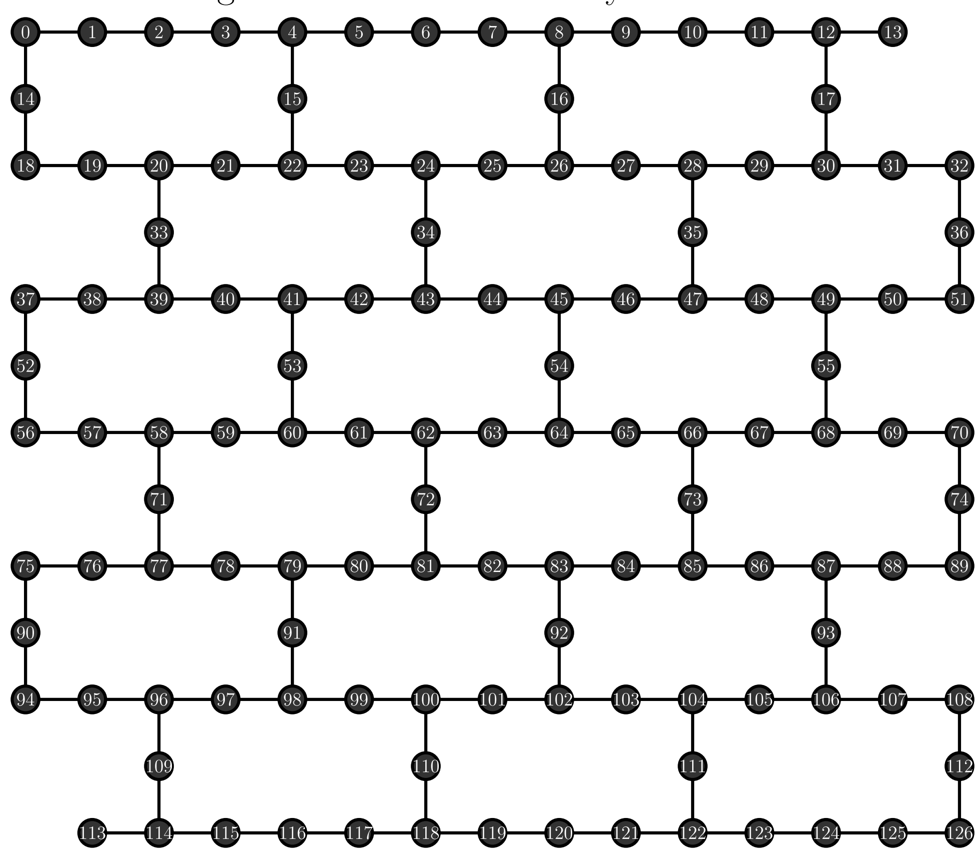
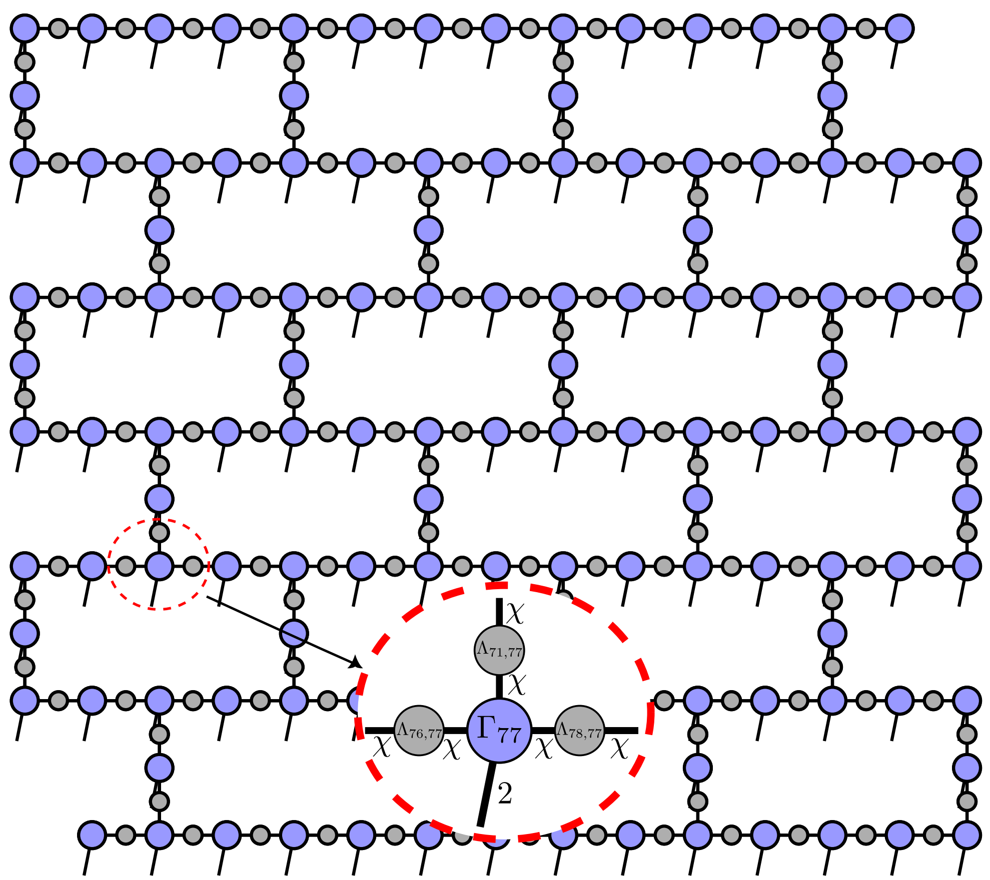
Quantum Computing on Classical Machines with Tensor Networks

Eagle Processor 6 × 3 Heavy − Hex Lattice



Classical Tensor Network Ansatz :



E.M. Stoudenmire

Jan 2024 - Brookhaven Natl. Lab

FLATIRON INSTITUTE
SIMONS FOUNDATION

Motivation

Great excitement for prospects of near-term **quantum computing**

Often making headlines:

Quantum computers could crack the cryptography that underpins financial stability

Disease control – Even though the novel coronavirus pandemic has not been curbed, quantum computing can help scientists and researchers discover vaccines in the future and address health

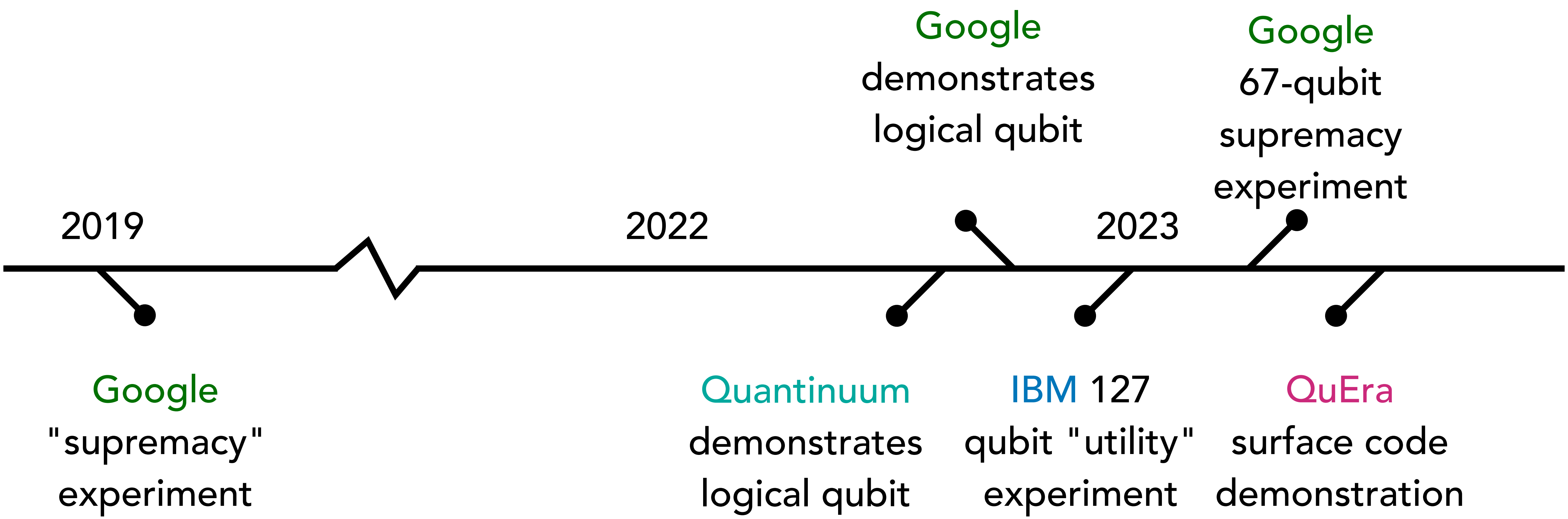
Cloud computing – Google plans to offer commercial cloud computing on its quantum computer process complicated problems and provide results to individual users.

Cryptography – Quantum cryptography can potentially change data security, creating tamper-pro cybersecurity measures.

in healthcare. Quantum computers have the potential to resolve problems of this complexity and magnitude across many different industries and applications, including finance, transportation, chemicals, and cybersecurity.

Motivation

Quantum hardware reaching impressive milestones



Motivation

Yet not clear what problems quantum computers can practically solve better than classical computers

Some candidates:

factoring (Shor's algorithm) or inverse problems (Grover's)

how robust to decoherence?

1000's of qubits needed? *time to solution?*

chemistry & physics simulation

can it scale? how accurate? sampling overhead?

Motivation

Amazing devices are being built...
we should research what they are best for

Simulating quantum computers clarifies line between easy and hard

Tensor networks are the most powerful simulators

Sometimes tensor networks are so powerful, we can flip the script: quantum algorithms become new "quantum inspired" classical algorithms

Today's Talk

- Motivation: Quantum Computing ✓
- Classical Methods and Tensor Networks for Quantum Systems
- Entanglement of Quantum Algorithms: the Quantum Fourier Transform (QFT)
- Assessing Quantum Utility Claims

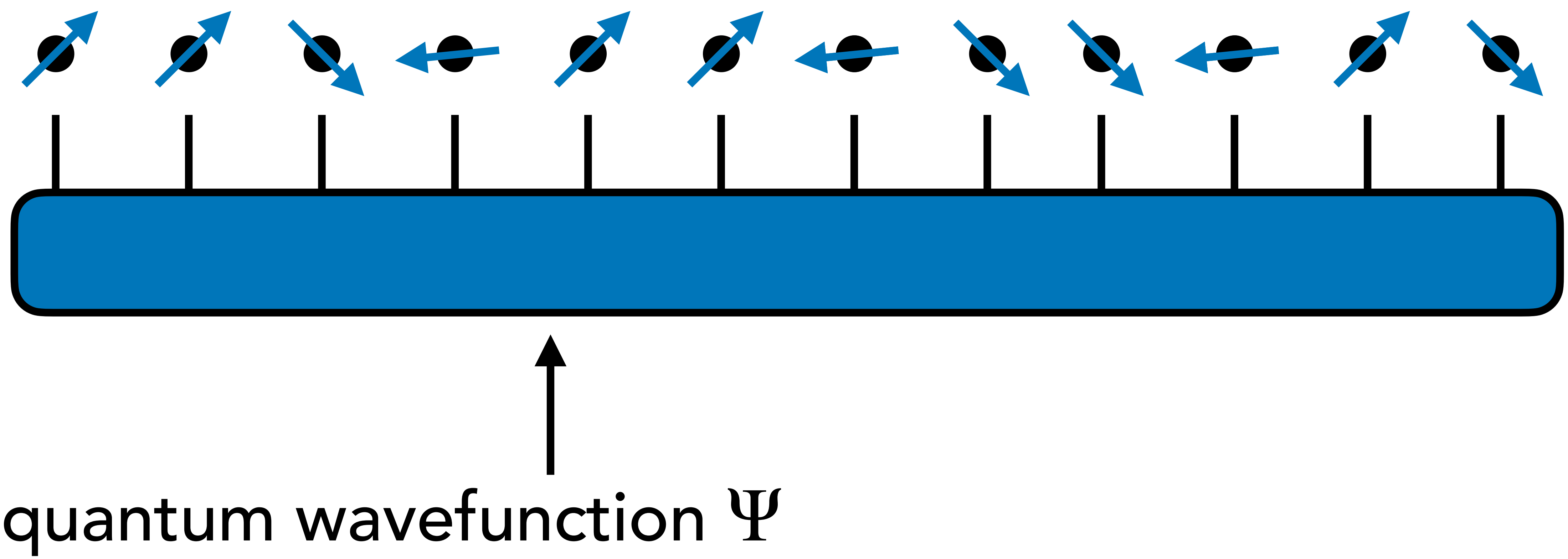
Classical Methods for Quantum Systems

How 'quantum' are classical computers?

Classical Methods for Quantum Systems

How hard is quantum mechanics?

Consider n quantum spins or qubits



2^n parameters inside

exponentially hard to store & manipulate

Classical Methods for Quantum Systems

What's going on at Flatiron Institute

Center for Computational Quantum Physics (CCQ)?

Classical Methods for Quantum Systems

Developing ways to break through the 2^n exponential quantum wall

quantum Monte Carlo

high-order perturbation theory

embedding (DMFT)

GW method

tensor networks

neural quantum states

density functional theory

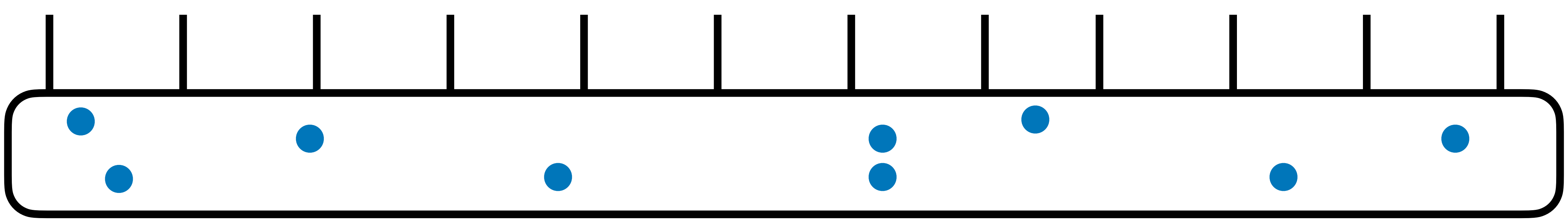
numerical renormalization group

Classical Methods for Quantum Systems

Developing ways to break through the 2^n exponential quantum wall

Quantum Monte Carlo

breaks exponential by sampling important configurations

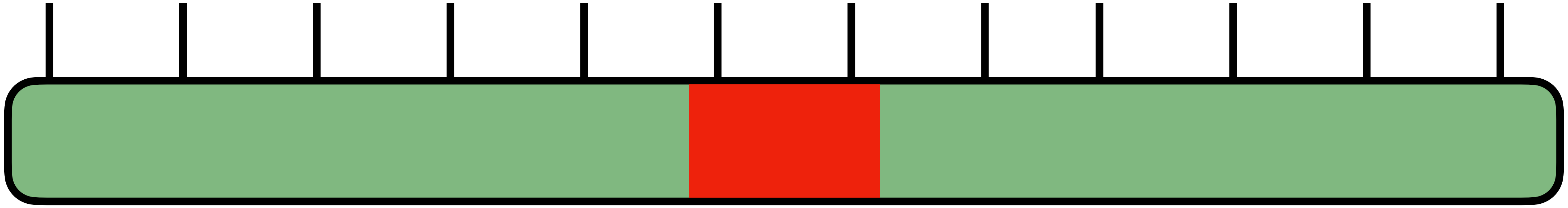


Classical Methods for Quantum Systems

Developing ways to break through the 2^n exponential quantum wall

Embedding / DMFT 🎯

treats small piece of system
inside solvable "bath" with mirrored properties



Classical Methods for Quantum Systems

Last but not least: **tensor networks**

Tensor networks:

- work directly with wavefunction
- use compression to store wavefunction
- closely mimic a quantum computer

Let's unpack these...

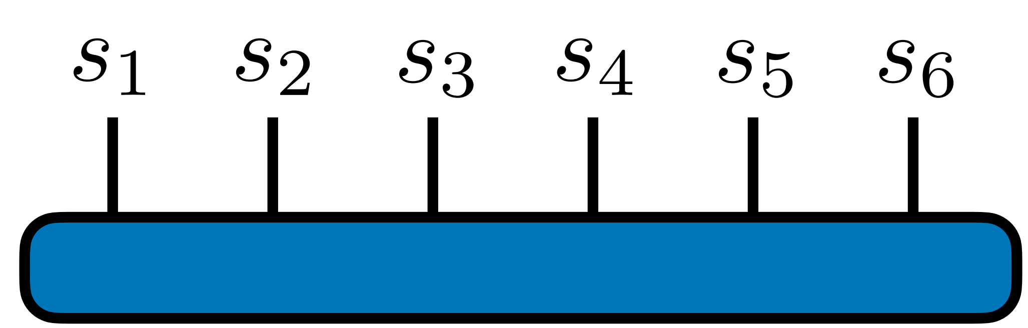
Classical Methods for Quantum Systems

General wavefunction of n qubits

$$|\Psi\rangle = \sum_{s_1 s_2 s_3 \cdots s_n} \Psi^{s_1 s_2 s_3 \cdots s_n} |s_1 s_2 s_3 \cdots s_n\rangle \qquad s_j \in 0, 1$$

Amplitudes form a big tensor!

$$\Psi^{s_1 s_2 s_3 s_4 s_5 s_6} =$$



Classical Methods for Quantum Systems

What is a tensor?

vector $$v = \begin{bmatrix} 2 \\ 3 \end{bmatrix} \qquad v_2 = 3$$

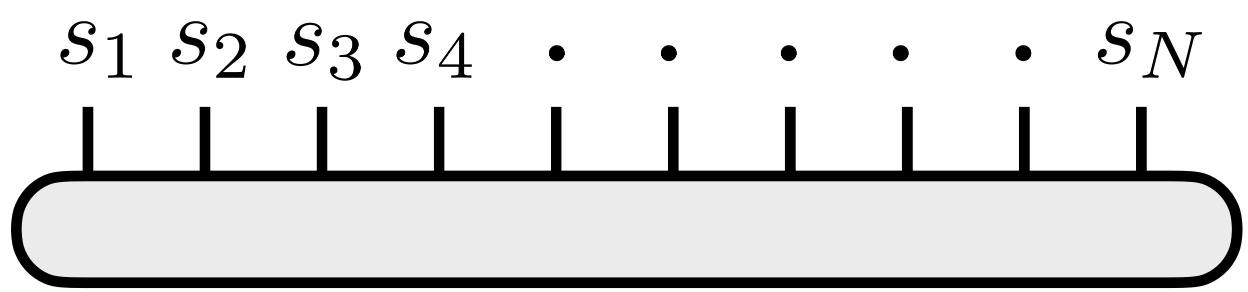
matrix $$M = \begin{bmatrix} 5 & 7 \\ 8 & 9 \end{bmatrix} \qquad M_{12} = 7$$

order-3 tensor $$T = \begin{bmatrix} 3 & \begin{bmatrix} 5 & 4 \\ 3 & 2 \end{bmatrix} & 7 \\ 1 & & 5 \end{bmatrix} \qquad T_{112} = 5$$

