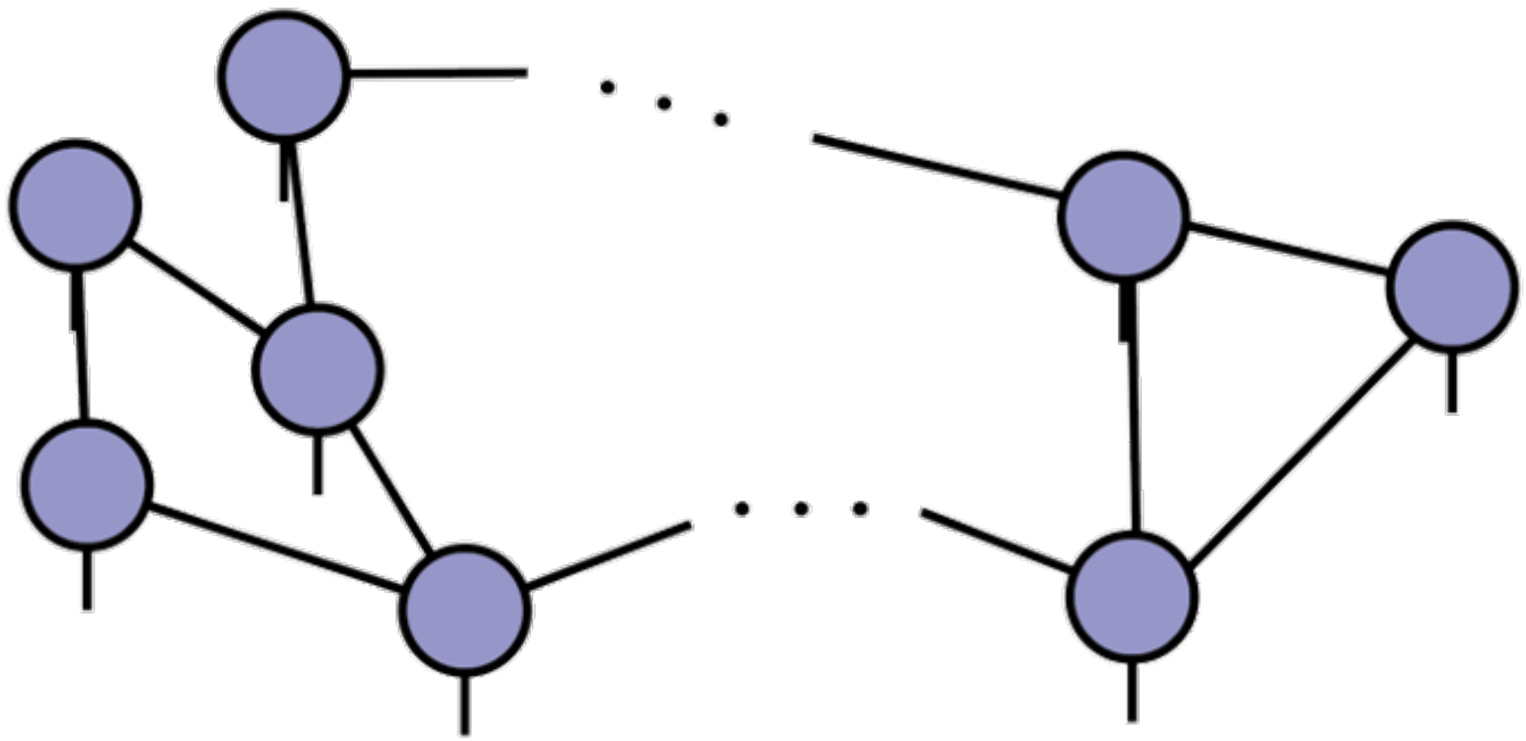
Tensor Networks Beyond One Dimension



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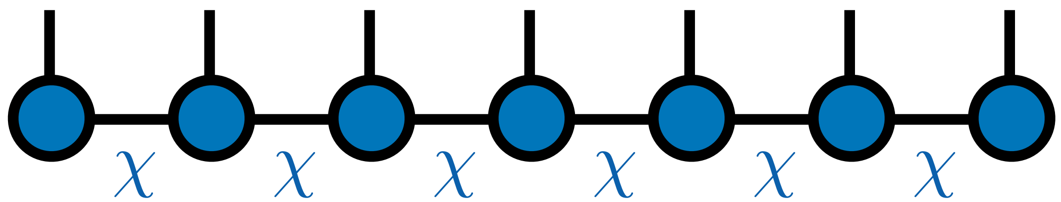
Motivation

