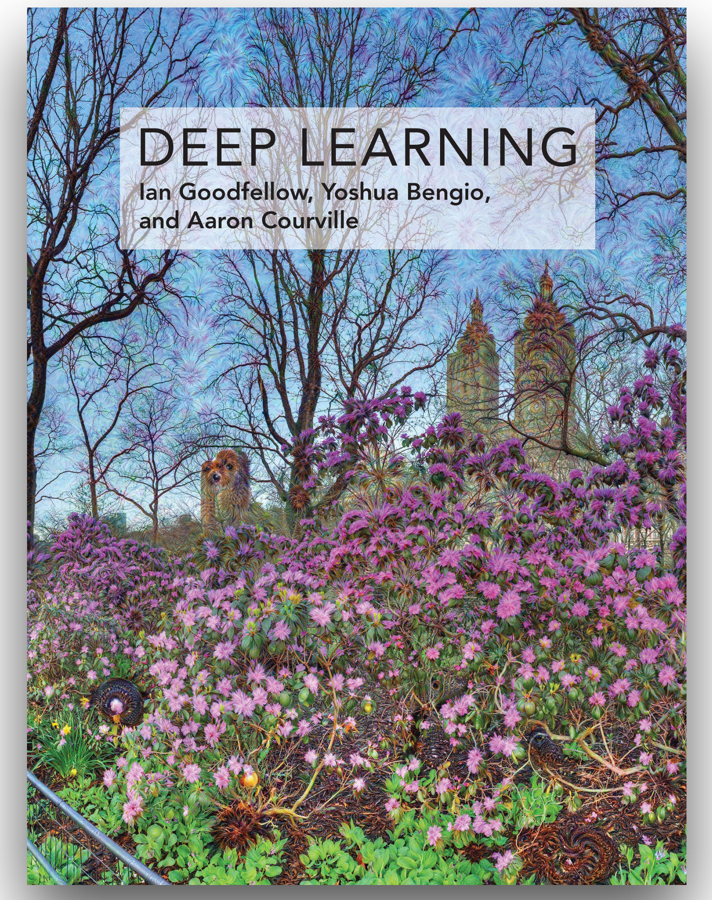
Li et al, PRL ’17, Mitarai et al, PRA ’18
J.-G.Liu, LW, PRA ’18, Xanadu, PRA ‘19

$$\nabla \langle H \rangle_\theta = \left(\langle H \rangle_{\theta+\pi/2} - \langle H \rangle_{\theta-\pi/2} \right) / 2$$

