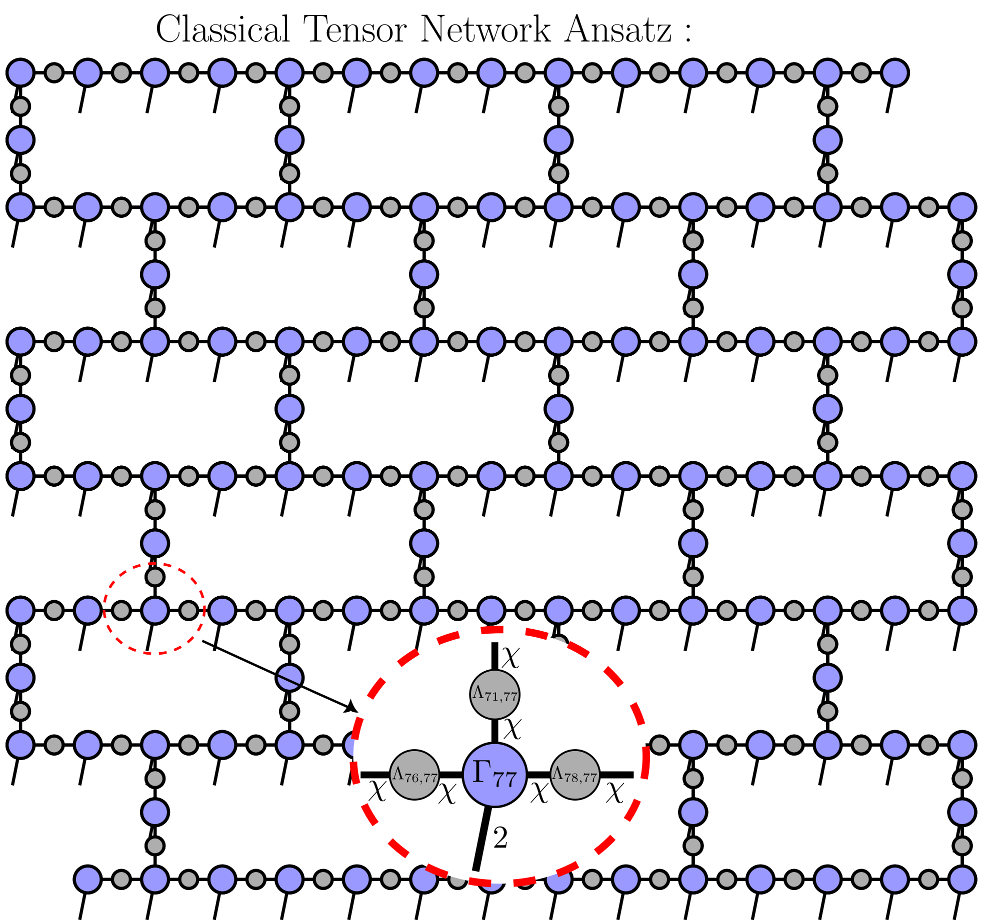
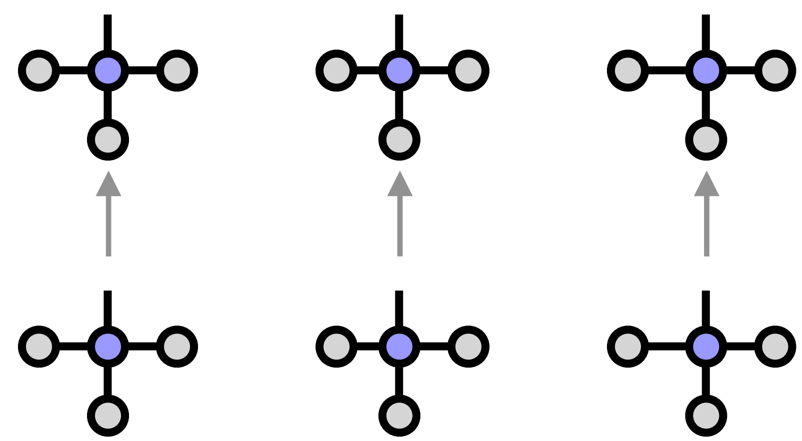
Dynamics of 2D and 3D Quantum Systems with Belief Propagation





E.M. Stoudenmire

May 2026 - Kyoto ExU Colloquium

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The mission of the Flatiron Institute is to advance scientific research through computational methods, including data analysis, modeling and simulation.

CCA: Center for Computational Astrophysics

CCB: Center for Computational Biology

CCQ: Center for Computational Quantum Physics

CCM: Center for Computational Mathematics

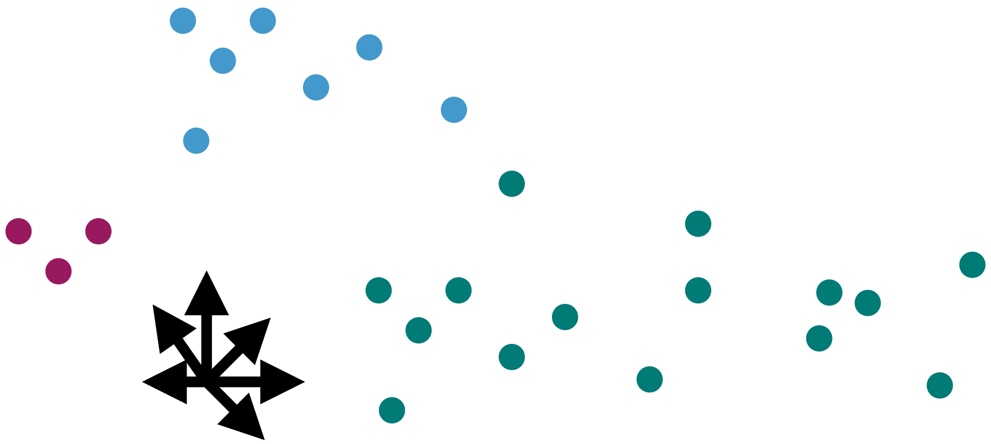
CCN: Center for Computational Neuroscience

ICC: Initiative for Computational Catalysis

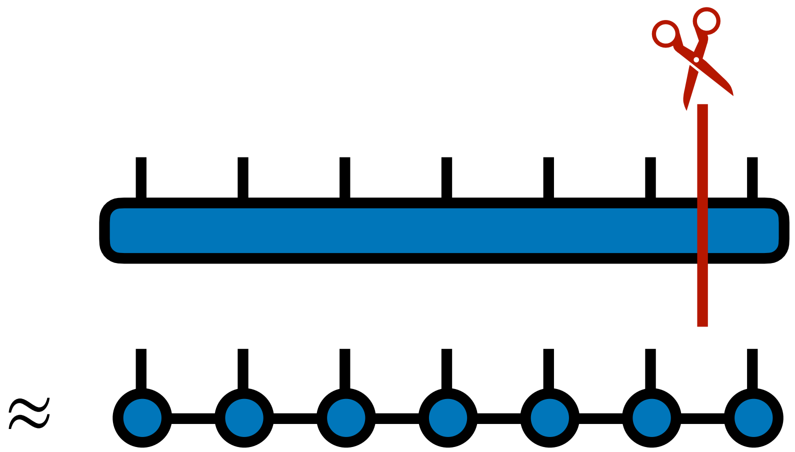
Motivation

Today's talk

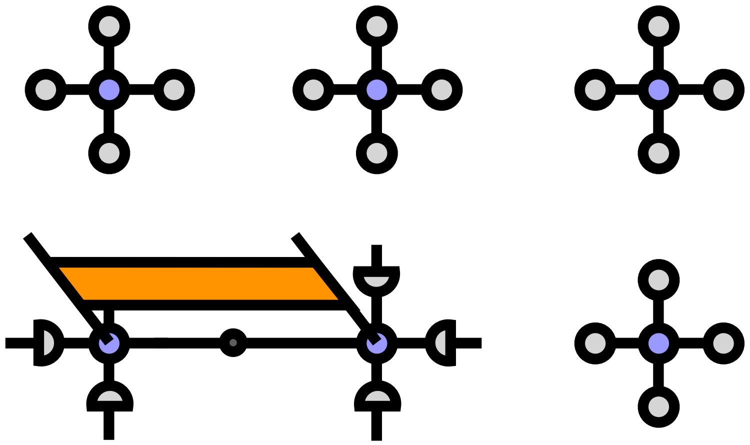
High-Dimensional Problems
as Tensors



Breaking the Curse of
Dimensionality

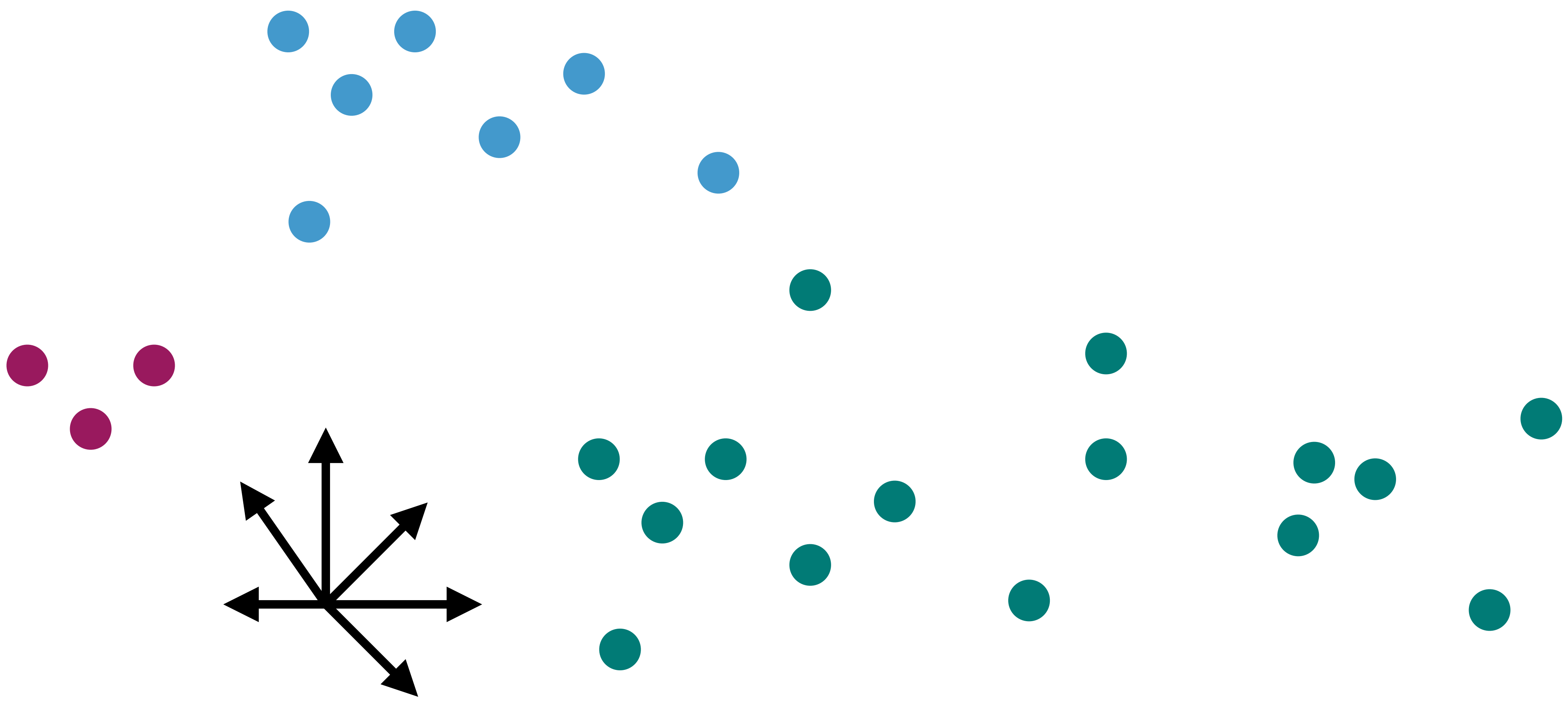


The Problem of Loops
& Belief Propagation



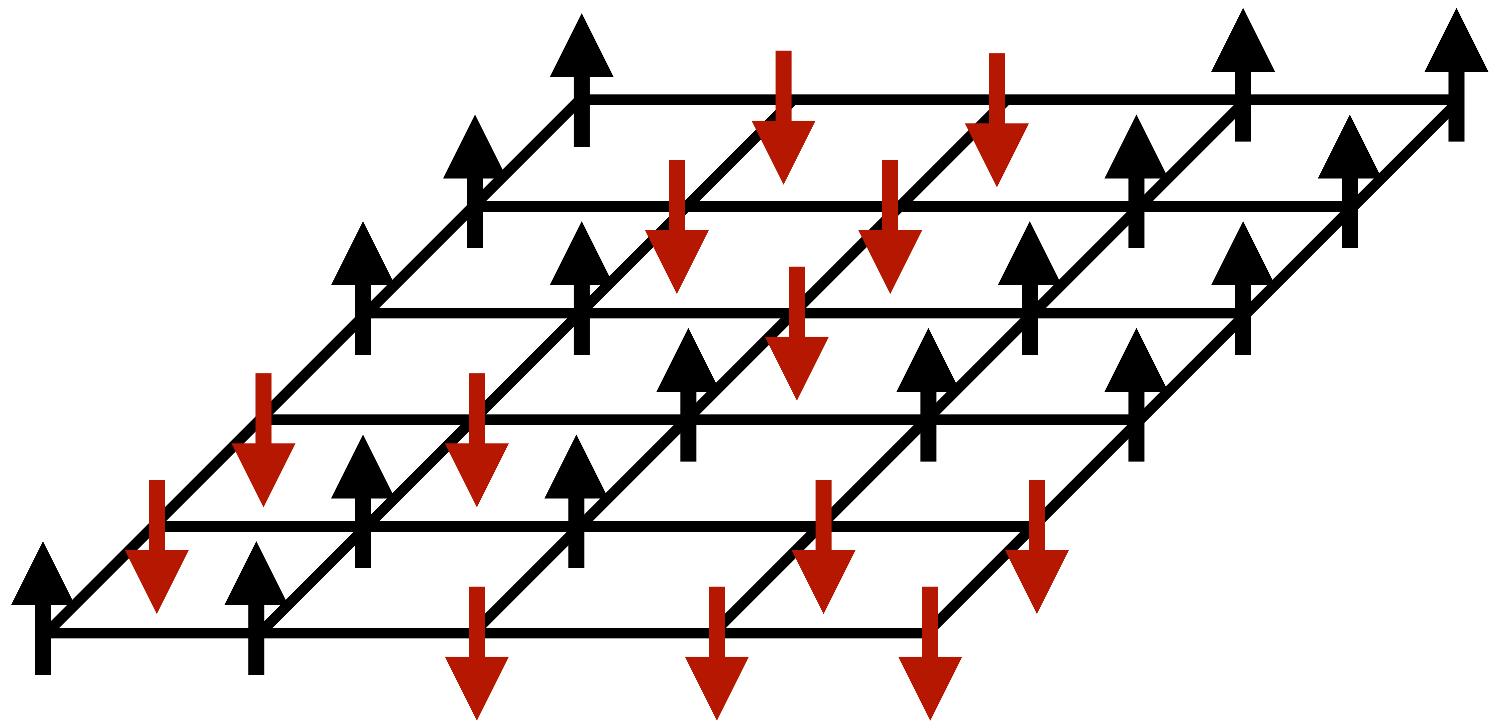
Motivation

High-dimensional problems are everywhere ...
from science to industry

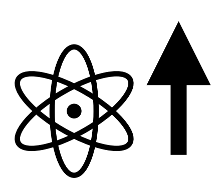


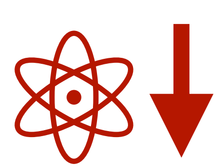
Motivation

Example: a **ferromagnet** ("fridge magnet")



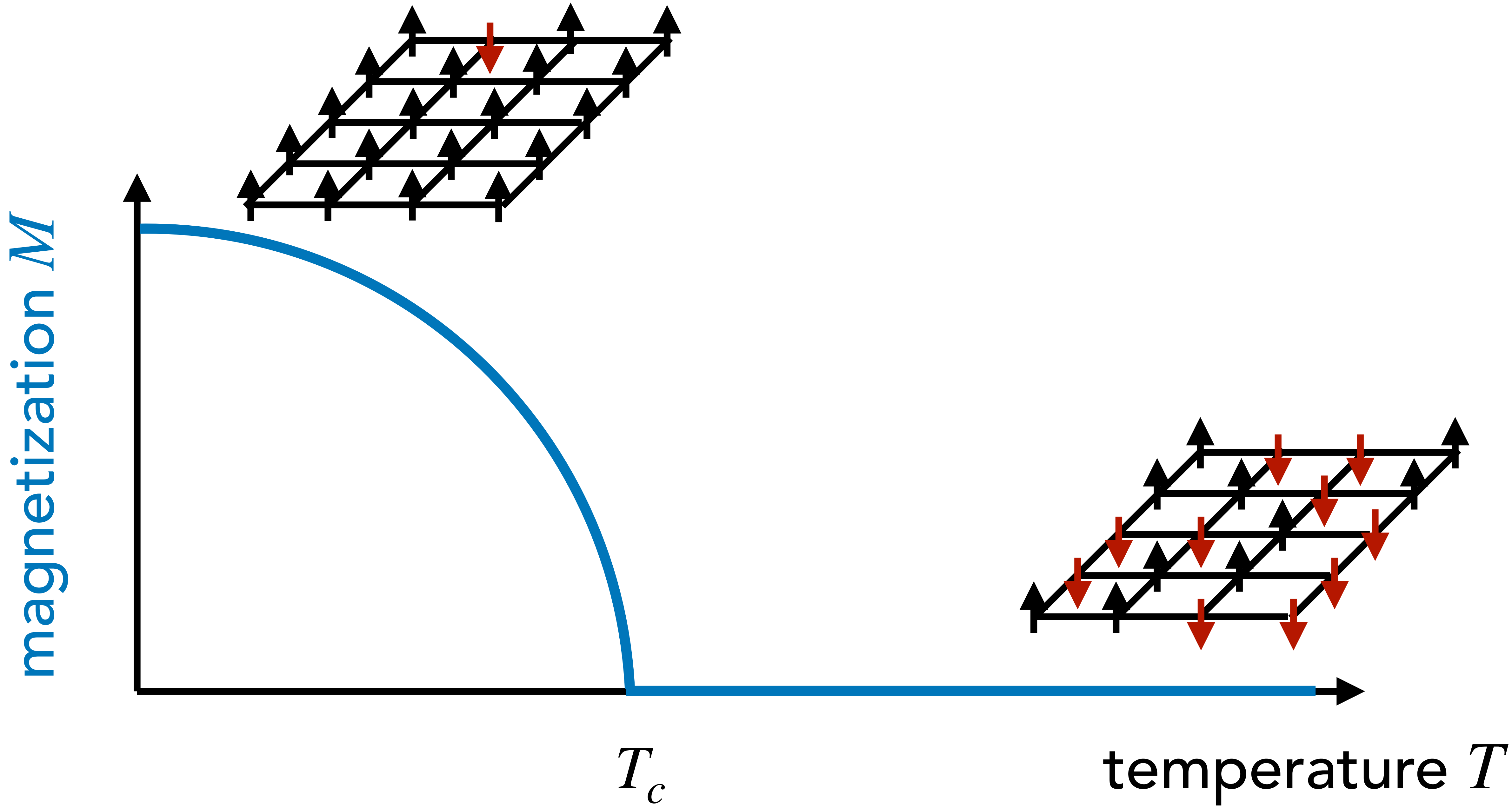
Atoms behave individually like small bar magnets ("spins")

 up or north orientation

 down or south orientation

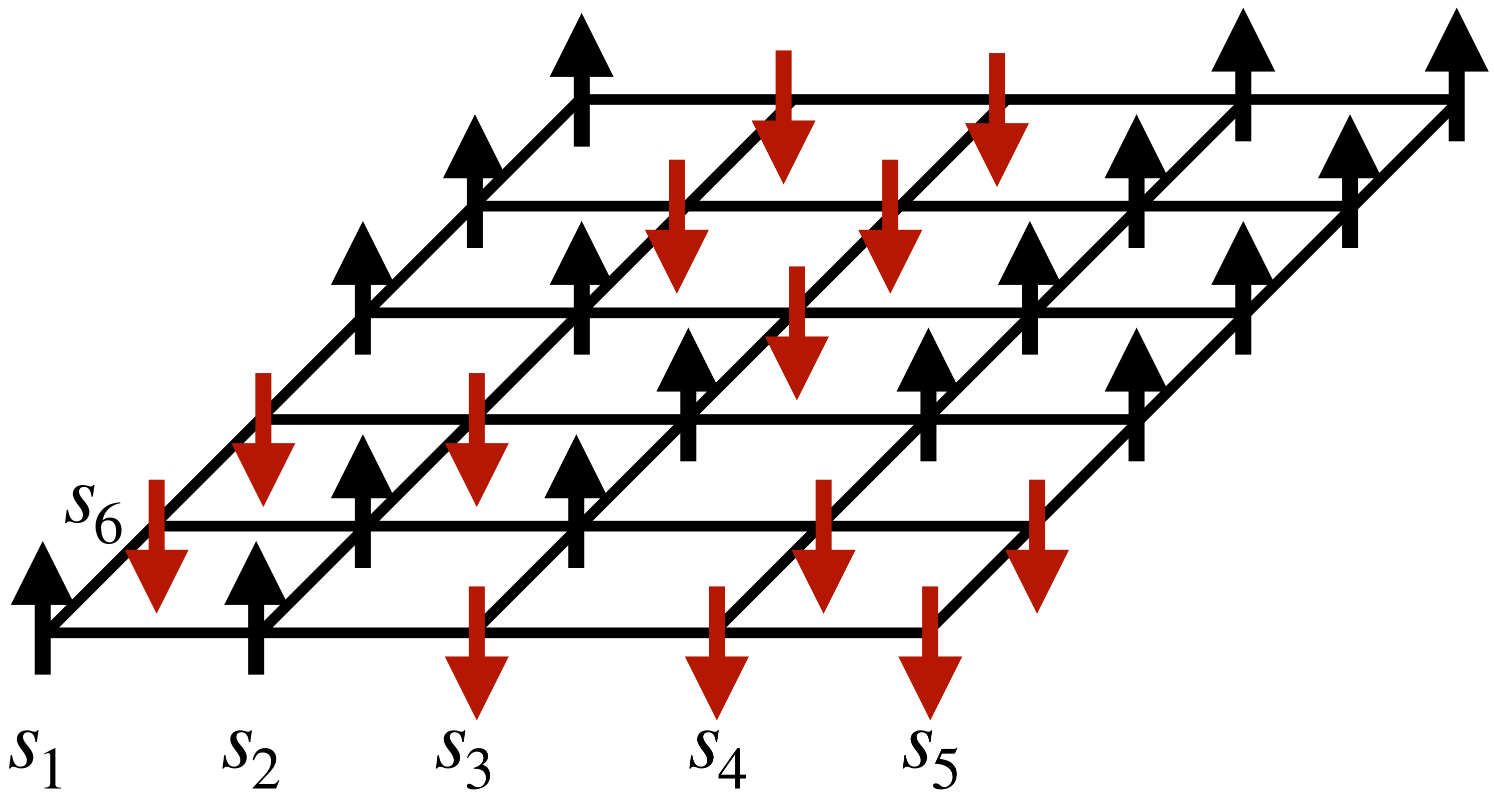
Motivation

Lowering or raising temperature
orders or disorders the magnet



Motivation

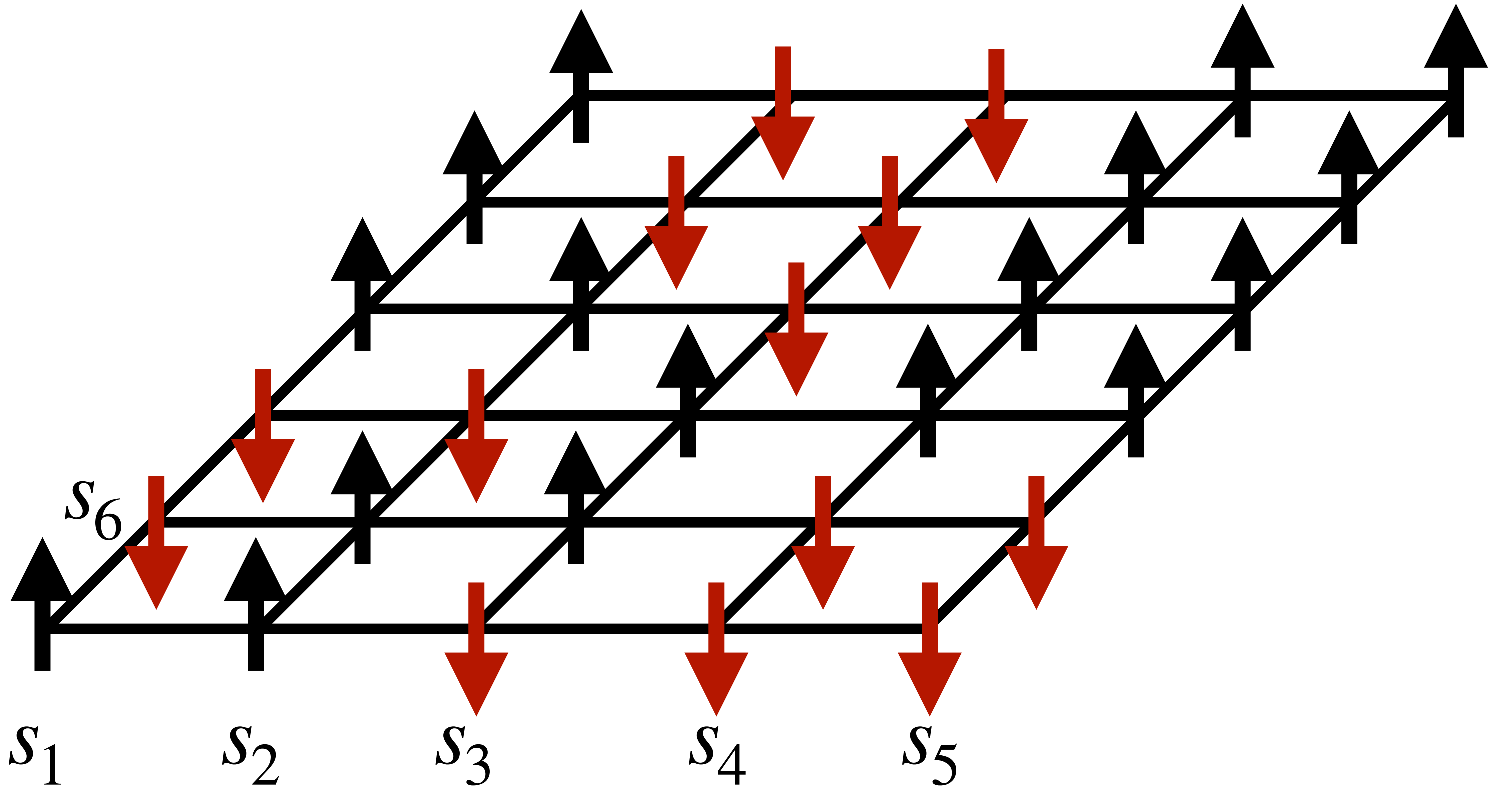
Why **high dimensional**?



Modeled as probability of spin configurations

$$P(s_1, s_2, s_3, \cdots, s_N)$$

Motivation



Probability of spin configurations

$$\left.\begin{array}{l} P(\uparrow,\uparrow,\uparrow,\ldots,\uparrow) = 0.1 \\ P(\downarrow,\uparrow,\uparrow,\ldots,\uparrow) = 0.001 \\ P(\uparrow,\downarrow,\uparrow,\ldots,\uparrow) = 0.003 \\ P(\uparrow,\uparrow,\downarrow,\ldots,\uparrow) = 0.007 \\ \qquad\qquad\vdots \end{array}\right\} 2^N \text{ of these for } N \text{ spins}$$

Motivation

How big is 2^N ?

$2^2 = 4$

$2^3 = 8$

$\vdots$

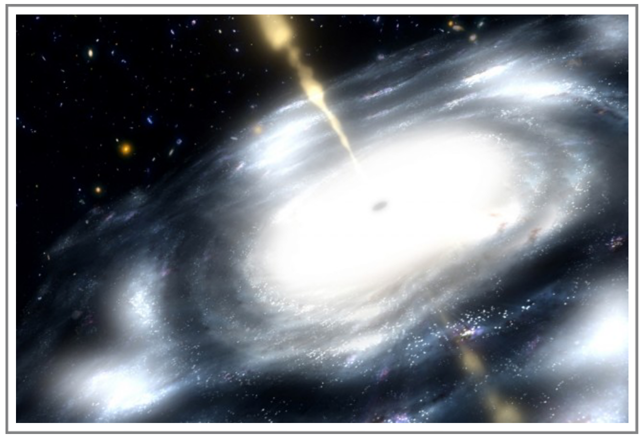
$2^{20} = 1{,}048{,}576$ (a million)

$\vdots$

$2^{100} = 1.2 \times 10^{30} \approx 1{,}000{,}000{,}000{,}000{,}000{,}000{,}000{,}000{,}000{,}000$

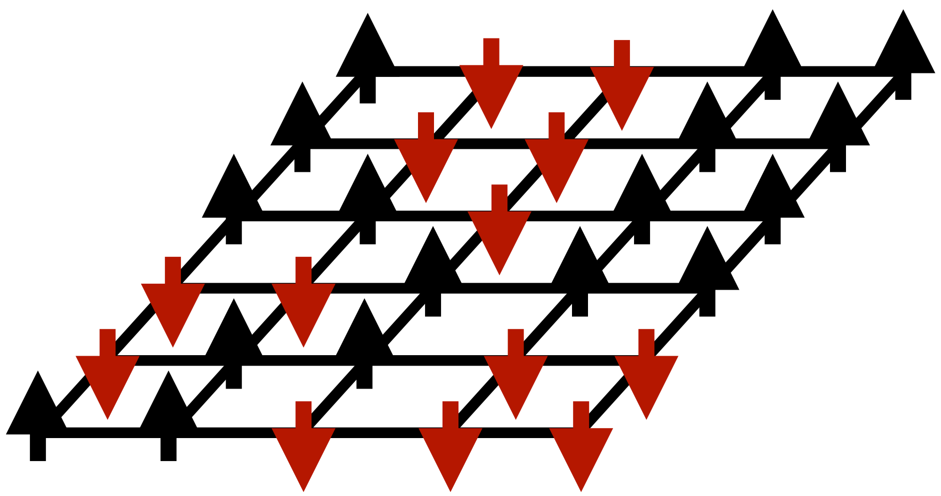
$\vdots$

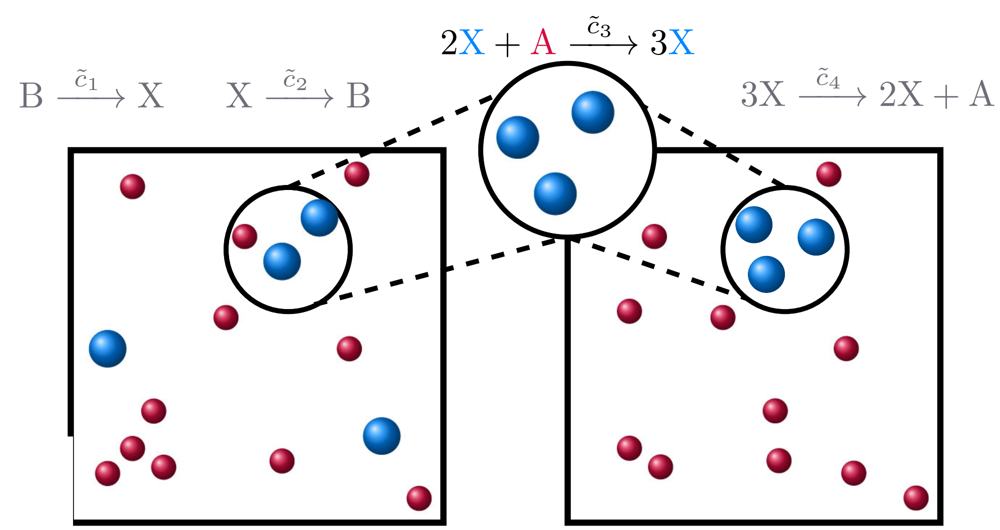
2^{300} greater than number of atoms in known universe!