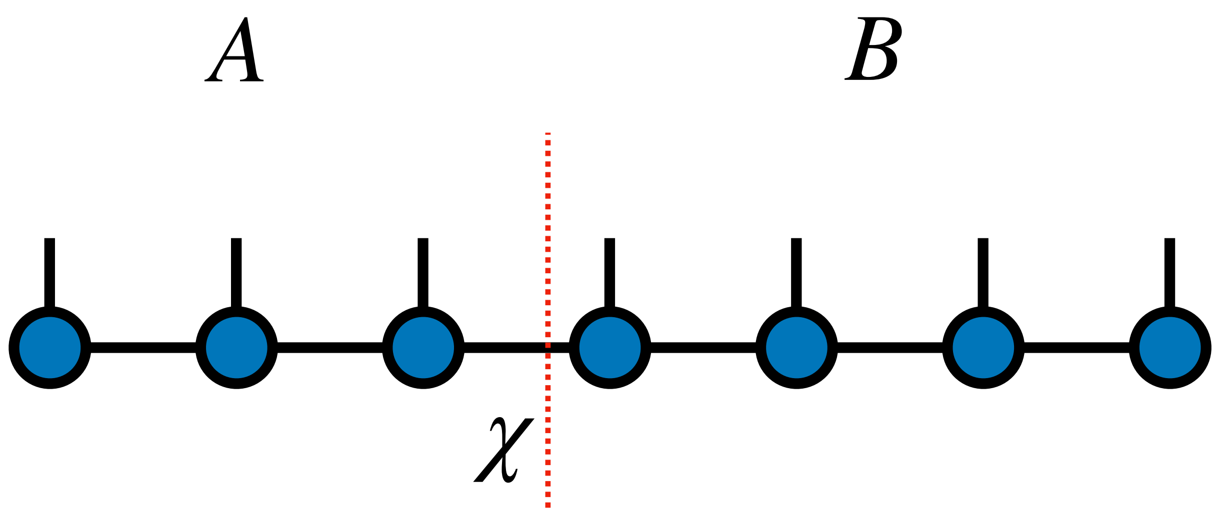
Earlier introduced tensor networks, but entirely focused on matrix product states



An MPS has a one-dimensional structure, making it powerful for 1D but weak for 2D and 3D systems

What tensor networks can we use in higher dimensions?
Alternatives to MPS?