Unbiased gradient estimator measured on the quantum circuit

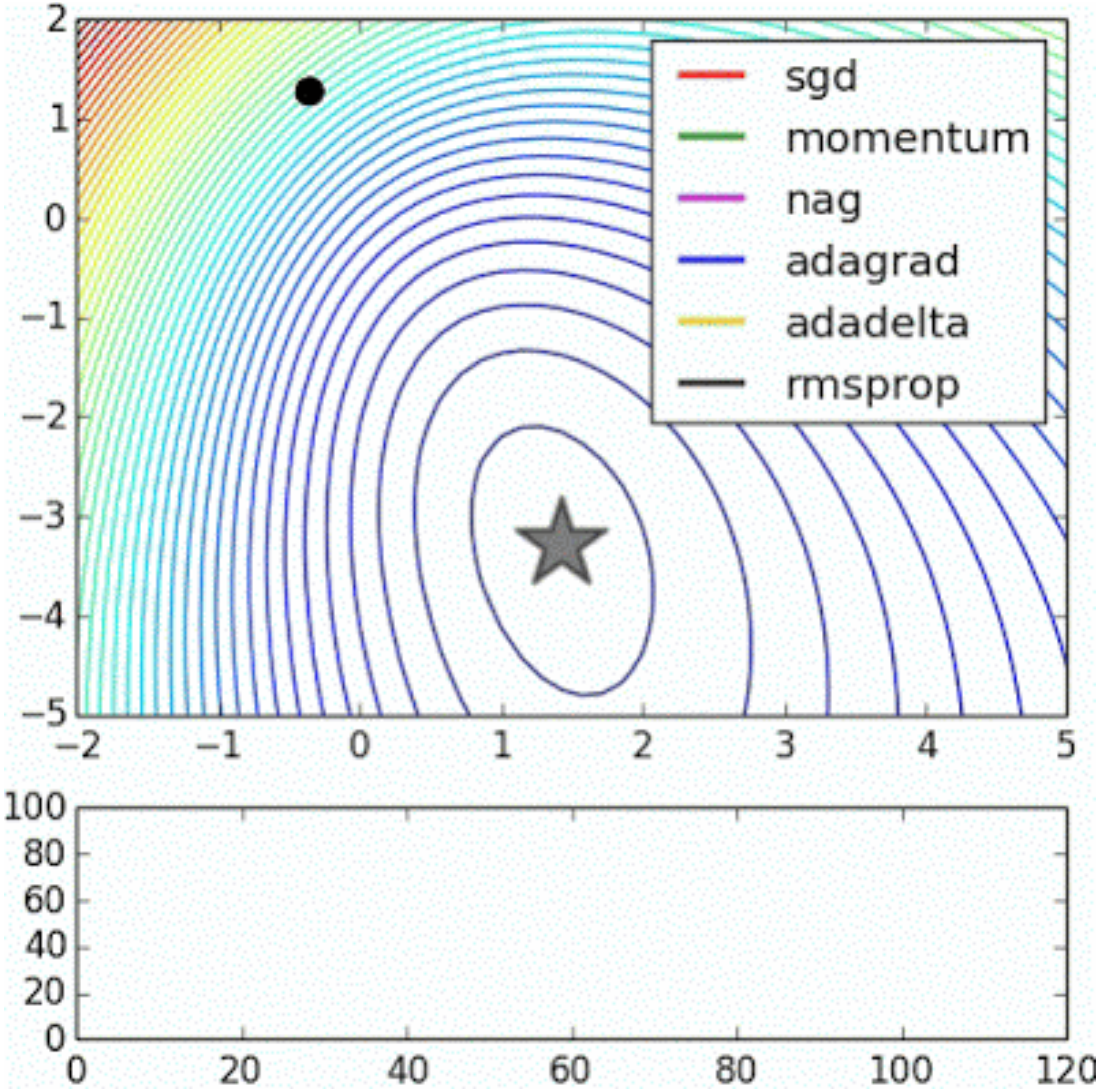
Optimization with noisy gradient

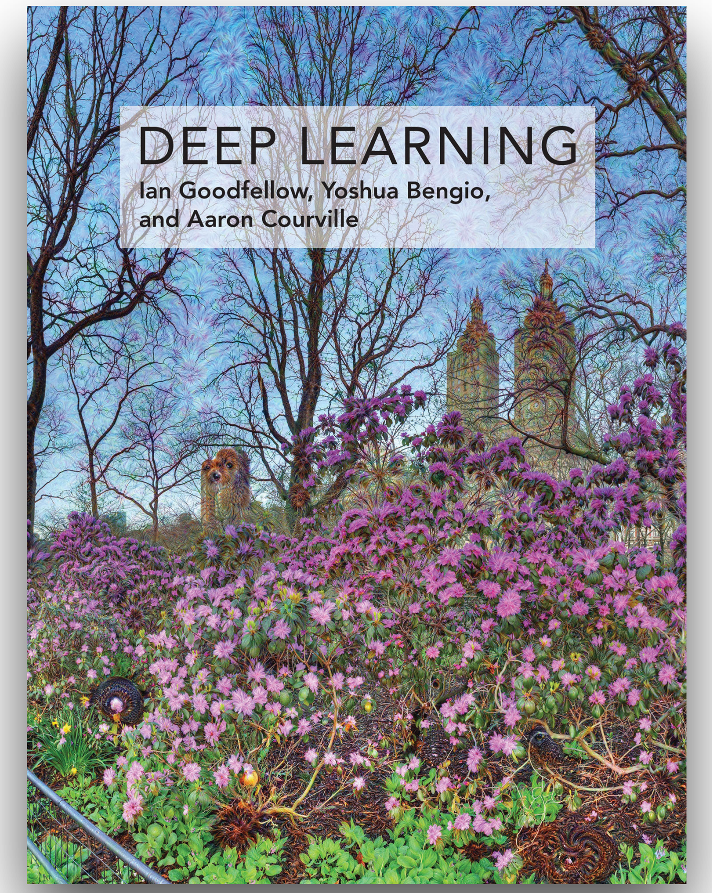




VQE encounters the same type of