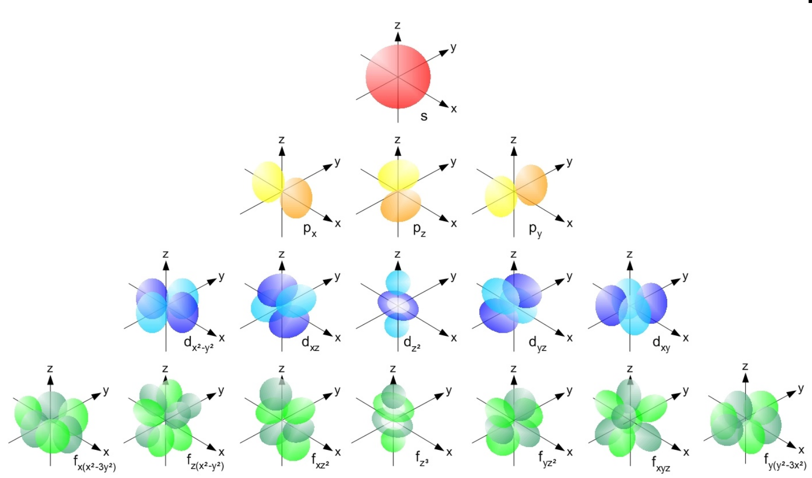


Motivation

Other examples of high-dimensional problems

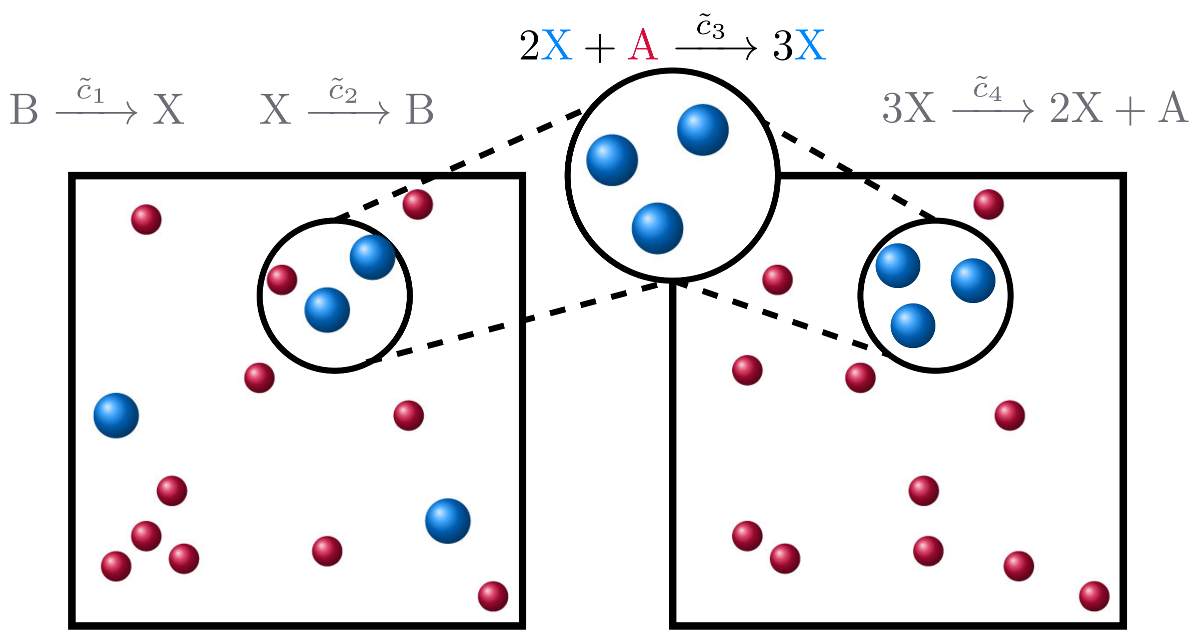






Motivation

Rate reaction equations of chemistry [*]



Dynamical problem (classical master equations)

A probability distribution of many variables

$$p(s_1, s_2, s_3, s_4, s_5, \ldots, s_n)$$

[*] Nicholson, Gingrich, Phys. Rev. X 13, 041006 (2023)

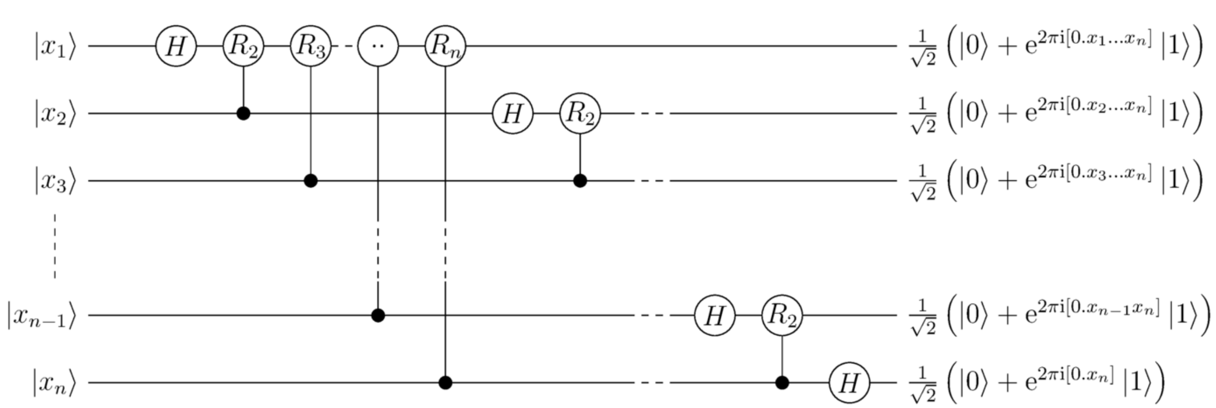
Motivation

Problems in **quantum physics** (many-body quantum)

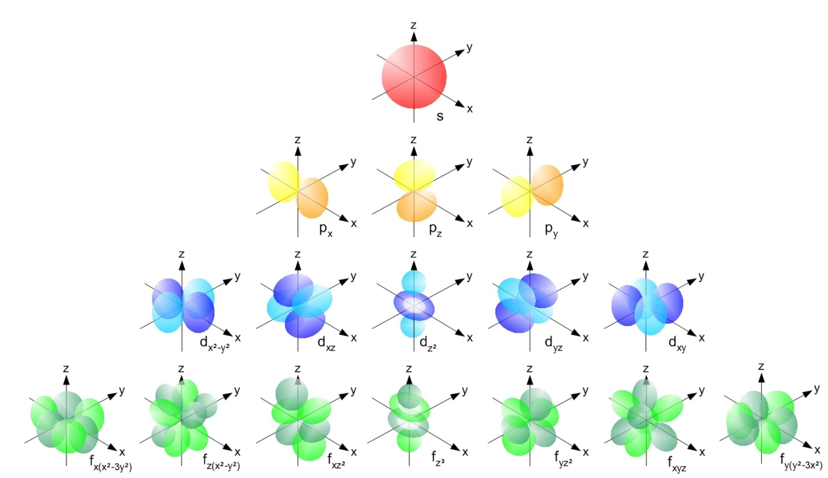
$$|\Psi\rangle = \sum_{s_1 s_2 s_3 \cdots s_n} \Psi^{s_1 s_2 s_3 \cdots s_n} |s_1 s_2 s_3 \cdots s_n\rangle \qquad s_j \in 0, 1$$

can describe

state of a quantum computer



state of many quantum particles



Tensors

Common language for high-dimensional problems

Function of N discrete variables:

$$f(s_1, s_2, s_3, \ldots, s_N)$$

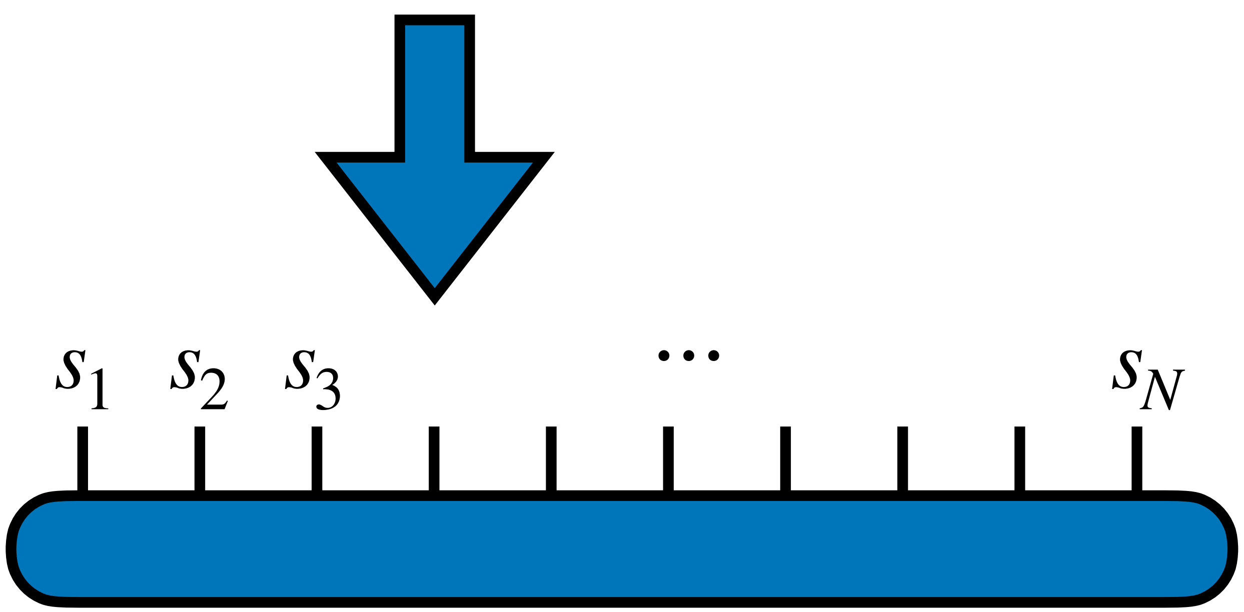
- Ferromagnet: spin probability $p(s_1, s_2, \ldots, s_N)$
- Network dynamics: probability $p(s_1, s_2, \ldots, s_N)$
- Quantum: wave function $\Psi(s_1, s_2, \ldots, s_N)$

Tensors

Evaluating function on all 2^N inputs:

$$F^{s_1 s_2 \cdots s_N} = f(s_1, s_2, s_3, \ldots, s_N)$$

$$F^{s_1 s_2 \cdots s_N} =$$



"tensorized" version of f – huge multi-dim. array

Motivation

Storing all configurations (full tensor) is an
exponential problem

Will never be solved by **brute force**...

2^{100} vector would take
as much memory (RAM cards)
as volume of Earth

Solving High-Dimensional Problems with Tensor Networks

We will encounter two main challenges –
and overcome them with tensor networks

1. **The Curse of Dimensionality**

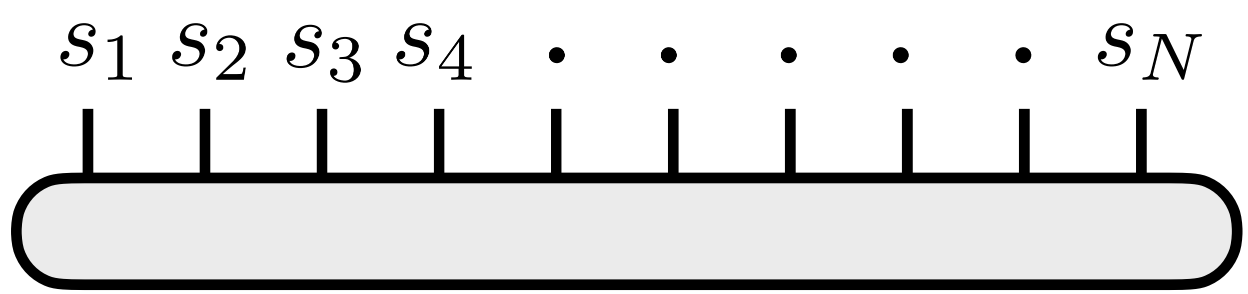
2. **The Problem of Loops**

Breaking the Curse of Dimensionality

Breaking the Curse of Dimensionality

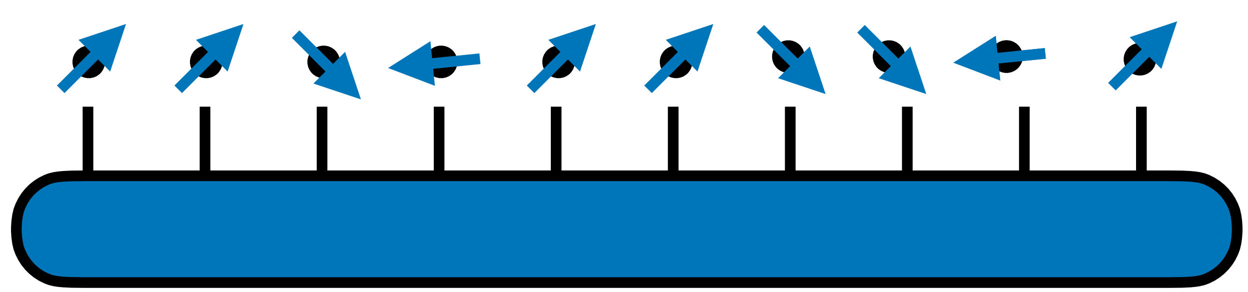
We have seen that states of high dimensional problems can be stored as **tensors** – high-dimensional arrays

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



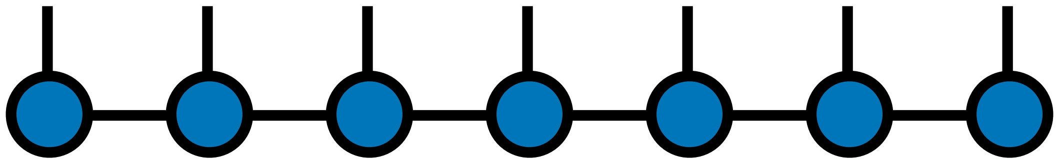
For example a quantum state of a spin system

$$|\Psi\rangle =$$



Tensor Networks

Diagrams actually precise notation:



Tensor diagram notation

Tensor Networks

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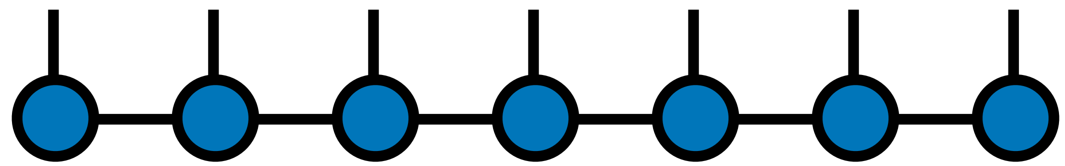
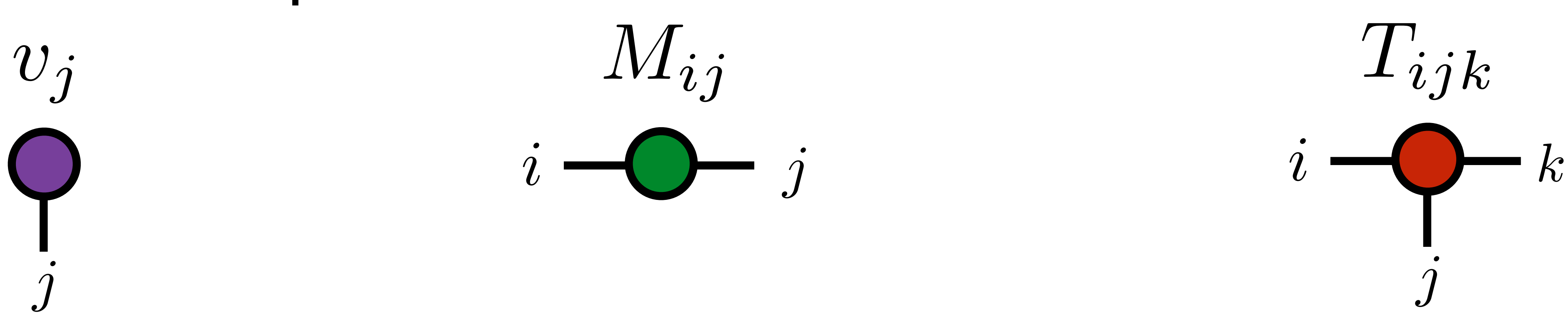


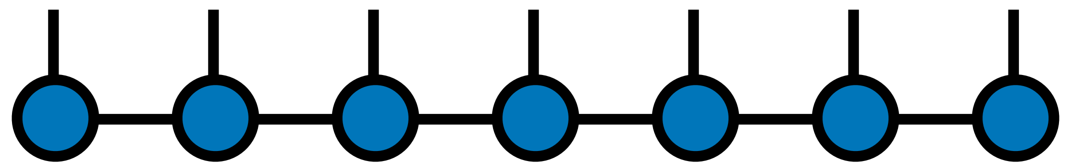
Tensor diagram notation

Low-order examples:



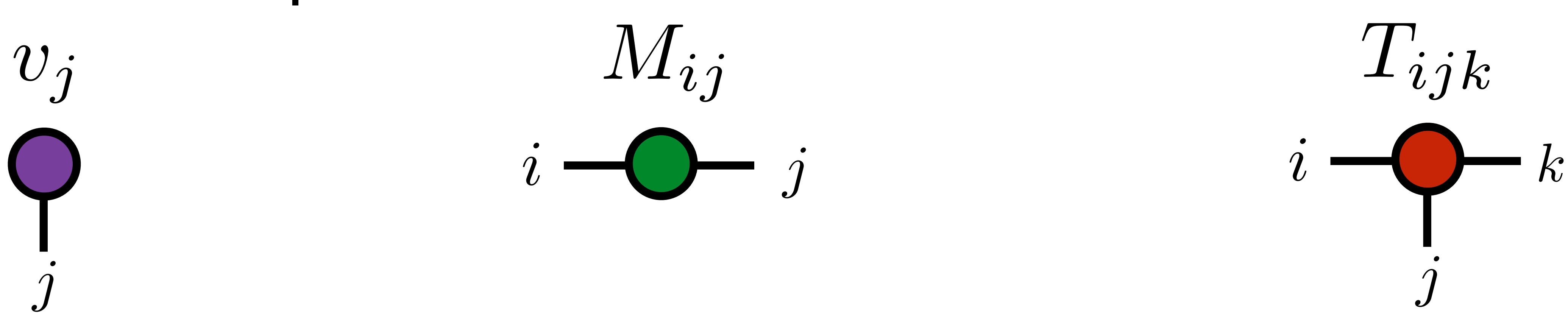
Tensor Networks

Diagrams actually precise notation:

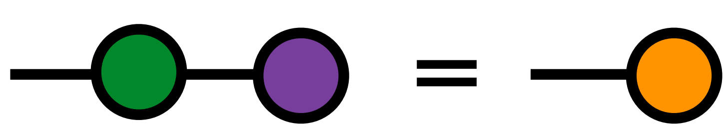


Tensor diagram notation

Low-order examples:



Joining wires means contraction:

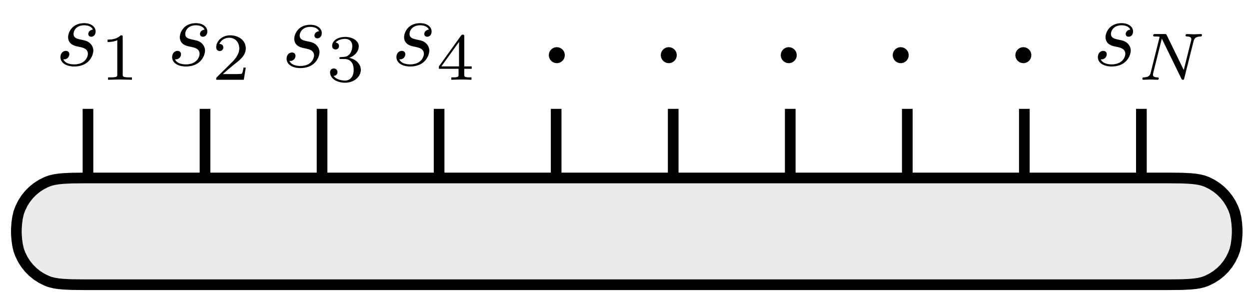


$$\sum_j M_{ij} v_j = w_i$$

Breaking the Curse of Dimensionality

But large tensors are useless on their own...

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



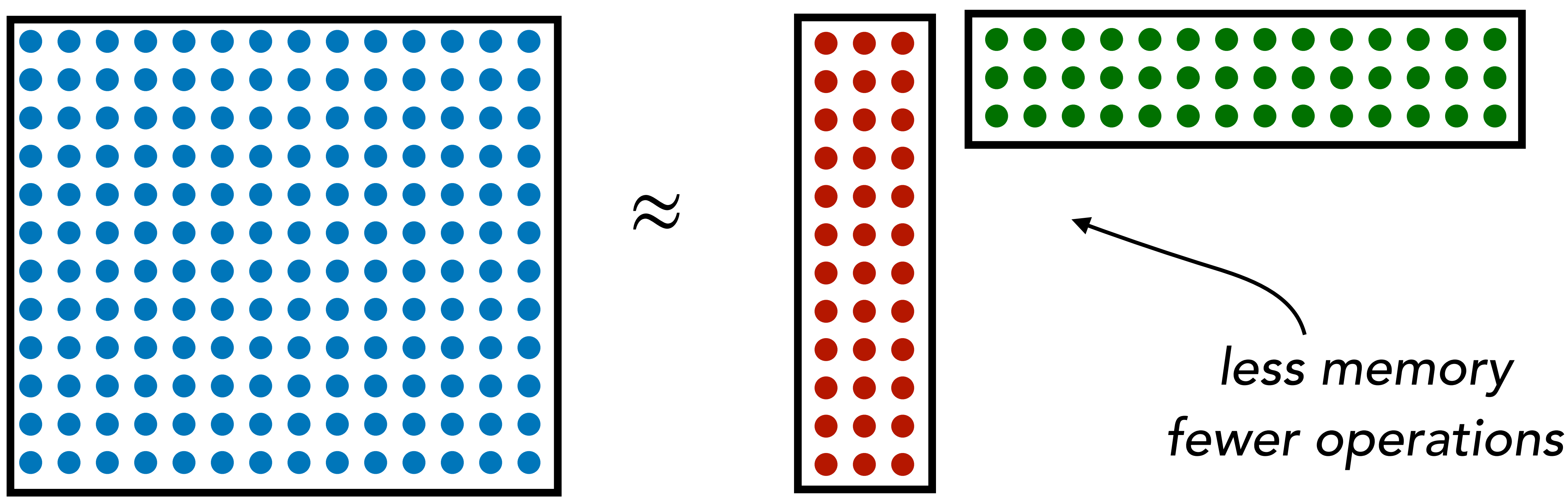
If each index has dimension d

Number of parameters is d^N - exponential memory cost

Called the "curse of dimensionality"

Breaking the Curse of Dimensionality

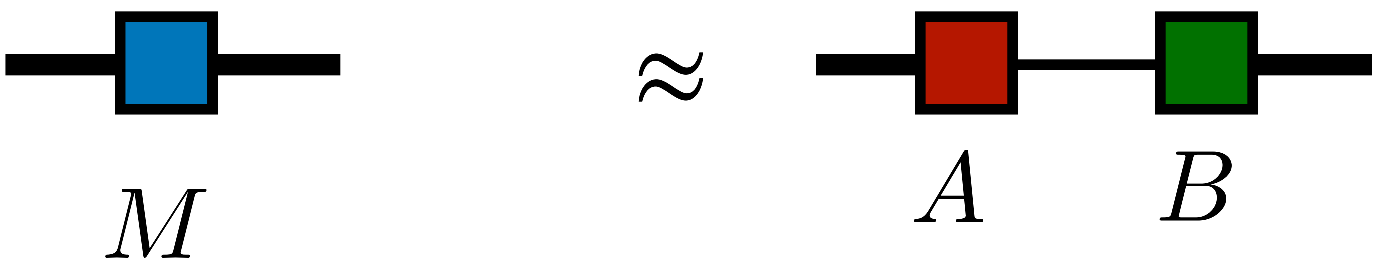
For matrices, we can break the curse via low-rank factorization



Low-rank form found by singular value decomposition (SVD), interpolative decomposition (ID), rank-revealing QR (RRQR)...

Breaking the Curse of Dimensionality

Example of a low-rank factorization:



$$\begin{bmatrix} 0.16 & 0.110 & 0.117 & 0.084 \\ 0.73 & 0.873 & 0.304 & 0.287 \\ 0.16 & 0.110 & 0.117 & 0.084 \\ 0.73 & 0.873 & 0.304 & 0.287 \end{bmatrix} \approx \begin{bmatrix} 1.0 & -1.0 \\ 1.0 & 1.0 \\ 1.0 & -1.0 \\ 1.0 & 1.0 \end{bmatrix} \begin{bmatrix} 0.445 & 0.492 & 0.211 & 0.186 \\ 0.285 & 0.381 & 0.094 & 0.101 \end{bmatrix}$$

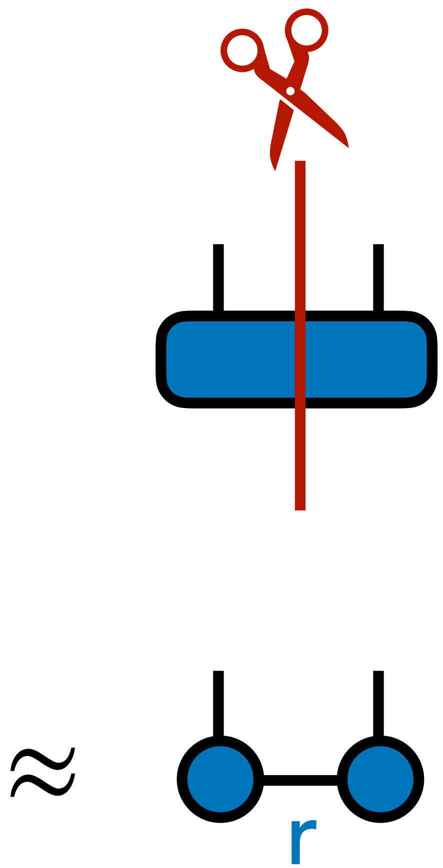
Matrices (and tensors) can have hidden structure

Breaking the Curse of Dimensionality

But how can we apply this to tensors?