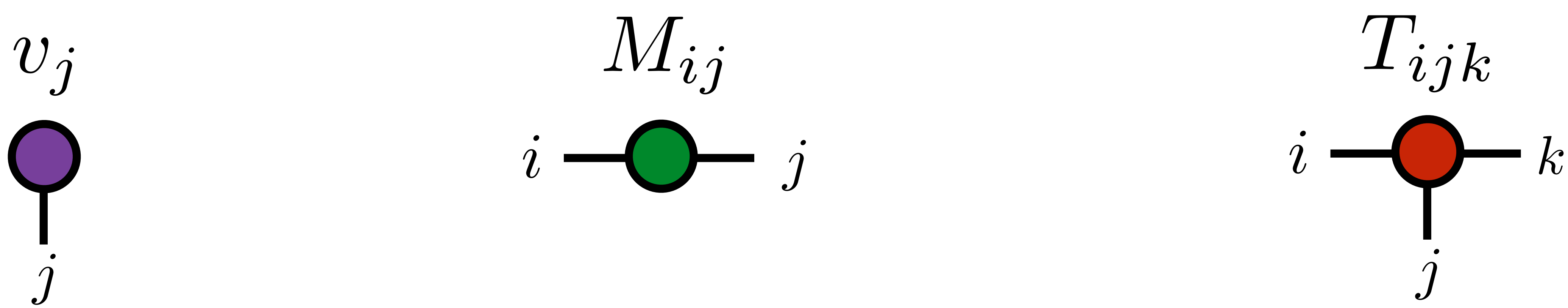
Classical Methods for Quantum Systems

N-index tensor = shape with N lines

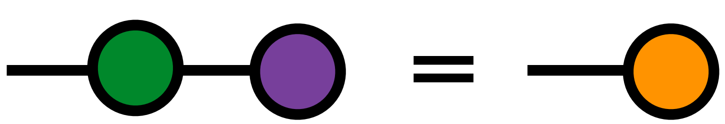
$$T^{s_1 s_2 s_3 \cdots s_N} =$$



Low-order examples:



Joining wires means contraction:

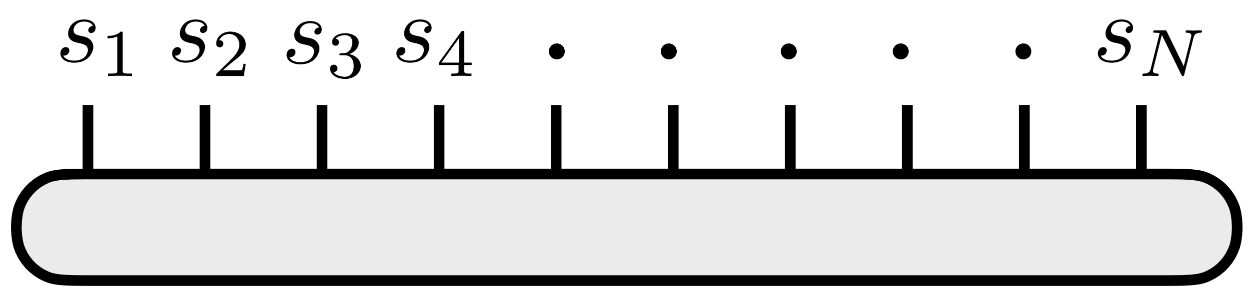


$$\sum_j M_{ij} v_j = w_i$$

Classical Methods for Quantum Systems

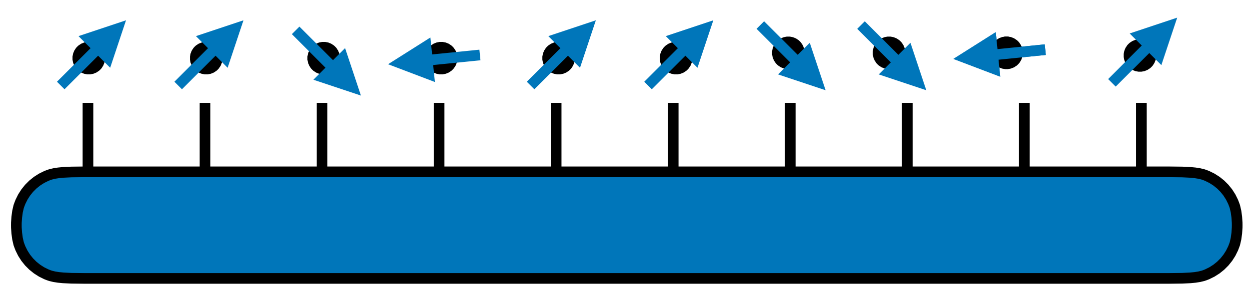
N-index tensor exponential to store

$$T^{s_1 s_2 s_3 \cdots s_N} =$$



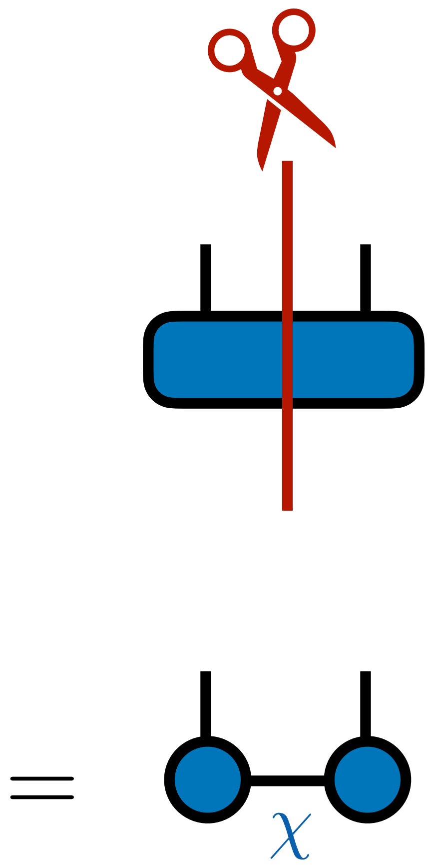
Tensor version of "many-body problem"

$$|\Psi\rangle =$$



Classical Methods for Quantum Systems

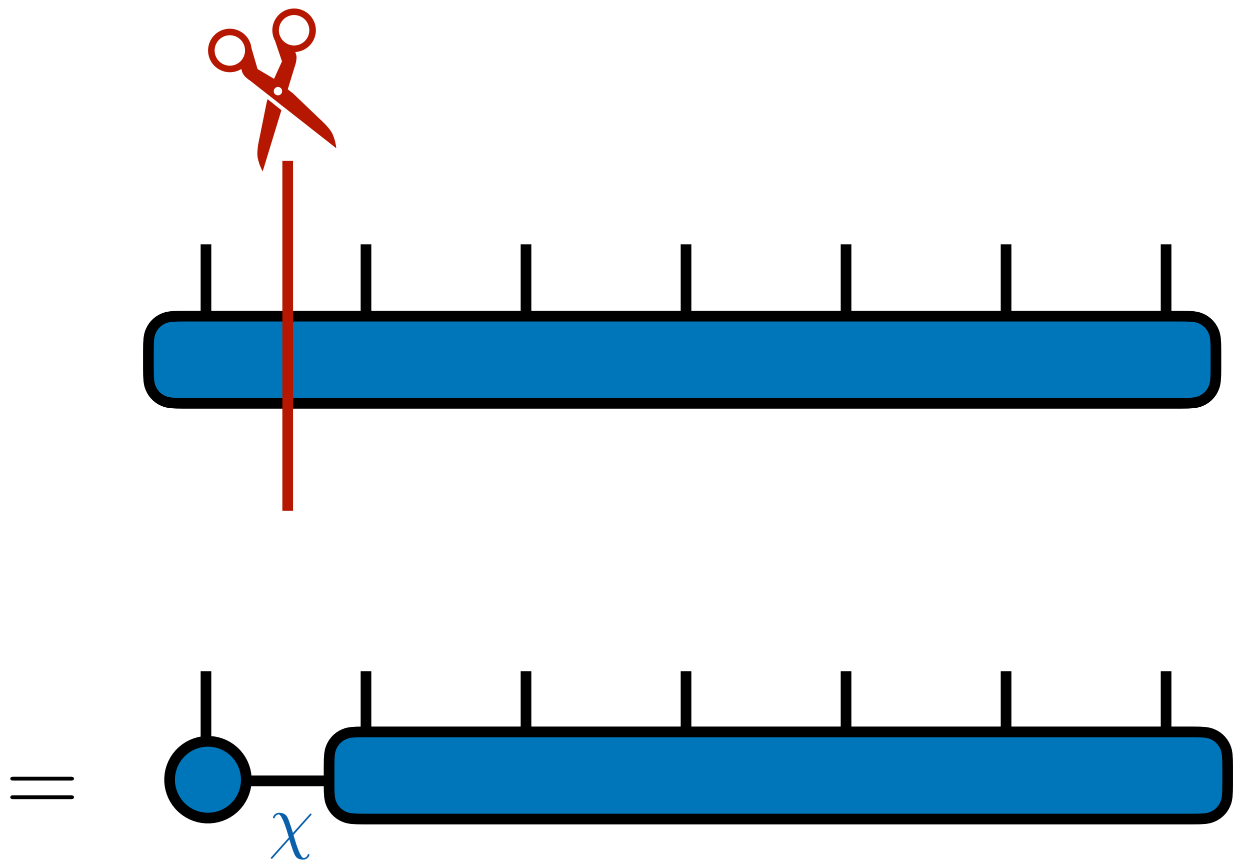
Just as factorizing a matrix reduces cost (memory and compute)



χ is matrix rank

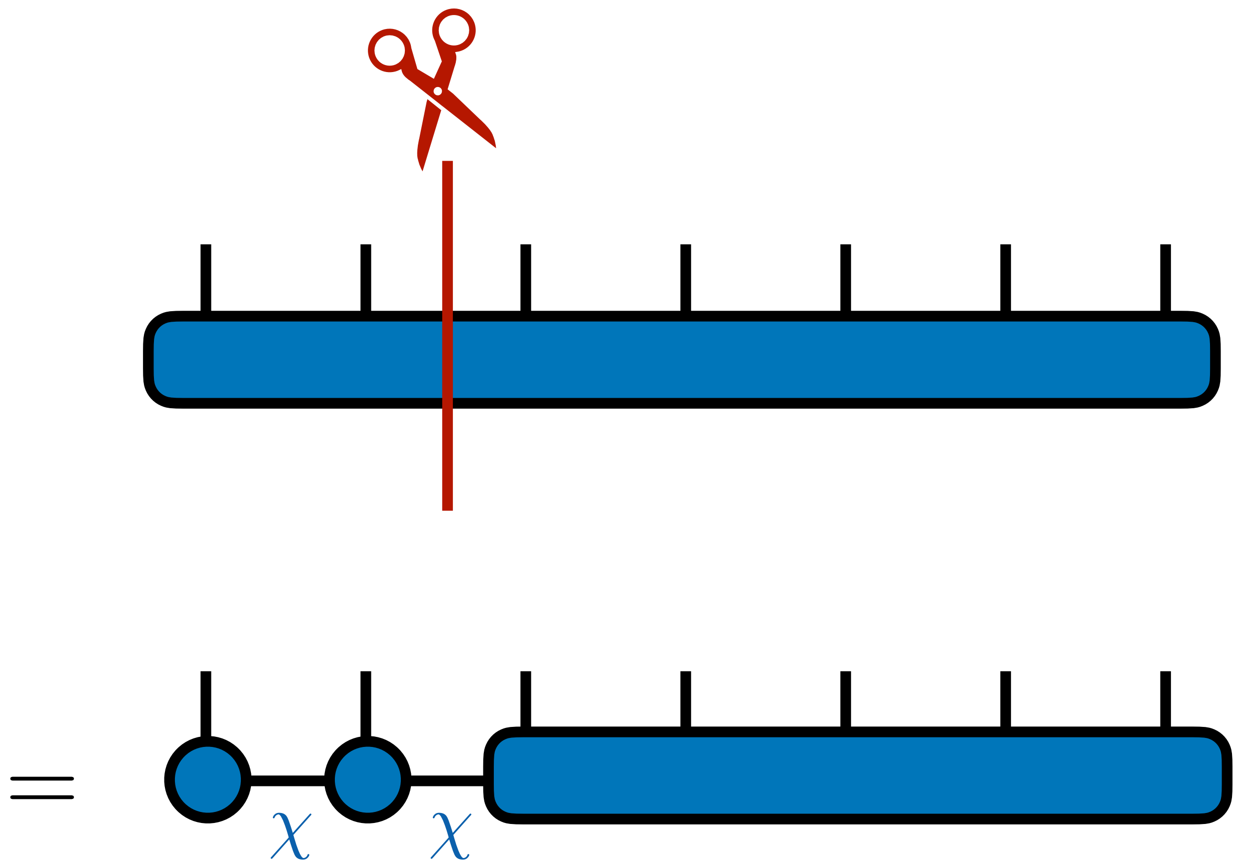
Classical Methods for Quantum Systems

Can recursively factor (compress) a tensor as well



Classical Methods for Quantum Systems

Can recursively factor (compress) a tensor as well



Classical Methods for Quantum Systems

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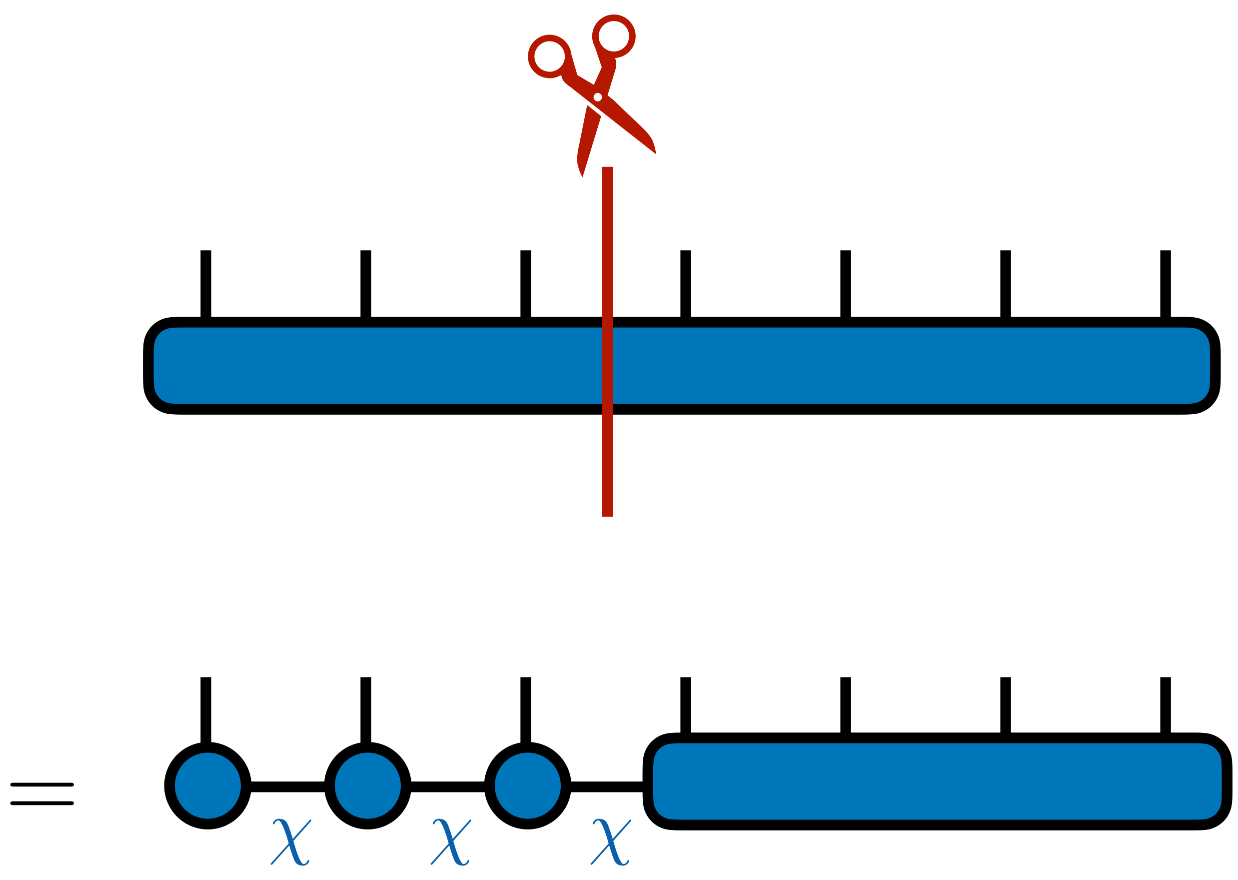

Classical Methods for Quantum Systems

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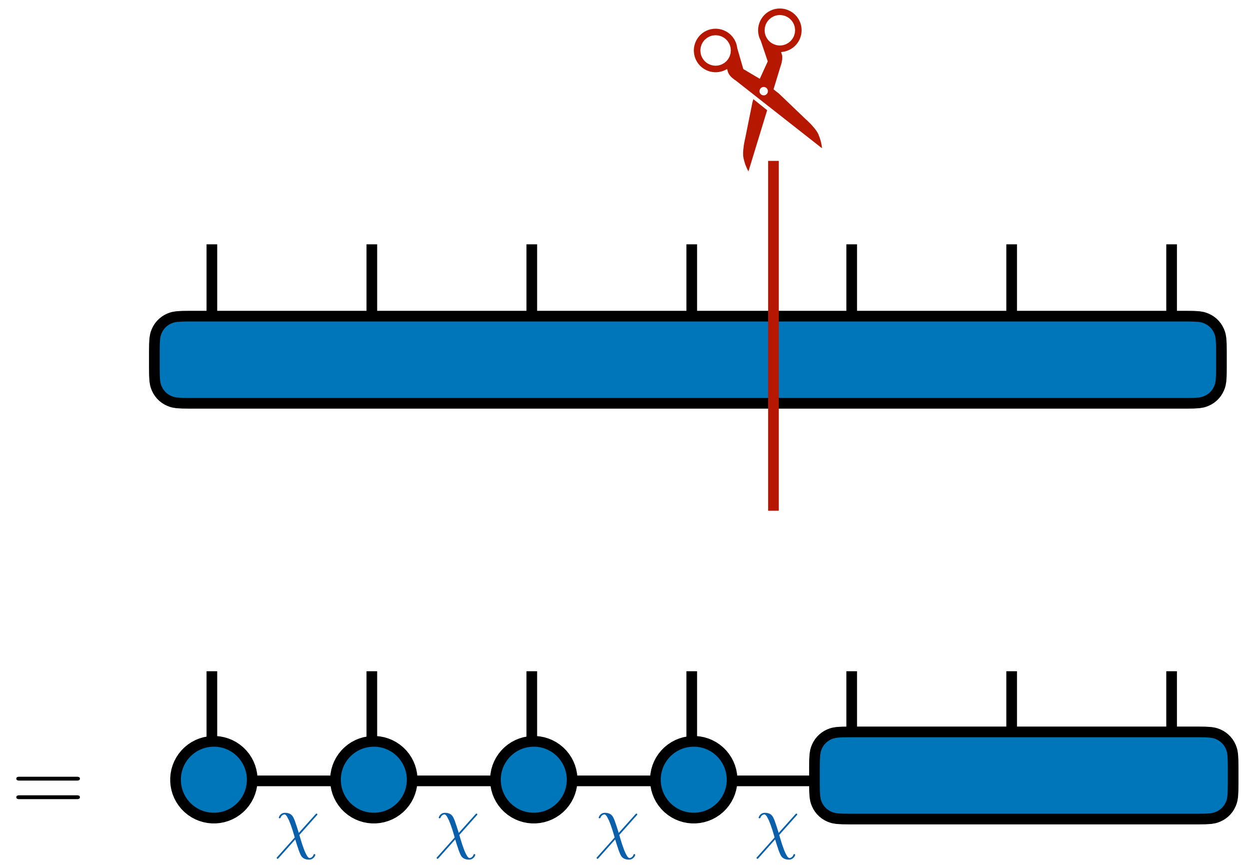