stochastic optimization in deep learning

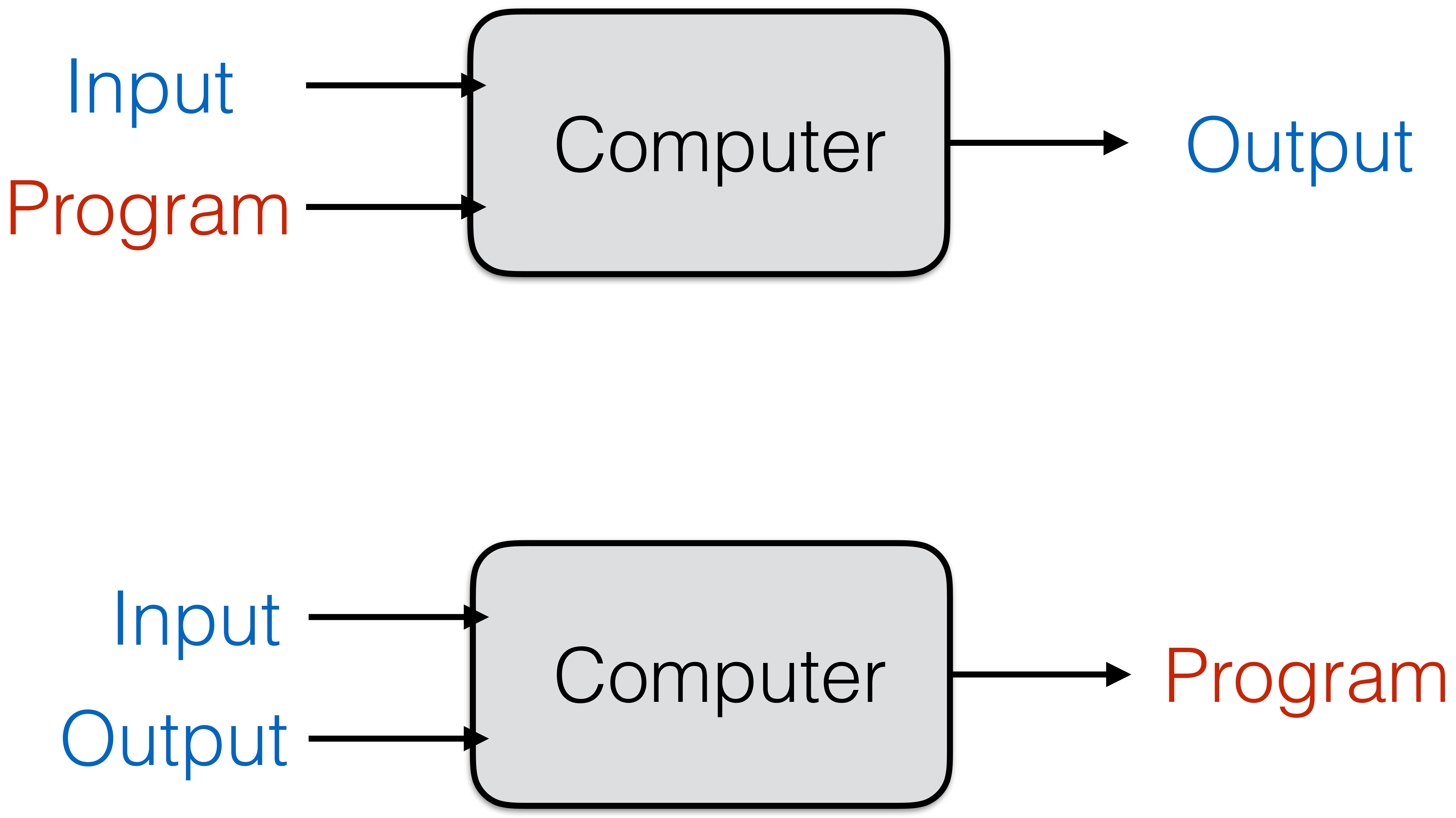
Optimization with noisy gradient





VQE encounters the same type of stochastic optimization in deep learning

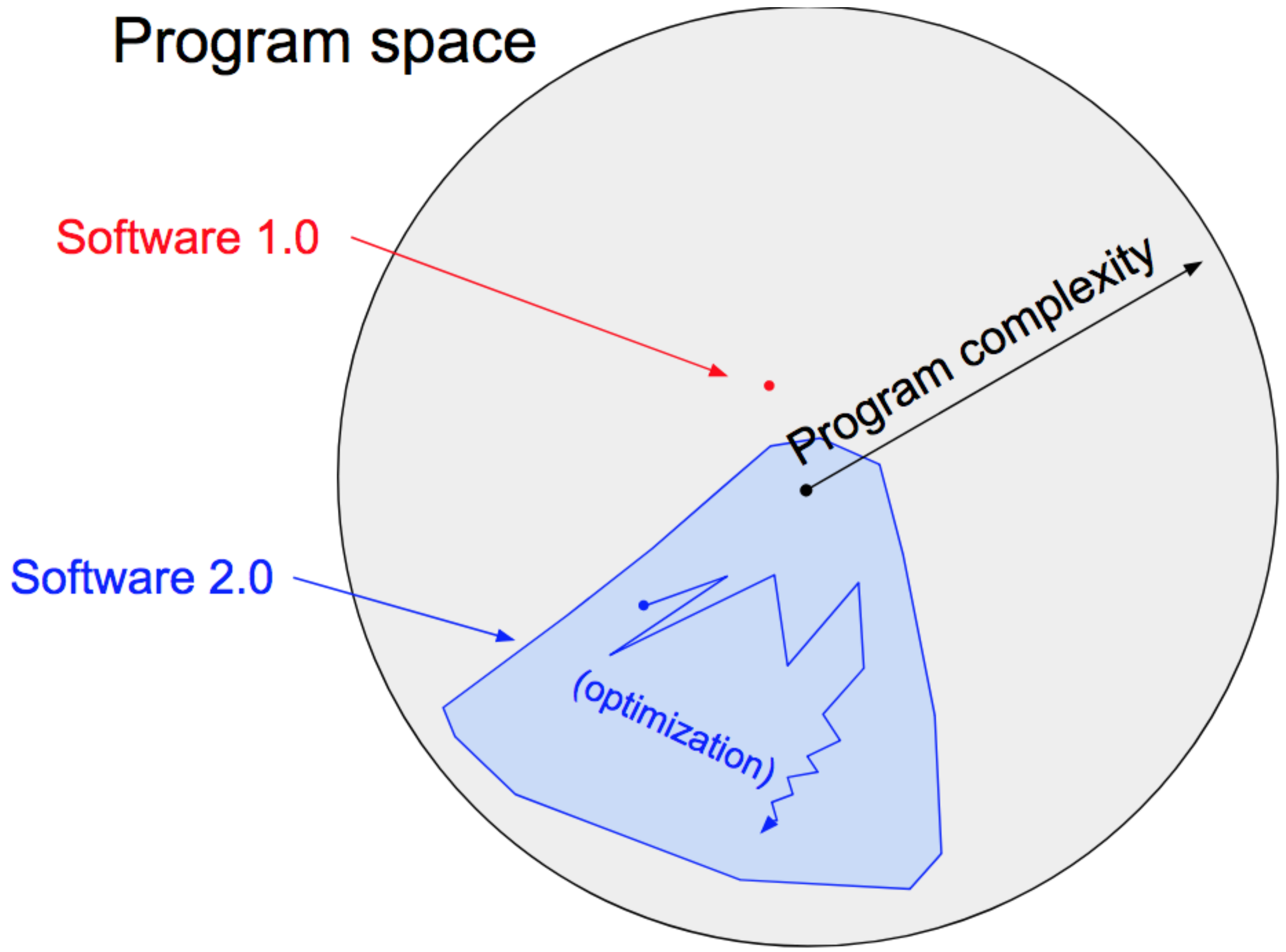
Differentiable Programming



Andrej Karpathy

Director of AI at Tesla. Previously Research Scientist at OpenAI and PhD student at Stanford. I like to train deep neural nets on large datasets.