Breaking the Curse of Dimensionality

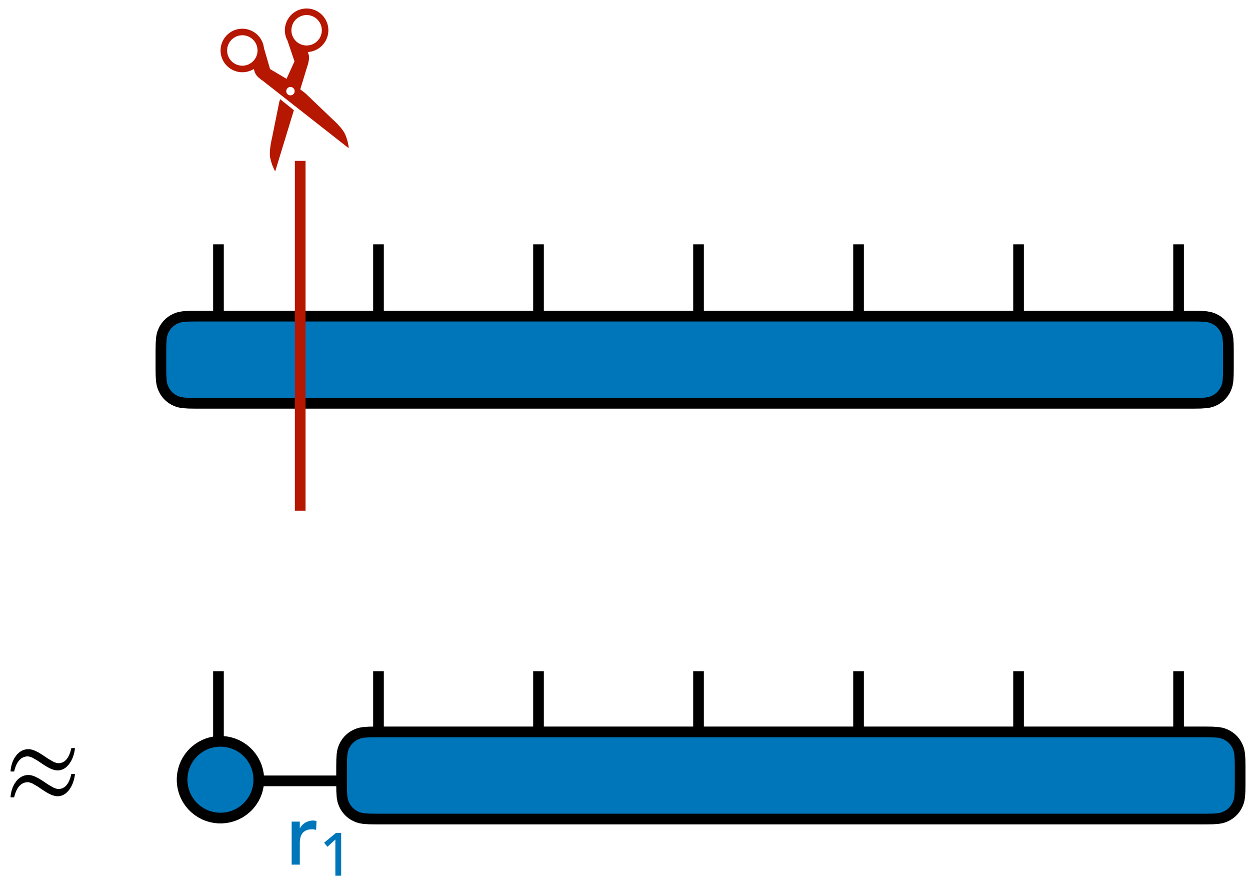
Just as factorizing a matrix reduces cost (memory and compute)



r is matrix rank

Breaking the Curse of Dimensionality

Can recursively factor & compress a tensor as well



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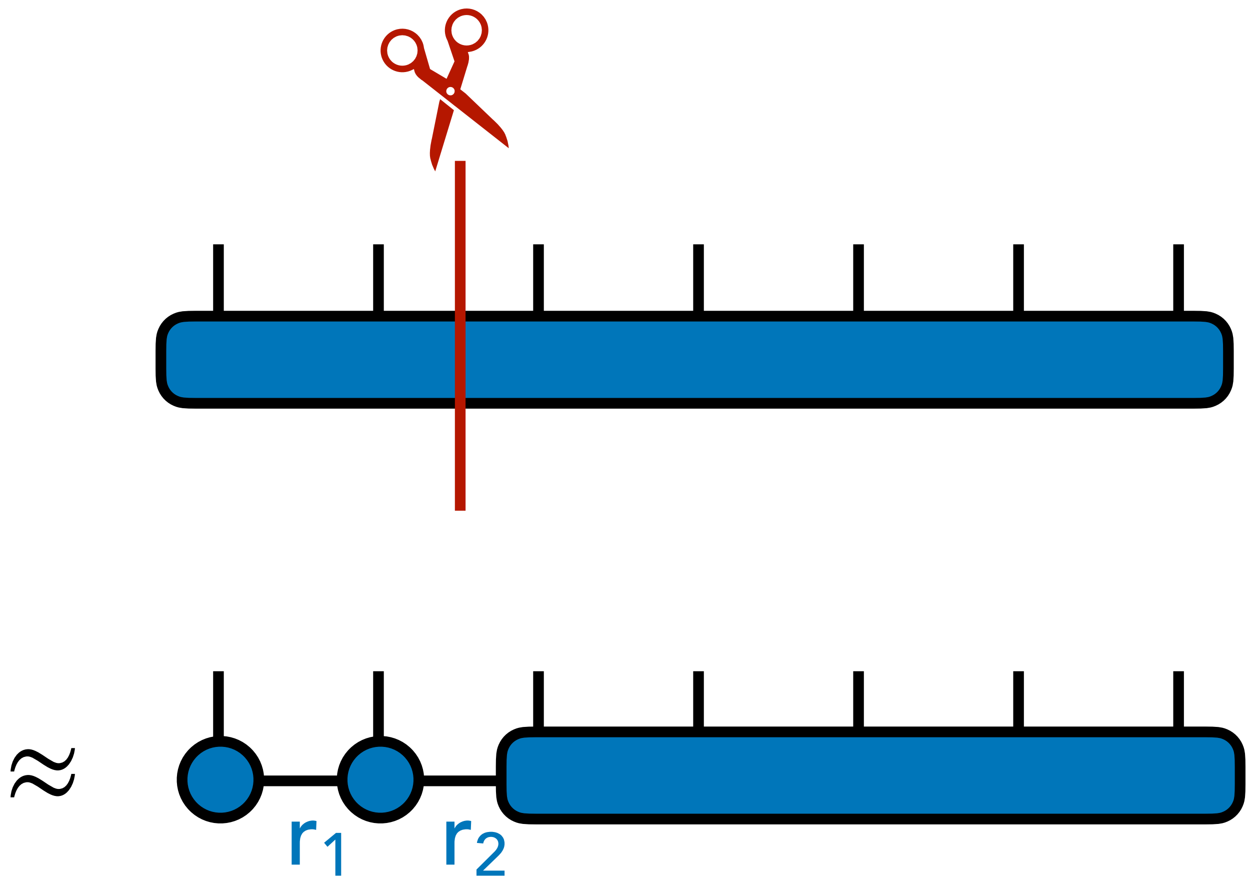

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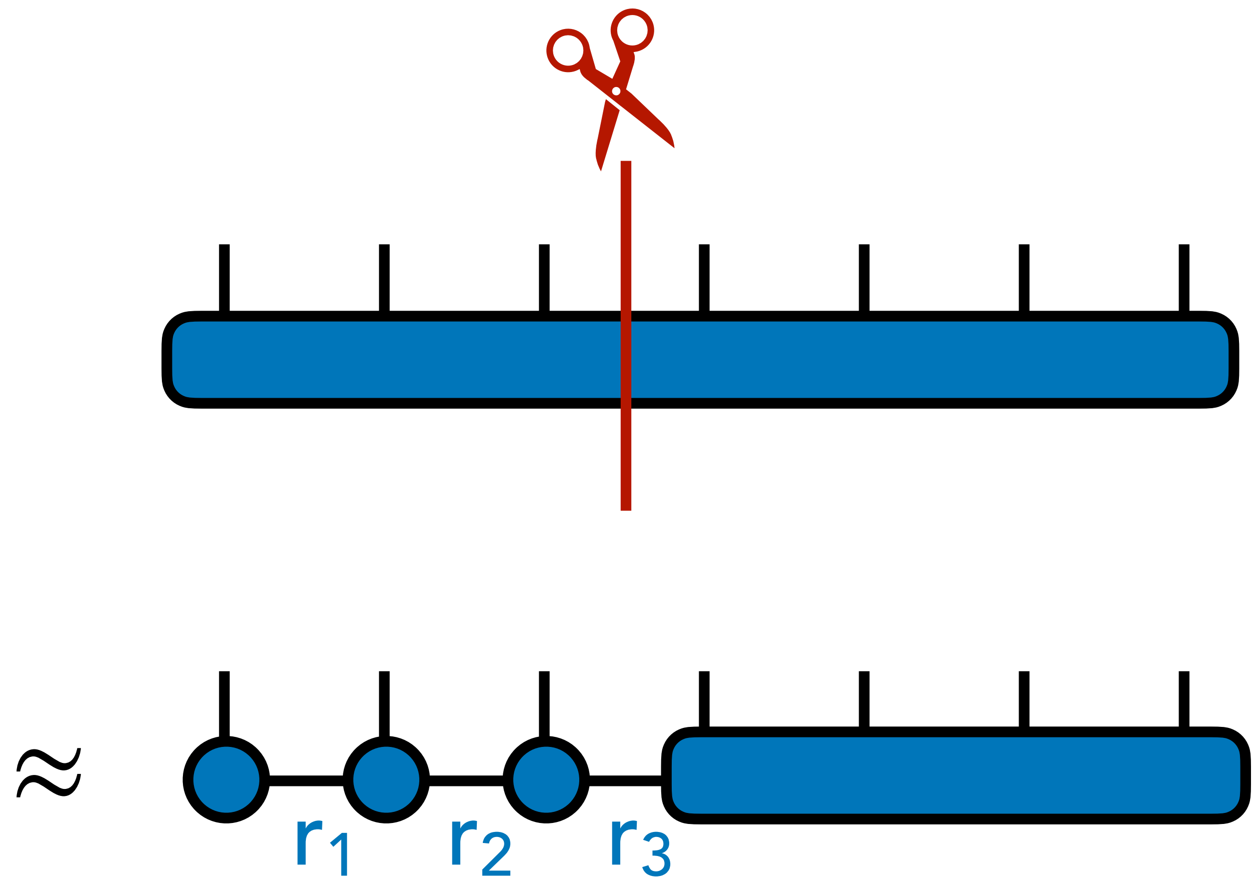

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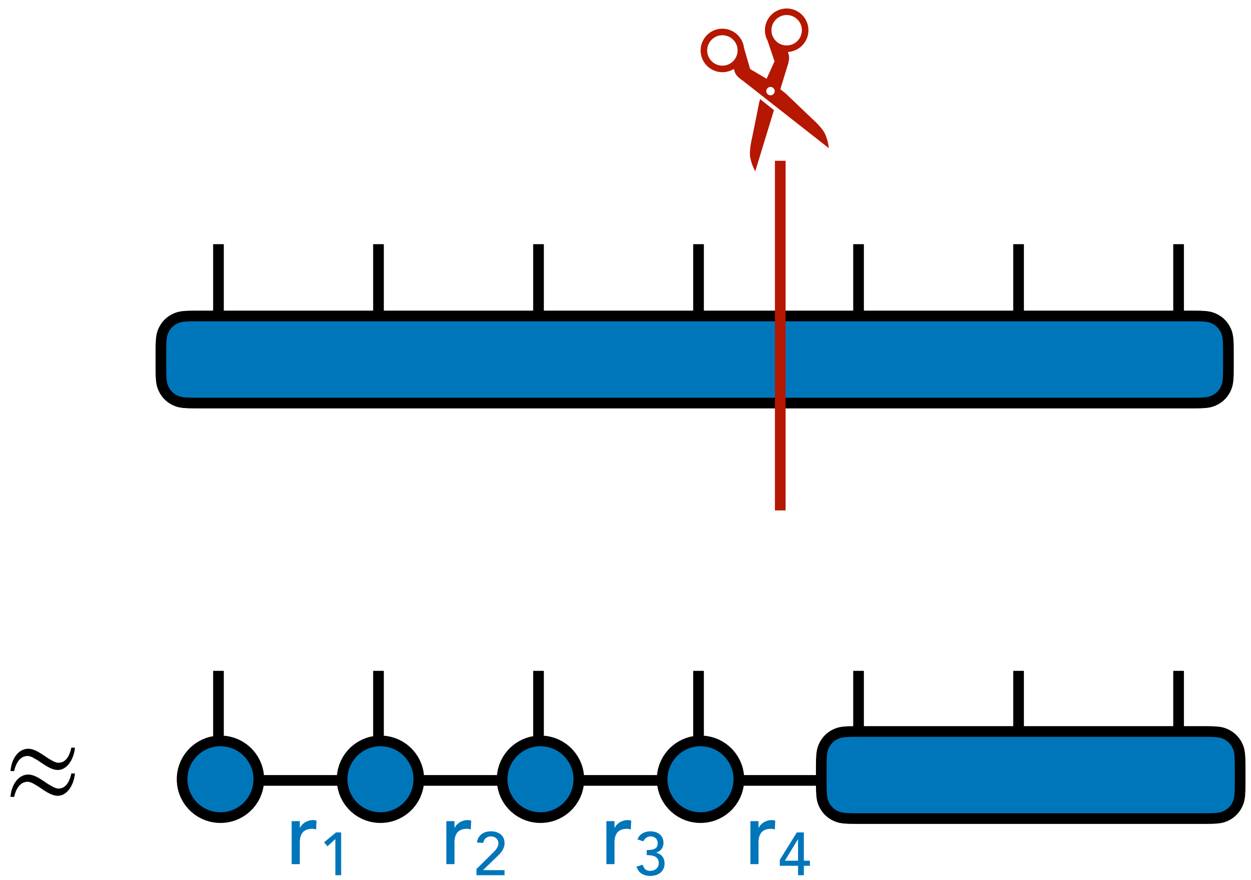

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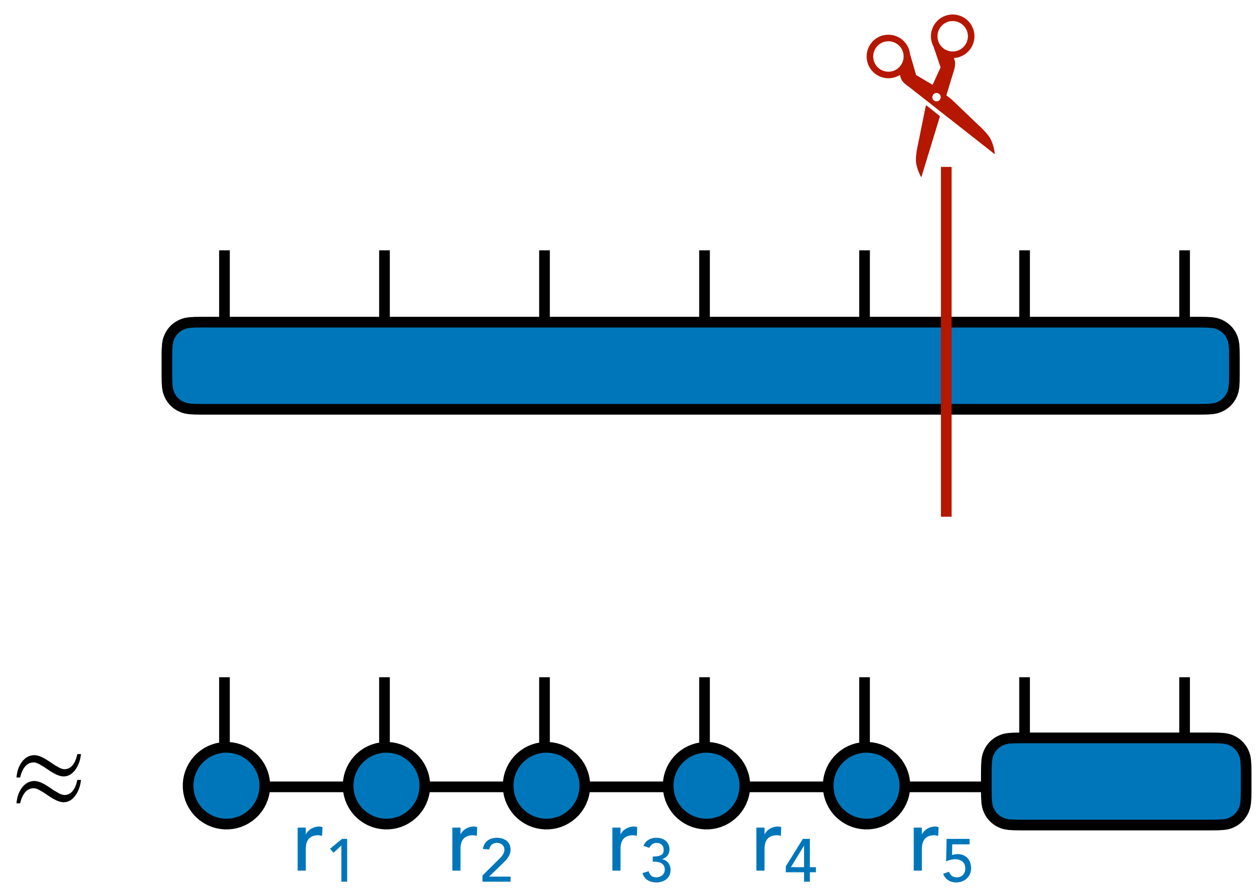

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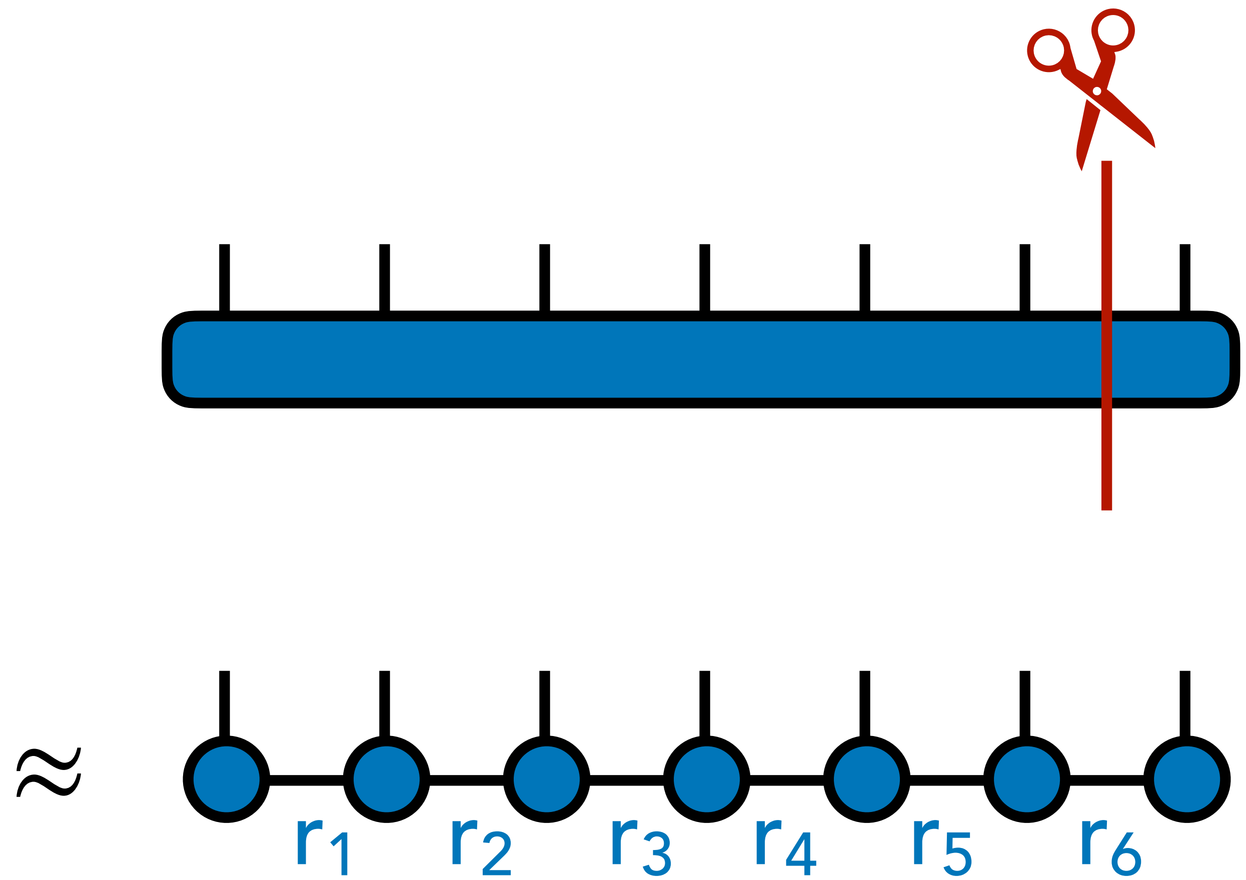

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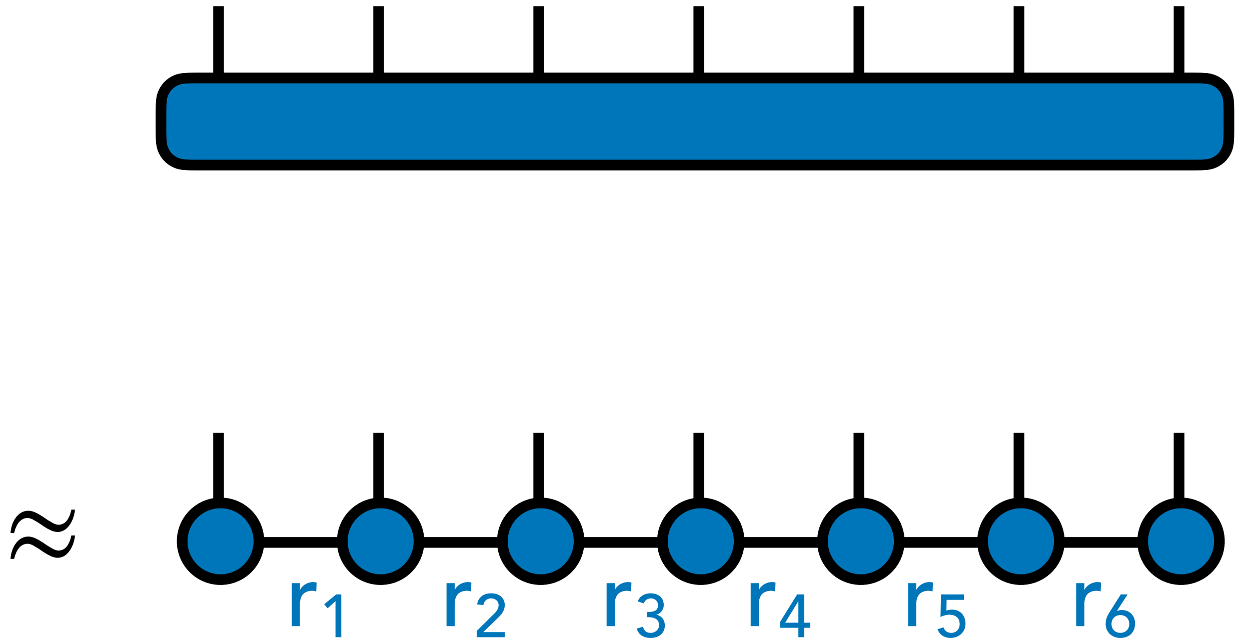
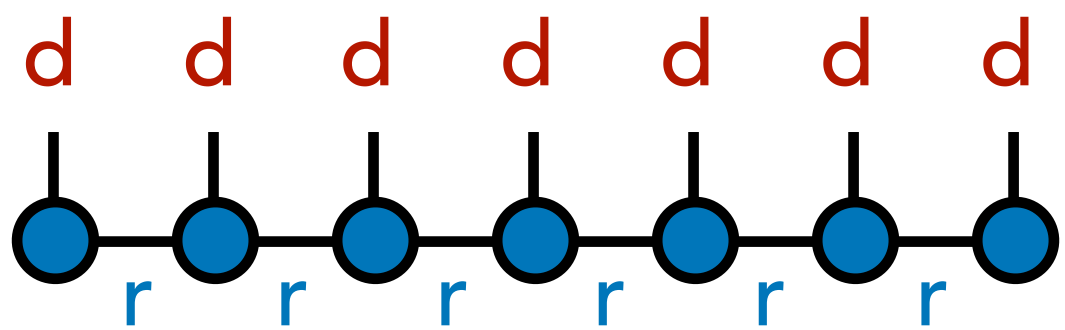


Massive gain if internal ranks (r_j's) small,
while accuracy remains good

Ranks often called "bond dimensions"

Breaking the Curse of Dimensionality

How much do we gain?



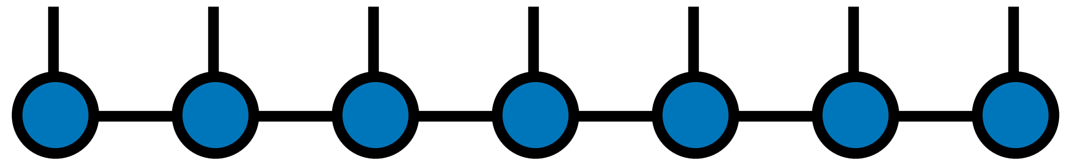
N tensors and $d\ r^2$ elements per tensor

$(N \cdot d \cdot r^2)$ versus d^N total parameters

Exponential improvement –
breaking the curse of dimensionality

Tensor Networks

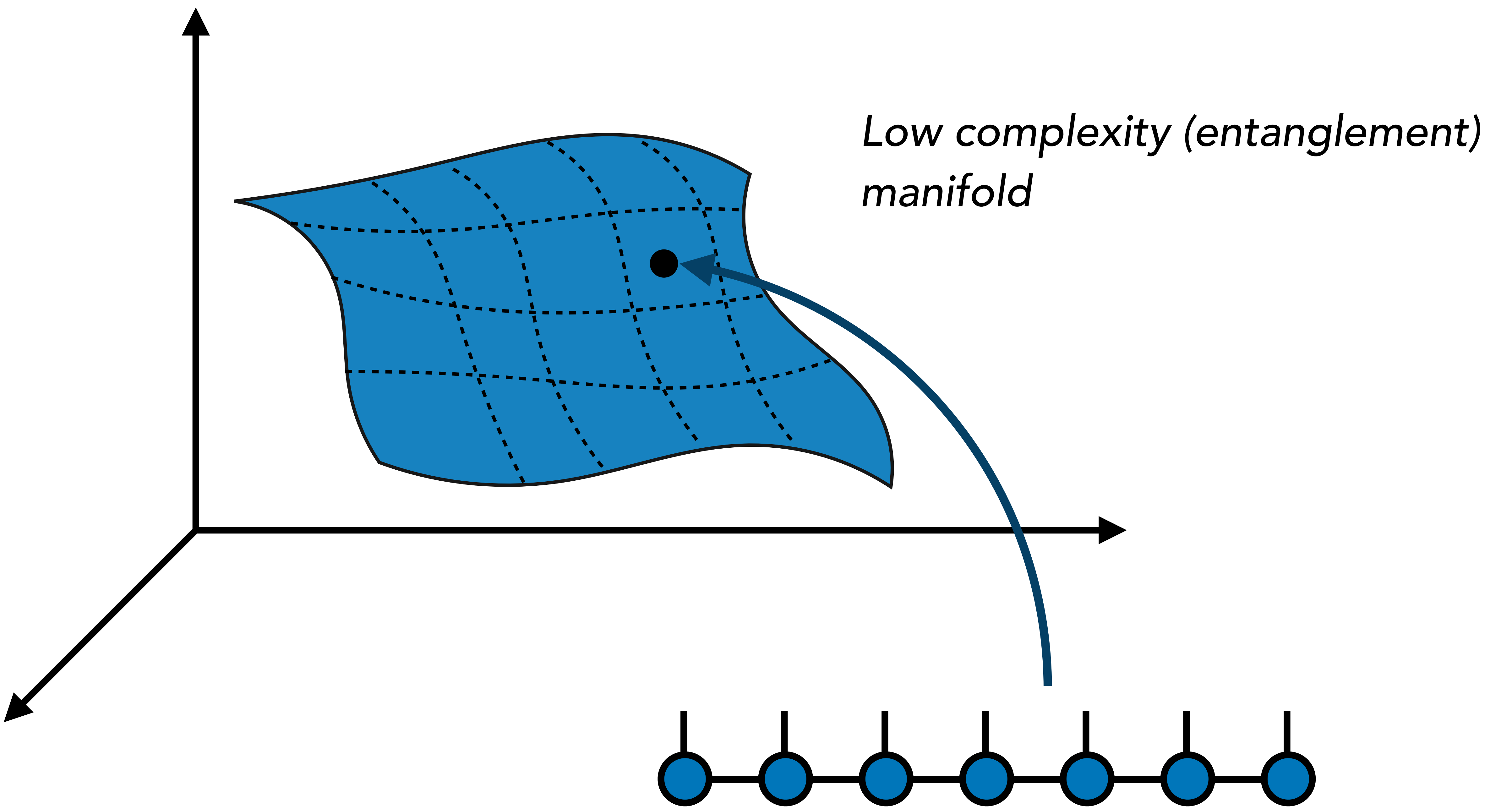
This format known as matrix product state (MPS)
or tensor train (TT)



Example of a tensor network
(network of tensors contracted together)

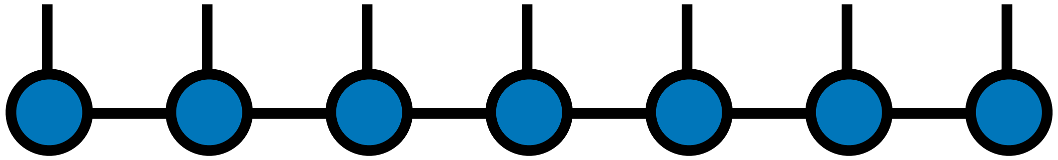
Tensor Networks

Parameters of a tensor network describe a manifold within exponential state space

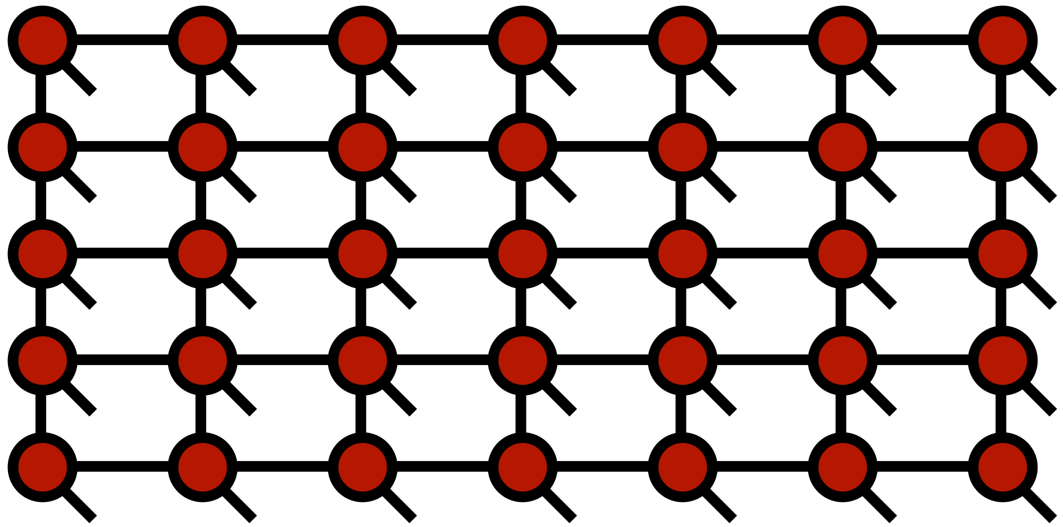


Tensor Networks

There are other types of tensor networks for 2D, 3D systems or multi-scale systems



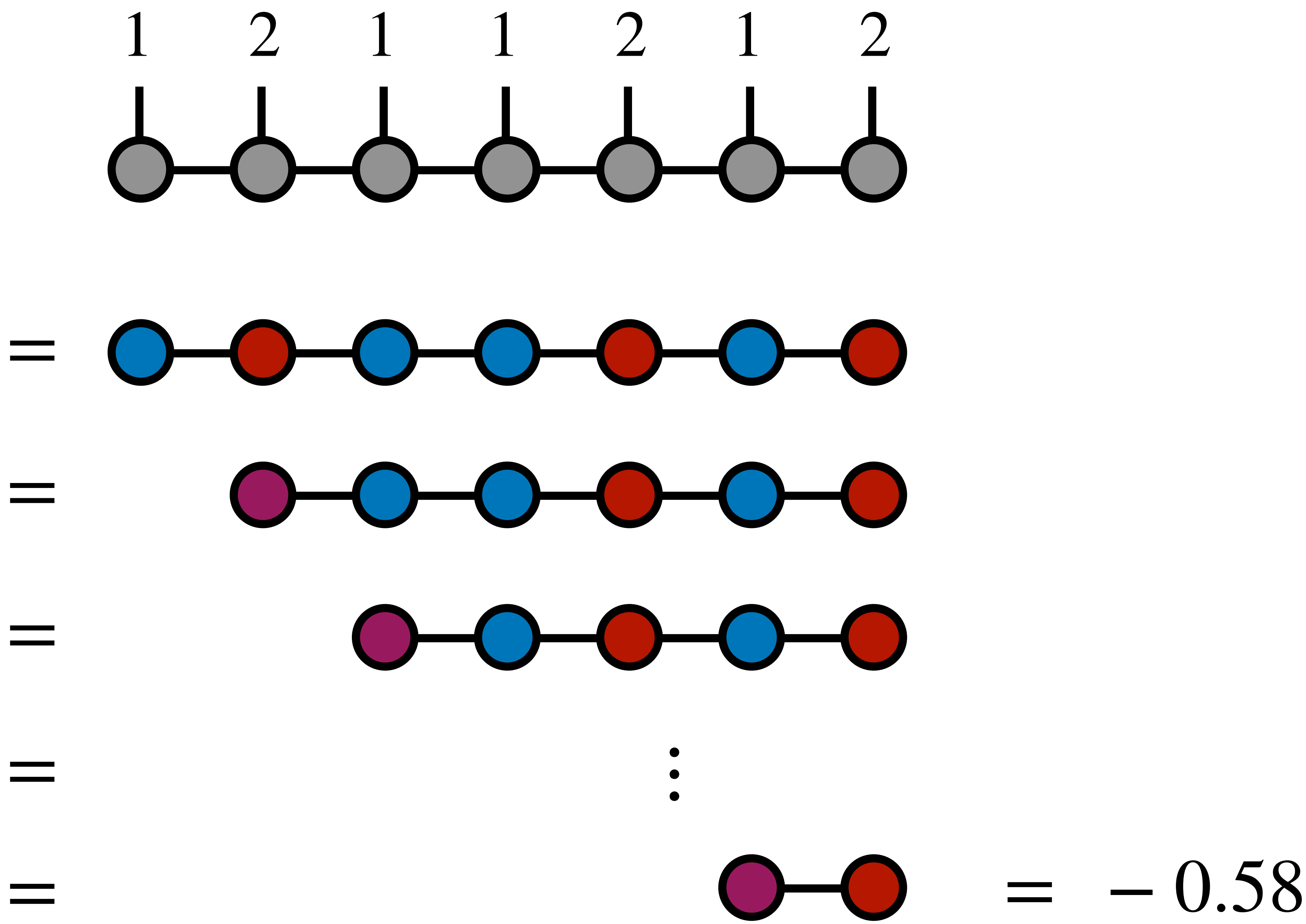
1D tensor network (MPS)