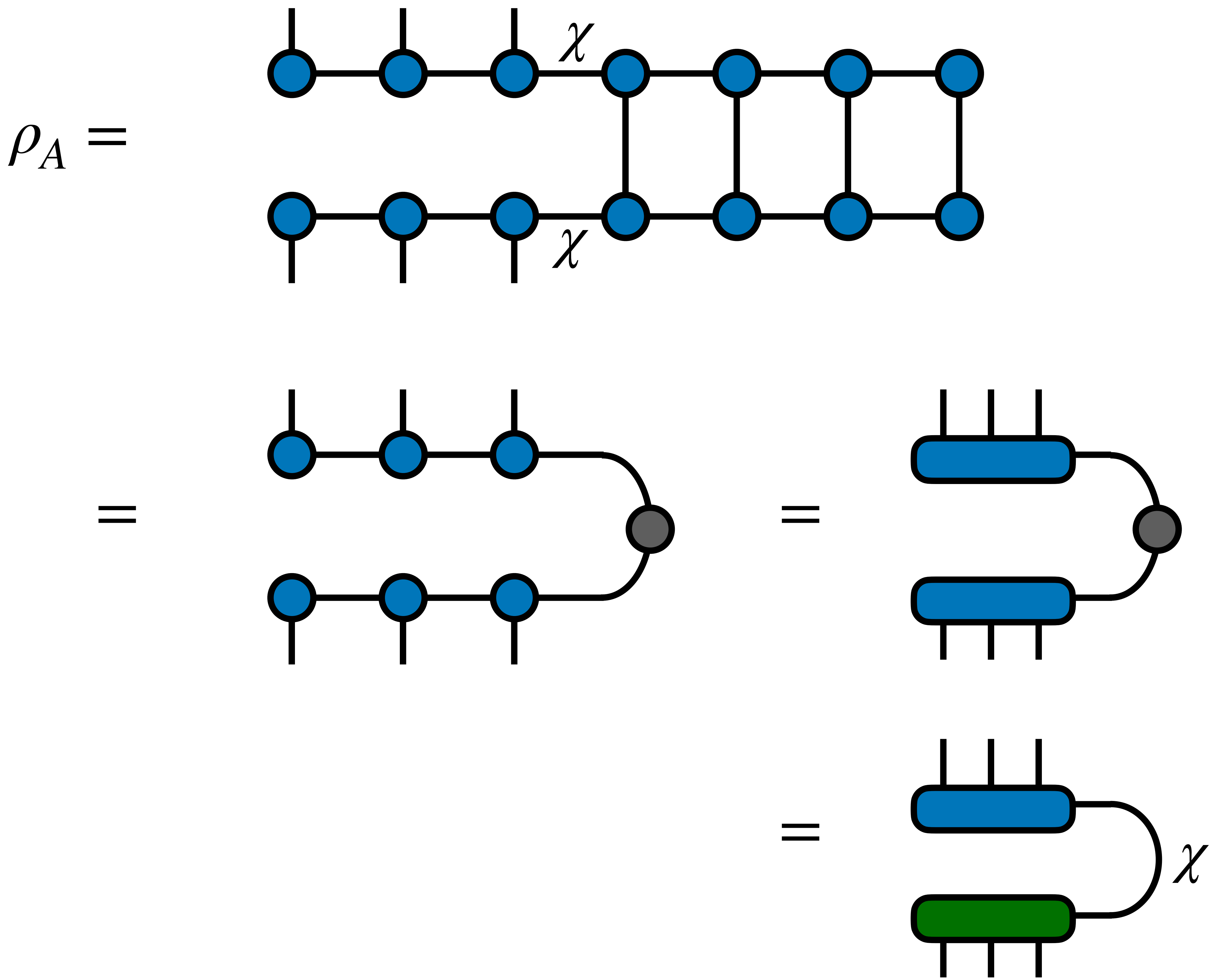
What is the entanglement capacity of an MPS tensor network?



Consider bipartition ("cut") across bond of dimension χ

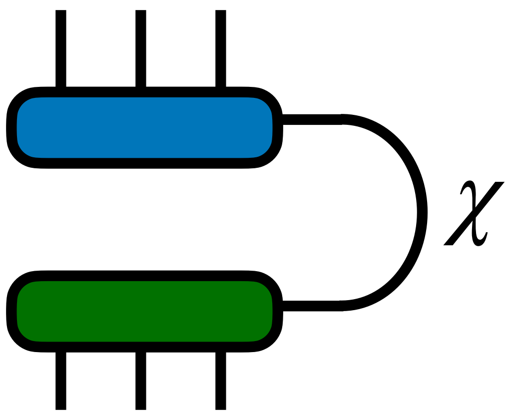
Compute reduced density matrix ρ_A

Entanglement capacity of an MPS



Entanglement capacity of an MPS

We have shown that ρ_A is a product of two matrices, contracted over an index of dimension χ