https://medium.com/@karpathy/software-2-0-a64152b37c35



Writing software 2.0 by gradient search in the program space

Differentiable Programming

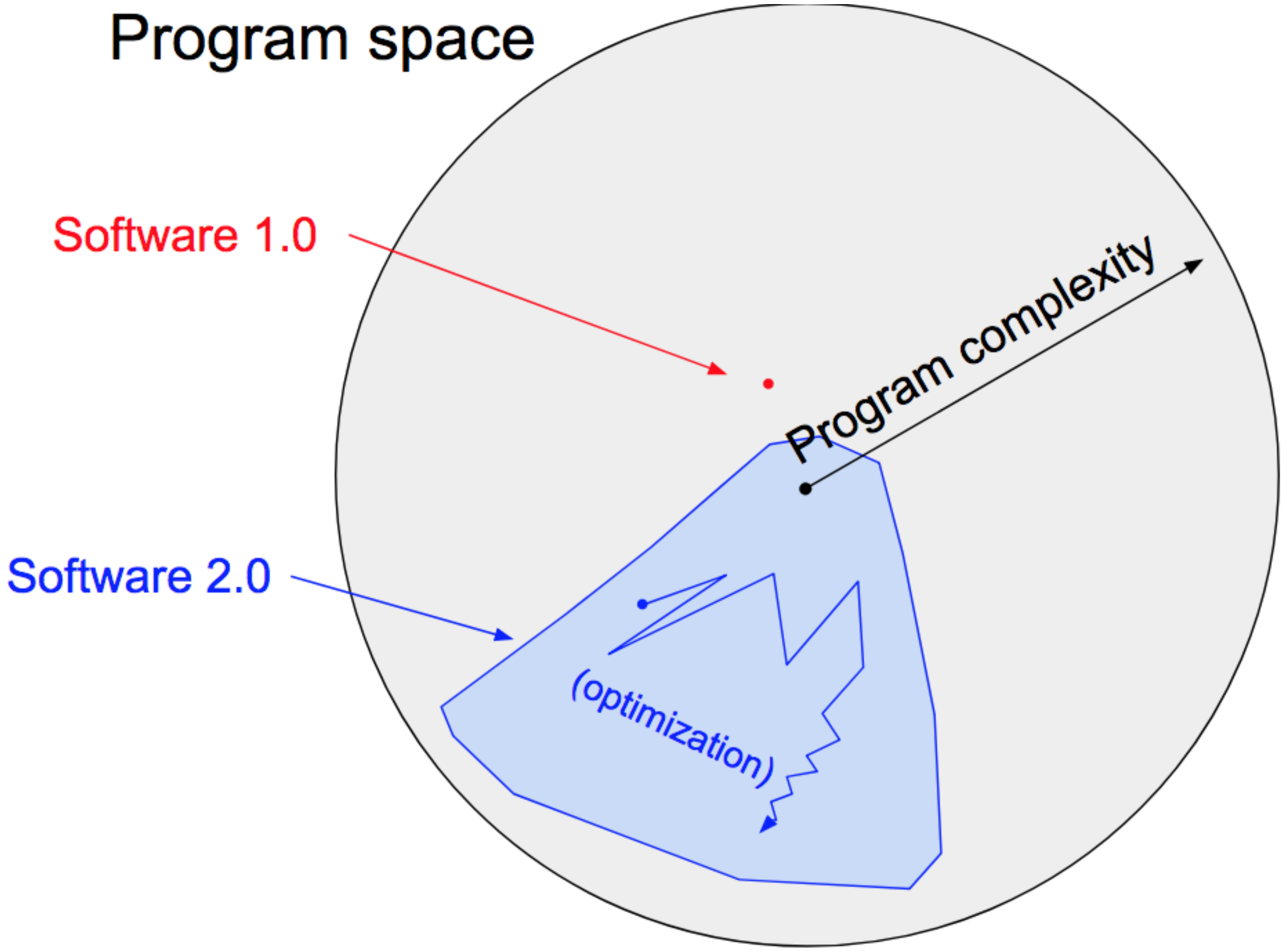
Benefits of Software 2.0

- Computationally homogeneous
- Simple to bake into silicon
- Constant running time
- Constant memory usage
- Highly portable & agile
- Modules can meld into an optimal whole
- **Better than humans**

Andrej Karpathy

Director of AI at Tesla. Previously Research Scientist at OpenAI and PhD student at Stanford. I like to train deep neural nets on large datasets.

https://medium.com/@karpathy/software-2-0-a64152b37c35

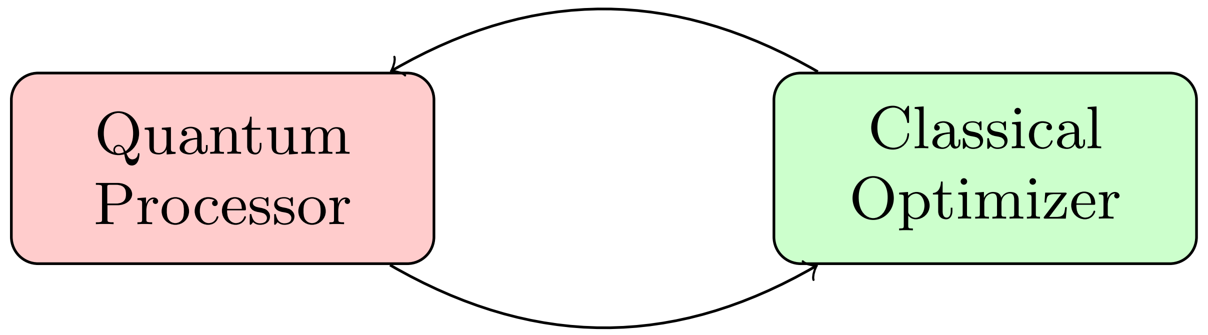