2D tensor network ("PEPS")

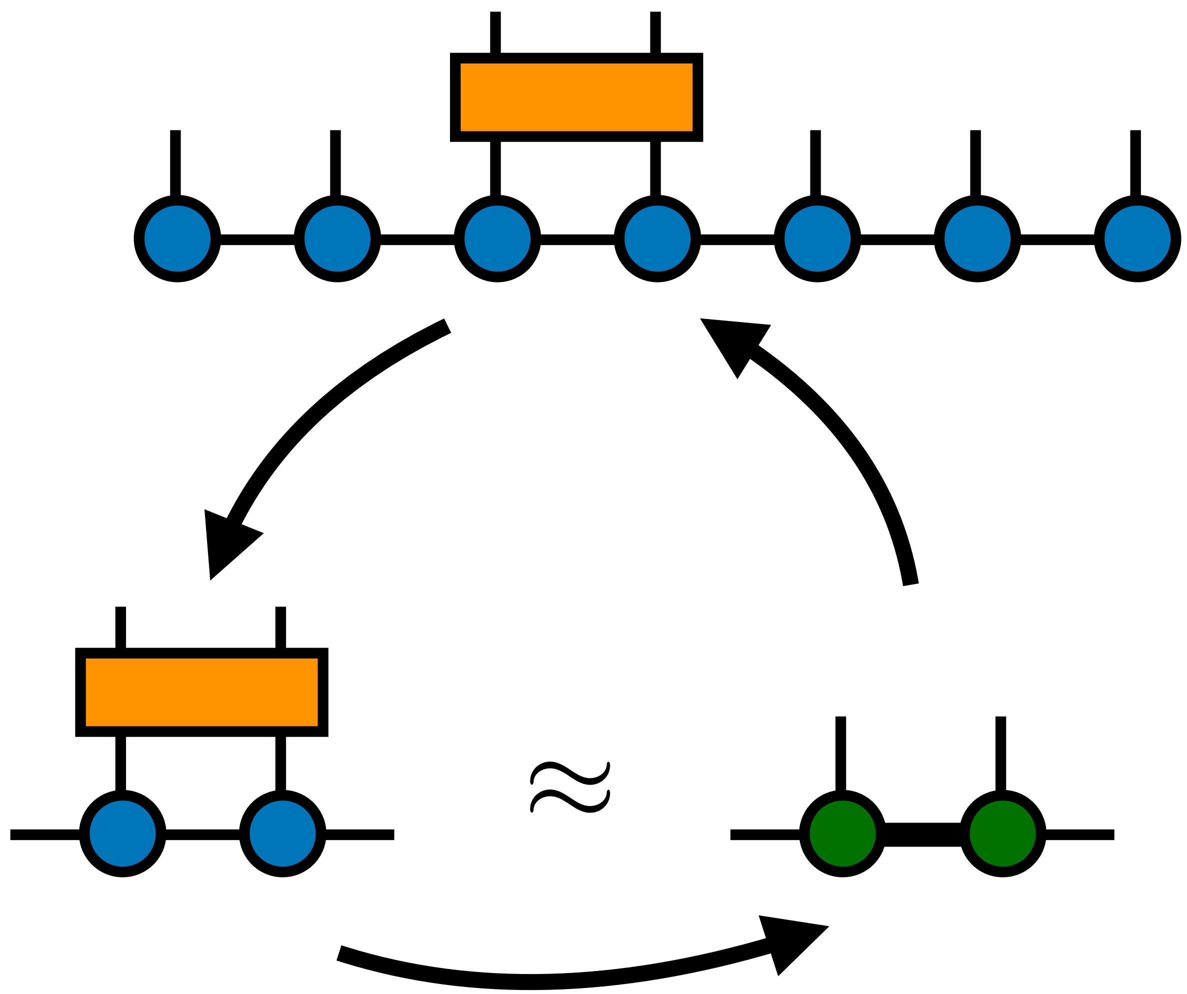
Tensor Networks

Can evaluate a single element of a tensor network, like a neural network



Tensor Network Algorithms

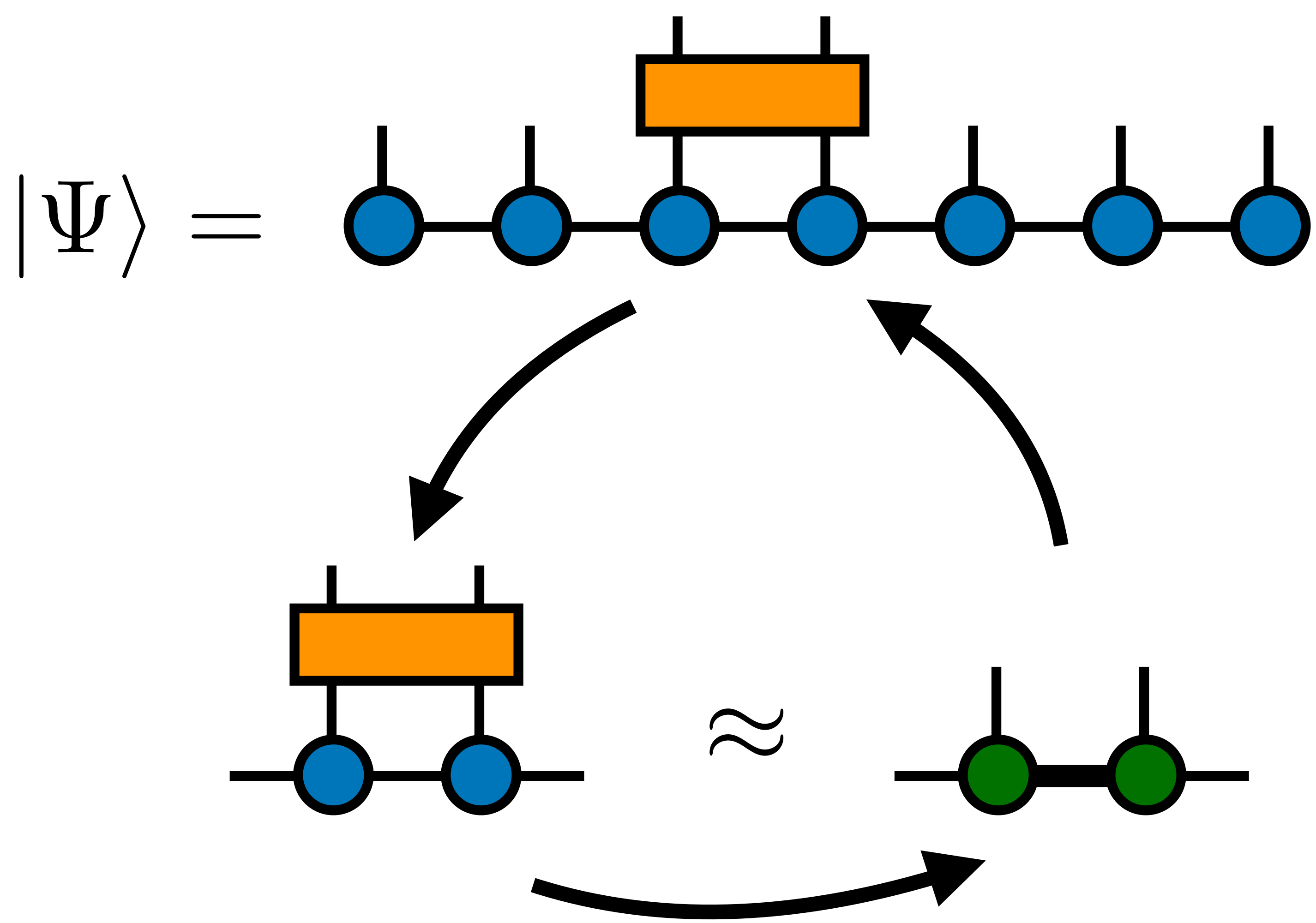
But key difference from neural networks or other high-dim. methods are novel **algorithms**



Tensor Network Algorithms

Tensor networks offer powerful algorithms

For example applying quantum gates
(imaginary or real time evolution)



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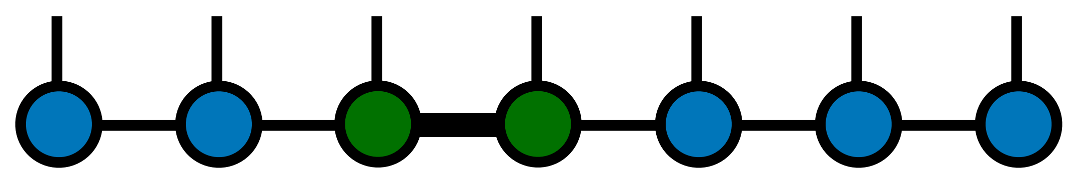
$$|\Psi\rangle =$$



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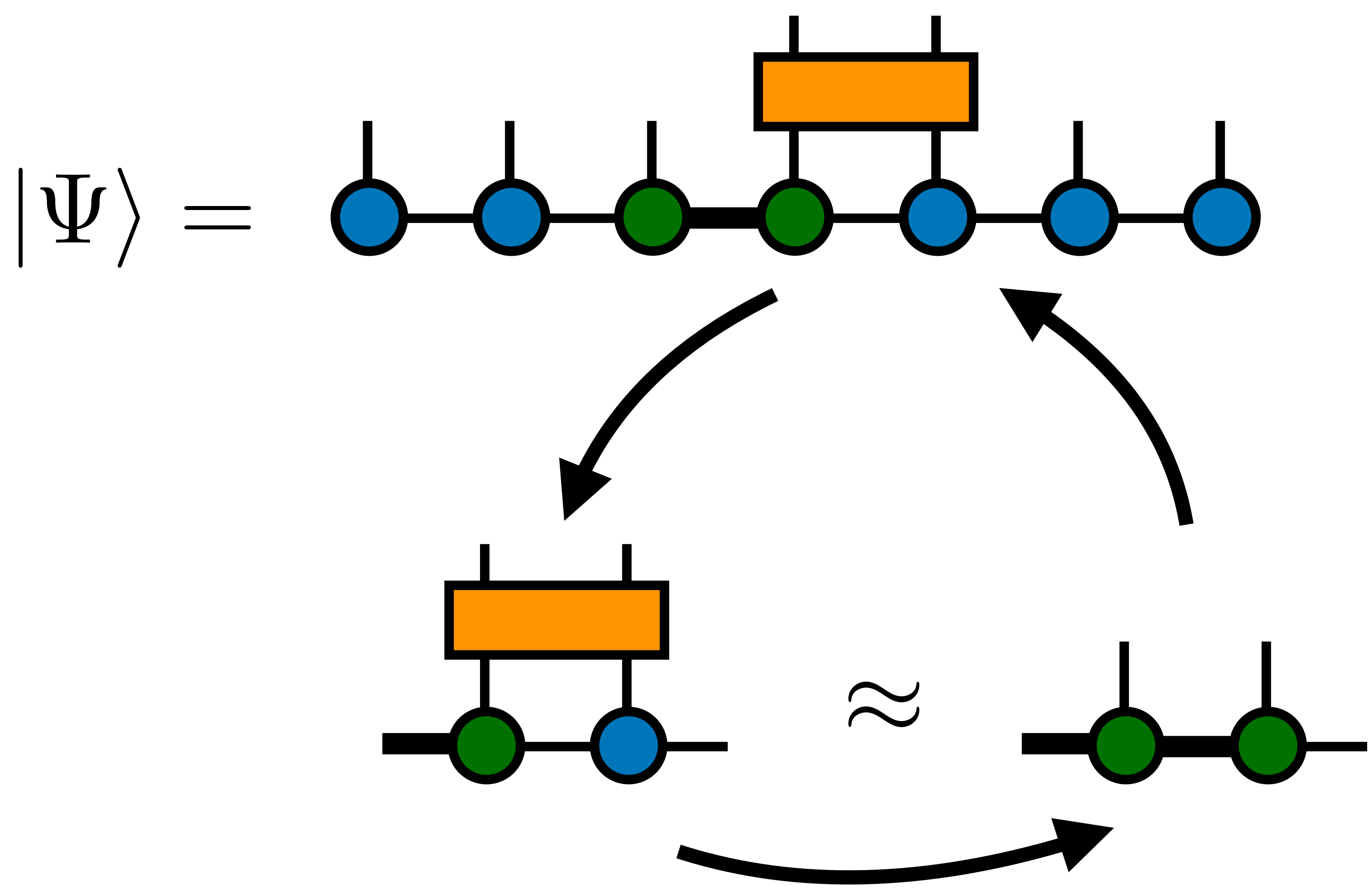

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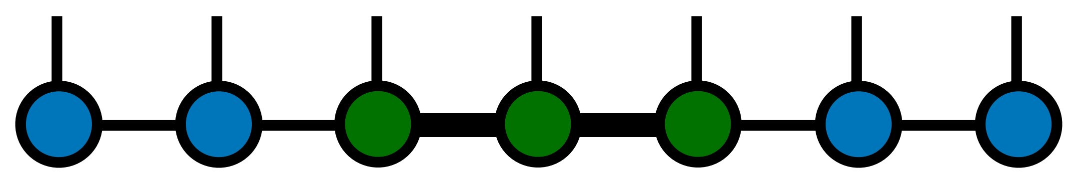
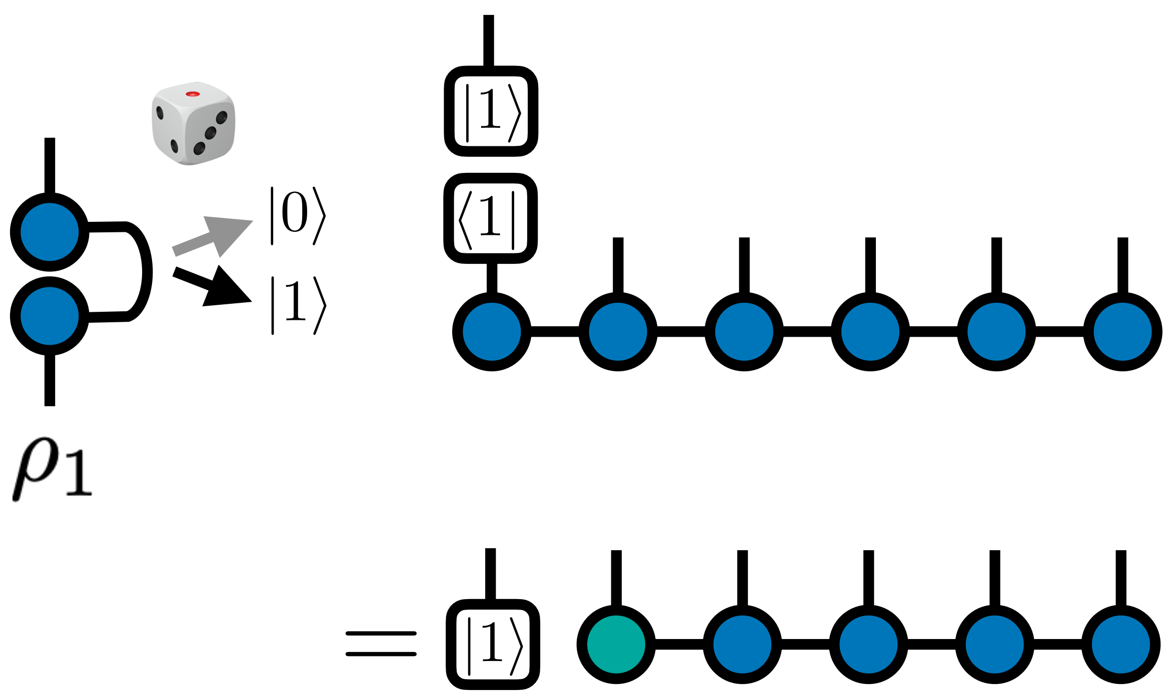


Tensor Network Algorithms

Tensor networks offer powerful algorithms

Can also "perfect sample" MPS tensor networks
No Markov chain / autocorrelation effects



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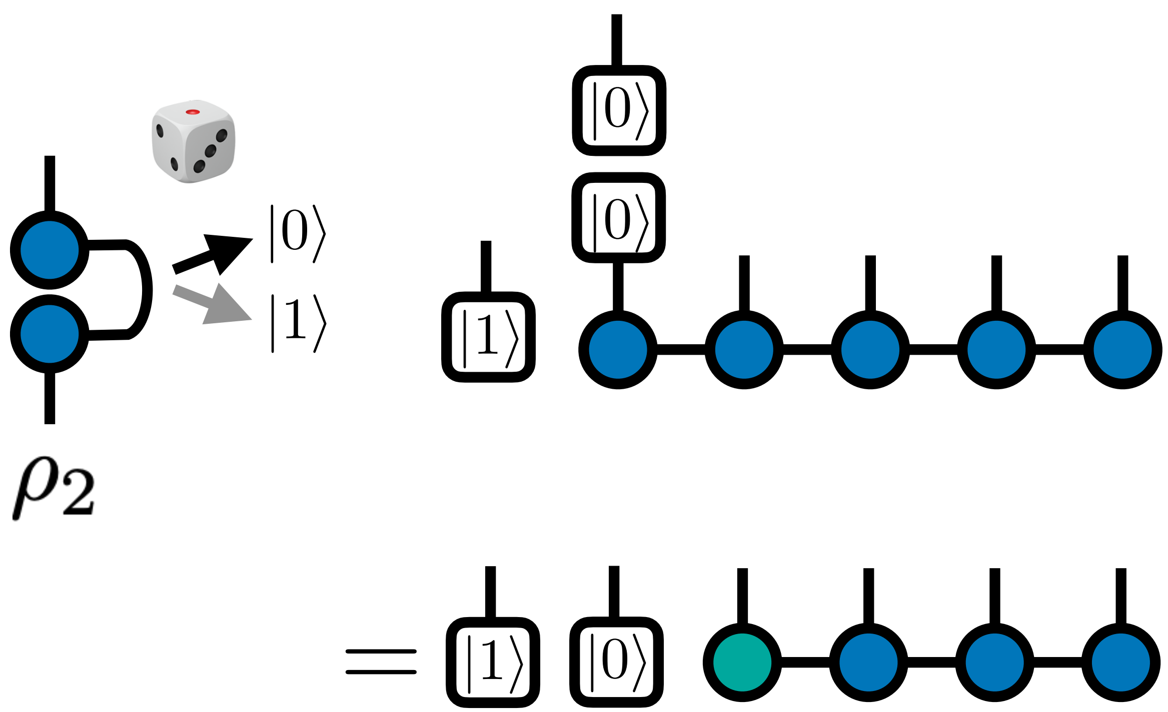

Tensor Network Algorithms

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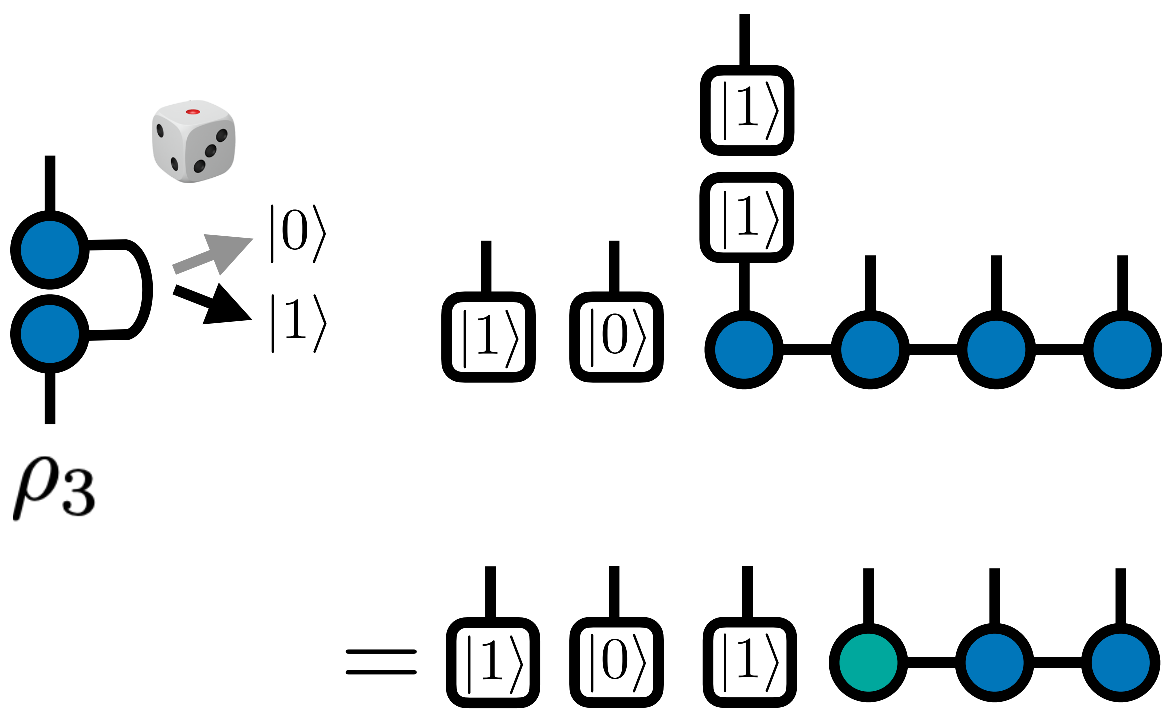
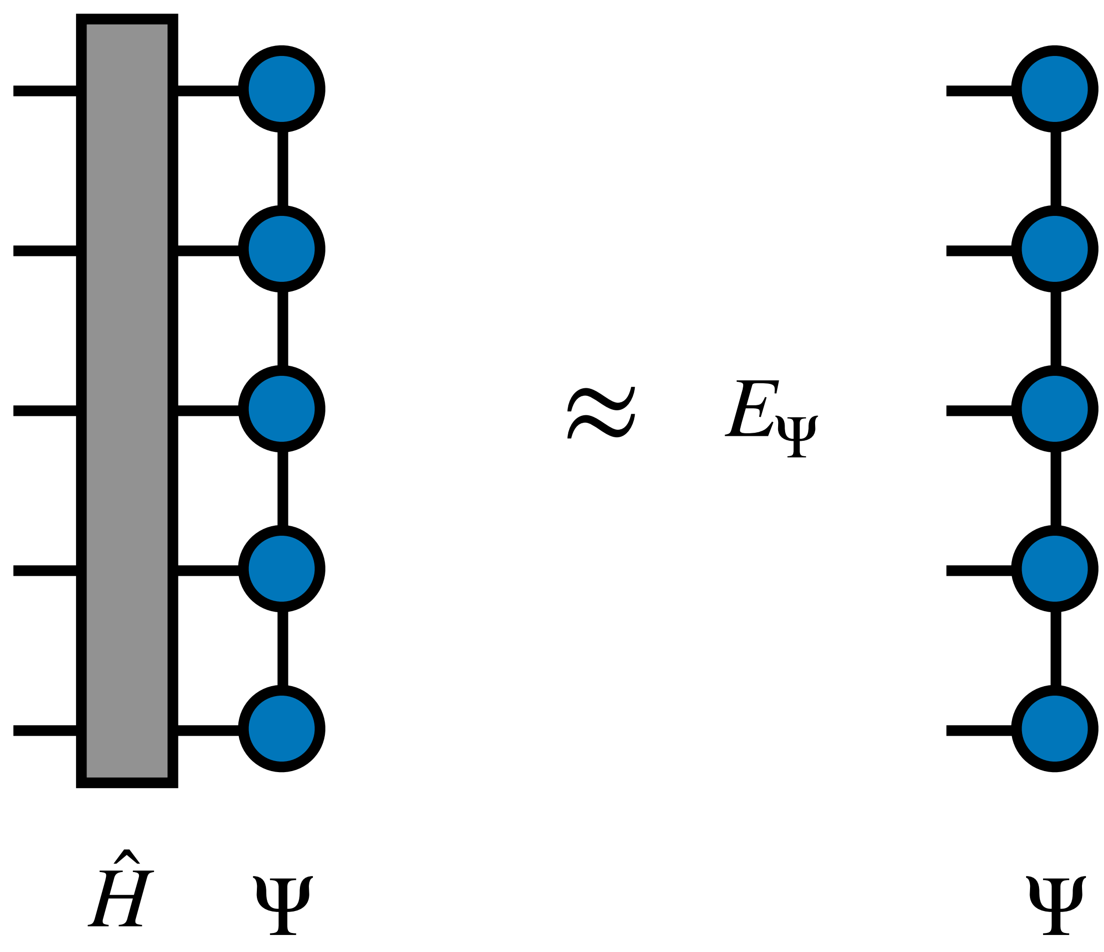


Tensor Network Algorithms

Tensor networks offer powerful algorithms

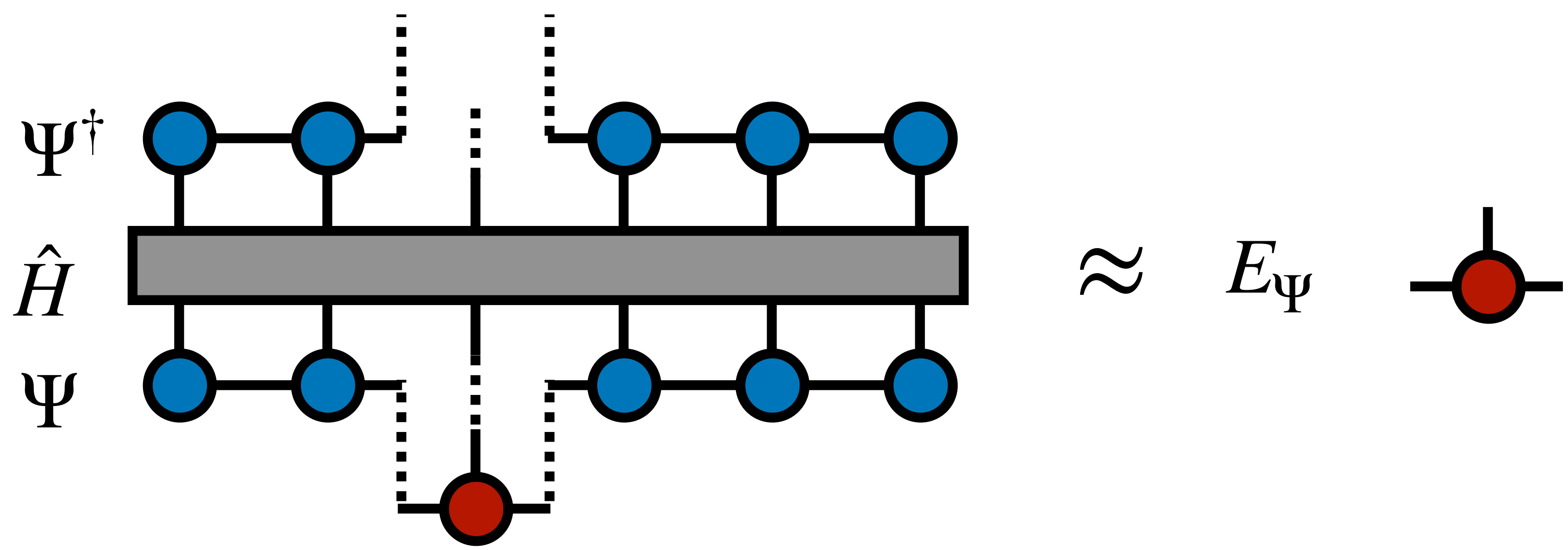
Seminal example is eigenvector finding
Known as "DMRG algorithm" in quantum phys. literature



Tensor Network Algorithms

Eigenvector-finding algorithm (DMRG)
extremely efficient

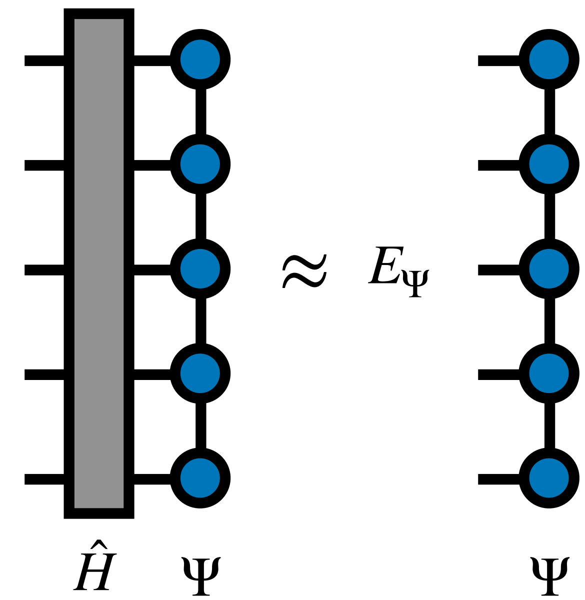
Each step solves a projected eigenvalue equation



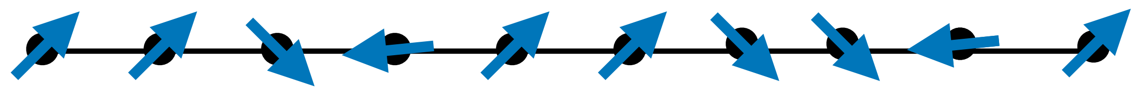
Can use fast methods (Lanczos, etc.)
Much faster than e.g. gradient optimization