Classical Methods for Quantum Systems

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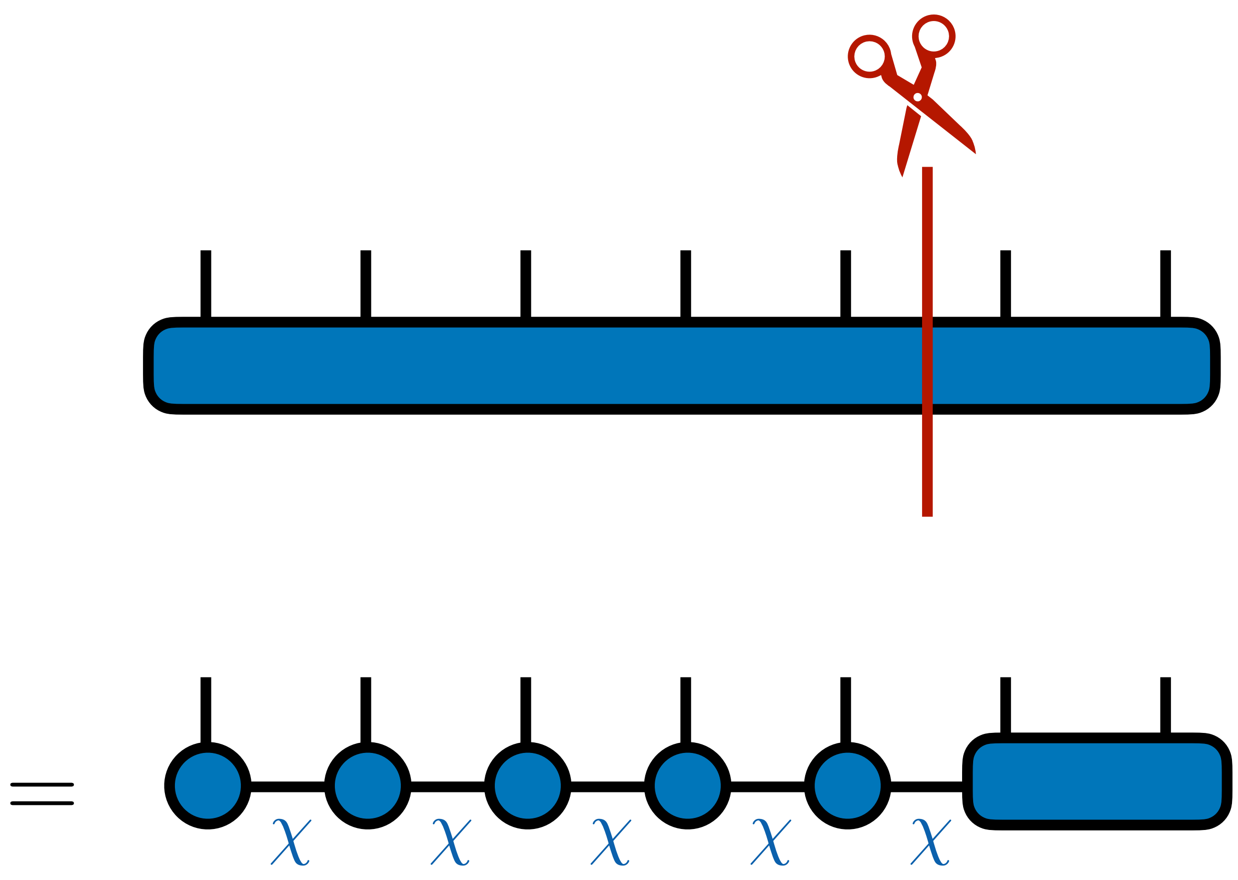

Classical Methods for Quantum Systems

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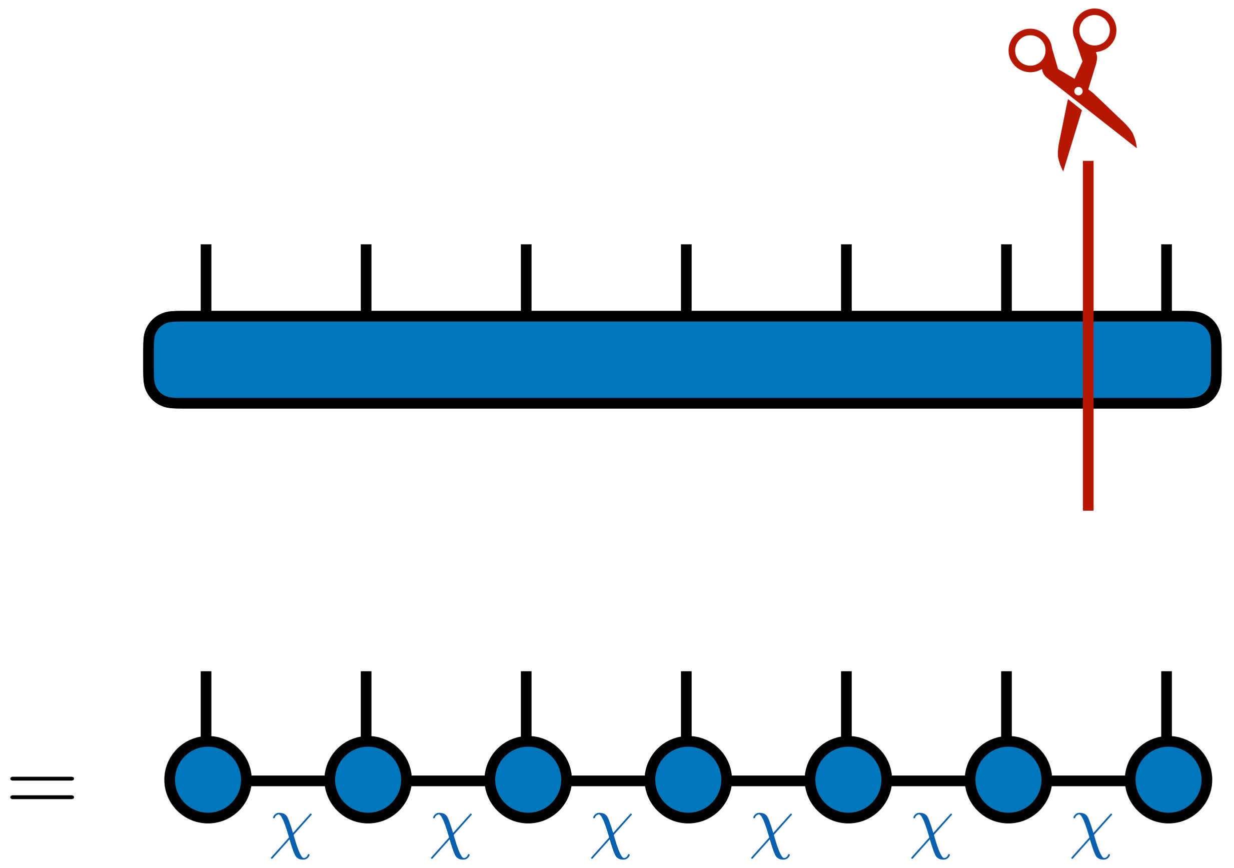

Classical Methods for Quantum Systems

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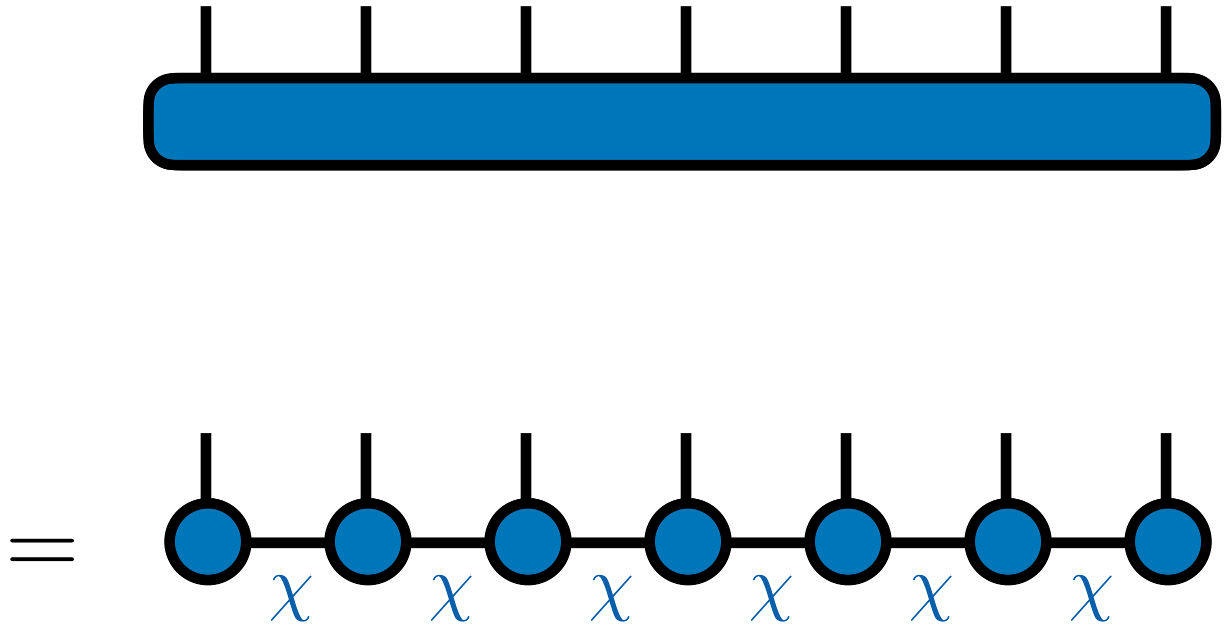
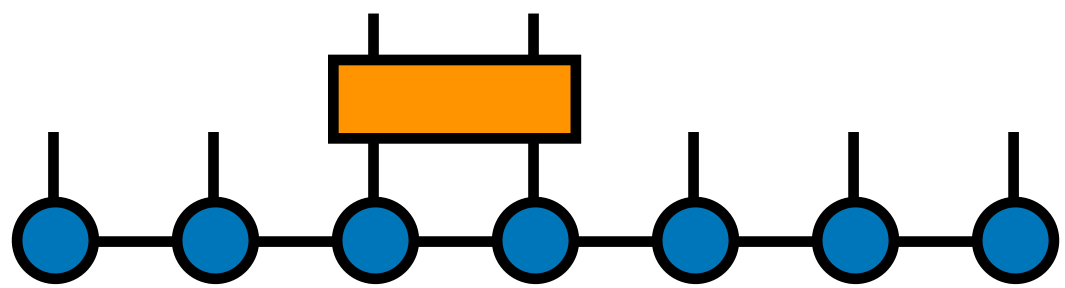


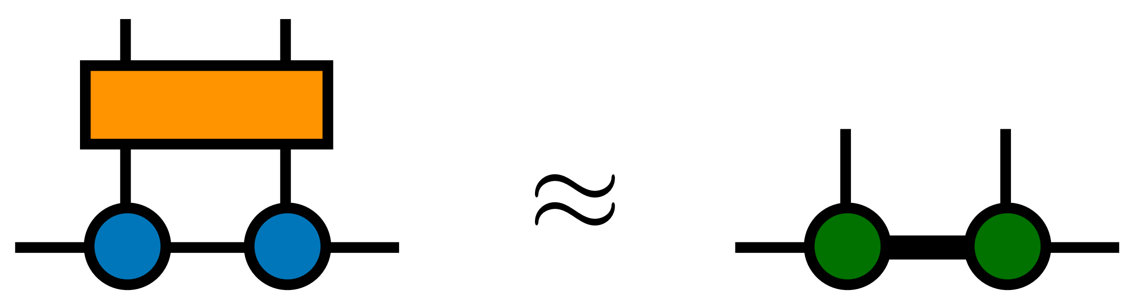
Advantage if internal indices small, yet accuracy is good (small "bond dimension" or "rank" χ)

Classical Methods for Quantum Systems

Optimize by e.g. applying quantum gates
(imaginary or real time evolution)

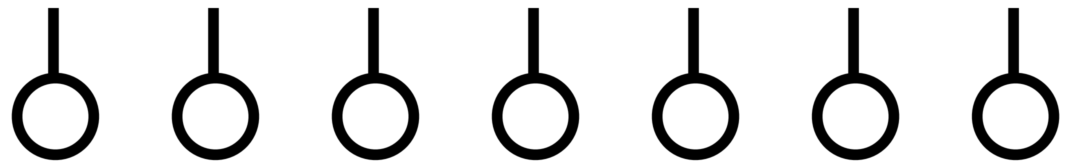
$|\Psi\rangle =$ 

Efficient – only touch three small tensors per gate



Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

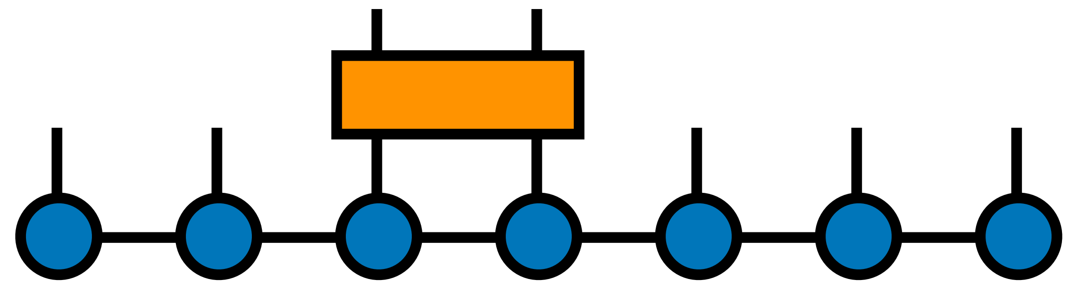
$$|\Psi\rangle =$$ 

	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓

Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

$$|\Psi\rangle =$$

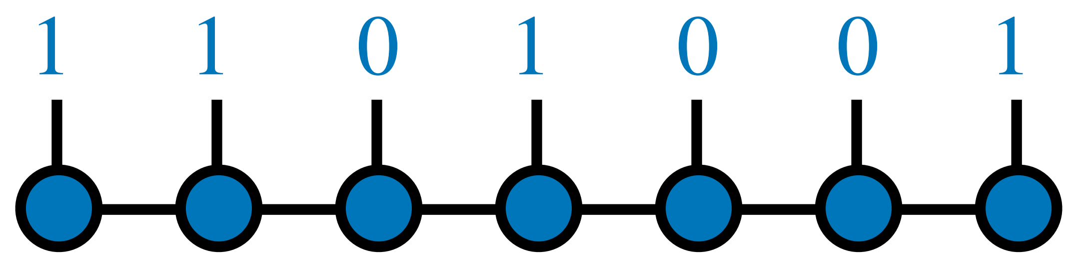


	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓
efficiently apply gates	✓	✓

Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

$$|\Psi\rangle =$$



	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓
efficiently apply gates	✓	✓
sample from wavefunction	✓	✓

Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

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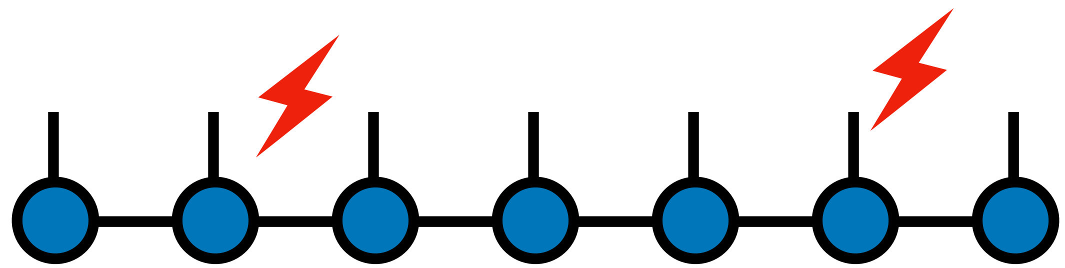
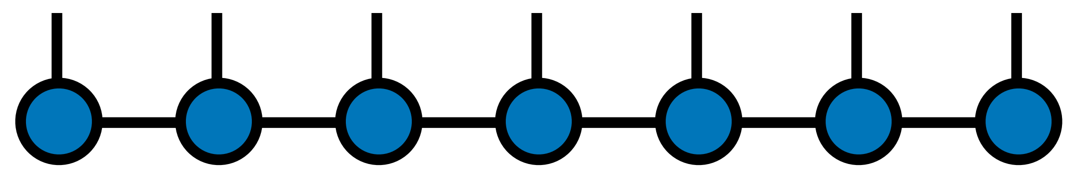


	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓
efficiently apply gates	✓	✓
sample from wavefunction	✓	✓
errors make handling easier	✓	✓

Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

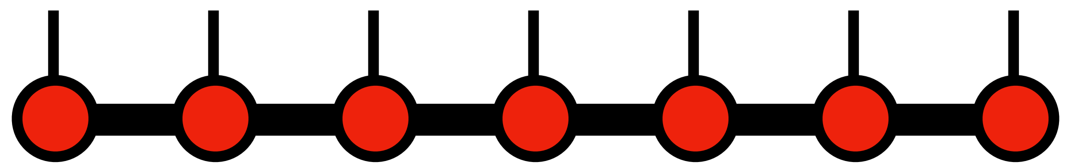
$$|\Psi\rangle =$$



	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓
efficiently apply gates	✓	✓
sample from wavefunction	✓	✓
errors make handling easier	✓	✓
non-unitary gates, post-selection, counting problems, ...	✗	✓

Classical Methods for Quantum Systems

How do tensor networks mimic quantum computers?

$$|\Psi\rangle =$$ 

	Quantum Computer	Tensor Network
prepare simple initial states	✓	✓
efficiently apply gates	✓	✓
sample from wavefunction	✓	✓
errors make handling easier	✓	✓
non-unitary gates, post-selection, counting problems, …	✗	✓
handle <u>high entanglement</u>	✓? or ✗?	✗

Classical Methods for Quantum Systems

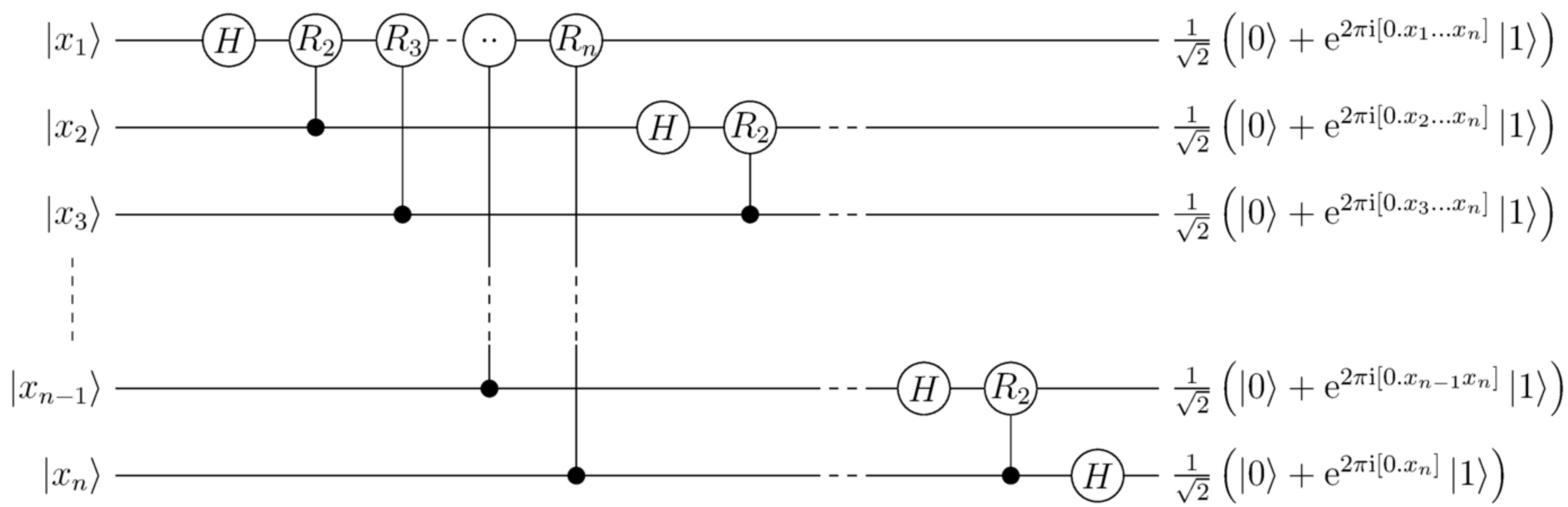
Thought experiment:
If we put a quantum computer and a tensor network in a box, for what problems could we tell them apart?