Writing software 2.0 by gradient search in the program space

Differentiable Quantum Programming

- Variational quantum eigensovler (VQE)
- Quantum approximate optimization algorithm (QAOA)
- Quantum circuit leanring (QCL)
- Quantum circuit Born machine (QCBM)

…



Original motivation:
What can we do with circuits of limited depth ?

Fundmental question:
Are we really good at programing quantum computers ?

It is a paradigm beyond quantum-classical hybrid

Differentiable Quantum Programming

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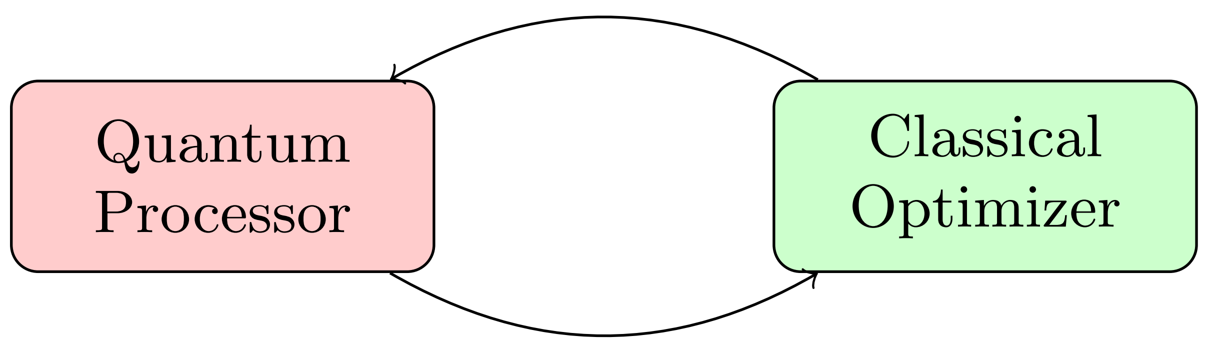
- Quantum circuit Born machine (QCBM)

…



Original motivation:
What can we do with circuits of limited depth ?