Tensor Network Algorithms

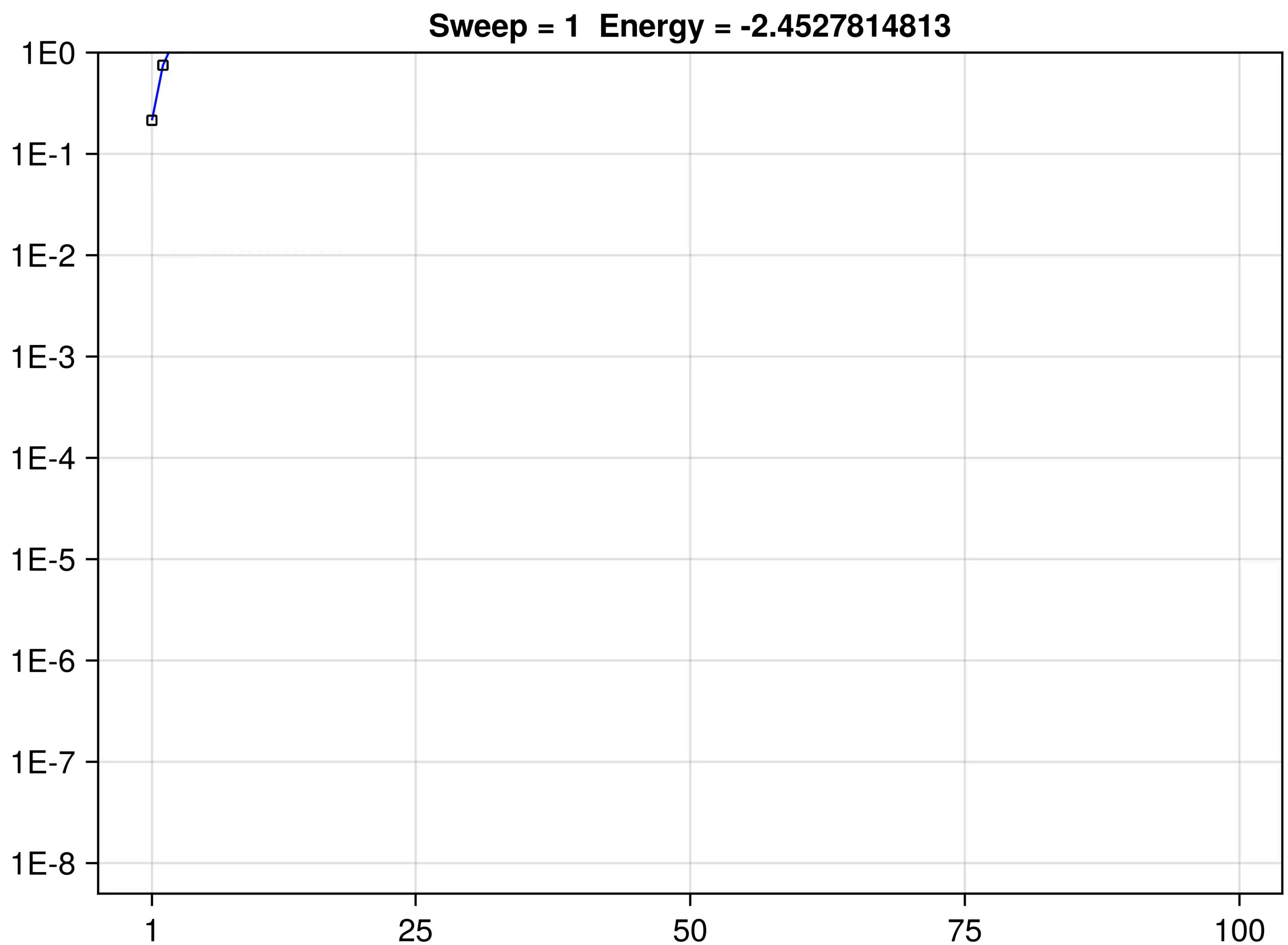
Movie of DMRG solving a one-dimensional quantum spin chain system (N=100, S=1)



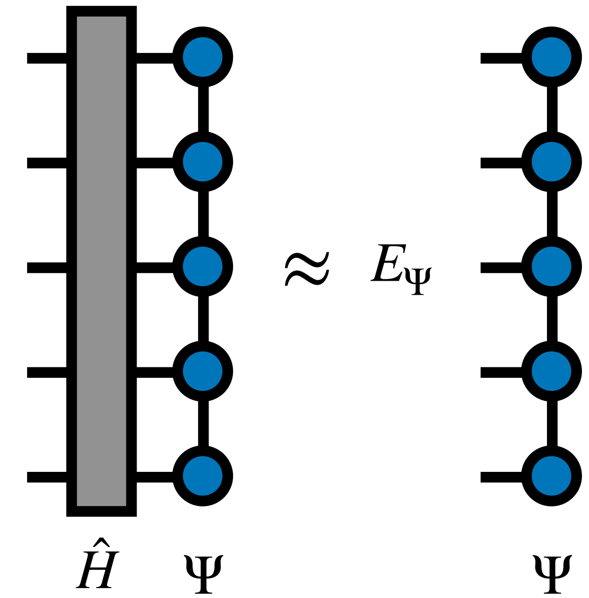
$$\hat{H} = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$$



Local energy error from converged result

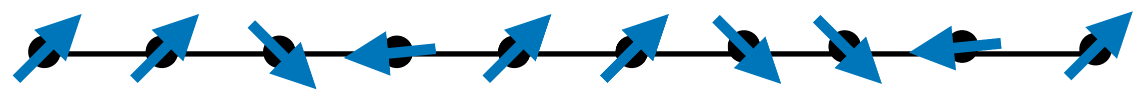


Tensor Network Algorithms

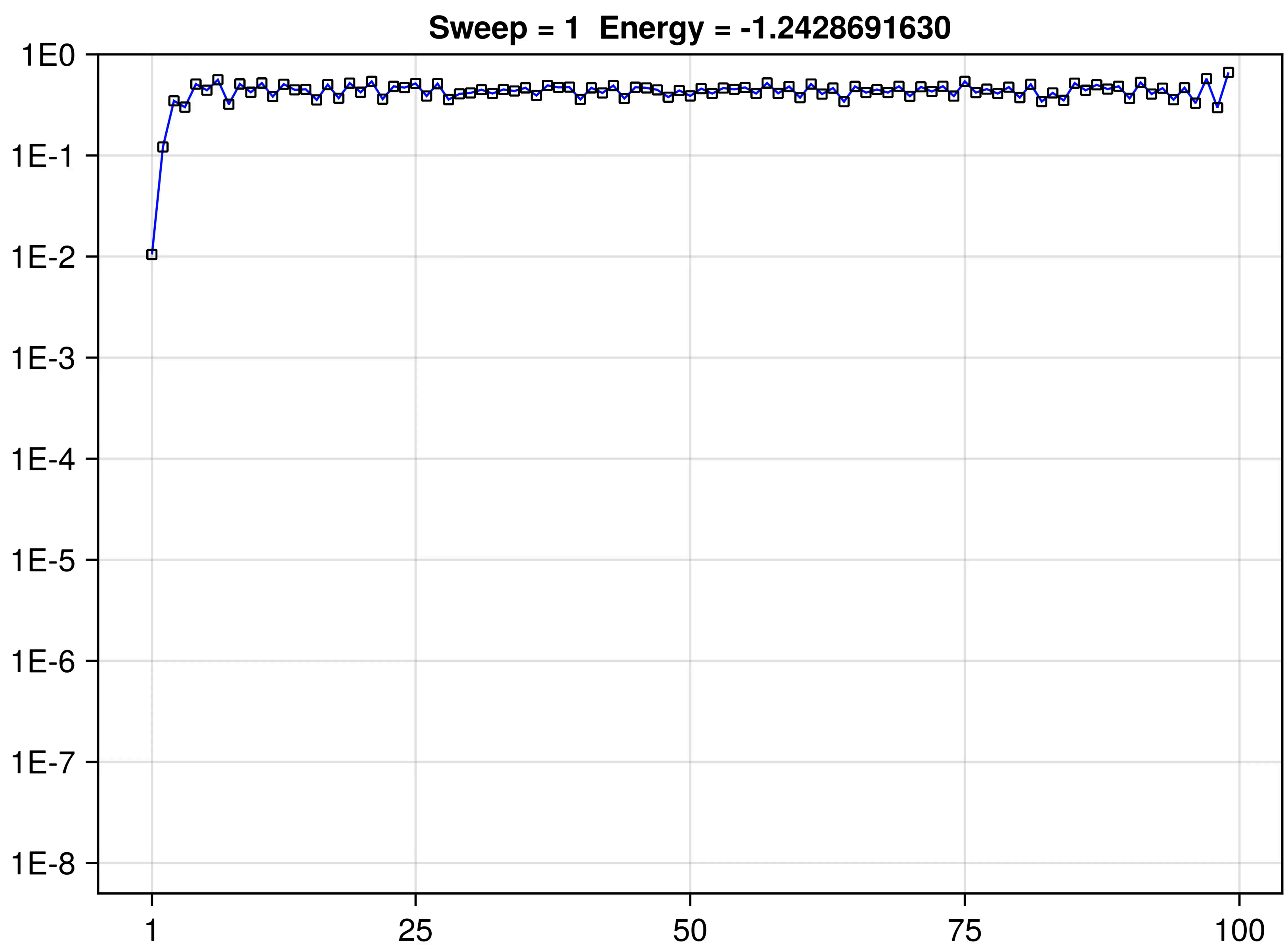


Movie of DMRG solving a one-dimensional quantum spin chain system (N=100, S=1/2)

$$\hat{H} = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$$



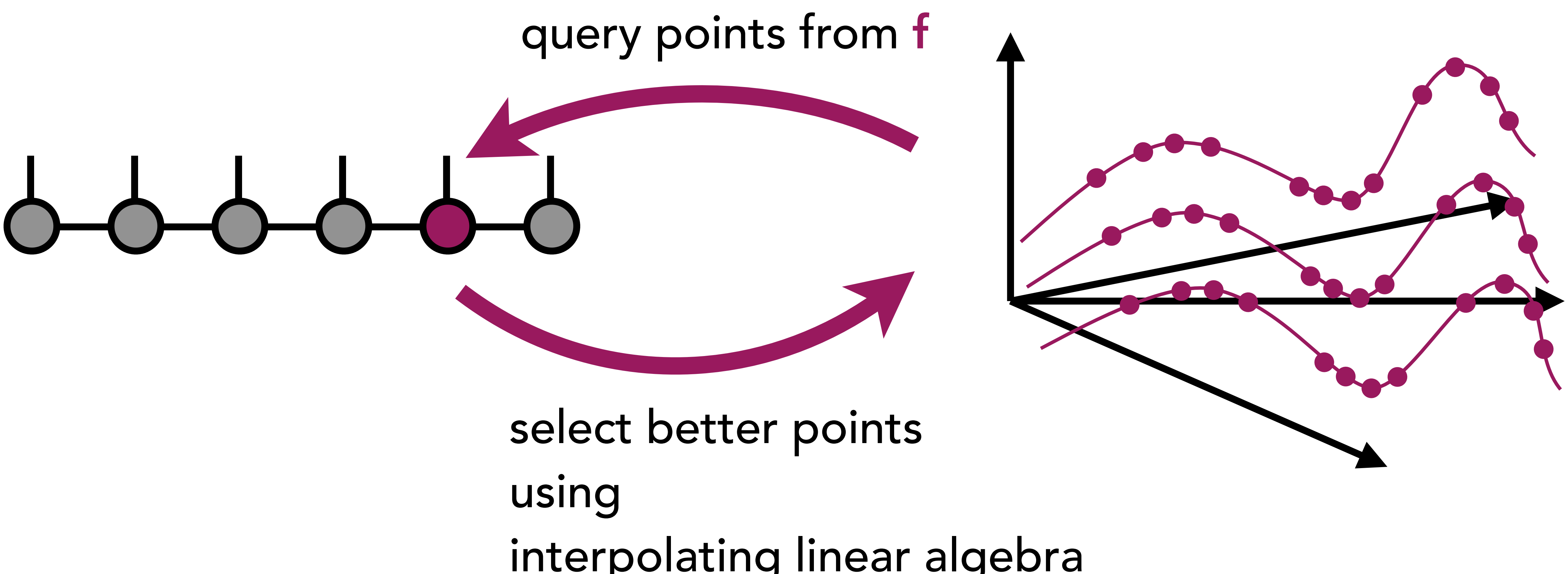
Local energy error from converged result



Tensor Network Algorithms

A lesser-known algorithm from math literature
is **tensor cross interpolation** (TCI) [1,2]

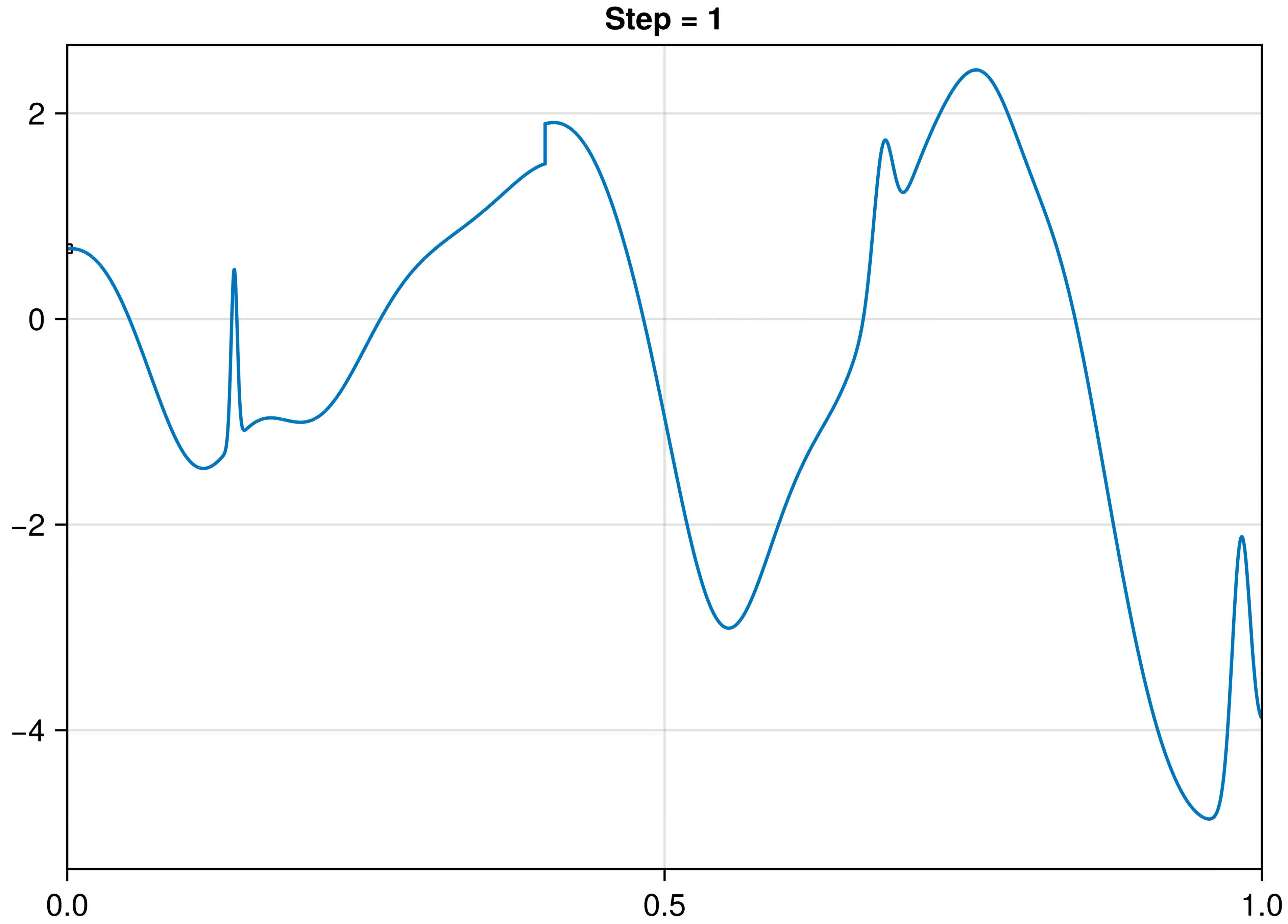
It is an **active machine learning** method for tensor networks



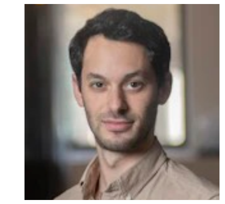
[1] I. Oseledets and E. Tyrtyshnikov, Linear Algebra Appl. 432, 70 (2010)
[2] Nunez Fernandez, et al. Phys. Rev. X 12, 041018 (2022)

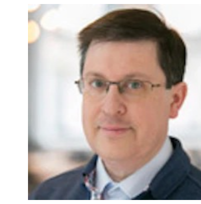
Tensor Network Algorithms

Demo of tensor cross interpolation (TCI)
for learning a function (sum of 40 Gaussians)

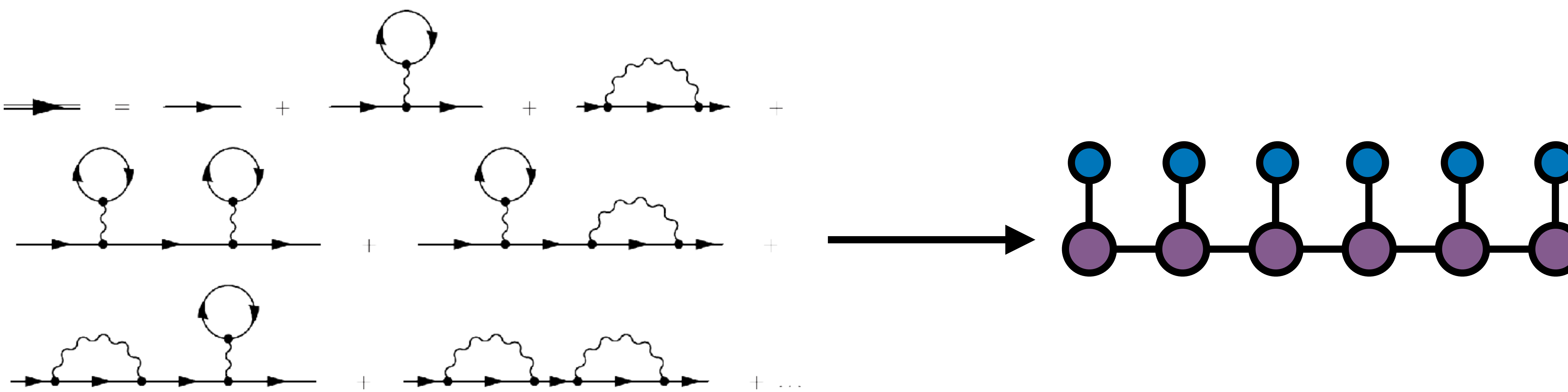


Tensor Network Algorithms


Jason Kaye
CCQ & CCM


Olivier Parcollet
CCQ

Researchers at Flatiron Institute and collegues used TCI algorithm to learn and sum entire orders of Feynman diagrams*



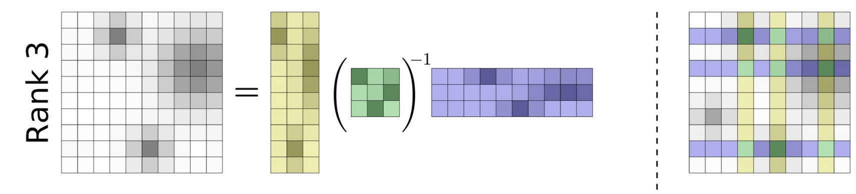
Result: time-dependent properties of *quantum dots*
Compute once for any driving protocol

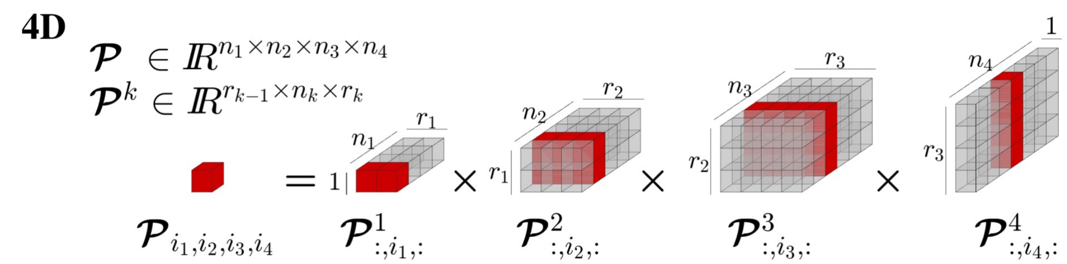
* Nunez Fernandez, et al. Phys. Rev. X 12, 041018 (2022)

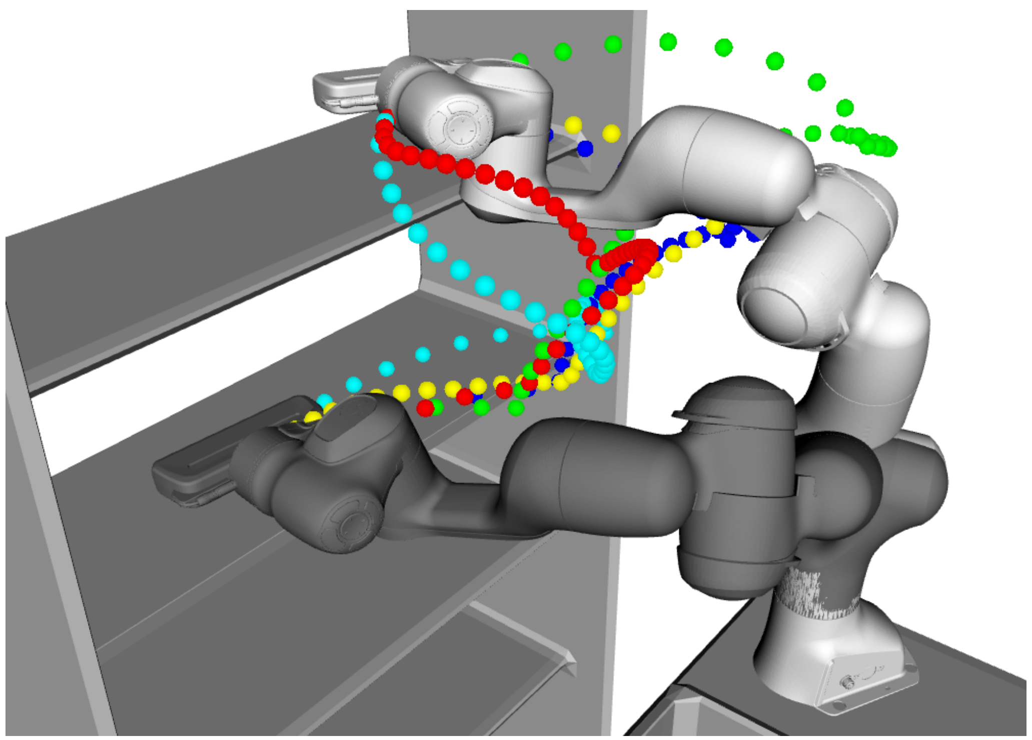
Tensor Network Algorithms

TCI can be harnessed for optimization too

Paper using TCI+optimization to control a robot arm! *







(a)

Figure 1. Solutions from TTGO for motion planning of a manipulator from a given initial configuration (white) to a final configuration (dark). The obtained joint angle trajectories result in different paths for the end.effector which are highlighted by dotted curves in different colors. The multimodality is clearly visible from these solutions.

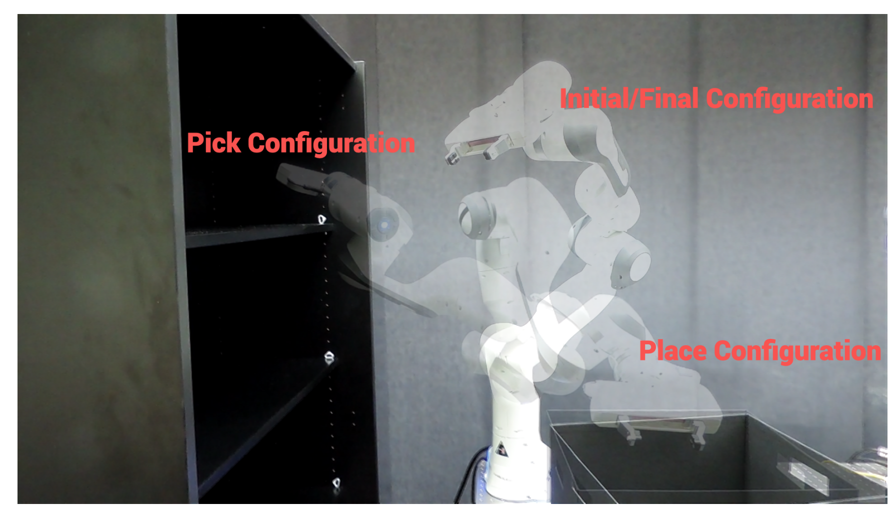


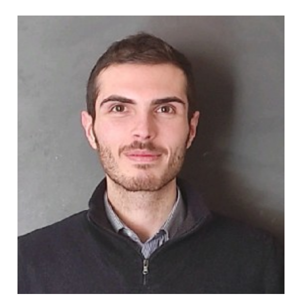
Figure 12. Real robot implementation of one of the TTGO solutions for the pick-and-place task. The motion from the initial configuration to the final configuration (same as the initial configuration in this case) via the picking configuration and placing configuration is depicted.

* Shetty, Lembono, Loew, and Calinon, Tensor Train for Global Optimization Problems in Robotics, Int. J. Robotics Research (2023)

Correcting the Problem of Loops

The "believers"

Joey Tindall



Antonio Mello

Matt Fishman

Dries Sels

Tindall, Mello, Fishman, EMS, Sels, arxiv:2503.05693 (2025)
J. Tindall, M. Fishman, EMS, D. Sels, PRX Quantum, 5, 010308 (2024)
J. Tindall, M. Fishman, SciPost Phys. 15, 222 (2023)

Correcting the Problem of Loops

Simulating dynamics frequently claimed as a source of quantum advantage or utility

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

"physics classical methods can't reach"

The New York Times

Quantum Computing Advance Begins New Era, IBM Says

A quantum computer came up with better answers to a physics

NewScientist

News Features Newsletters Podcasts Video Comment Culture Crosswords | This week's magazine

Health Space Physics Technology Environment Mind Humans Life Mathematics Chemistry Earth Society

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

2023

"beat a supercomputer"

THE WALL STREET JOURNAL.

D-Wave Claims 'Quantum Supremacy,' Beating Traditional Computers

The company said classical computers can't beat its quantum computer in magnetic materials simulation. Some physicists disagree.

By Belle Lin

SCIENTIFIC AMERICAN

MARCH 12, 2025 | 3 MIN READ

Controversial 'Quantum Advantage' Claim Made by Computing Firm D-Wave

The company says it has solved the first problem of scientific relevance with a quantum processor faster than could be done with classical computers—but others disagree

BY DAVIDE CASTELVECCHI & NATURE MAGAZINE

2024

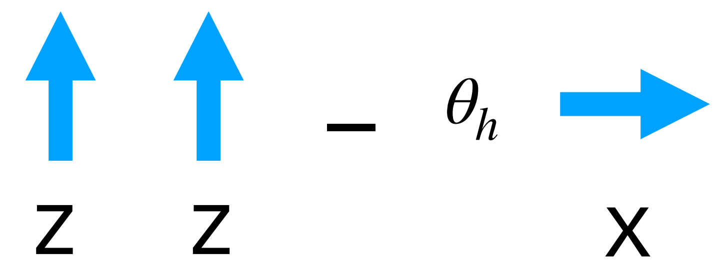
"beating traditional computers"

Correcting the Problem of Loops

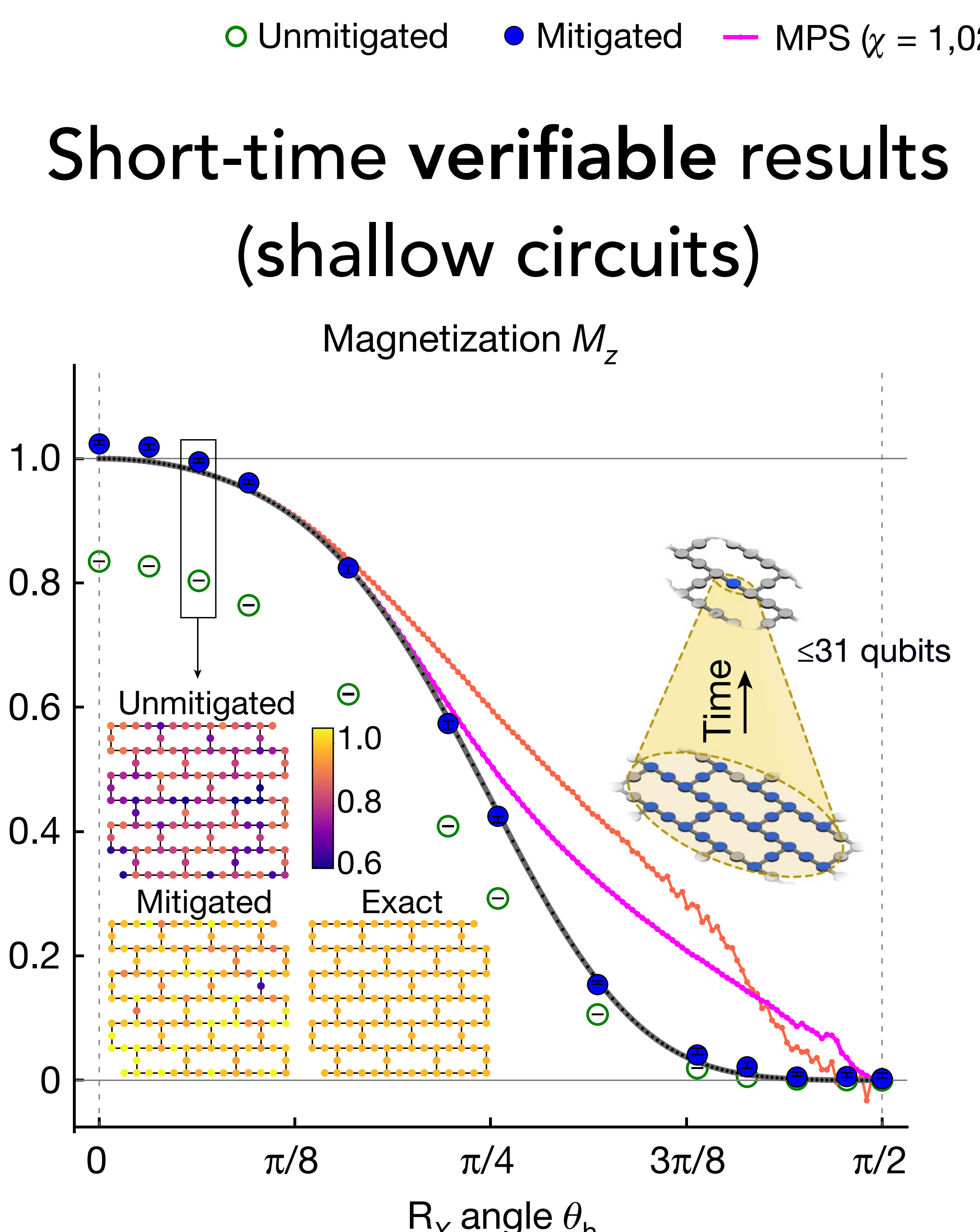
What did such experiments do?