Application #1:
The Quantum Fourier Transform

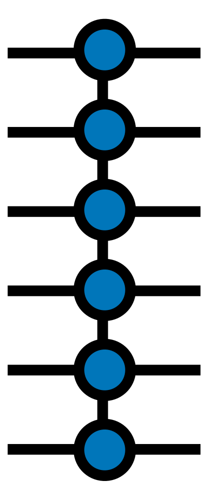
How 'quantum' are
quantum algorithms?

Analogy between quantum and classical so precise, some quantum algorithms have been classical all along

Quantum Fourier transform (QFT):



$\approx$



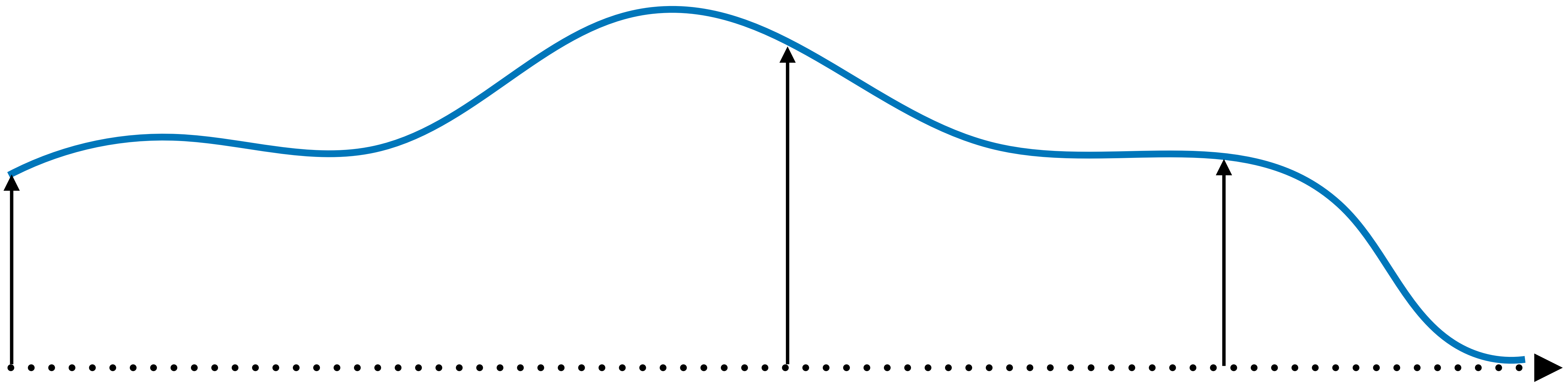
Equal to network of small tensors ("MPO" tensor network)

Chen, Stoudenmire, White, PRX Quantum, arxiv:2210.08468

What does the QFT do?

Consider function discretized on grid of spacing $\frac{1}{2^n}$

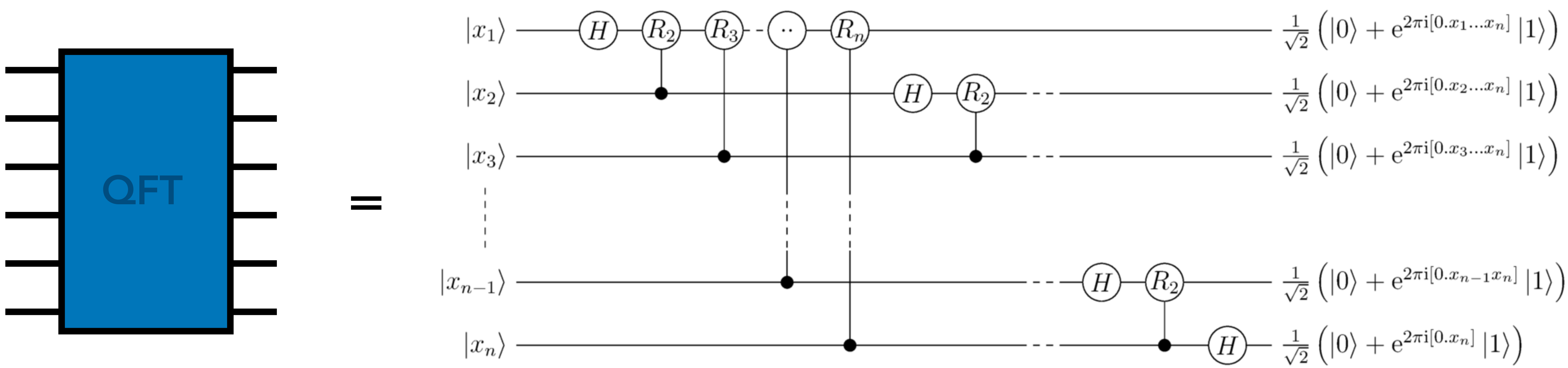
Encode as tensor network state of n qubits



"amplitude encoding"

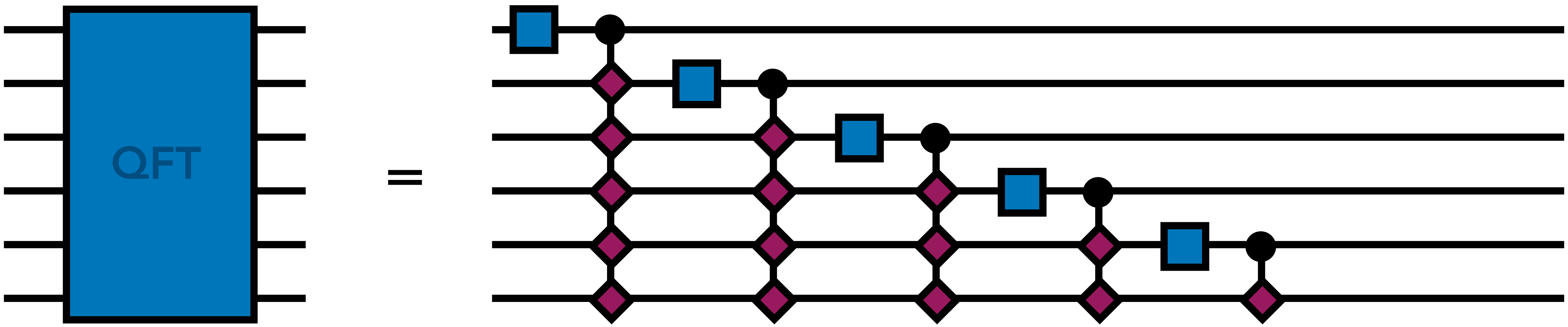
Quantum Fourier Transform

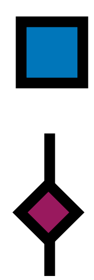
Performs a discrete Fourier transform on a quantum state (viewed as a large vector)



Quantum Fourier Transform

Circuit for QFT can be interpreted as a tensor network





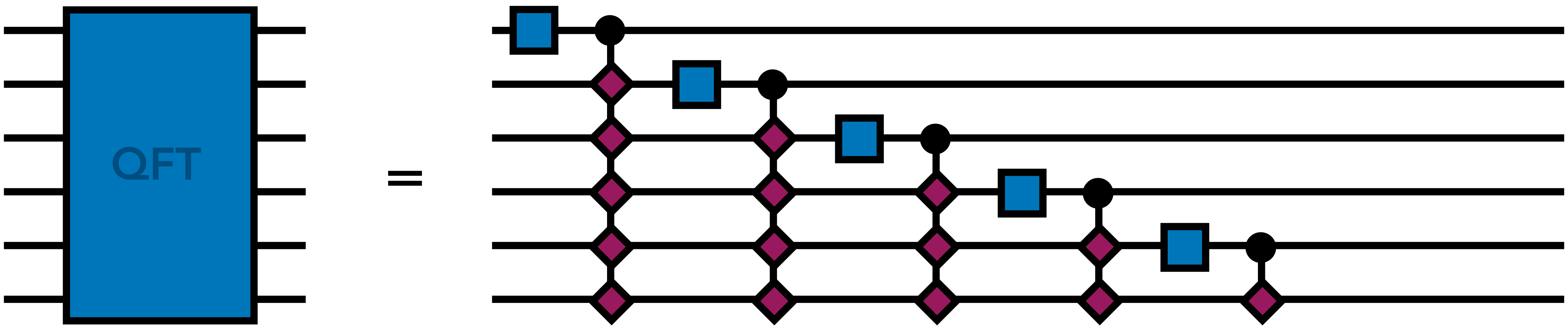
= Hadamard gates

= controlled phase gates

Treat each column as an MPO and multiply together

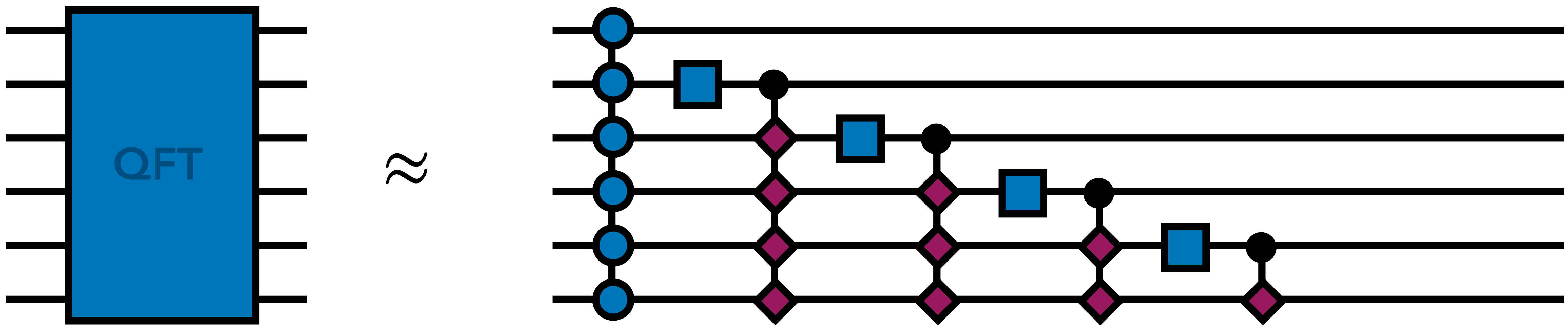
Quantum Fourier Transform

Treat each column as an MPO tensor network and multiply these together:



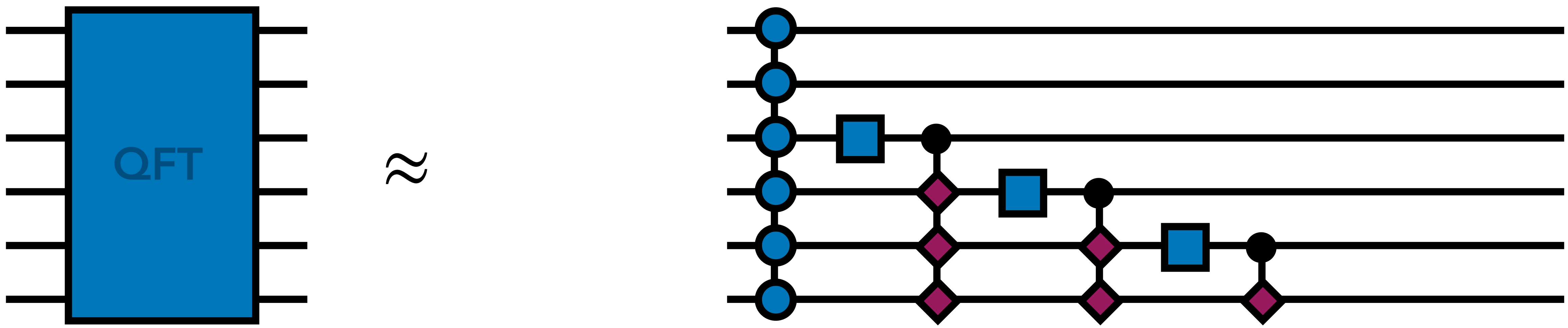
Quantum Fourier Transform

Treat each column as an MPO and multiply together



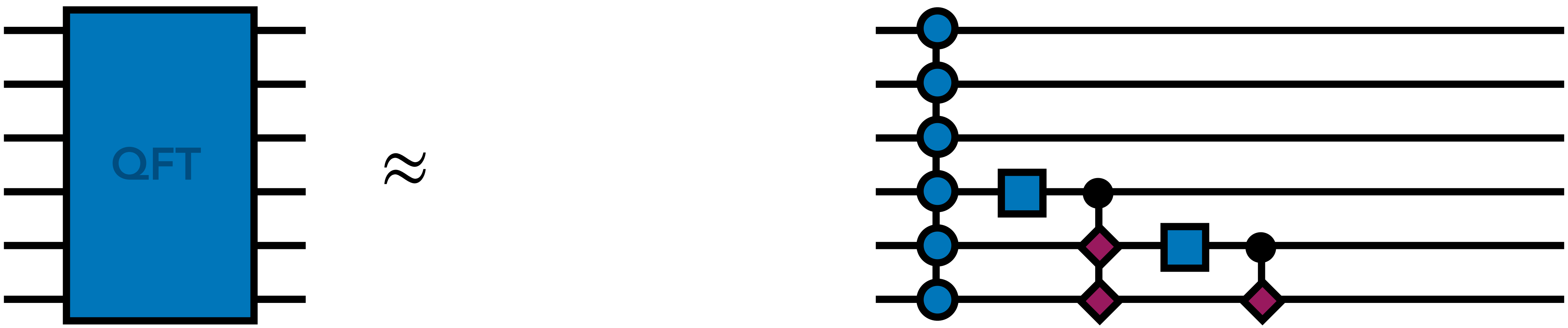
Quantum Fourier Transform

Treat each column as an MPO and multiply together



Quantum Fourier Transform

Treat each column as an MPO and multiply together



Quantum Fourier Transform

Treat each column as an MPO and multiply together

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Quantum Fourier Transform

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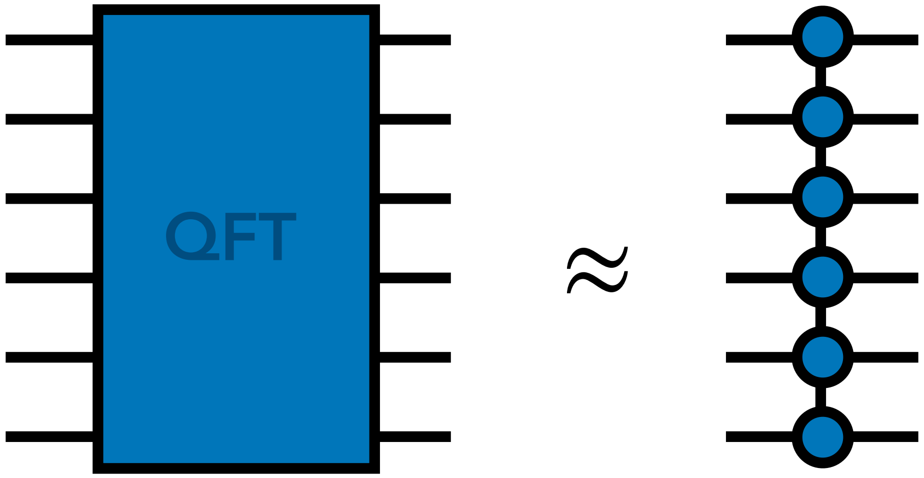
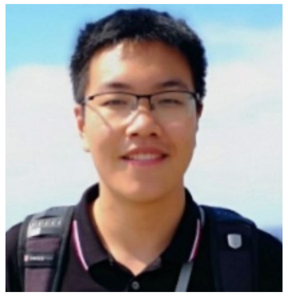


Result is MPO of internal dimension $\chi = 8$!
(When working to double precision)*

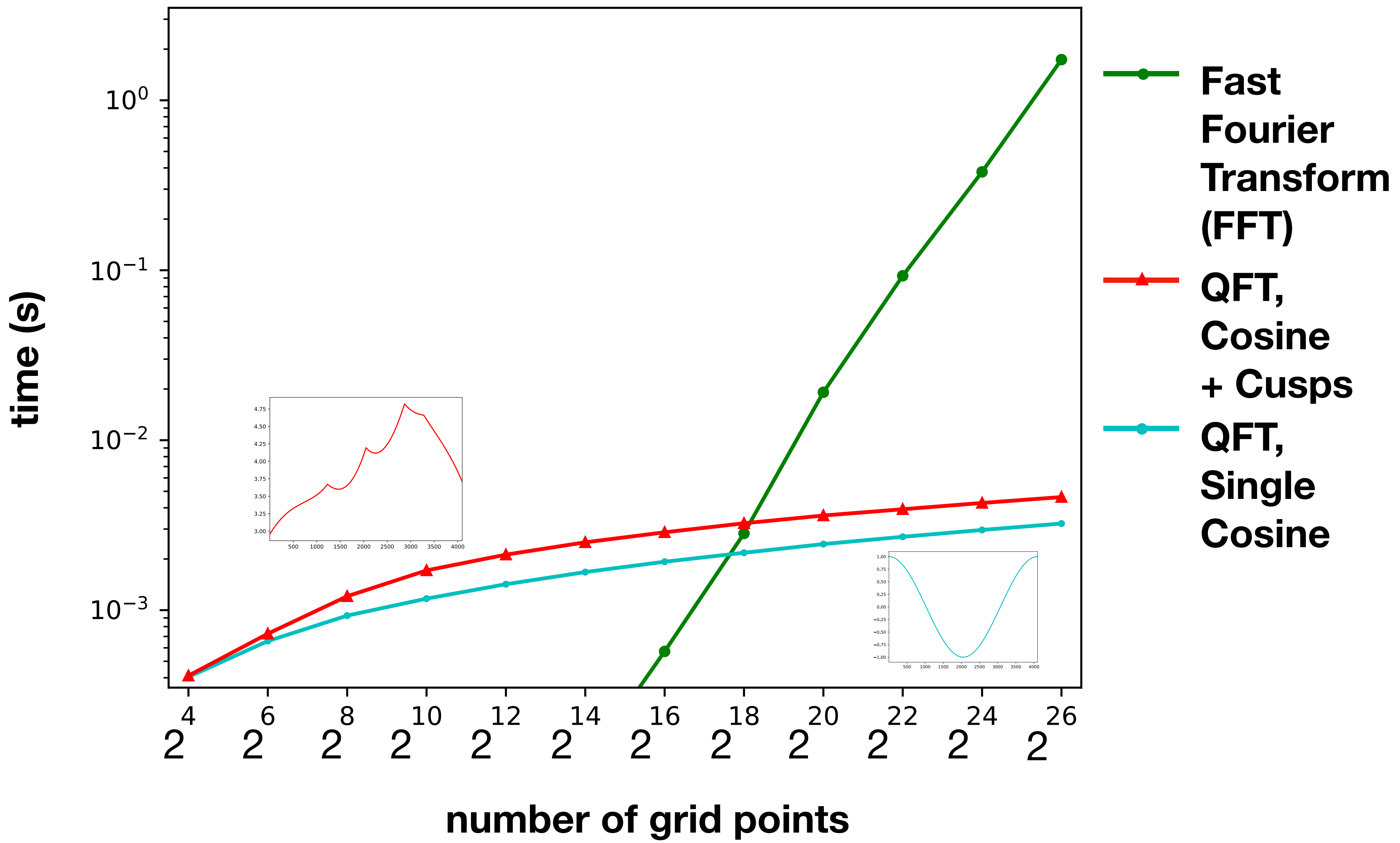


Jielun Chen

Chen, Stoudenmire, White, PRX Quantum, arxiv:2210.08468

Classical Methods for Quantum Systems

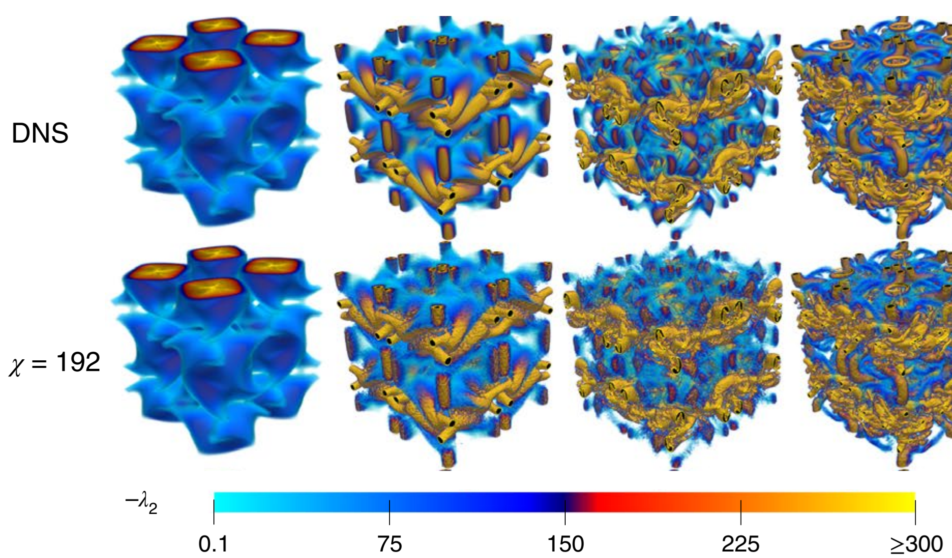
Compressed quantum Fourier transform beats "fast Fourier transform" (FFT)