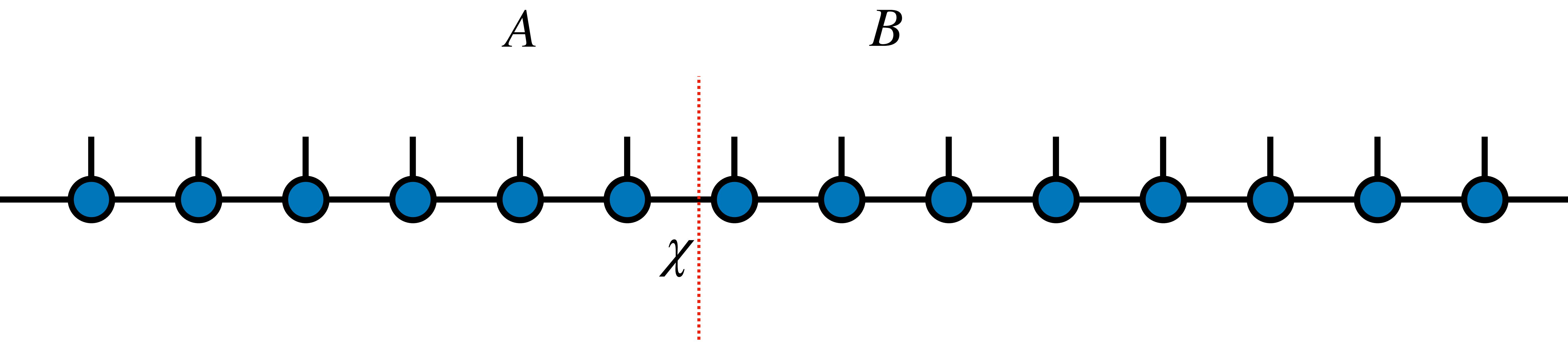
$\rho_A =$ 

Thus ρ_A has maximum rank χ, i.e. at most χ non-zero singular values

Recall $S_{vN} = -\,\mathrm{Tr}(\rho \log(\rho))$

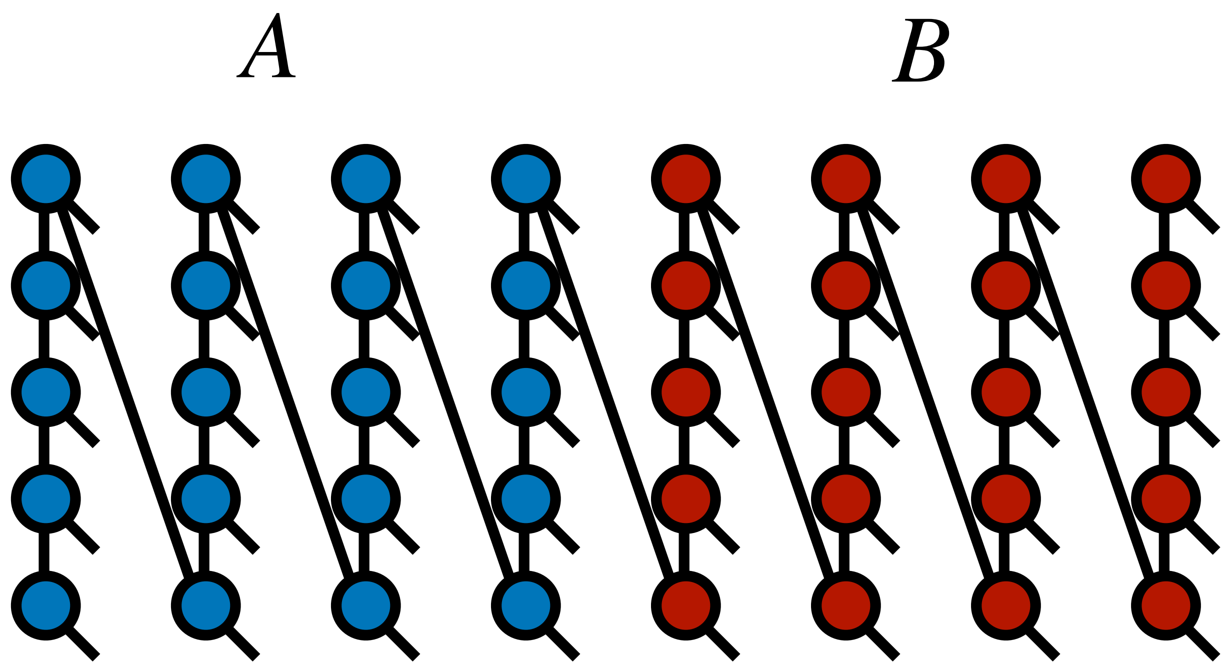
Maximum entropy if all eigenvalues $p_n = 1/\chi$, implies an upper bound $S_{vN} \leq \log(\chi)$