IBM experiment:

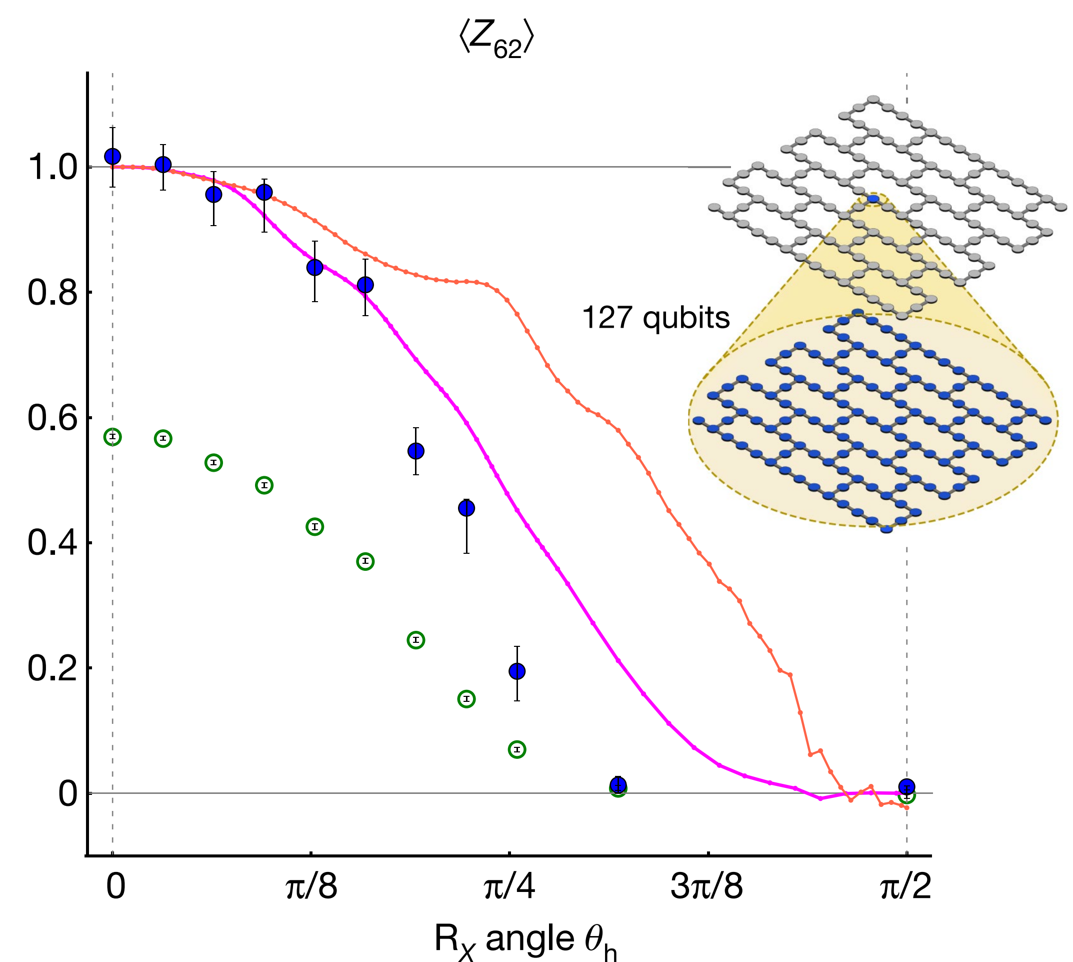
Qubits as quantum Ising "spins":



Short-time **verifiable** results (shallow circuits)



Longer time results (deeper circuits)



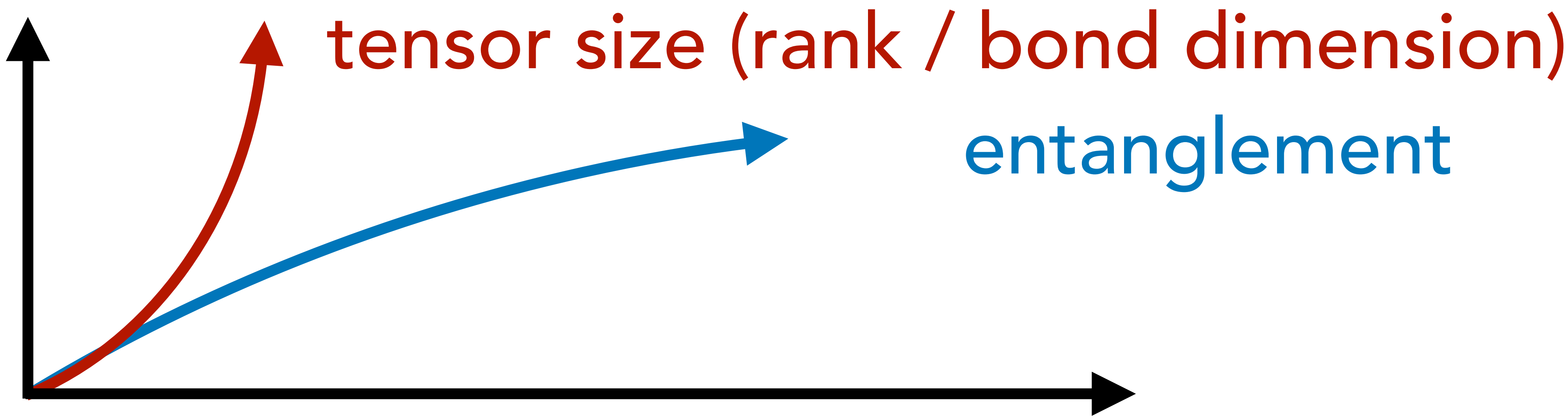
Correcting the Problem of Loops

What's behind such claims?

1. Quantum **dynamics is challenging** for classical approaches

Quantum Monte Carlo 🎲 → complex phase / sign problem

Tensor networks – growth of entanglement in time

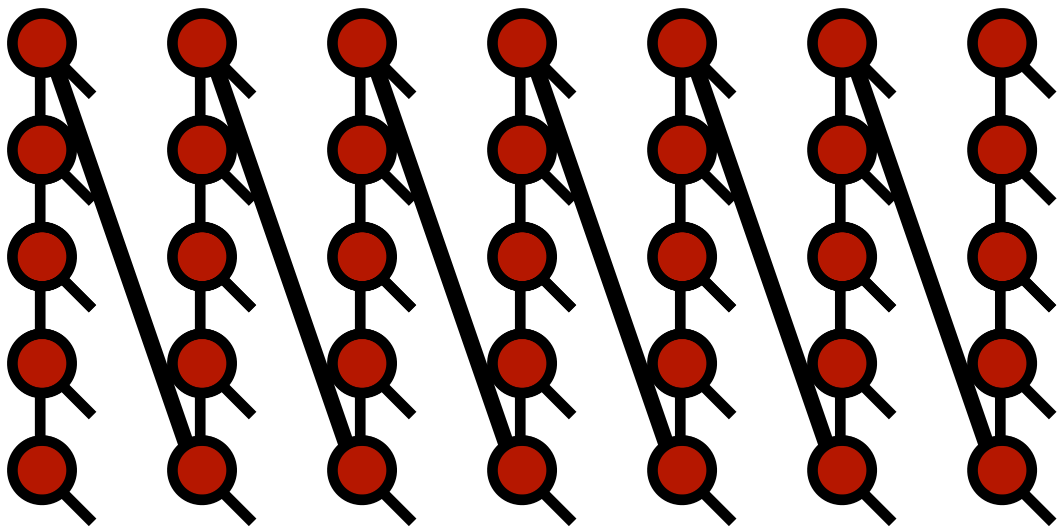


More entanglement = larger tensors, more expensive

Correcting the Problem of Loops

What underlies such claims?

2. **Two-dimensional systems** more challenging for tensor networks

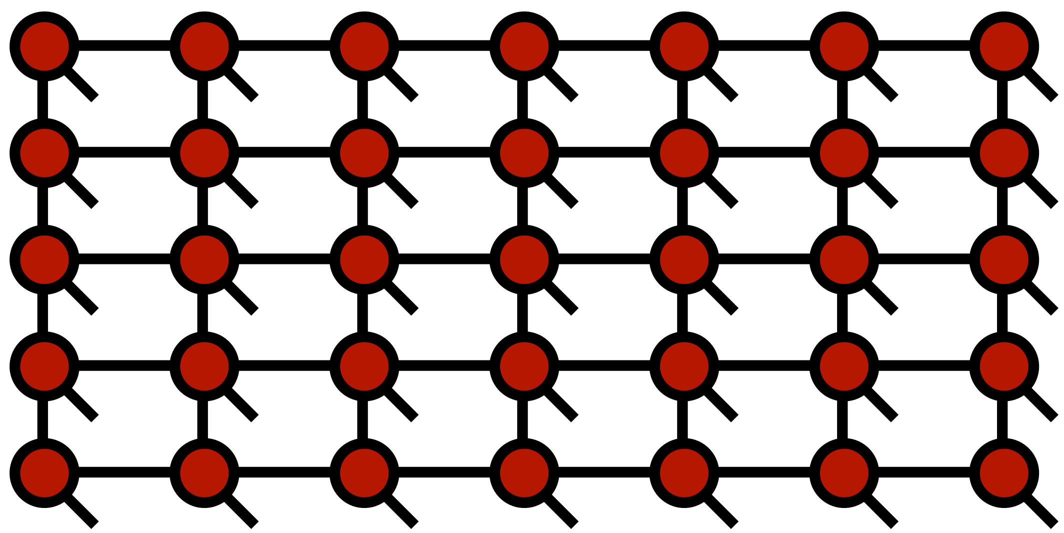


1D MPS tensor network – blowup of bond size necessary to capture 2D correlations

Correcting the Problem of Loops

What underlies such claims?

2. **Two-dimensional systems** more challenging for tensor networks



2D tensor network – popular optimization algorithms often scale poorly

Correcting the Problem of Loops

Will 2D dynamics always be hard for classical?
The situation is rapidly changing...

The key, as always, is
new algorithms... just have to "believe"

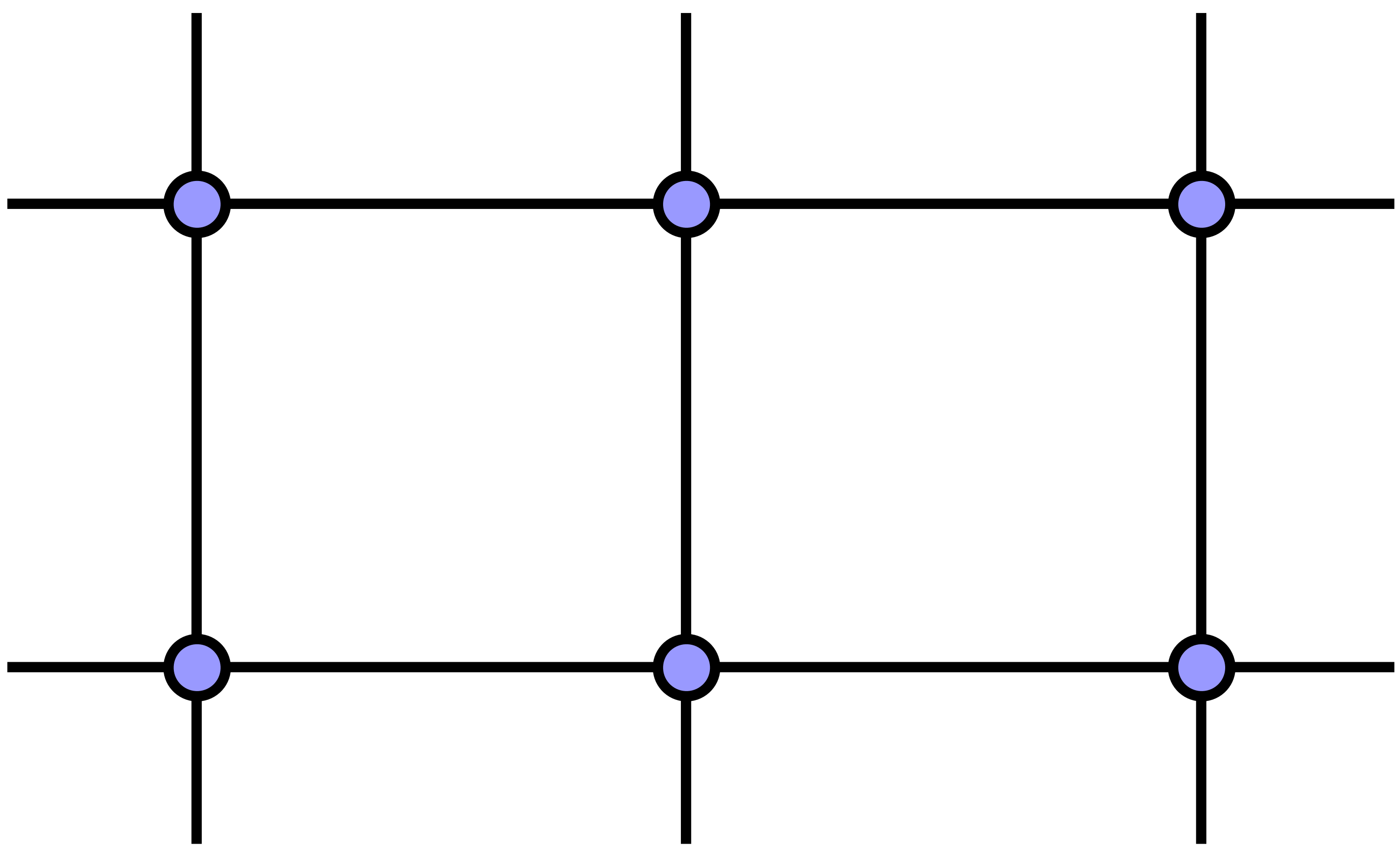
Correcting the Problem of Loops

New algorithm:

belief propagation (very old algorithm)

+ tensor networks

= very affordable 2D and 3D quantum dynamics



Correcting the Problem of Loops

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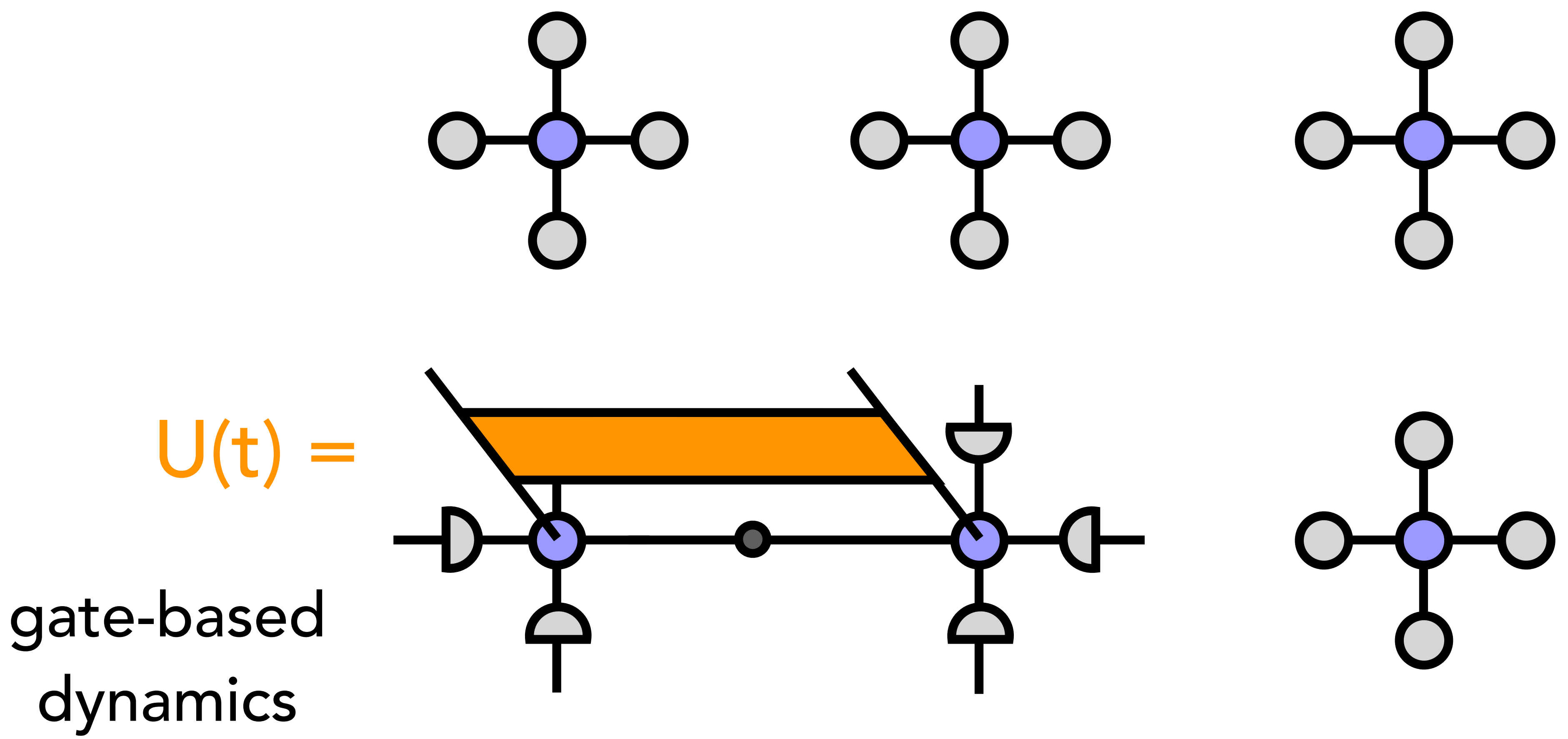


Belief propagation has been around for some time

Hans Bethe
statistical mechanics (1935)

Statistical Theory of Superlattices

By H. A. Bethe, H. H. Wills Physical Laboratory, University of Bristol

(*Communicated by W. L. Bragg, F.R.S.—Received February* 13, 1935)

Judea Pearl
probabilistic inference (1982)

REVEREND BAYES ON INFERENCE ENGINES: A DISTRIBUTED HIERARCHICAL APPROACH(*)(**)

Judea Pearl
Cognitive Systems Laboratory
School of Engineering and Applied Science
University of California, Los Angeles

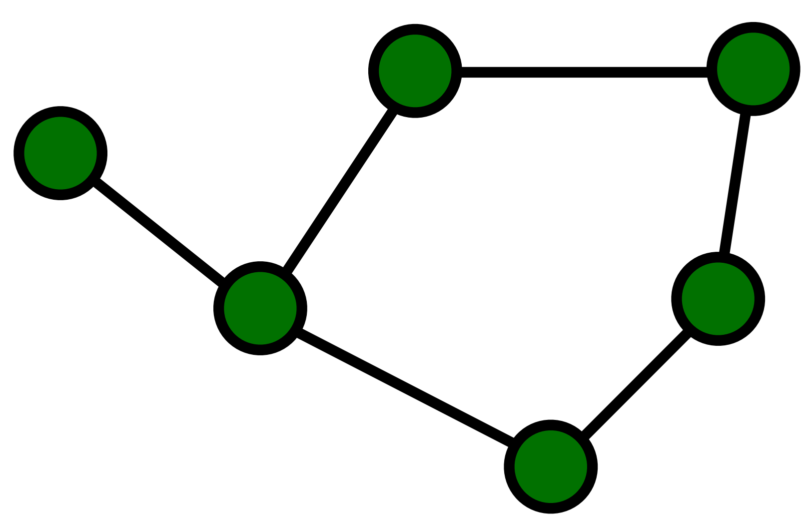
Mezard, Parisi, Virasoro
spin glass physics (1985)

J. Physique Lett. **46**, 217-222 (1985)
DOI: 10.1051/jphyslet:01985004606021700

Random free energies in spin glasses

M. Mézard, G. Parisi et M.A. Virasoro

Originally approximates *marginals* of
locally tree-like graphs (e.g. stat mech models)



Recently adapted to quantum wavefunctions

PHYSICAL REVIEW RESEARCH **3**, 023073 (2021)

Tensor networks contraction and the belief propagation algorithm

R. Alkabetz and I. Arad
Department of Physics, Technion, 3200003 Haifa, Israel

[Submitted on 9 Jun 2022]

Efficient tensor network simulation of quantum many-body physics on sparse graphs

Subhayan Sahu, Brian Swingle

SciPost Physics

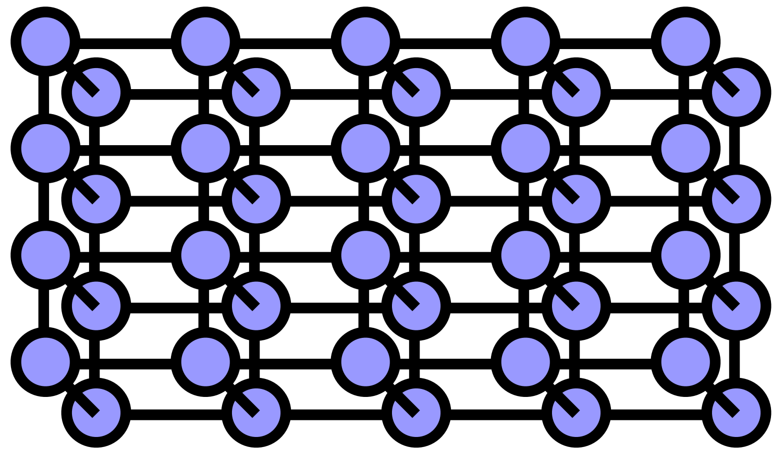
Gauging tensor networks with belief propagation

Joseph Tindall, Matt Fishman

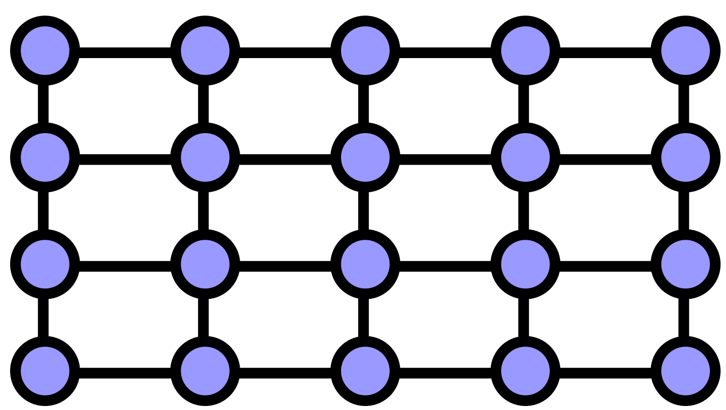
SciPost Phys. 15, 222 (2023) · published 1 December 2023

Alkabetz, Arad, Phys. Rev. Research 3, 023073 (2021
Sahu, Swingle, arxiv:2206.04701
Guo, Poletti, Arad, Phys. Rev. B, **108**, 125111 (2023)
Tindall, Fishman, SciPost Phys. **15**, 222 (2023)

To apply belief propagation to quantum systems, start from "⟨ bra | ket ⟩" network ("norm network")

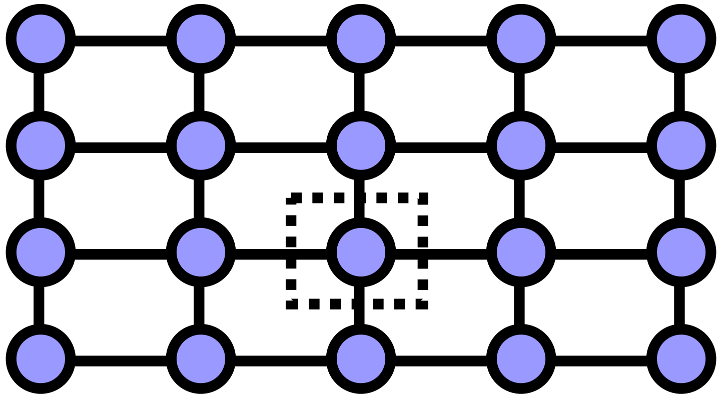


Top-down view



Ideally compute exact "environment"

Defined as network with one tensor removed



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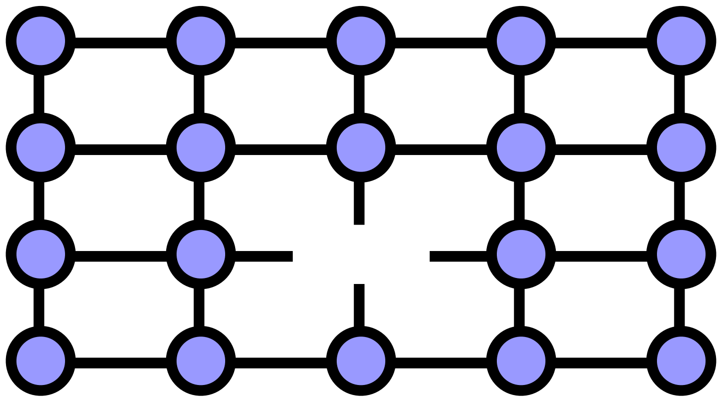
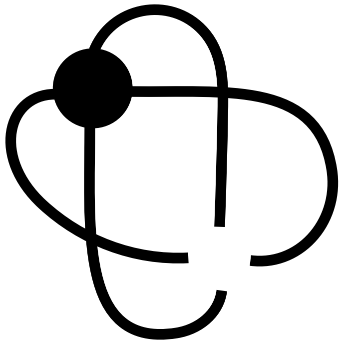


=



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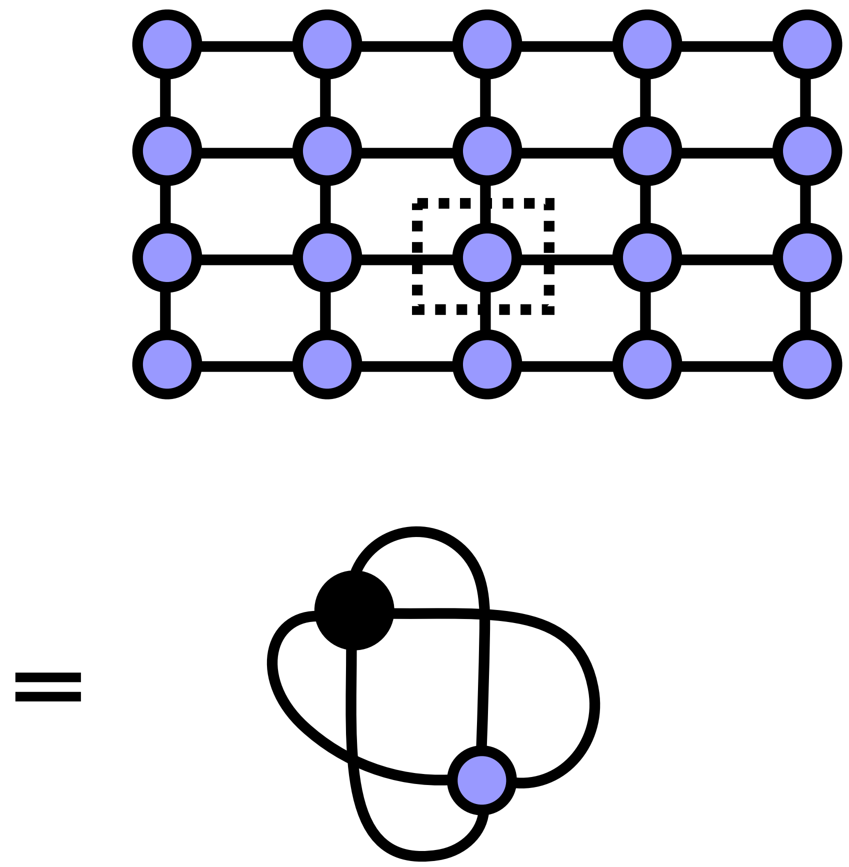
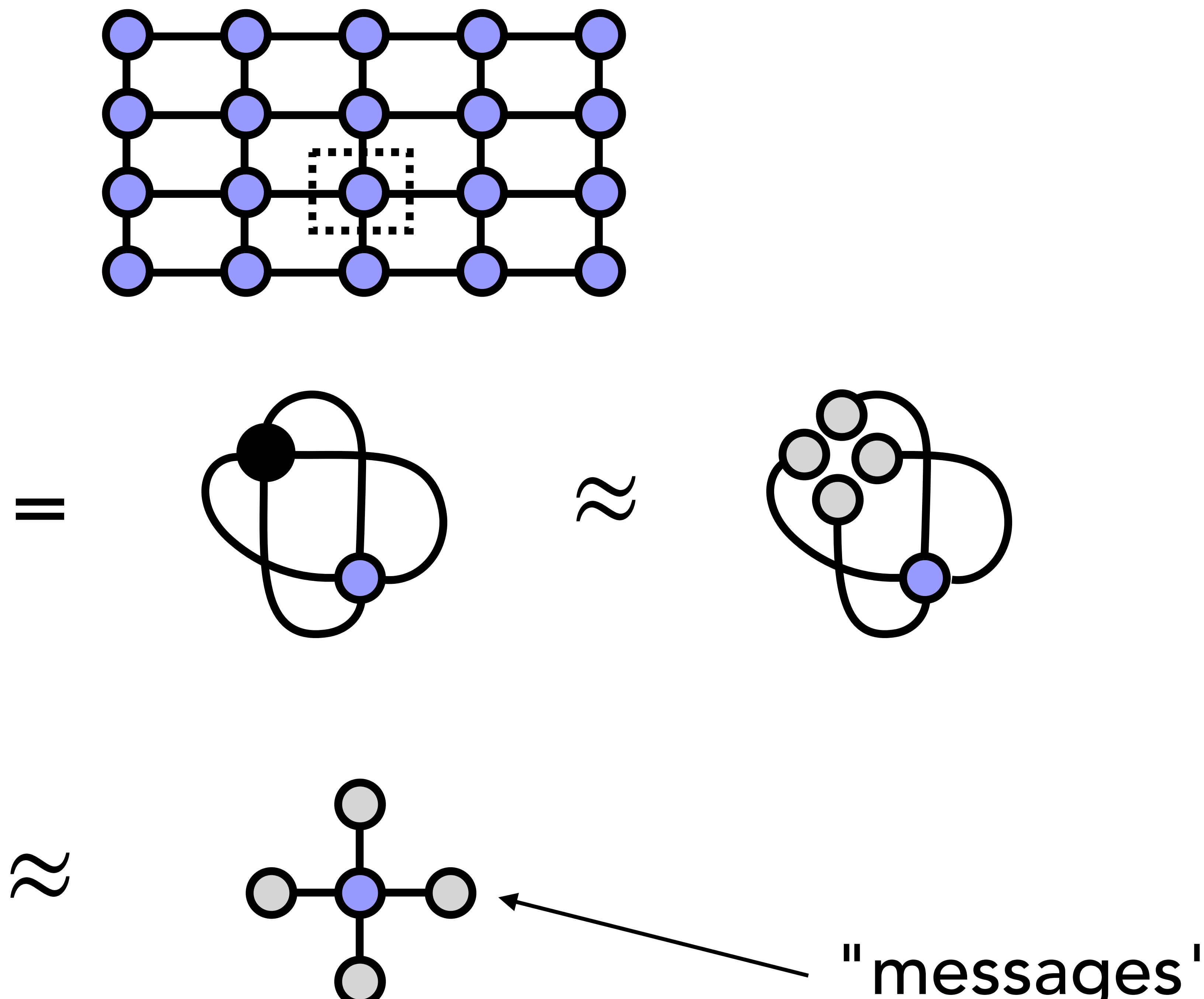
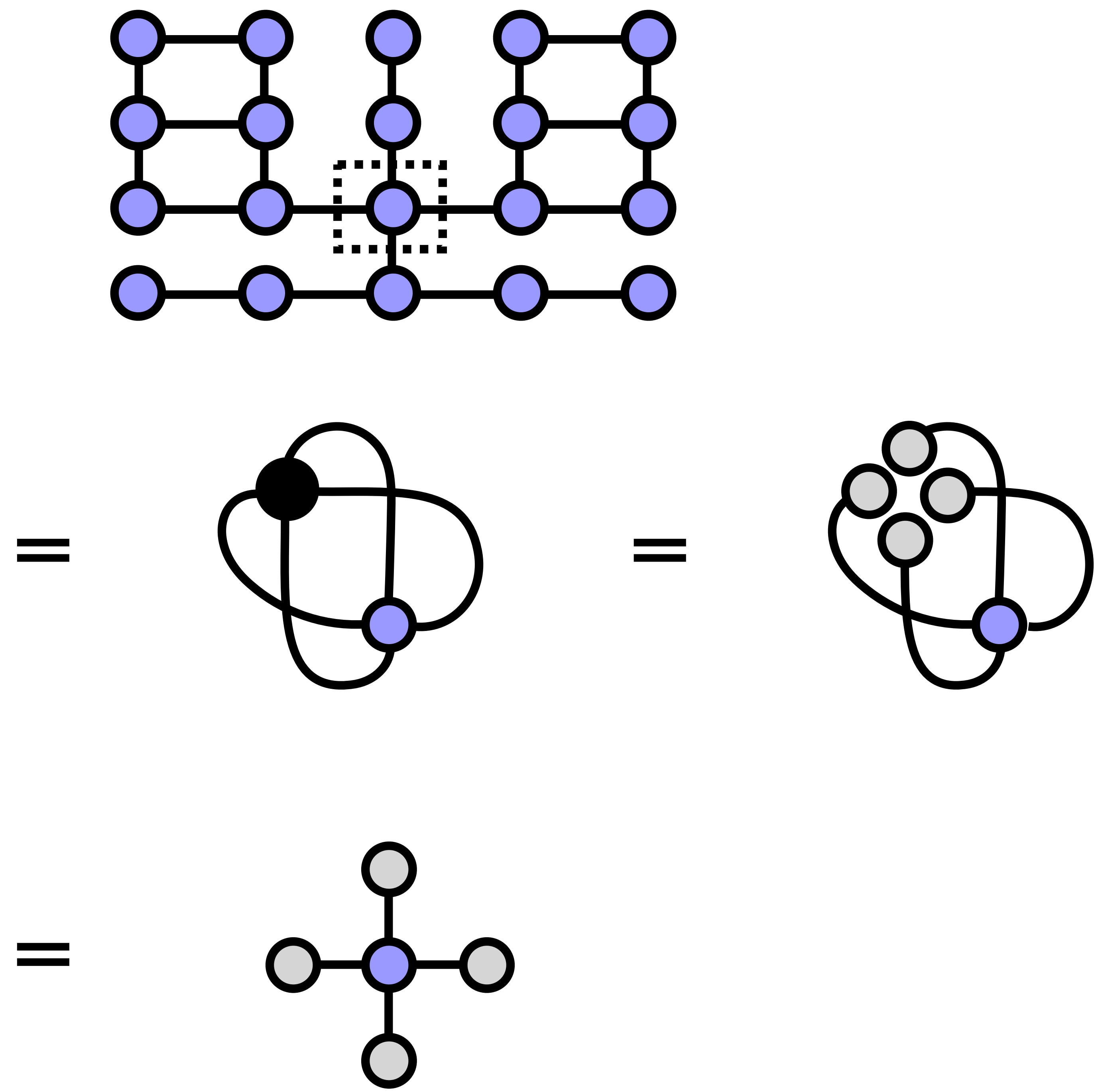