Chen, Stoudenmire, White, PRX Quantum, arxiv:2210.08468

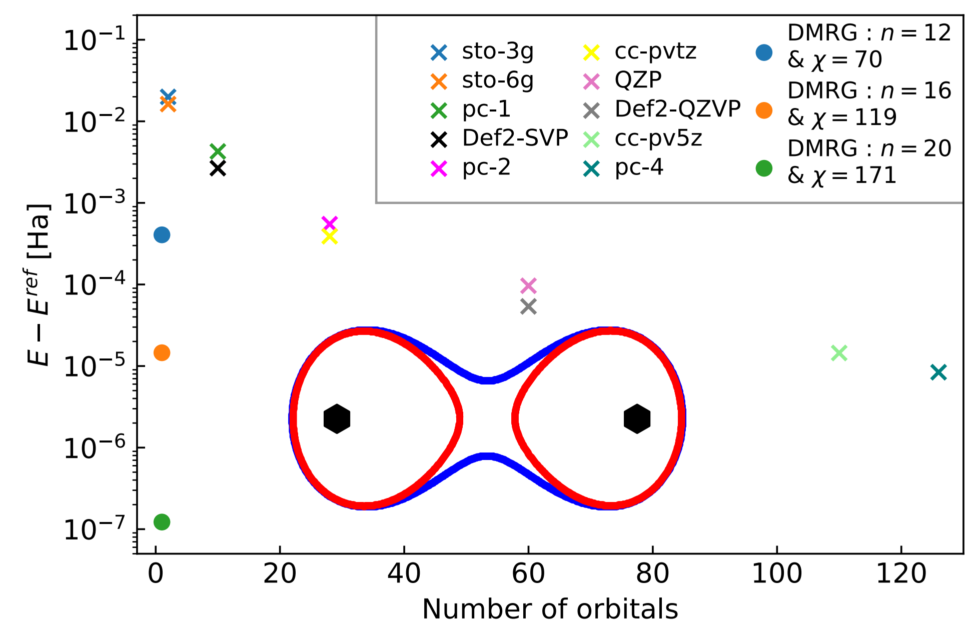
Classical Methods for Quantum Systems

Rapidly developing topic of
"quantum-inspired classical algorithms"



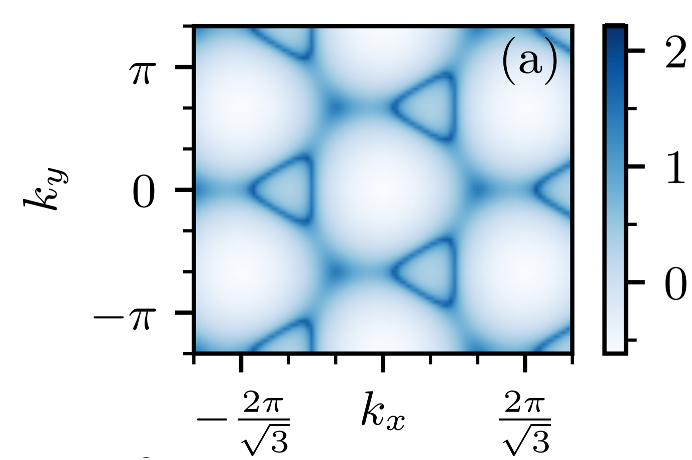
fluid simulations

Gourianov et al., Nature Comp. Sci., 2, 30-37 (2022)



quantum chemistry

Jolly, Núñez Fernández, Waintal, arxiv:2308.03508



function representations

*Shinaoka et al., Phys. Rev. X **13**, 021015 (2023)*

Application #2:
Physics Simulation
(Ising Dynamics on Heavy-Hex Lattice)

Have quantum computers demonstrated utility?

This work – collaboration with:

Joey Tindall

Flatiron CCQ

Matt Fishman

Flatiron CCQ

Dries Sels

Flatiron CCQ

New York University

J. Tindall, M. Fishman, EMS, D. Sels, PRX Quantum, arxiv:2306.14887

J. Tindall, M. Fishman, SciPost Phys. 15, 222 (2023)

Motivation

Last June, sudden coverage of a new quantum experiment:

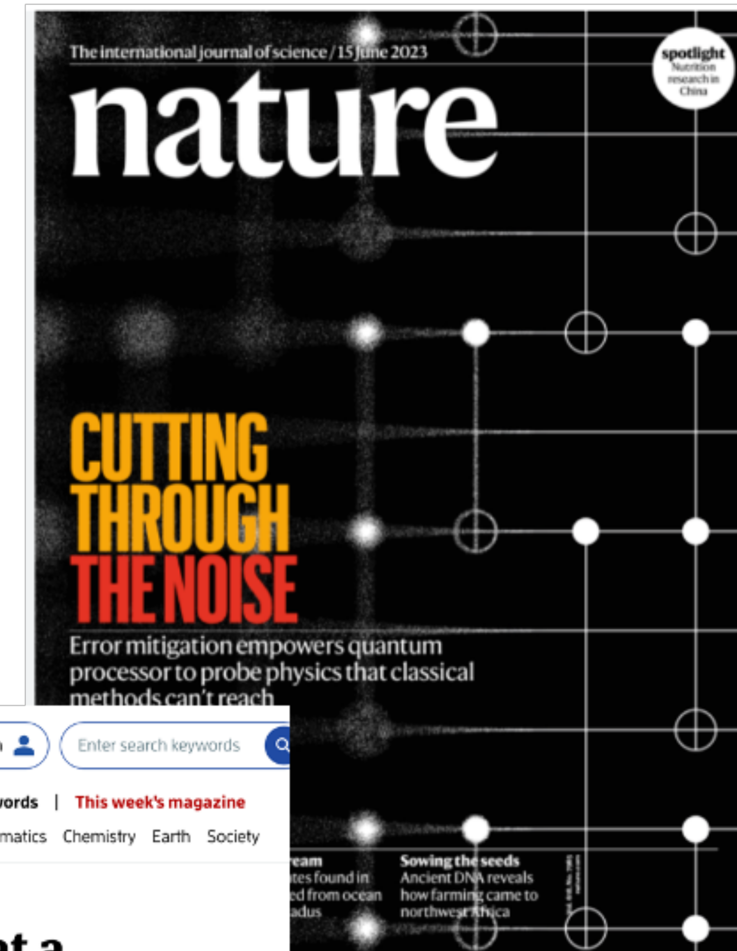

Article | Open Access | Published: 14 June 2023

Evidence for the utility of quantum computing before fault tolerance

Youngseok Kim, Andrew Eddins, Sajant Anand, Ken Xuan Wei, Ewout van den Berg, Sami Rosenblatt, Hasan Nayfeh, Yantao Wu, Michael Zaletel, Kristan Temme & Abhinav Kandala

Nature **618**, 500–505 (2023) | Cite this article

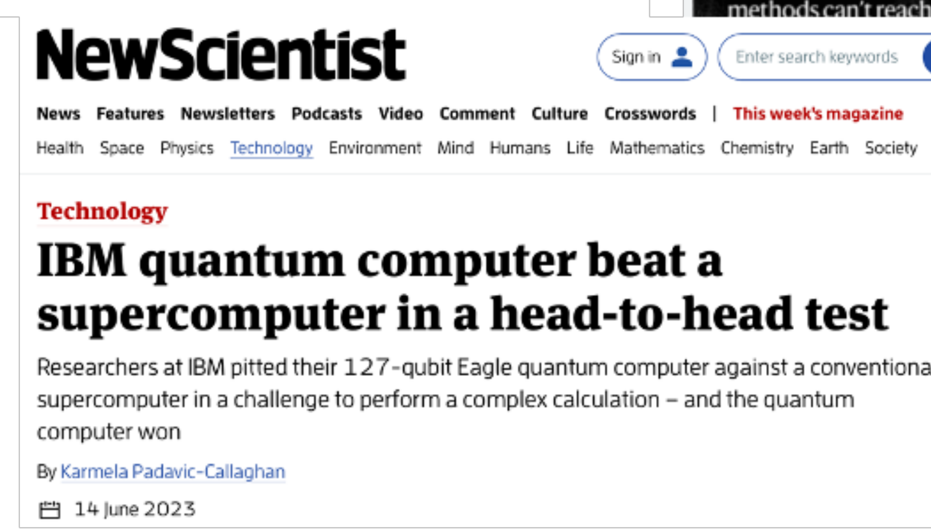
77k Accesses | **1** Citations | **609** Altmetric | Metrics




The New York Times

Quantum Computing Advance Begins New Era, IBM Says

A quantum computer came up with better answers to a physics problem than a conventional supercomputer.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Technology

IBM quantum computer beat a supercomputer in a head-to-head test

Researchers at IBM pitted their 127-qubit Eagle quantum computer against a conventional supercomputer in a challenge to perform a complex calculation – and the quantum computer won

By Karmela Padavic-Callaghan

14 June 2023

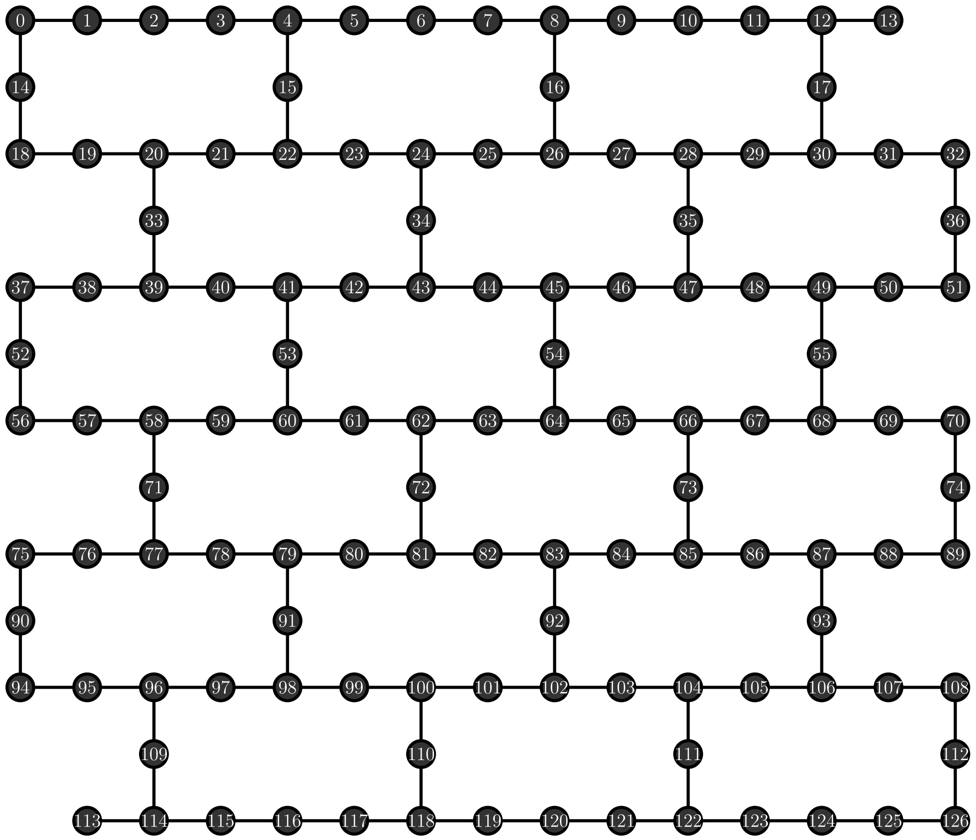
"beat a supercomputer"

"classical methods can't reach"

Experiment

What did the experiment compute?

Eagle Processor 6 × 3 Heavy − Hex Lattice



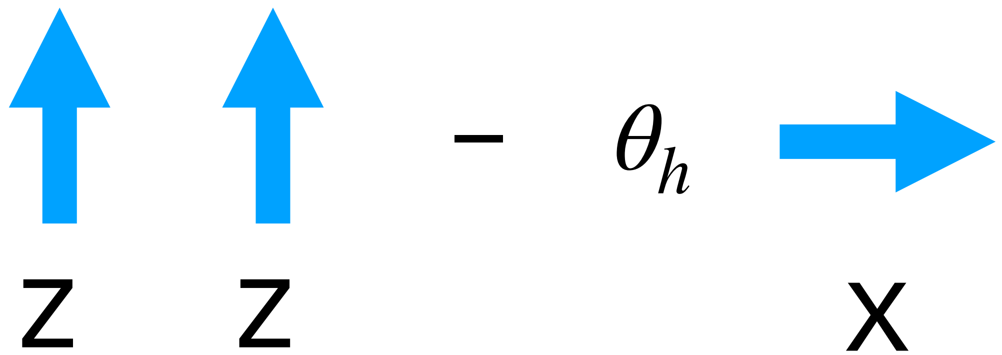
Heavy-hexagon lattice

"Kicked" quantum Ising Floquet dynamics

$$U(\theta_h) = \left(\prod_{\langle v,v' \rangle} \exp\left(\mathrm{i}\frac{\pi}{4} Z_v Z_{v'}\right)\right) \left(\prod_v \exp\left(-\mathrm{i}\frac{\theta_h}{2} X_v\right)\right)$$

Repeatedly apply $U(\theta_h)$

Qubits as quantum Ising "spins":



Kim, Youngseok, et al. "Evidence for the utility of quantum computing before fault tolerance." *Nature* 618.7965 (2023): 500-505

Experiment

Zero-noise extrapolation to mitigate hardware errors

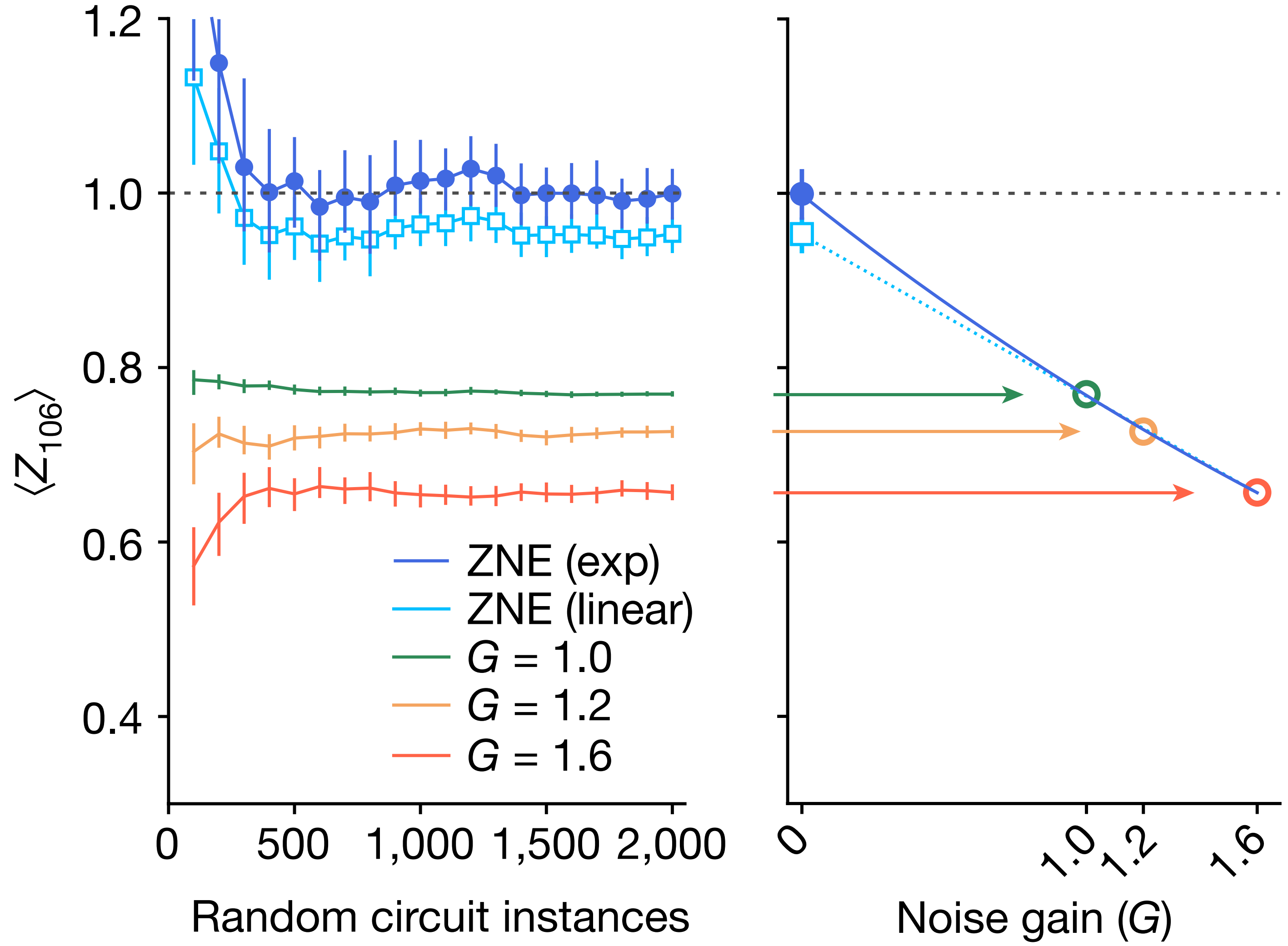
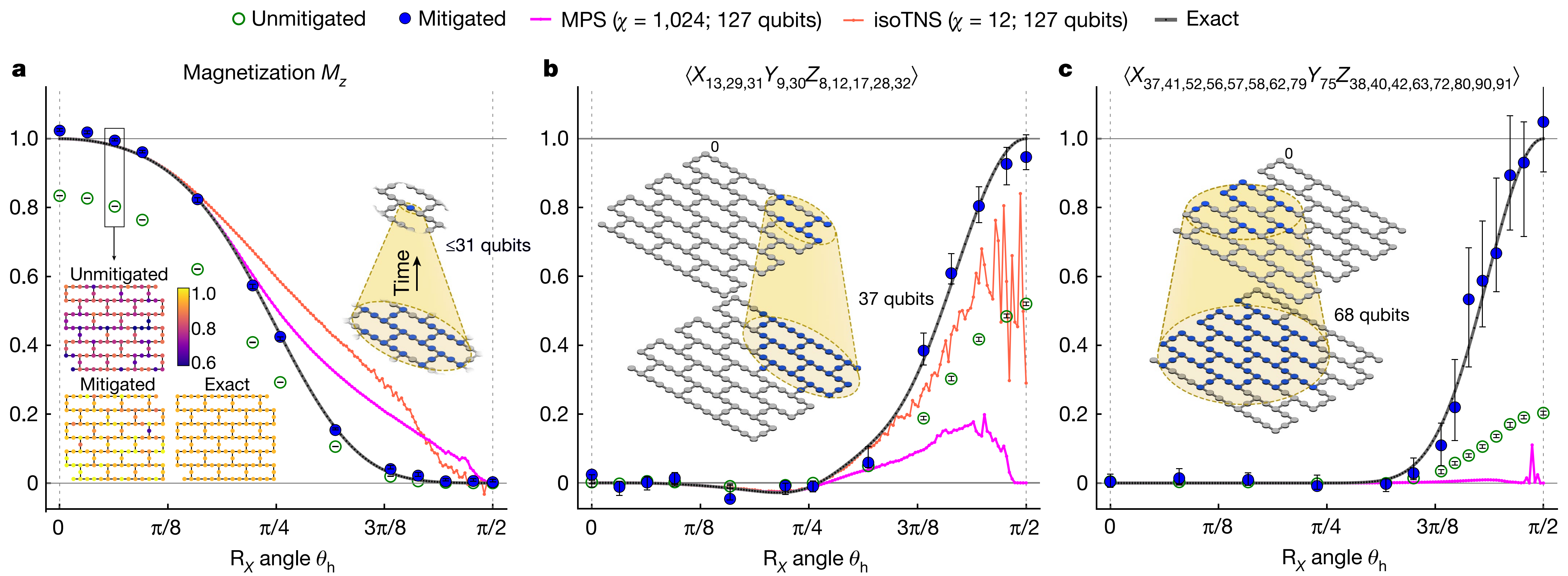