We therefore see MPS with $\chi \sim \mathcal{O}(1)$ obey a 1D area law



Entropy bounded $S_{vN} \leq \log(\chi) \ \sim N^0$ (i.e. const with system size)

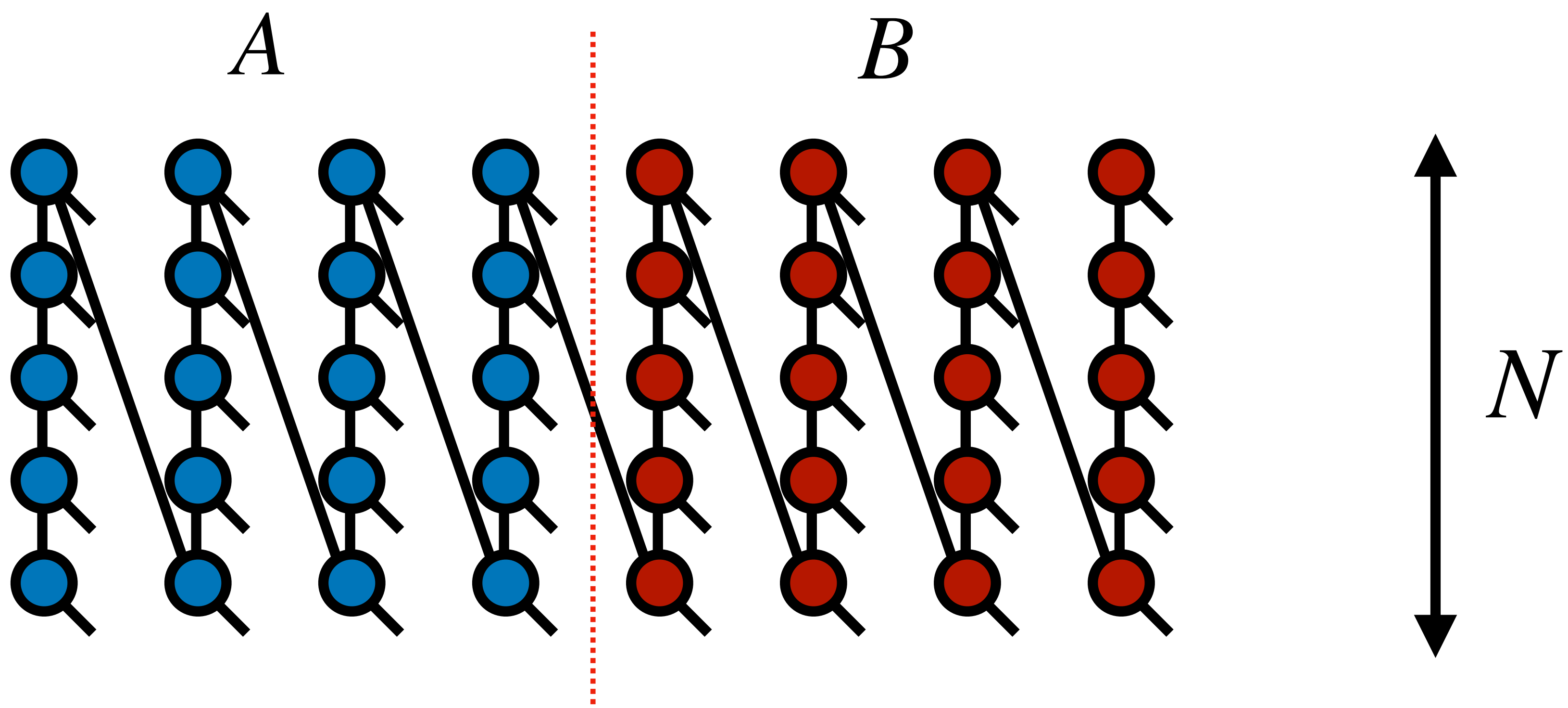
If we use MPS for a two-dimensional system (2D)



we can treat the 2D system using a "zig-zag" or "snaking" pattern to visit all the sites