Small (4-index) environment tensor sufficient to contract whole network, but just as hard to compute

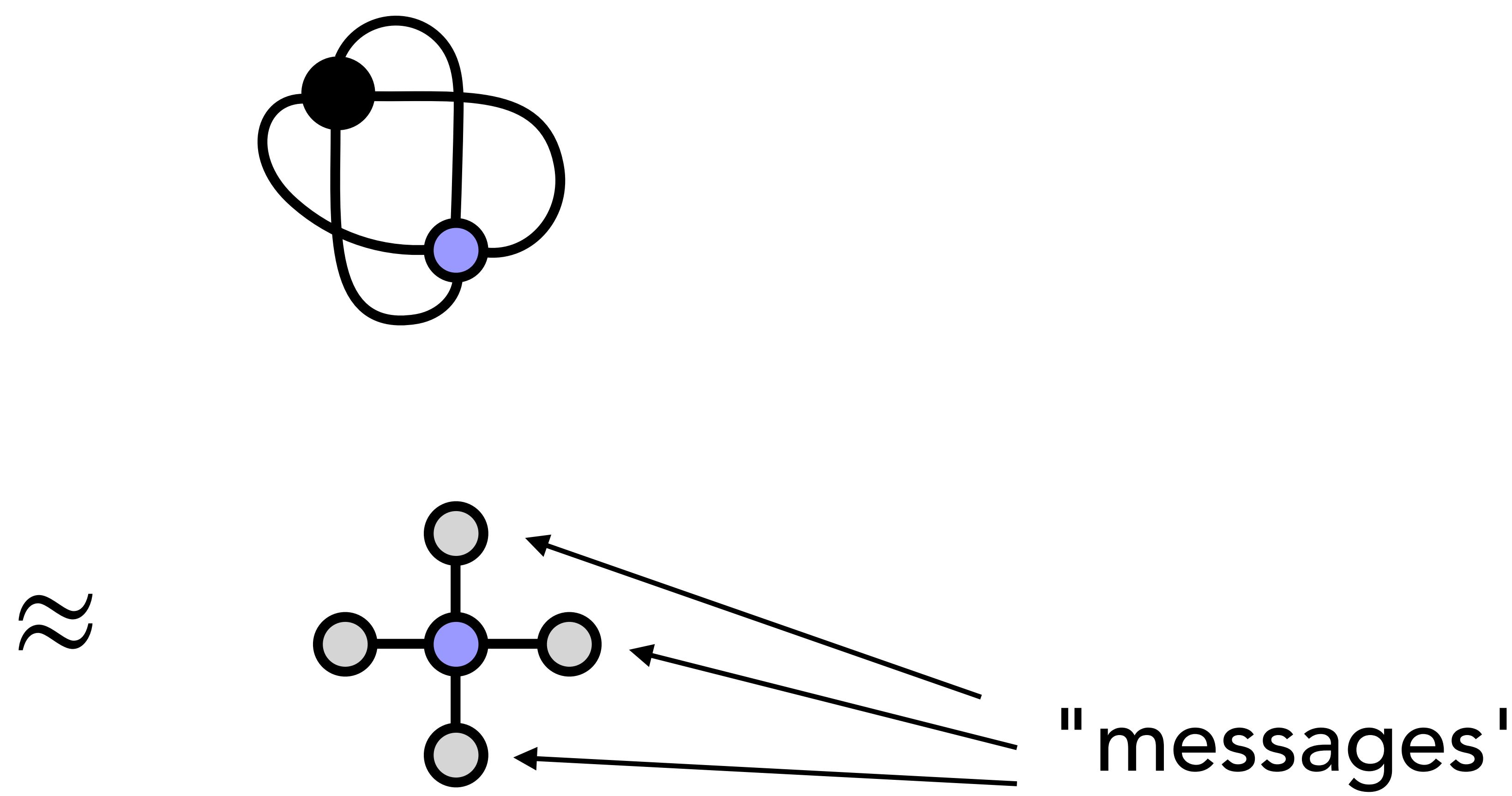
Make seemingly *drastic* approximation



Would be exact if certain loops don't contribute

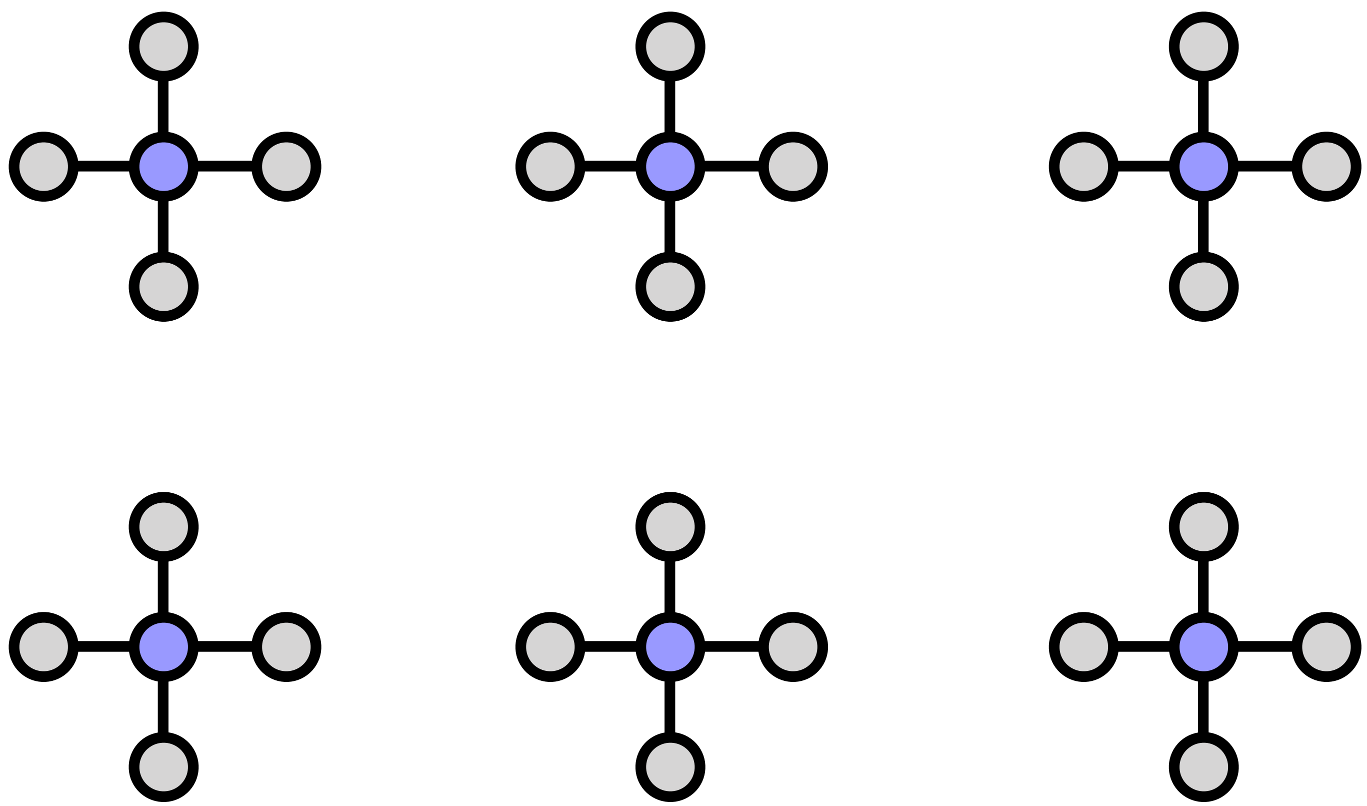


How to find "messages" in practice?



Message Passing

Use "message passing" to converge the messages until self-consistency



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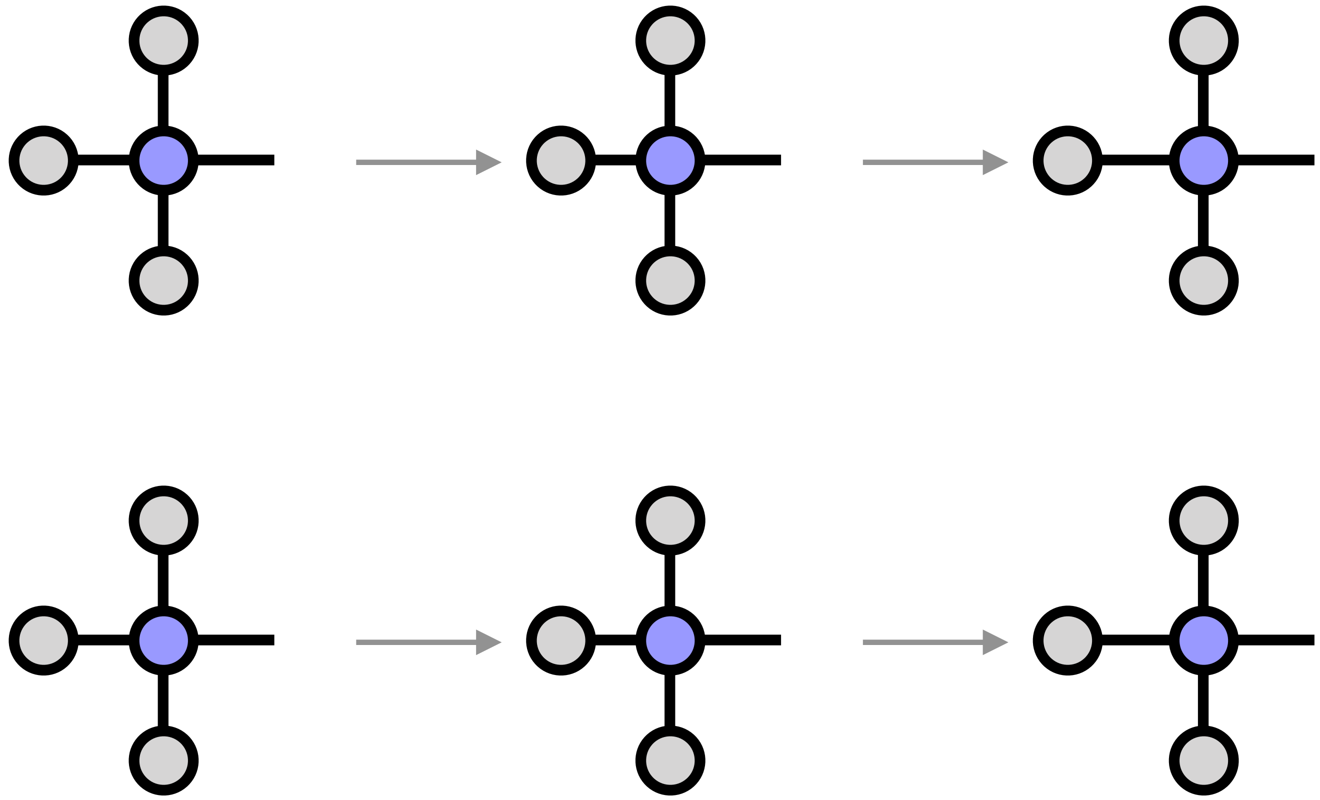

Message Passing

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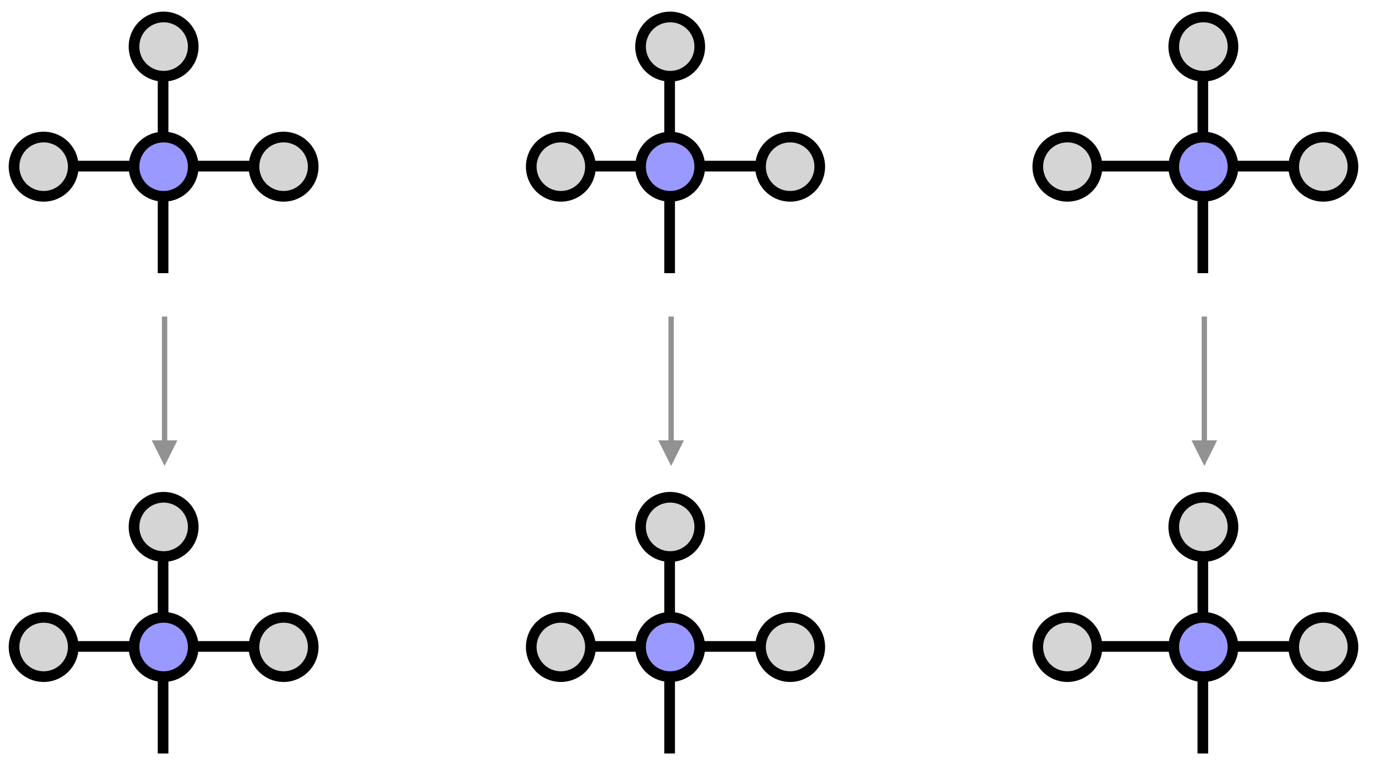

Message Passing

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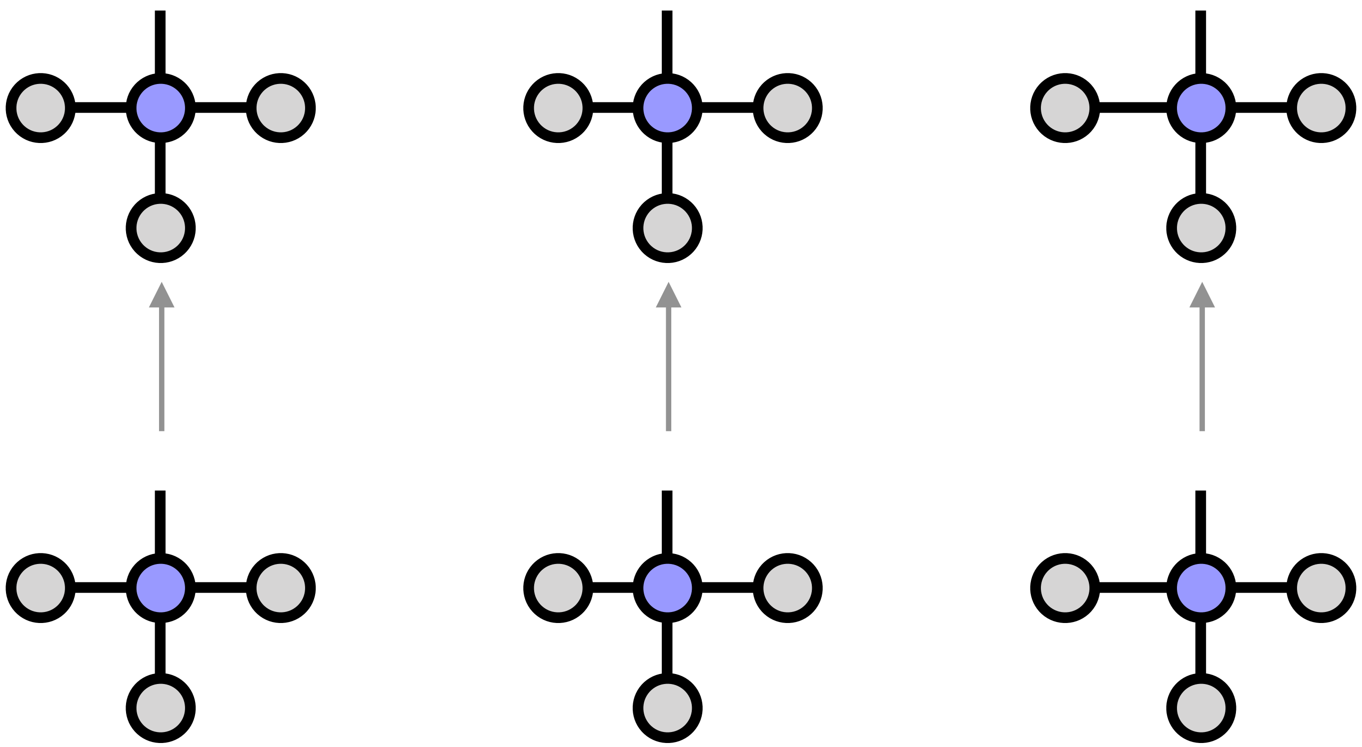
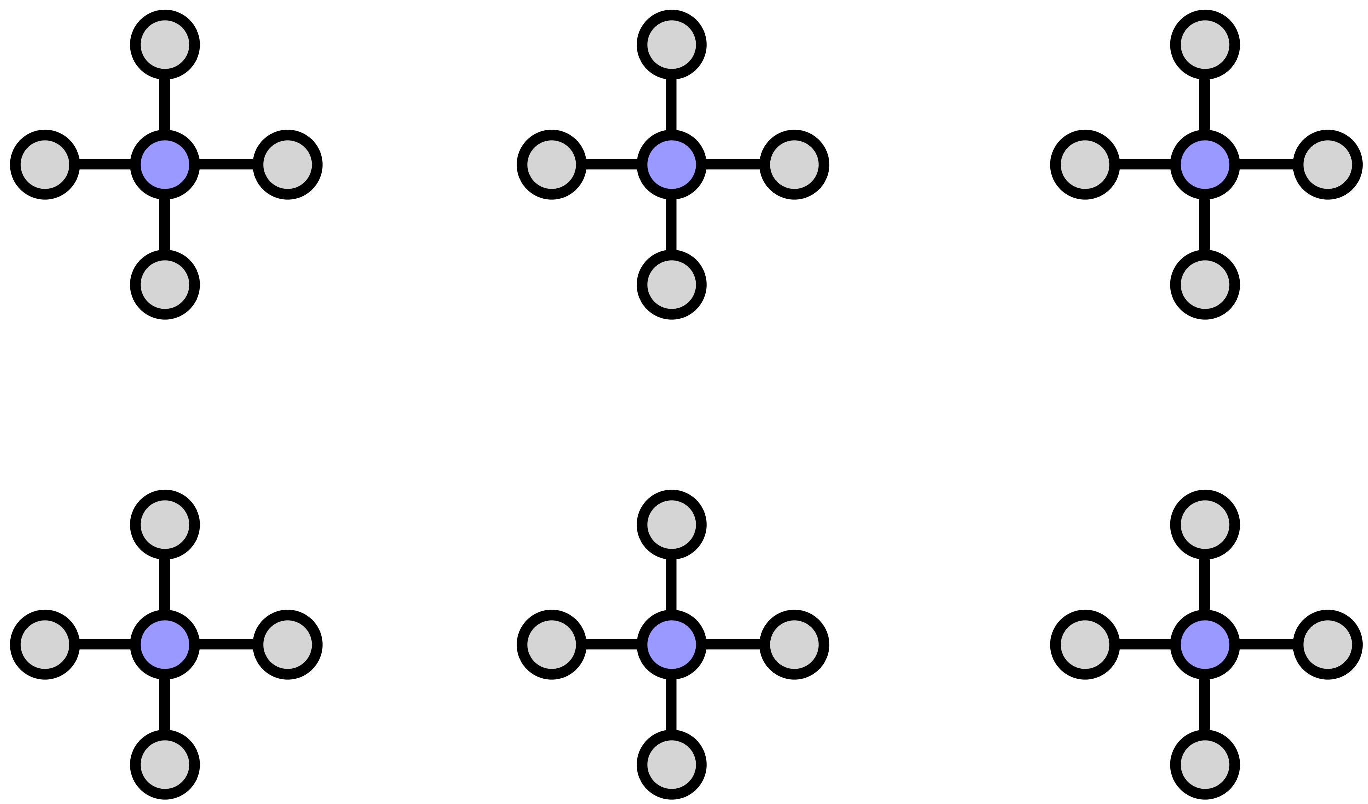
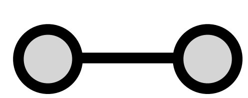


Belief Propagation

After messages converged,
can compute BP estimate of norm ("partition function")

$\langle\psi|\psi\rangle \approx$



Under condition that  $= 1$ for all messages

Belief Propagation

Scaling of quantum belief propagation is

$$O(\chi^{z+1})$$

where z is the *number of neighbors* of the lattice

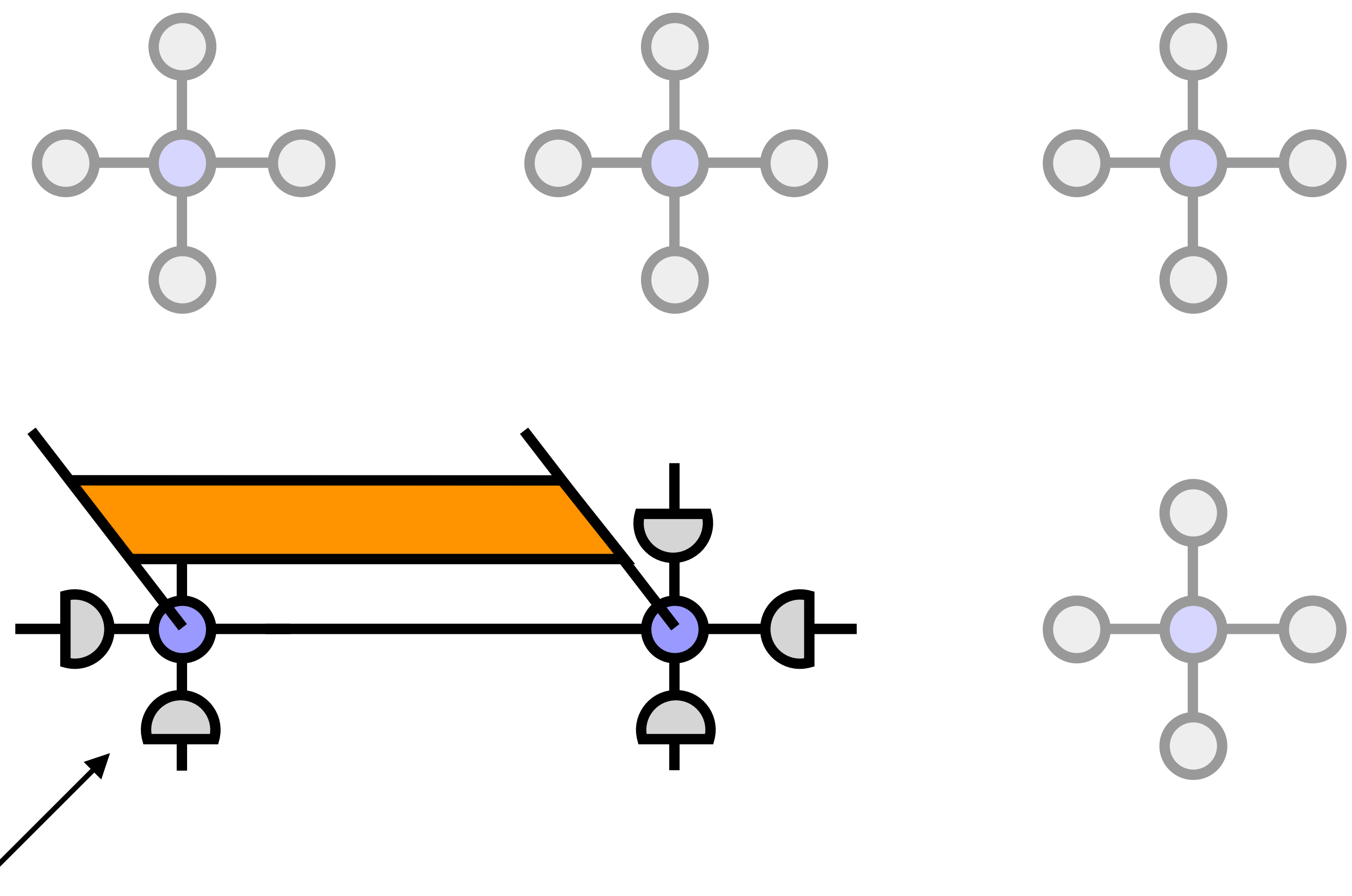
So for square lattice, scaling is $O(\chi^5)$
Compared to scaling and prefactors of other TNS algorithms, generally much better (others $\chi^6 - \chi^{10}$)

More neighbors (higher z) costs more, but lower bond dimensions usually needed (mean field like)