Figure from: Kim, Youngseok, et al. "Evidence for the utility of quantum computing before fault tolerance." *Nature* 618.7965 (2023): 500-505

Experiment

Measure expected values of Pauli operators



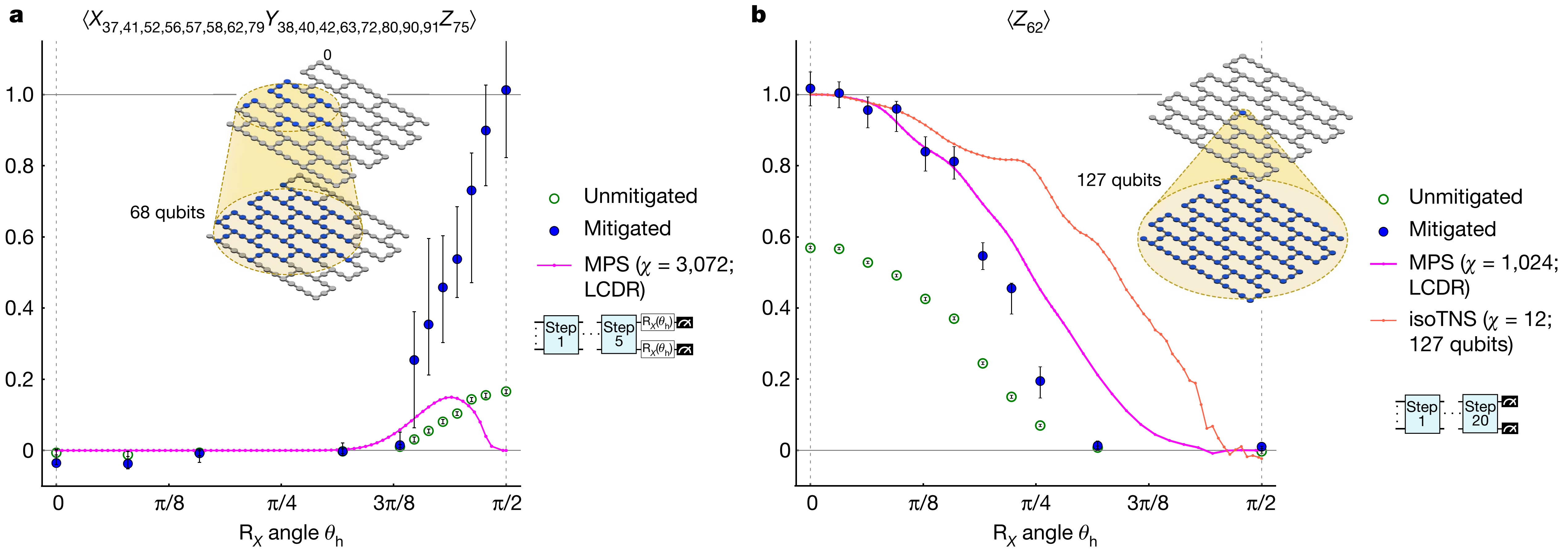
Short times: exact results available

Certain tensor network methods already struggling

Figure from: Kim, Youngseok, et al. "Evidence for the utility of quantum computing before fault tolerance." *Nature* 618.7965 (2023): 500-505

Experiment

Longer times (deeper circuits) with quantum processor



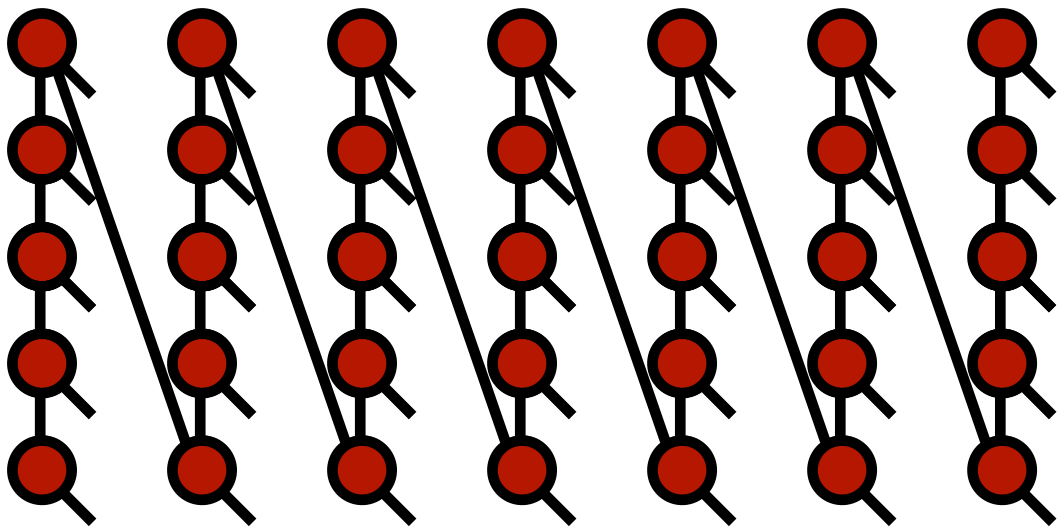
These tensor methods cannot keep up

Figure from: Kim, Youngseok, et al. "Evidence for the utility of quantum computing before fault tolerance." *Nature* 618.7965 (2023): 500-505

Tensor Networks for Two Dimensions

Challenges for 2D tensor networks

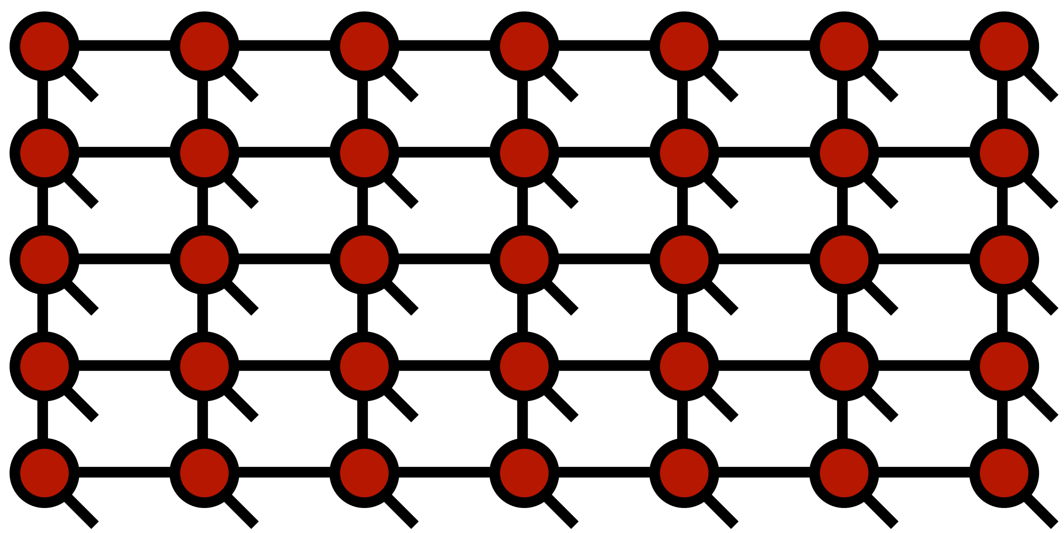
- Can use 1D tensor networks (MPS), however cost grows exponentially



Tensor Networks for Two Dimensions

Challenges for 2D tensor networks

- There are 2D tensor networks ("PEPS" or "TNS")

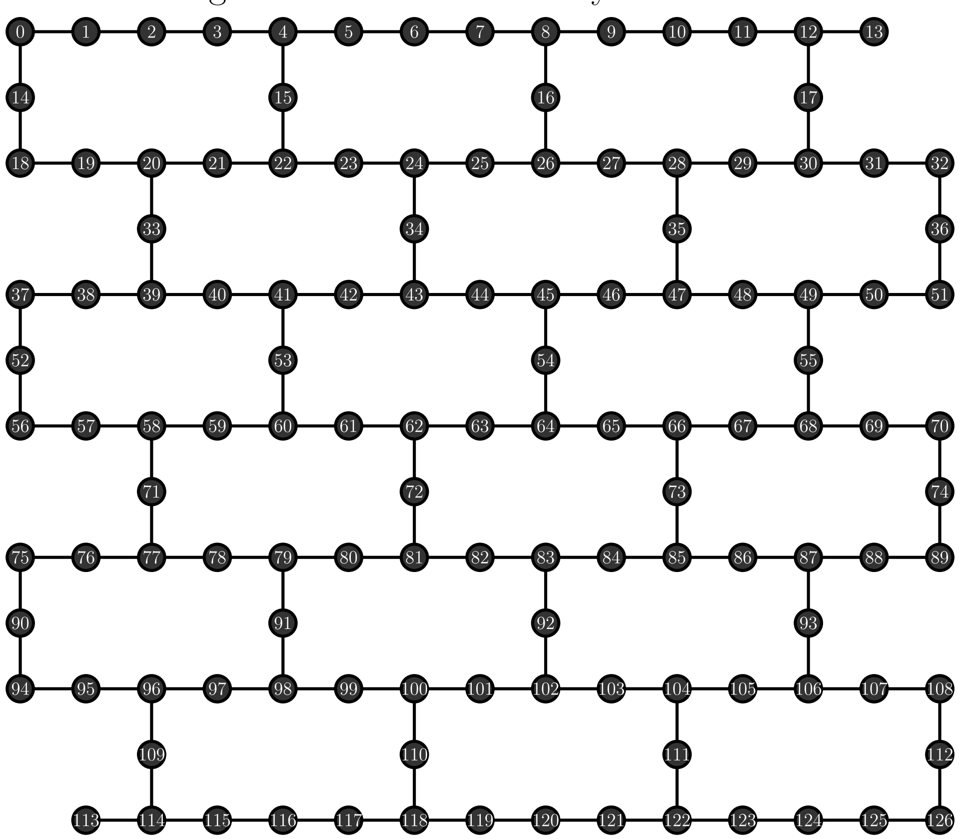


but most algorithms expensive to reach high accuracy

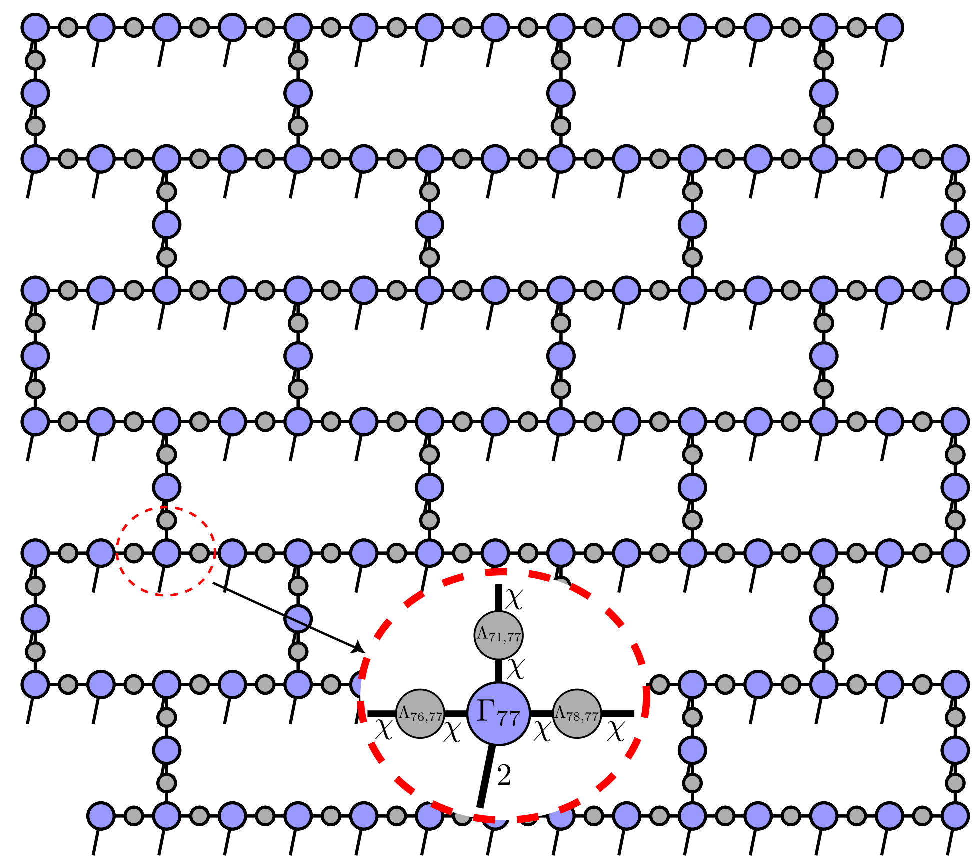
Tensor Networks for Two Dimensions

However, we were able to simulate the same 2D lattice to high accuracy – how?

Eagle Processor 6×3 Heavy $-$ Hex Lattice

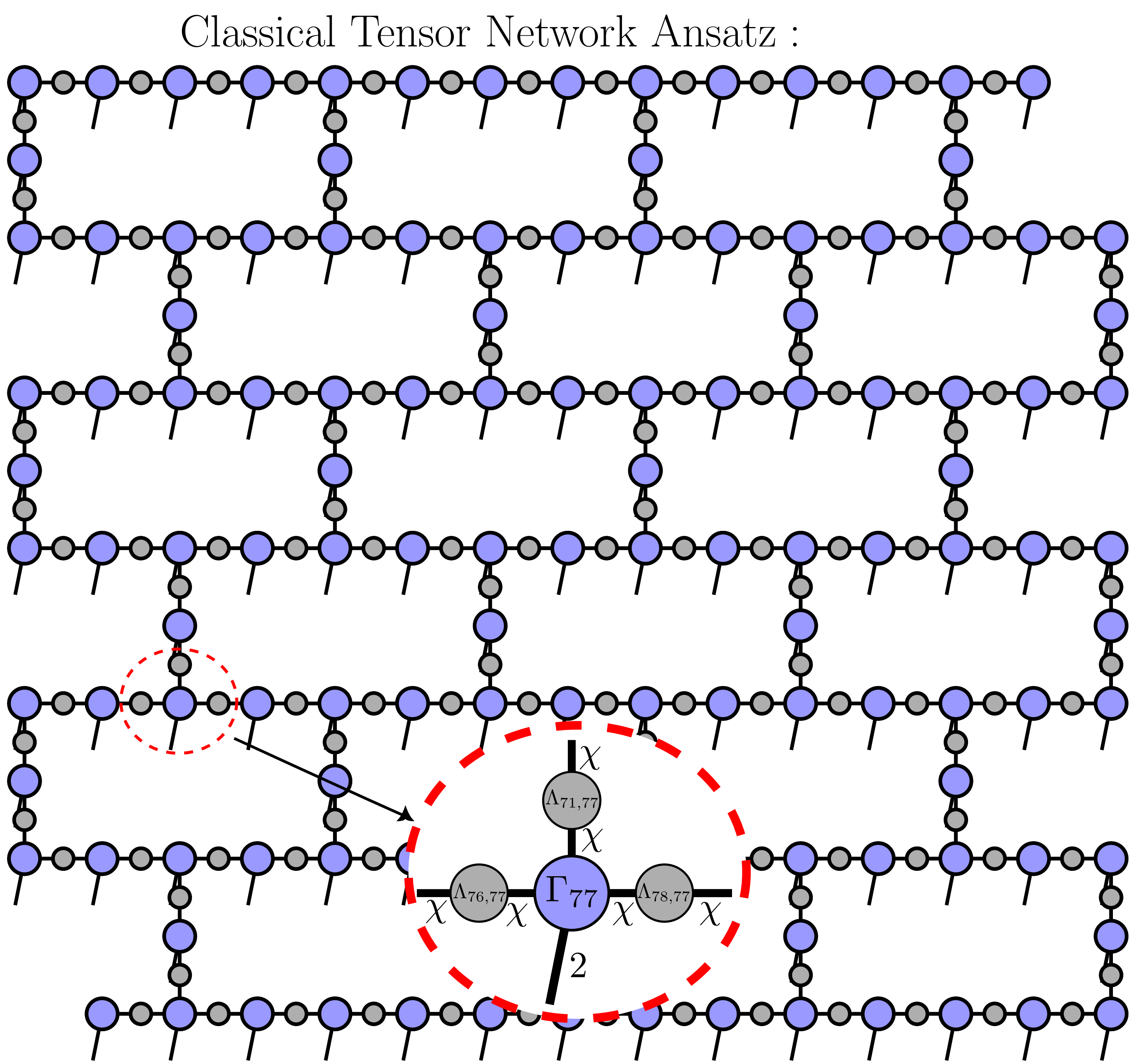


Classical Tensor Network Ansatz :