Fundmental question:
Are we really good at programing quantum computers ?

It is a paradigm beyond quantum-classical hybrid

Quantum circuit classifier	Farhi, Neven, 1802.06002, Wilson et al, 1806.08321
Quantum kernel learning	Schuld, Killoran, 1803.07128, Havlicek et al, 1804.11326
Learn state overlap algorithm	Cincio, Subaşı, Sornborger, Coles, 1803.04114
Quantum variational autoencoder	Khoshaman, Vinci, Denis, Andriyash, Sadeghi, Amin, 1802.05779
Quantum adversarial training	Dallaire-Demers, Lloyd, Benedetti, 1804.08641,1804.09139, 1806.00463

Differentiable Quantum Programming

- Variational quantum eigensovler (VQE)
- Quantum approximate optimization algorithm (QAOA)
- Quantum circuit leanring (QCL)
- Quantum circuit Born machine (QCBM)

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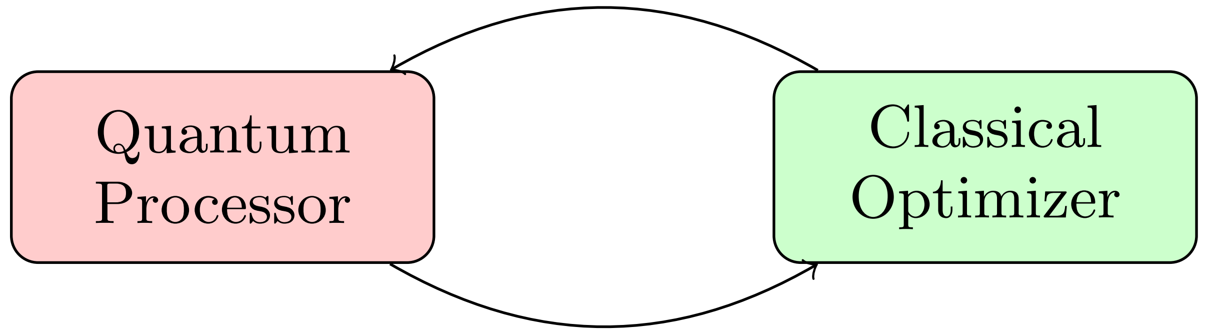

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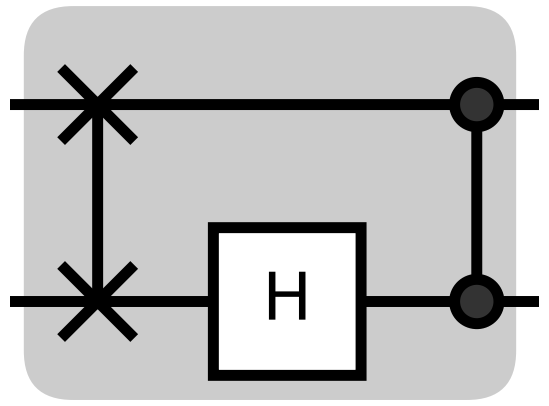
Quantum Software 2.0

Karpathy, Medium '17

Be prepared for Quantum Software 2.0

https://github.com/QuantumBFS/Yao.jl

julia +



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罗秀哲 Xiu-Zhe Luo: USTC—>IOP—>Waterloo
刘金国 Jin-Guo Liu: NJU—>IOP—> ???

Features:

- Strong focus on variational quantum algorithms
- Differentiable programming of quantum circuits
- Batch parallelization with GPU acceleration

Thank You!

Variational quantum eigensolver with fewer qubits

Jin-Guo Liu, Yi-Hong Zhang, Yuan Wan, LW, 1902.02663

Neural Networks | **Tensor Networks** | **Quantum Circuits**