Belief Propagation

Use converged messages to apply gates

U(t) =



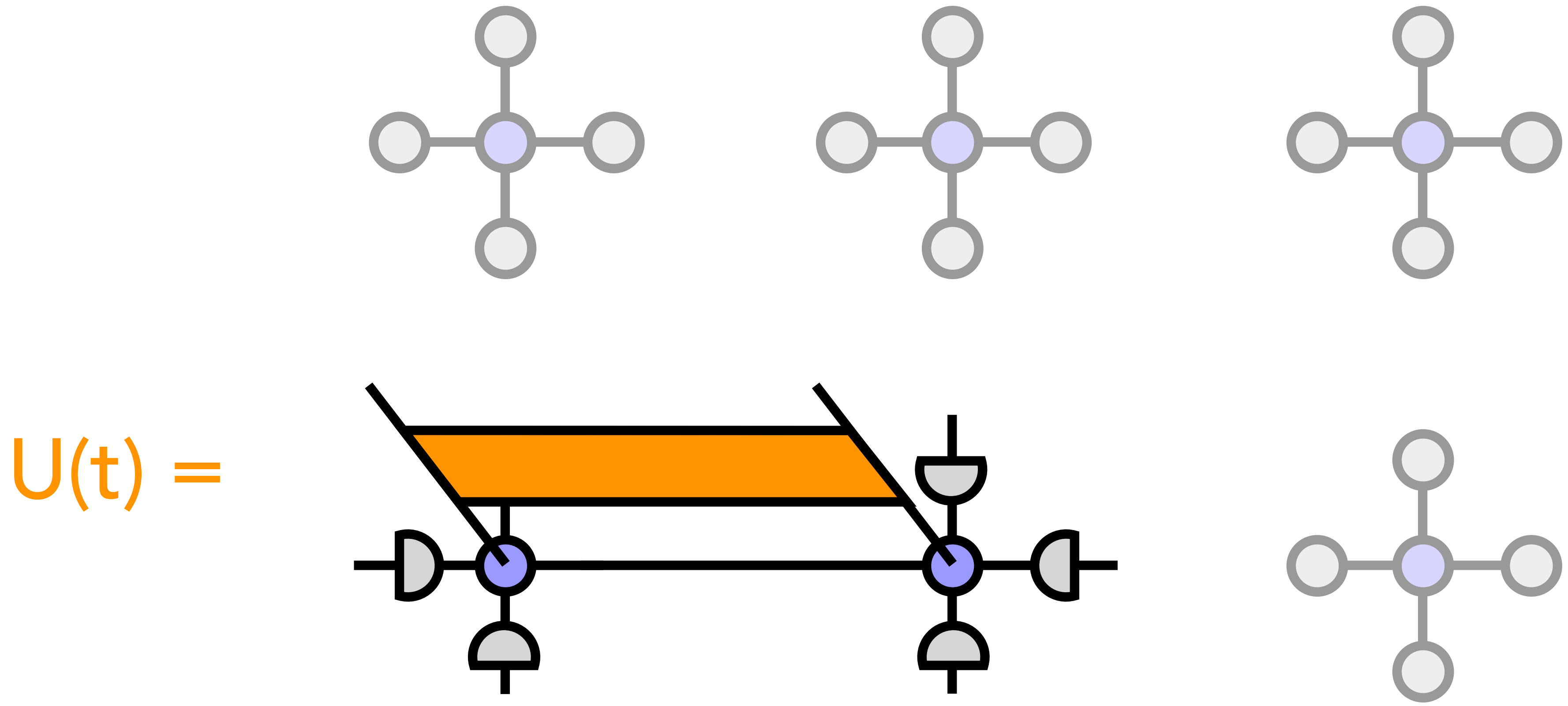
square roots
of messages

Belief Propagation

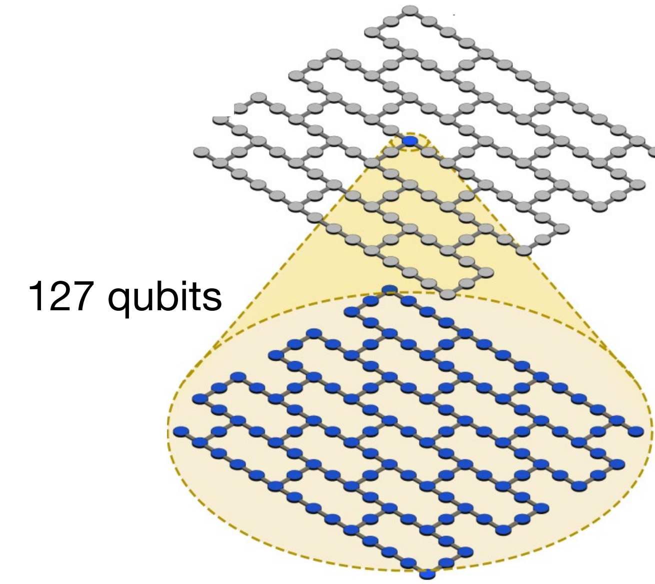
Applying gates lets us:

1) compute ground states & thermal states (imaginary time)

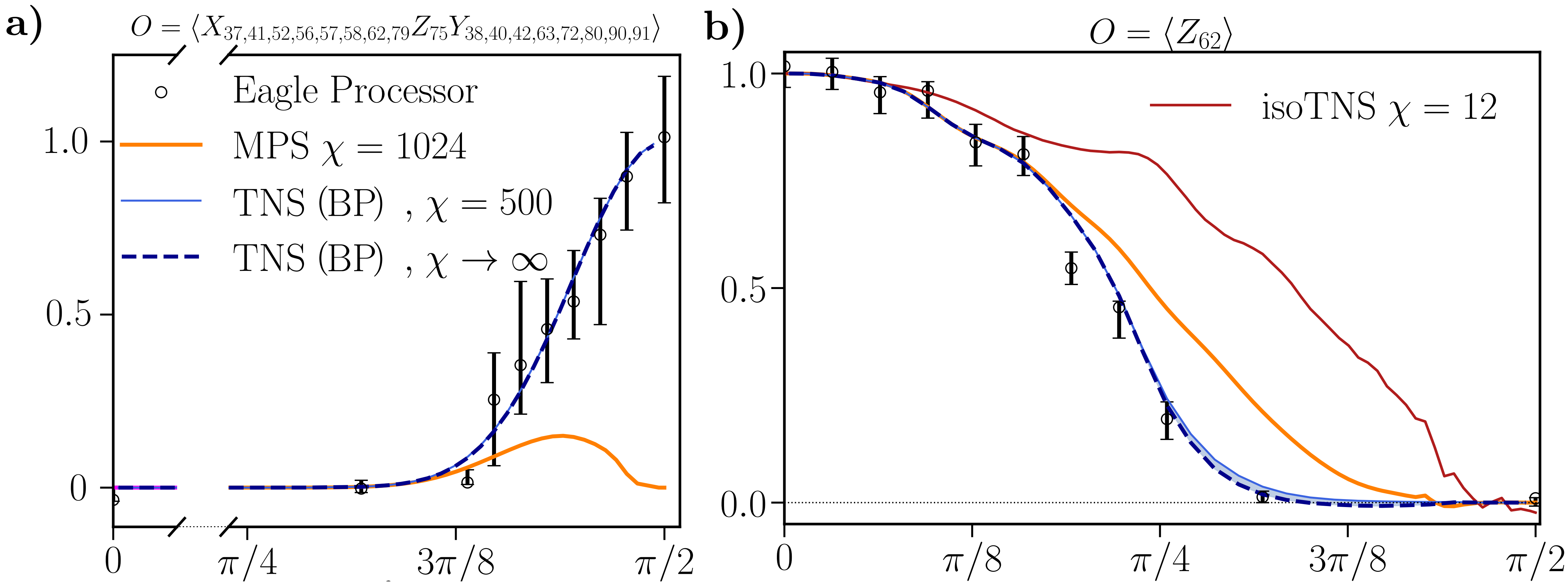
2) compute dynamics (real time)



How well does it work?



Can compute same results as IBM quantum device to large depths / long times:



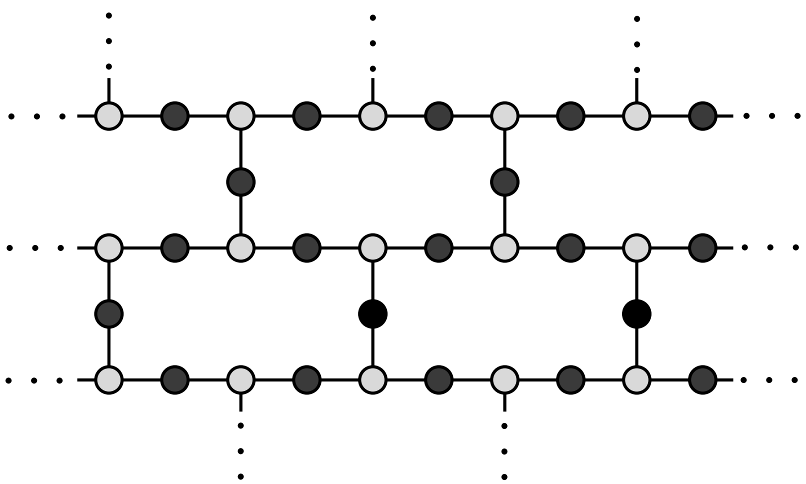
Running times from 5 secs to ~1 day on single cluster node

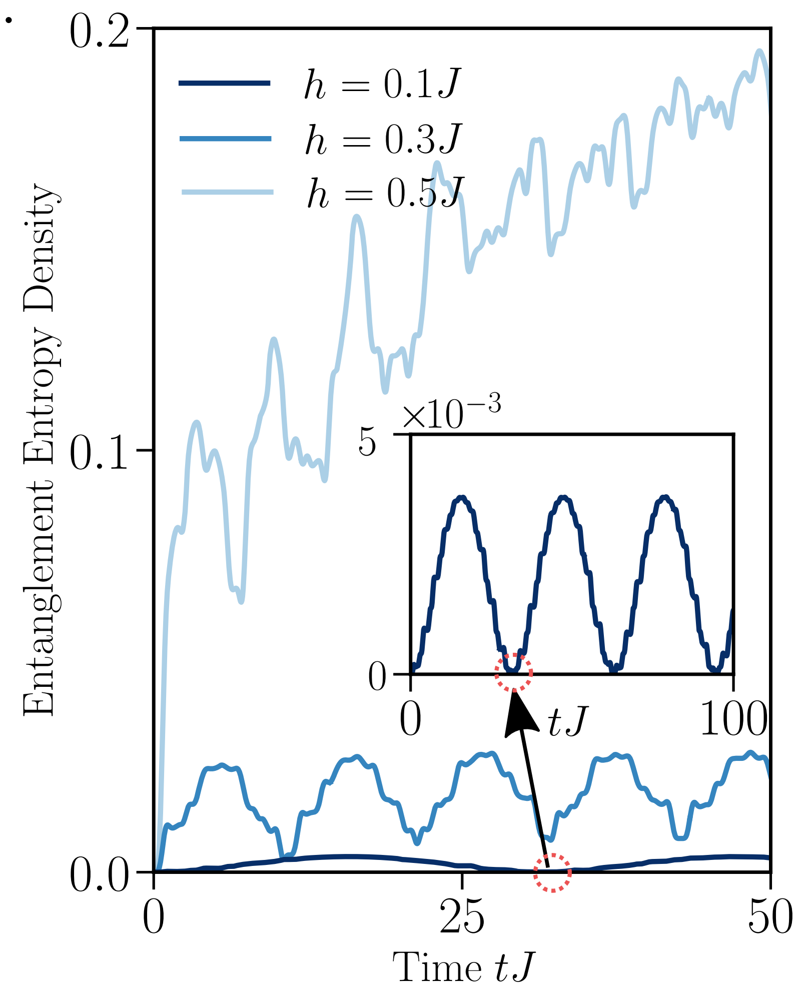
Confinement Physics

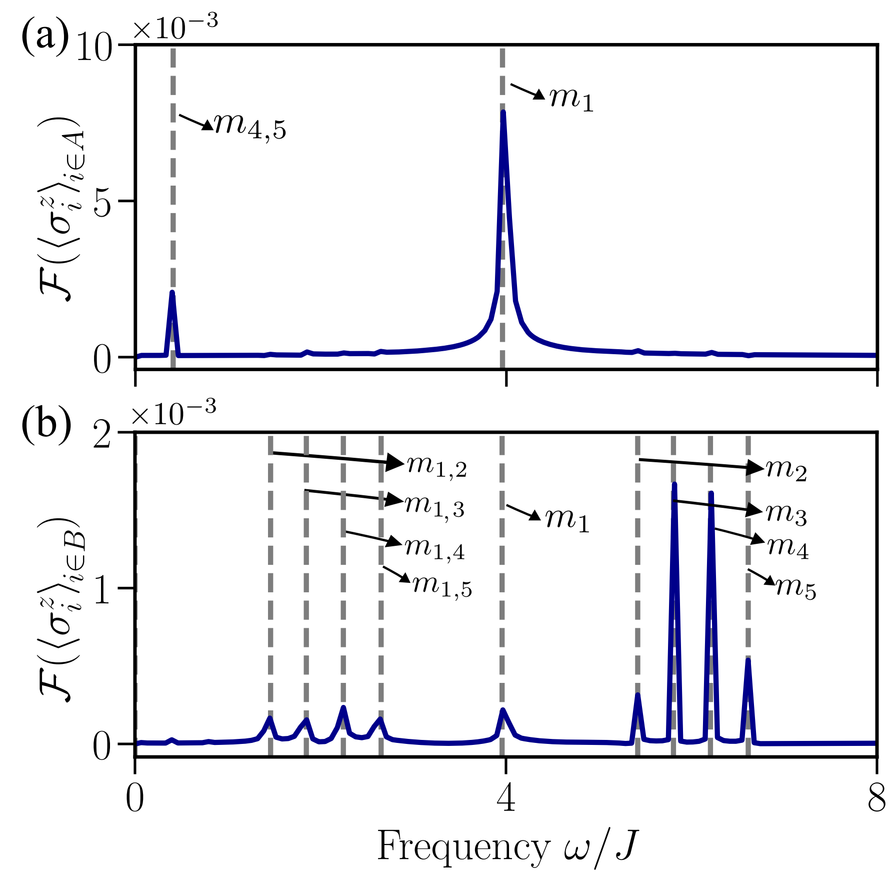
In-depth understanding of the physics

Joey Tindall
Flatiron CCQ

Dries Sels
Flatiron CCQ
NYU



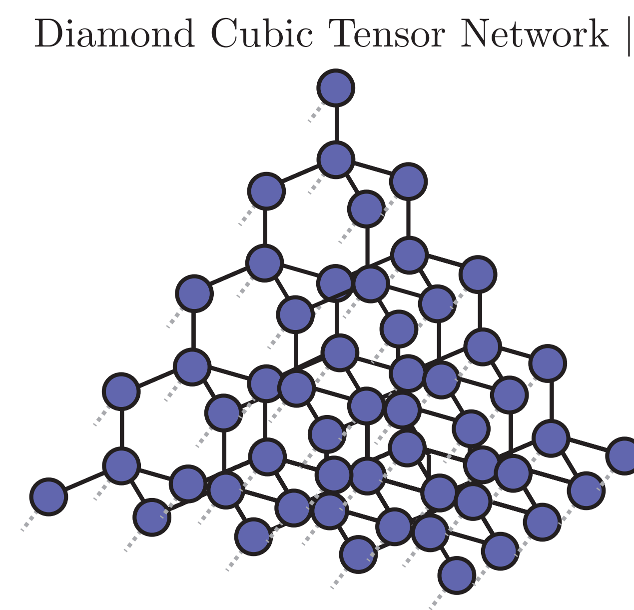




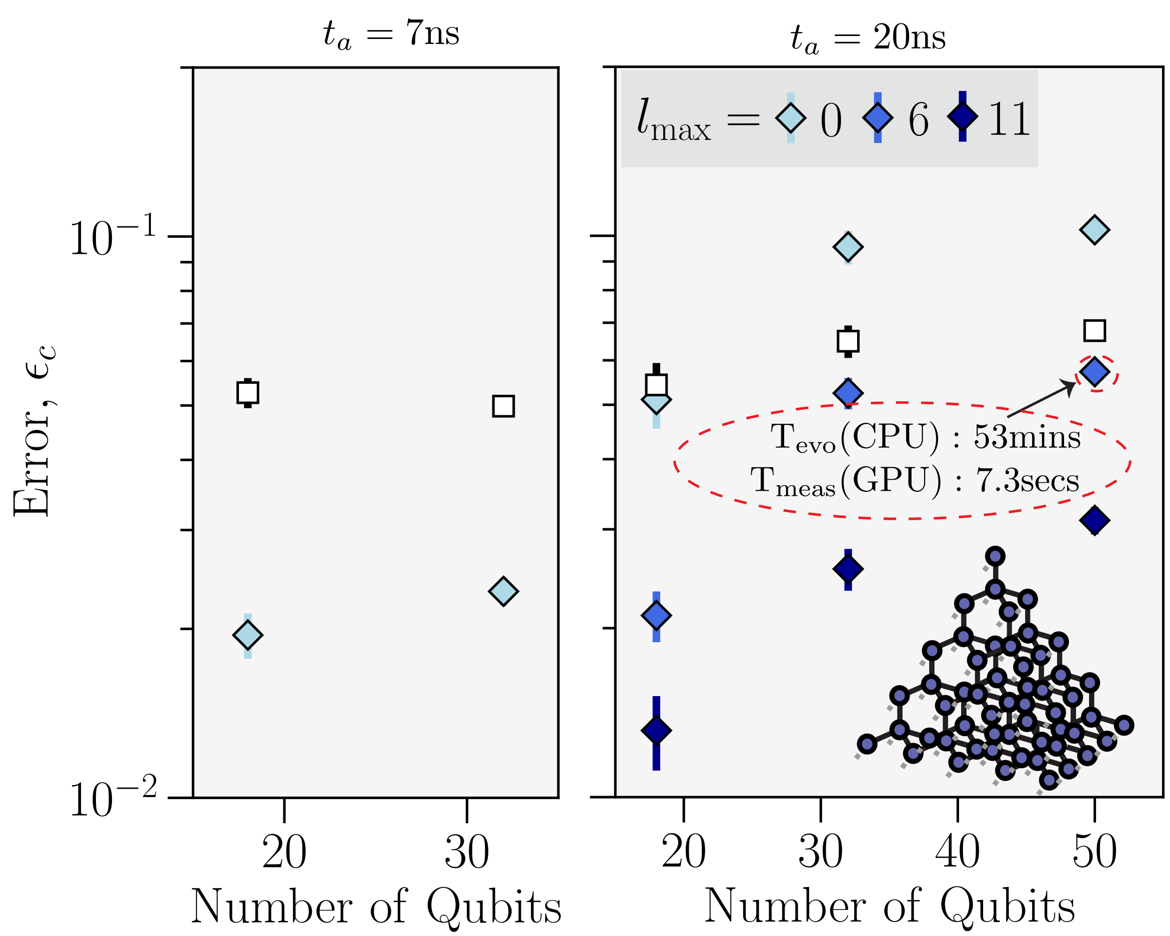
Tindall, Sels, "Confinement in the TFIM on the Heavy Hex Lattice", PRL **133**, 180402 (2024)

Quantum Dynamics – New Algorithms

Compute **3D quantum dynamics** with these tools [1]



Correlator errors:



Quantum annealer

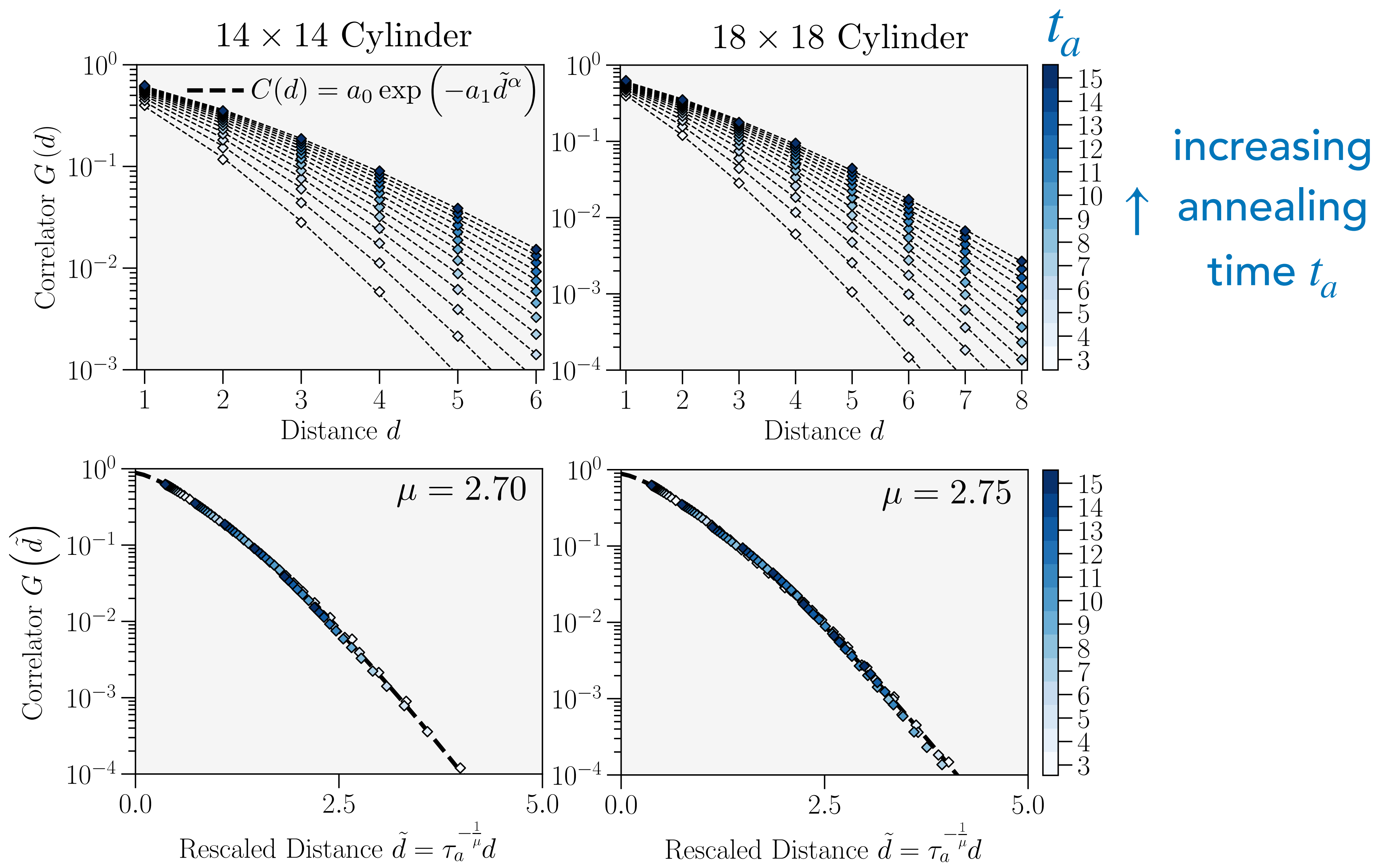
Loop corrected BP method

Competitive with quantum hardware, using scalable methods

[1] Tindall, Mello, Fishman, EMS, Sels, arxiv:2503.05693 (2025)

Quantum Dynamics – New Algorithms

Kibble-Zurek physics through correlator collapse



Tindall, Mello, Fishman, EMS, Sels, arxiv:2503.05693 (2025)

Summary

Prediction: claims of quantum advantage on **structured** problems are premature

Examples of **structure** – all benefiting simulations

hydrodynamics
low-dimensional (MPS)
smooth functions
analytic functions
decay of correlations / gap
high-dimensional (mean field / BP)
scale separation
Kibble-Zurek physics
low circuit depth
sign problem free
large loops / tree-like (BP)
light cone
symmetries
weak correlation / Gaussianity
finite temperature
dualities
low entanglement
dissipation
Cliffordness / low magic
self-similar
locality of interactions
self-averaging
universality / continuum limit
equivalence of ensembles
semi-classical
symmetry breaking
dual unitary

New Possibilities

arxiv:2504.07344

Simulating quantum dynamics in two-dimensional lattices with tensor network influence functional belief propagation

Gunhee Park (박건희),[1] Johnnie Gray,[2] and Garnet Kin-Lic Chan[2]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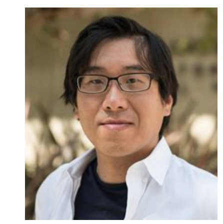
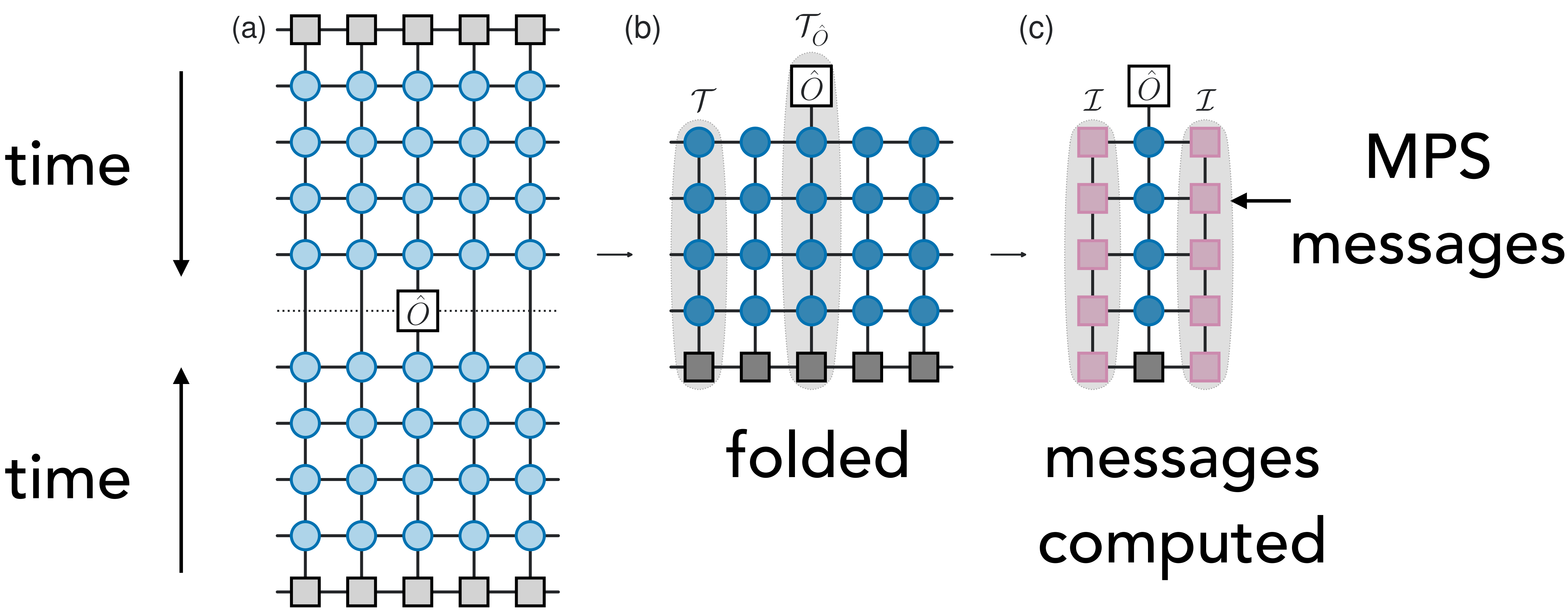

G. Chan

Belief propagation hybridized with "influence functional"

Space + time combined method



Thoughts & Future Directions

Tensor networks helping define boundary between hard vs. easy high-dimensional problems

Radically new algorithms

New tools for

- dynamics of 2D and 3D quantum systems

  - as well as -

- learning tensor networks from data
- high-dimensional functions (PDE's, large-scale Hartree-Fock)

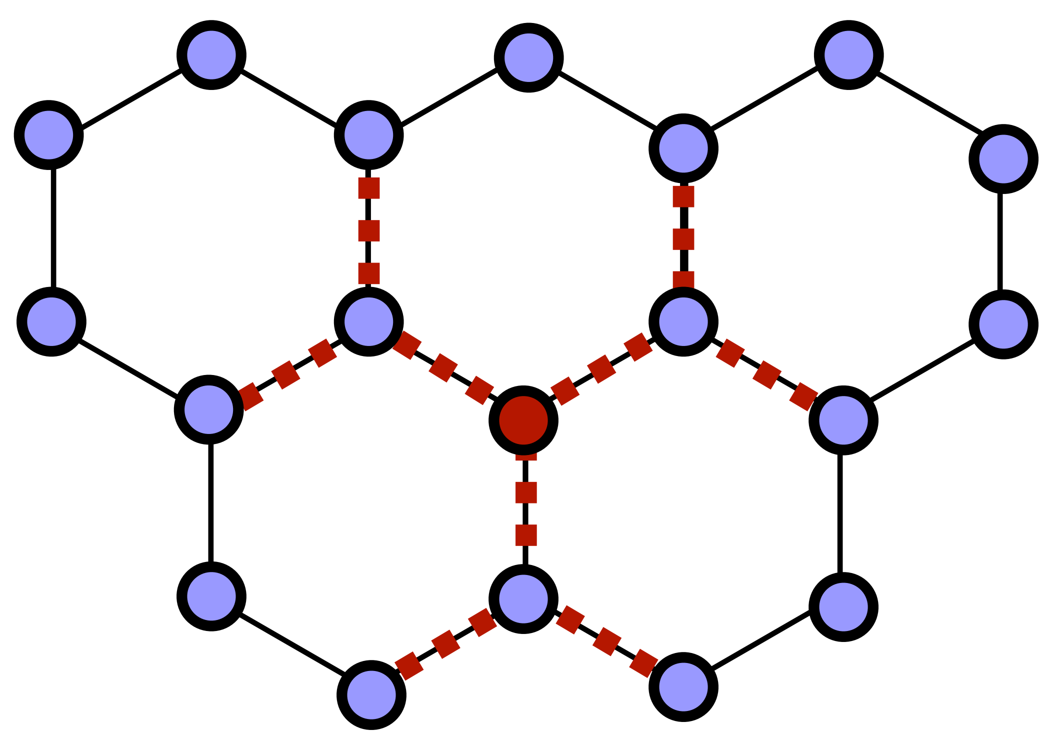
Exciting physics and science do

Thanks for your attention!

BP Approximation

Intuitive understanding of BP approximation is viewing its convergence as

$$\epsilon_{BP} \sim e^{-a\,\xi/L_{\mathrm{loop}}}$$



honeycomb lattice

$$\xi = 2$$

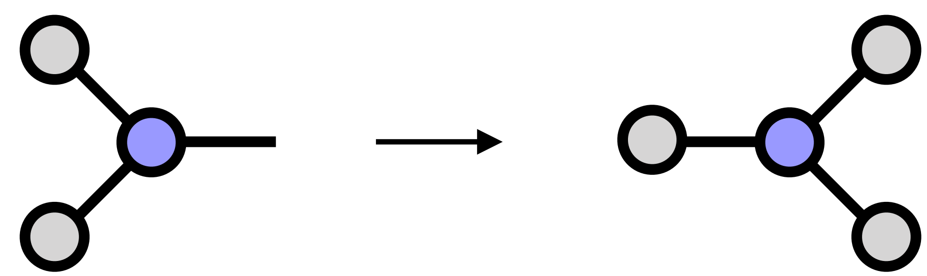
$$L_{\mathrm{loop}} = 6$$

If correlations do not transit around a loop, loop might as well not be there

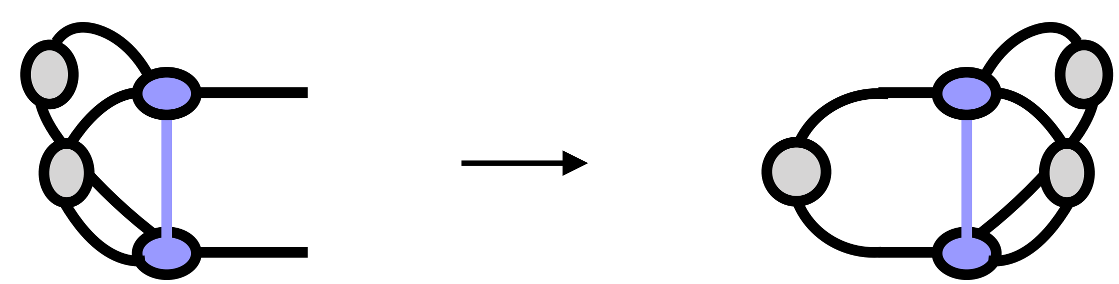
Belief Propagation

Side-on view helpful to understand quantum case

Top view:



Side view:



Quantum messages are **matrices**