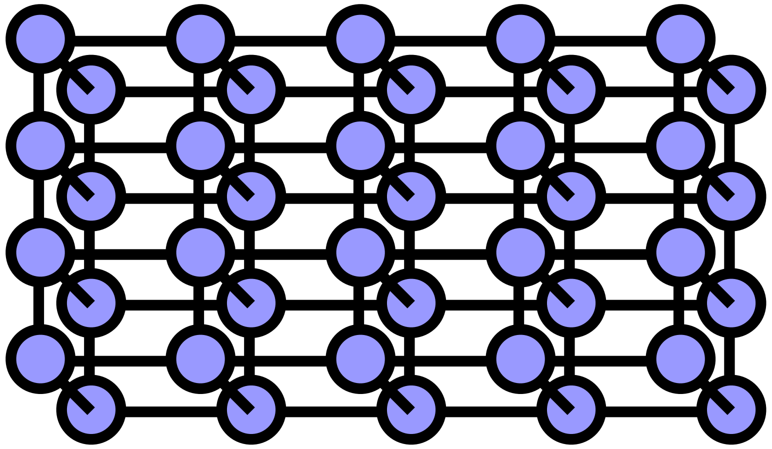
Tensor Networks for Two Dimensions

Start from tensor network state (TNS) with same topology as experiment

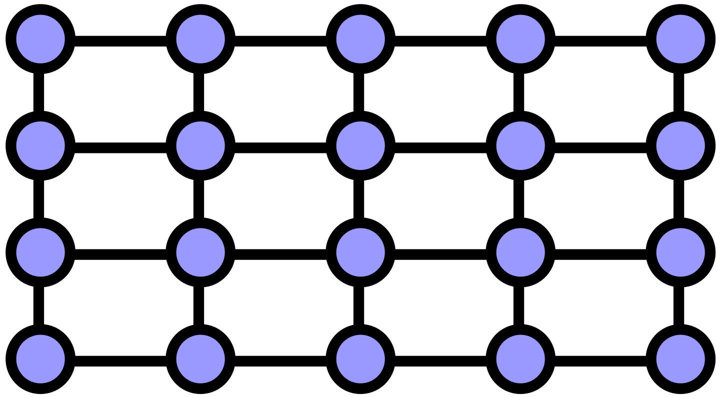


Tensor Networks for Two Dimensions

Ideally, for computing properties, want to fully contract "bra & ket" copies of network

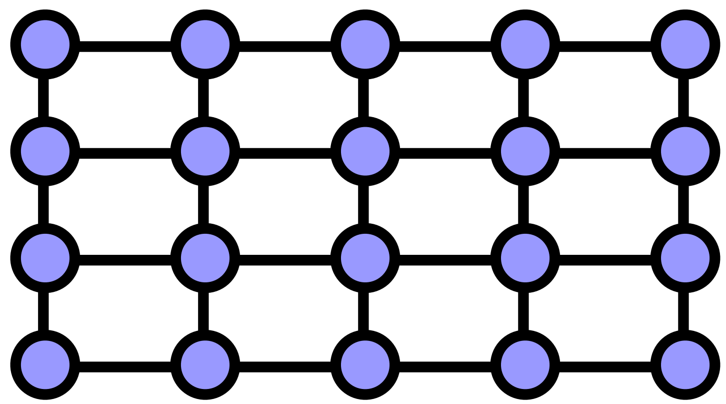


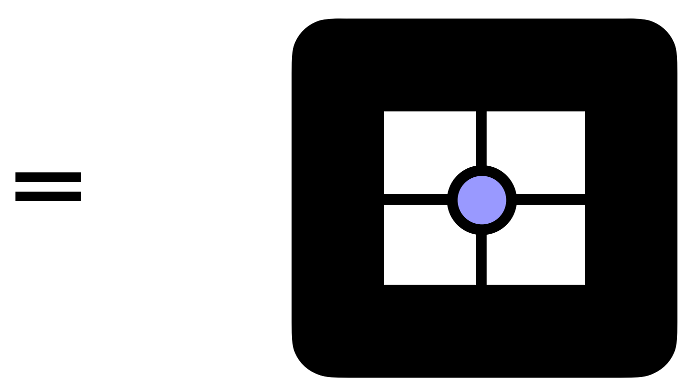
Top-down view



Tensor Networks for Two Dimensions

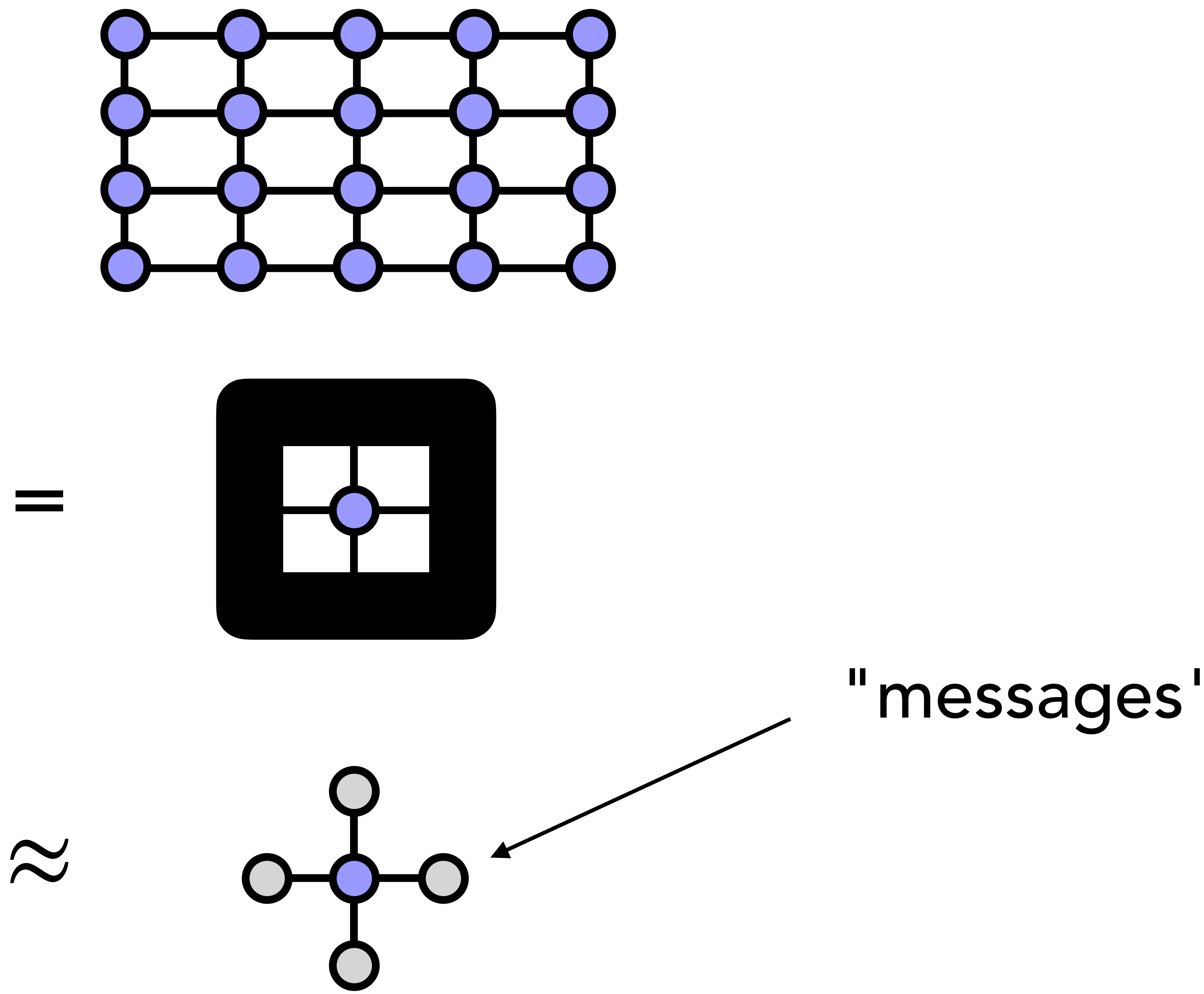
Ideally would get "full environment"
(contraction with tensor to optimize removed)





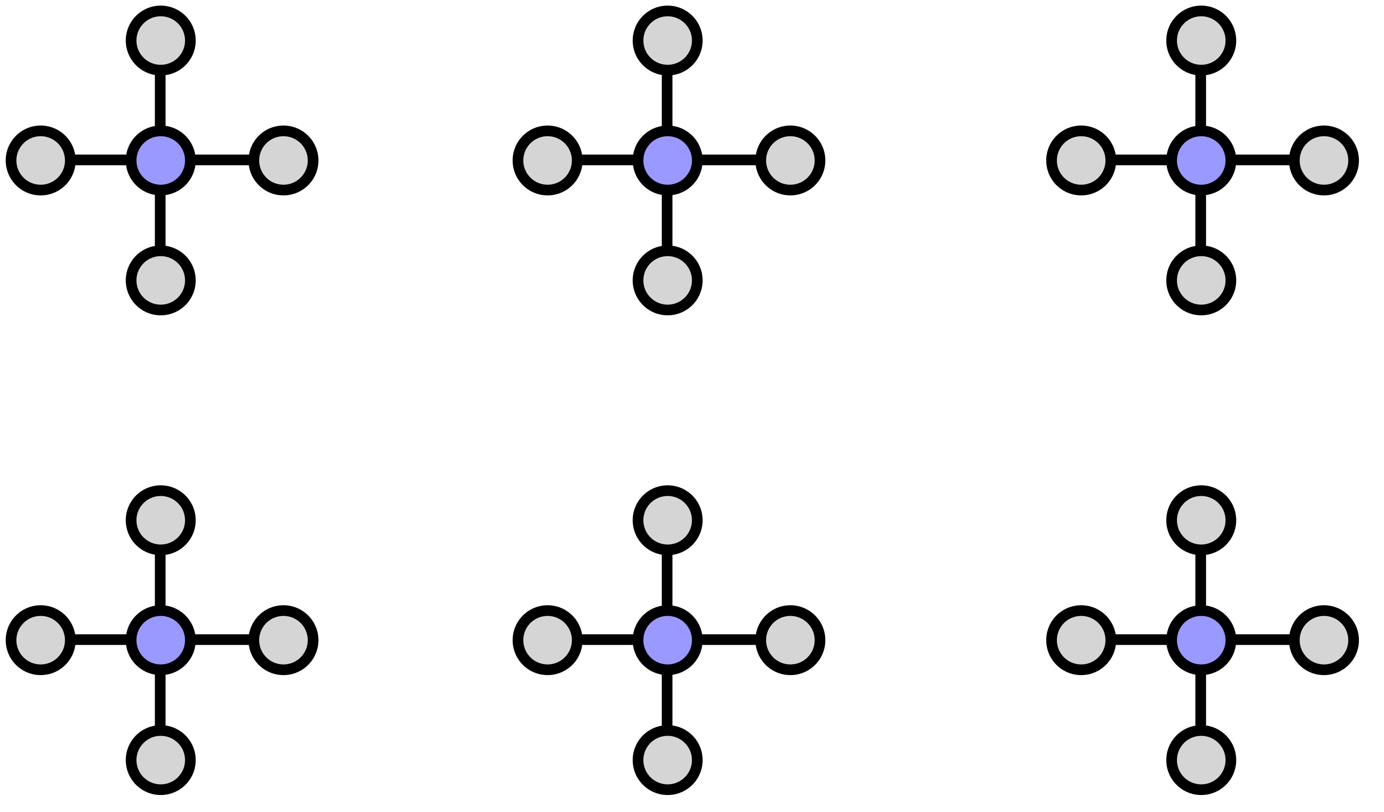
Tensor Networks for Two Dimensions

We will make a seemingly drastic approximation



Belief Propagation

Use "belief propagation" to converge the messages until self-consistency



Belief Propagation

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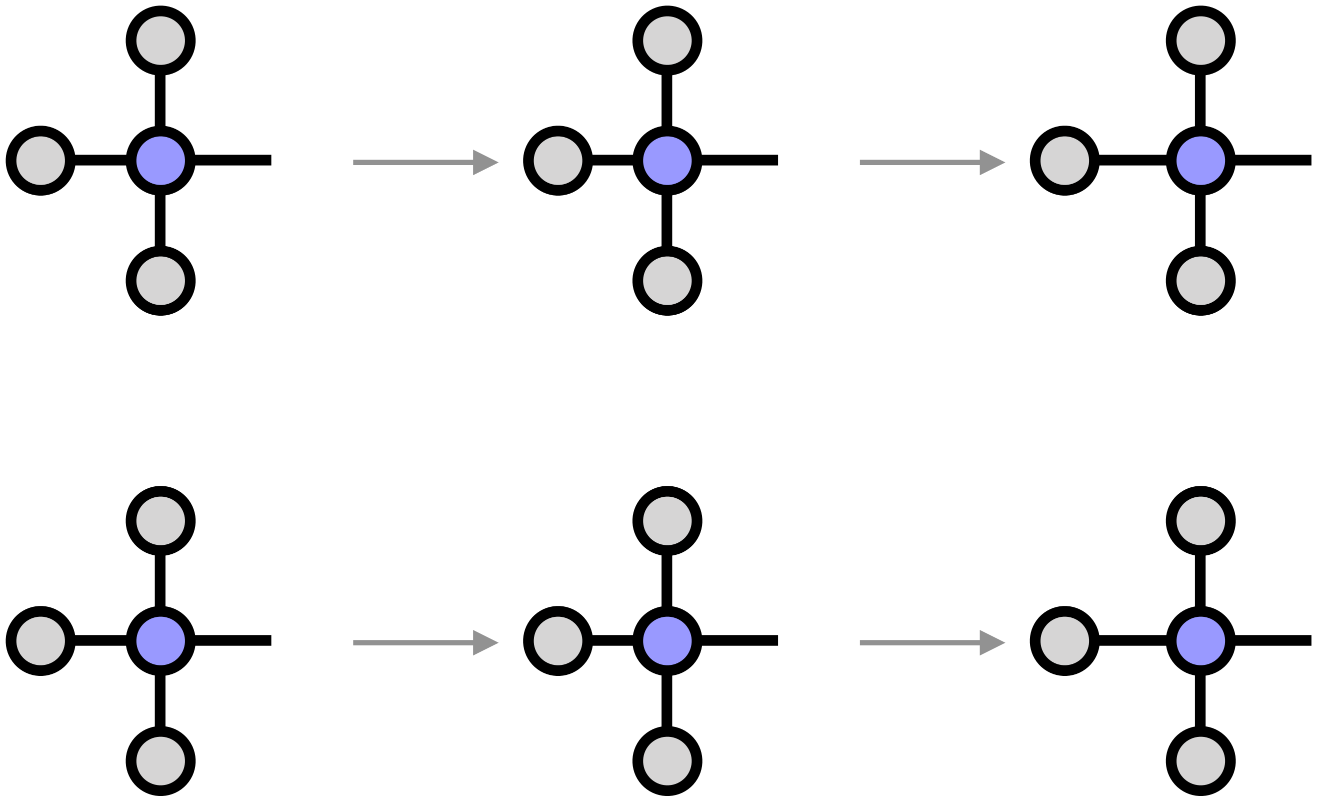

Belief Propagation

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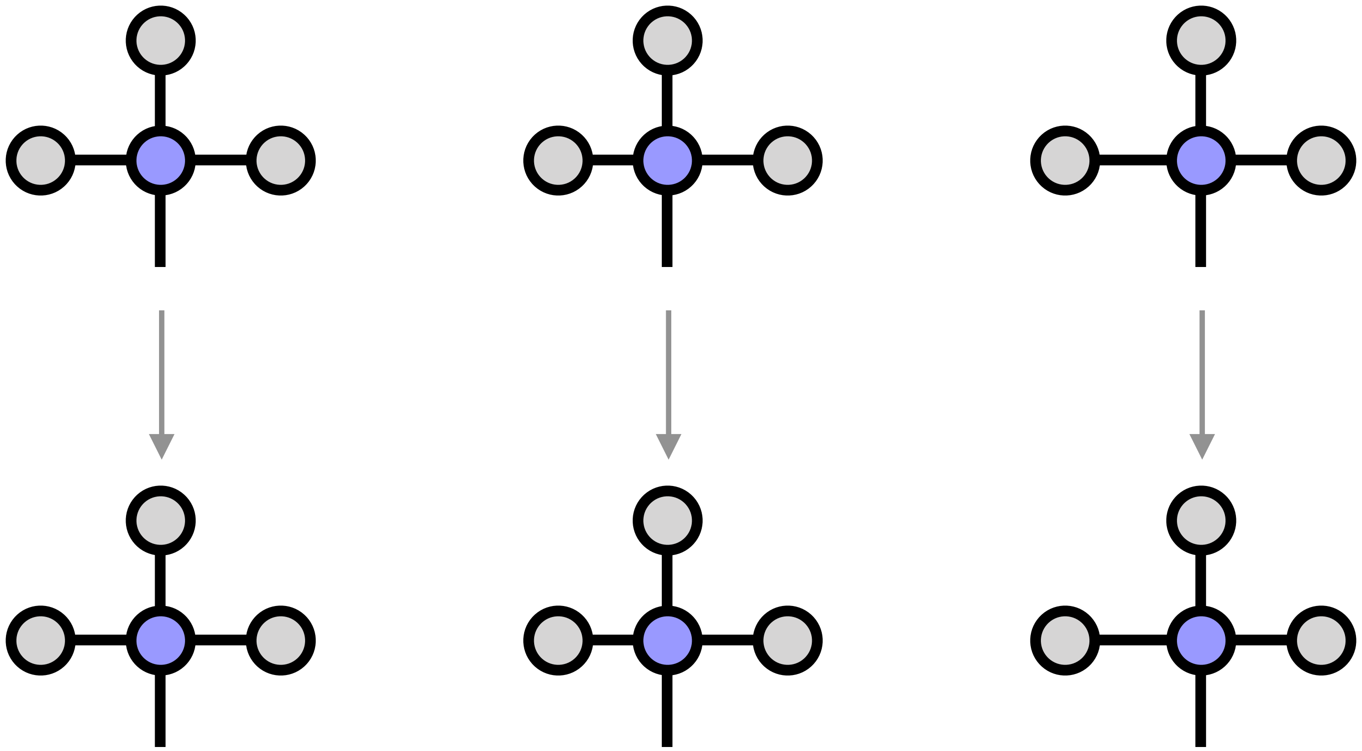