Basis of 2D-DMRG approach that has been successful on *thin* 2D systems

But importantly, scaling of entanglement is still that of an MPS

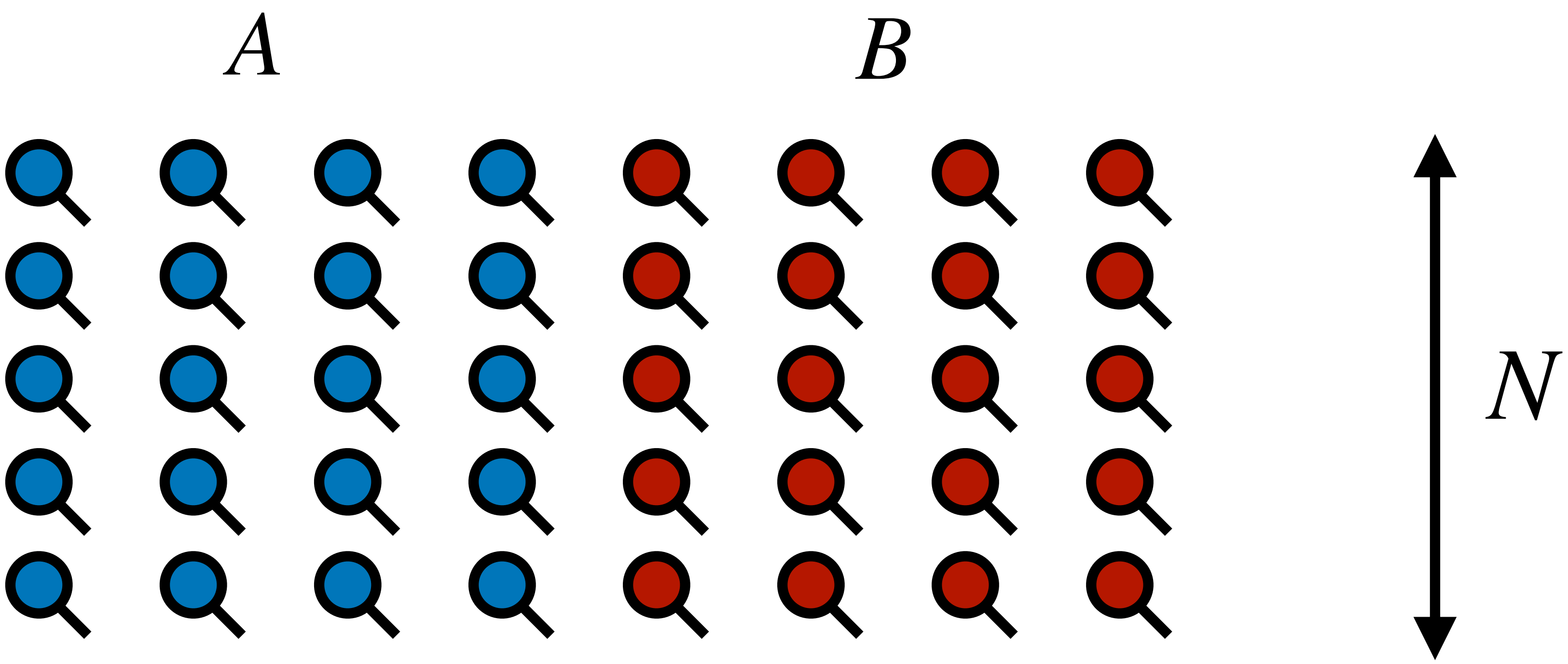


$S_{vN} \leq \log(\chi)$

If we assume 2D wavefunction is “nice” and obeys 2D area law, where $S_{vN} \sim aN$