Belief Propagation

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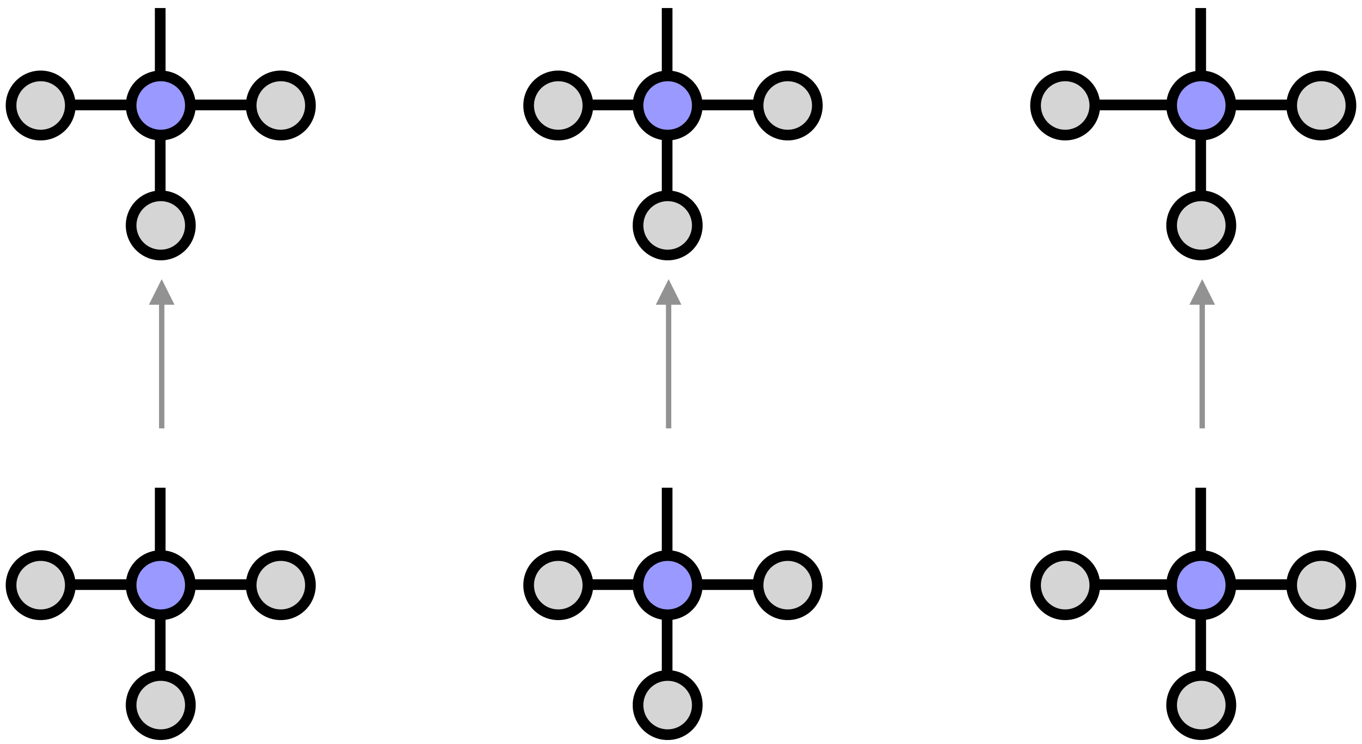
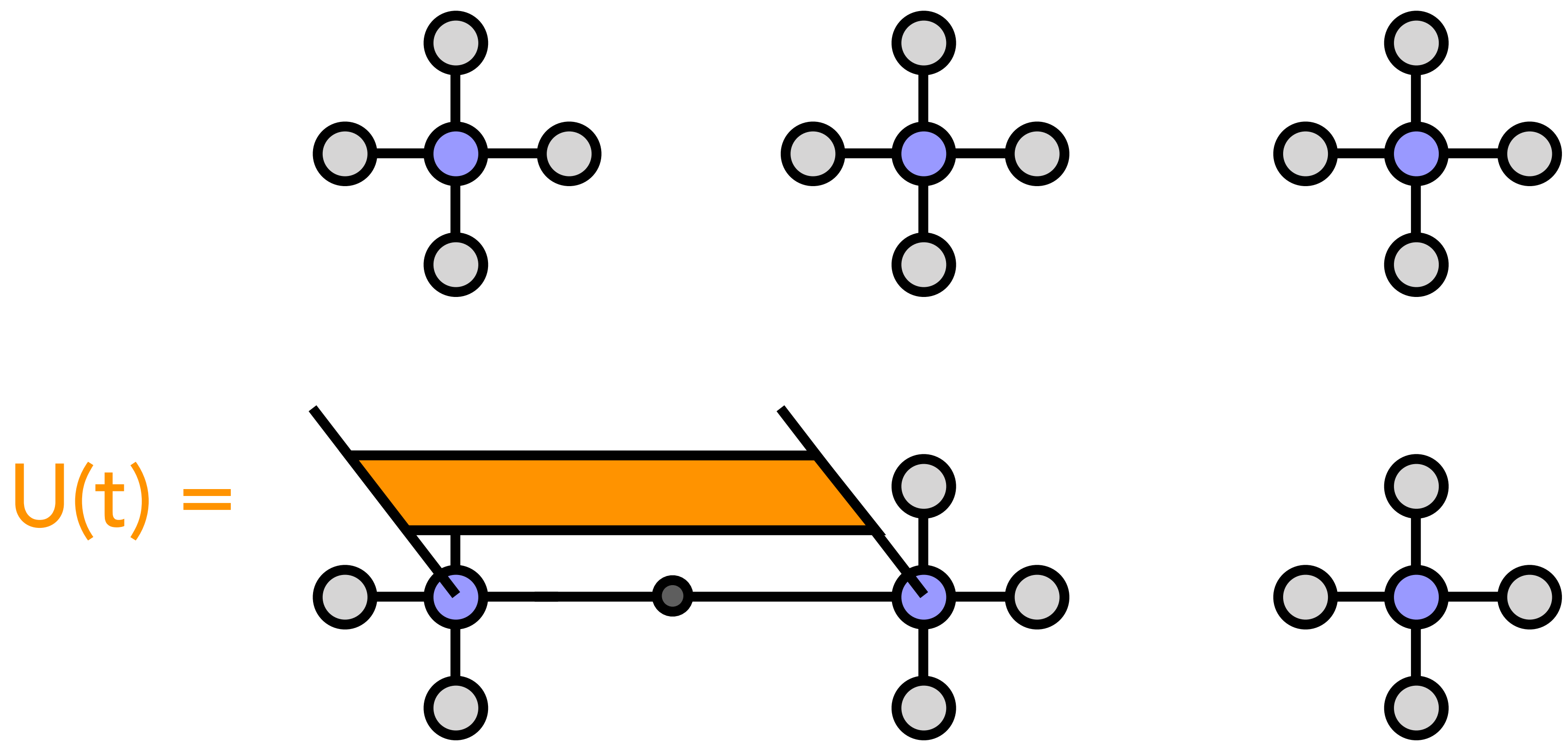
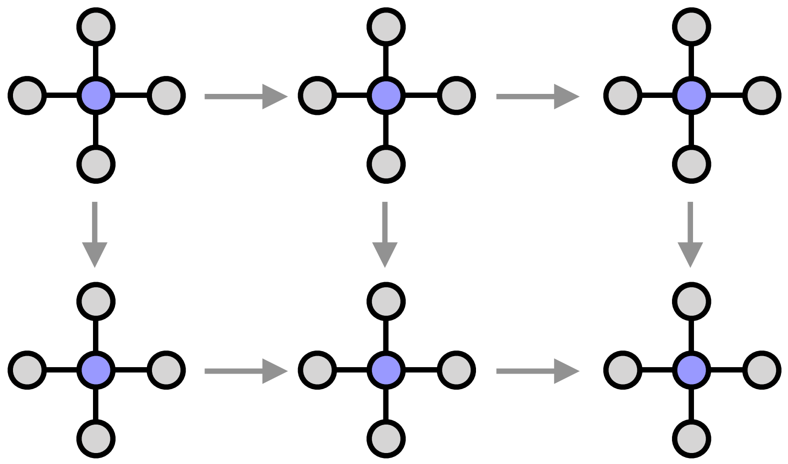


Belief Propagation

After messages converged, apply gates to evolve one step in time



Belief Propagation



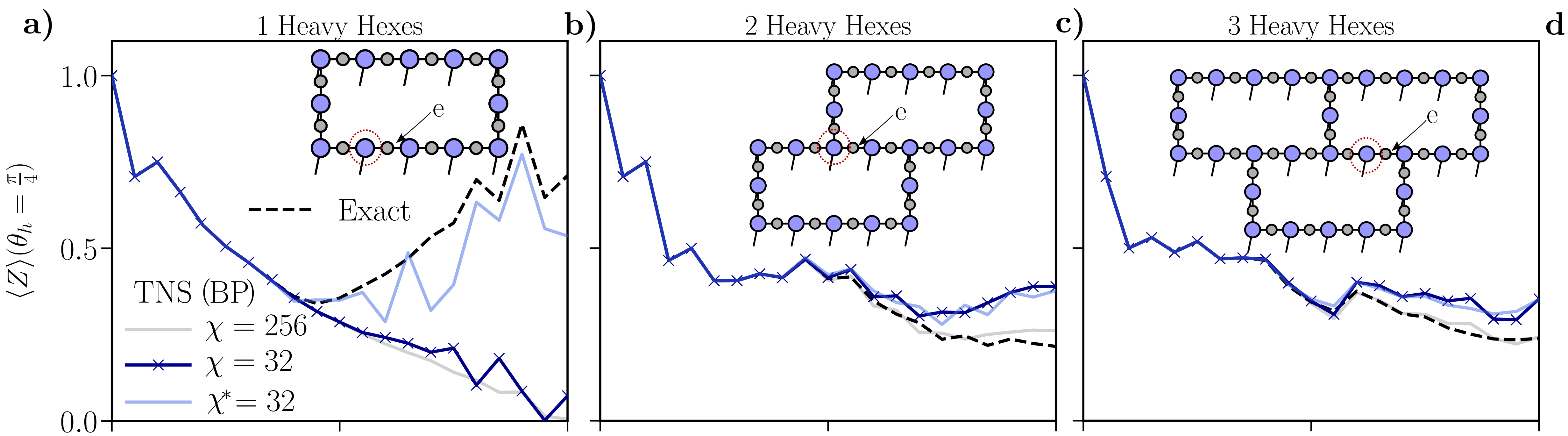
Belief propagation method aspects:

- if lattice has no loops, fully controlled
- can run on any lattice
- cheap: use *huge* internal bond dimensions χ
- similar to mean-field theory, but likely much more accurate
- can do dynamics on top

Sahu, Swingle, arxiv:2206.04701
Guo, Poletti, Arad, arxiv:2301.05844
Tindall, Fishman, arxiv:2306.17837

How well does it work?

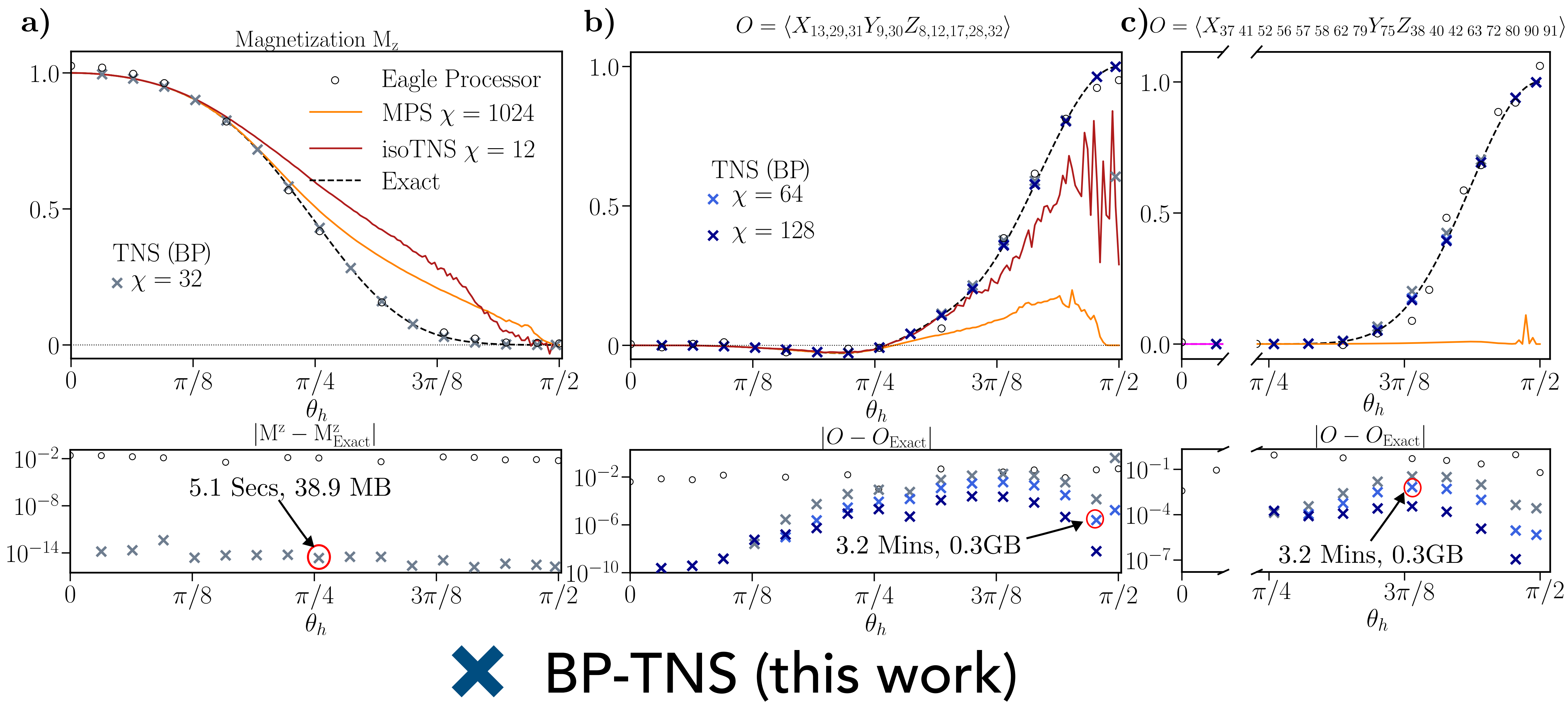
Test on verifiable, small systems



Larger lattices help!

How well does it work?

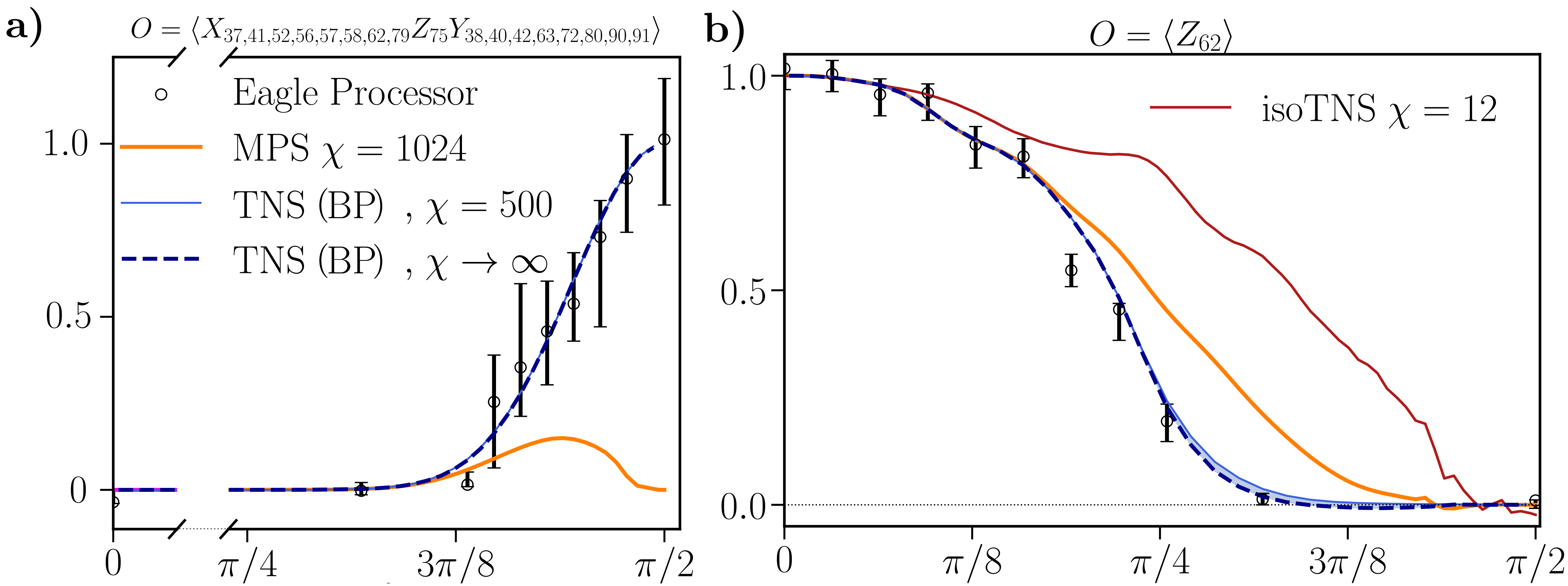
Nearly exact for verifiable regime (5 time steps)



Only minutes running on M1 Macbook Pro

How well does it work?

Remains highly accurate for larger depths



Larger χ requires ~day on cluster node

Use trick involving extra evolution to get 3-Pauli operators

How well does it work?

Many other simulations have come out!

- Kechedzhi et al., arxiv:2306.15970 — finite-size & lightcone extrapolations
- Begušić, Chan, arxiv:2306.16372 — Clifford perturbation theory
- Anand et al. arxiv:2306.17839 — tensor networks
- Begušić, Gray, Chan, arxiv:2308.05077 — tensor networks
- Liao et al., arxiv:2308.03082 — tensor networks

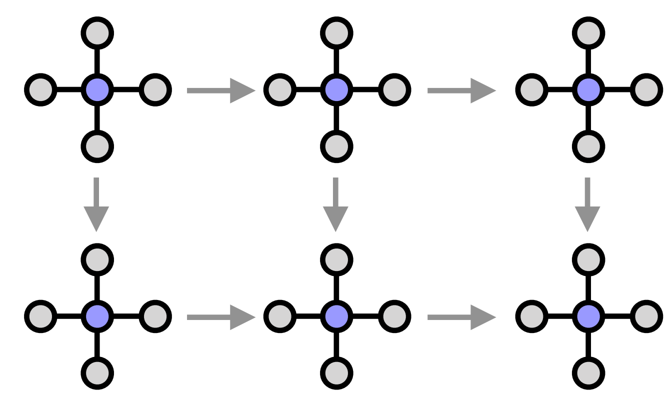
All agree with our results, some very closely

Based on more detailed per-time-step analysis & MPS comparison, we believe ours are highly accurate

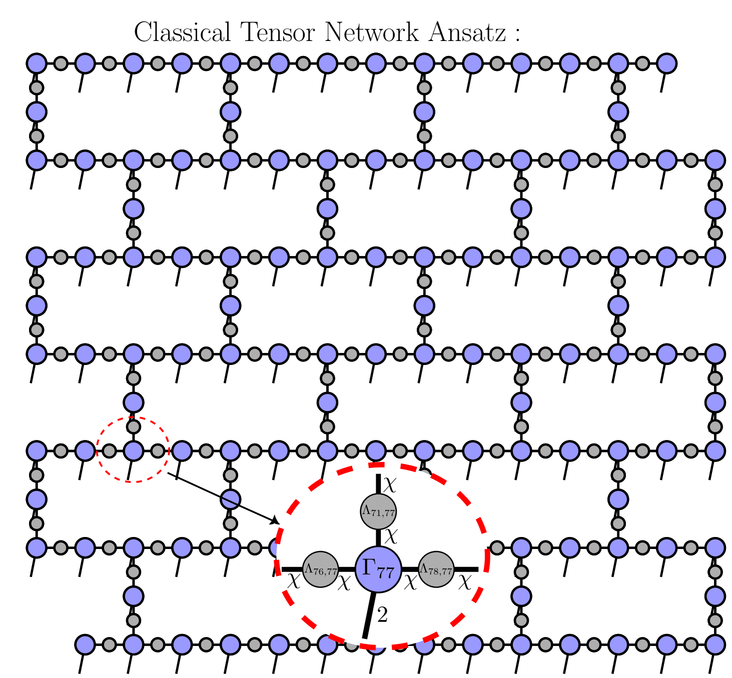
Summary: Ising on Heavy-Hex

Apparently Ising on 2D heavy-hex lattice has "tree-like" correlations (as if loops played no role)

Belief propagation tensor network method very effective for dynamics in this case



Can study large 2D quantum systems evolving in time



Thoughts & Future Directions

Tensor networks defining boundary between hard vs. easy quantum problems

Helping to quantum computing to focus on problems with greatest opportunity

On classical side, how many quantum algorithms can be brought into classical world, becoming "quantum-inspired classical"

Can get benefits of certain quantum algorithms today, on existing computers