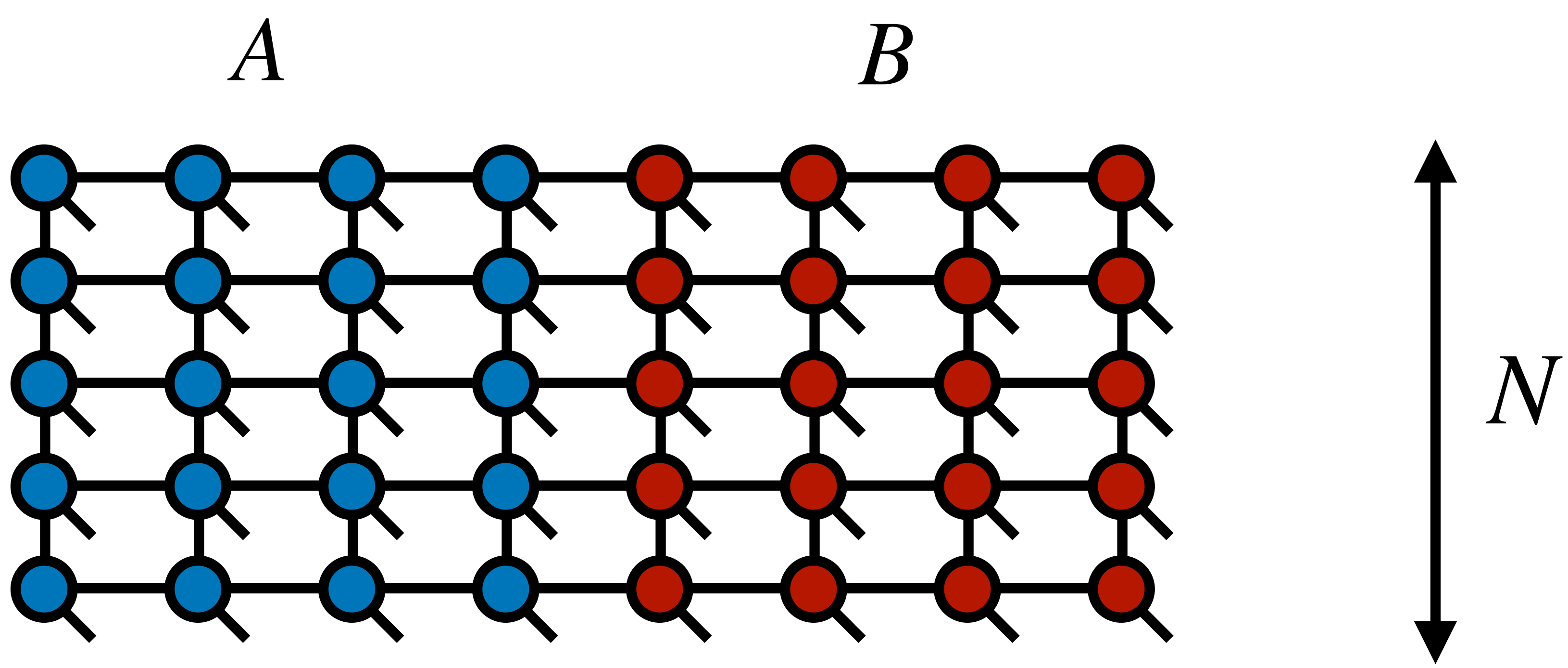
Then requires $\chi \sim e^{aN}$ to capture the state

Intuition: each bond of size χ contributes ~$\log(\chi)$ entanglement



Want total $S_{vN} \sim N$, so put N bonds across the cut (i.e. connecting regions A and B)

Intuition: each bond of size χ contributes ~$\ln(\chi)$ entanglement



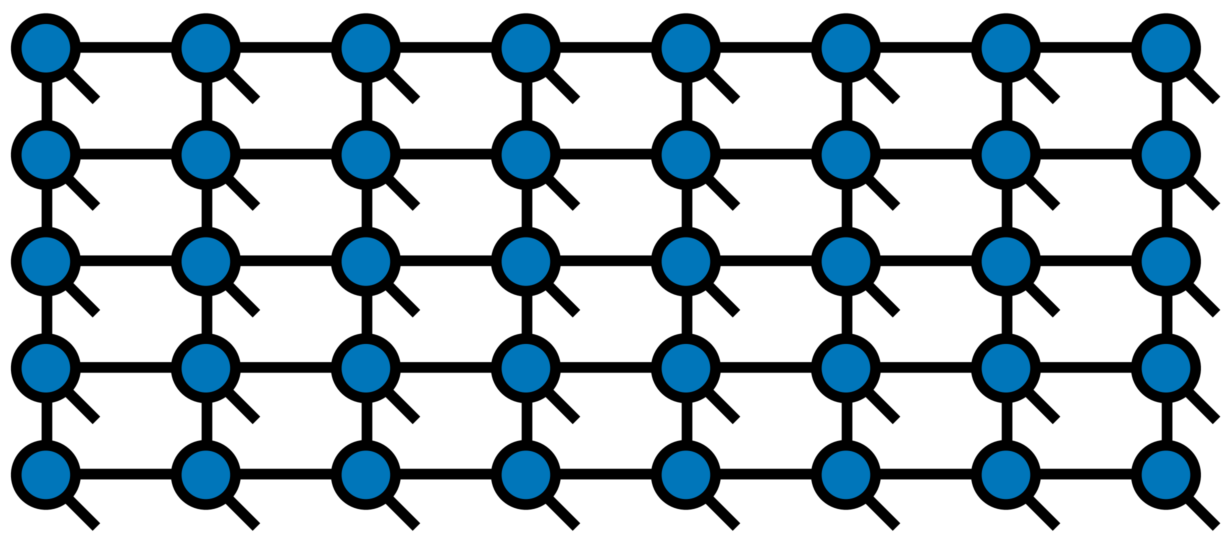
Want total $S_{vN} \sim N$, so put N bonds across the cut
(i.e. connecting regions A and B)

Motivates 2D tensor network state (TNS)
also called projected entangled pair state (PEPS)

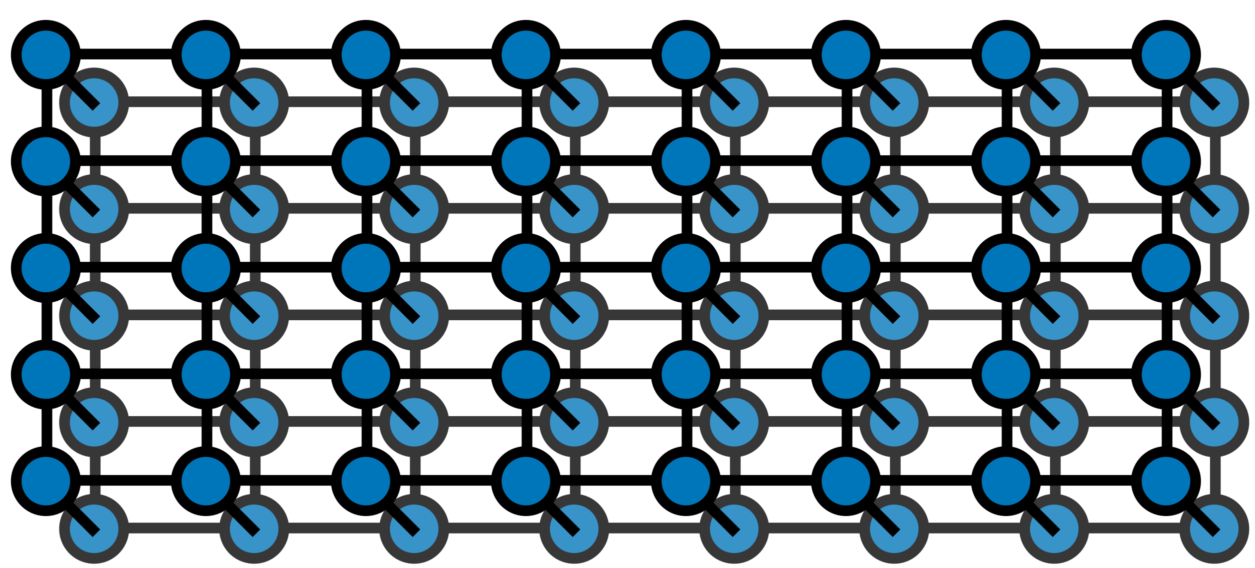
The Belief Propagation Algorithm for General Tensor Networks

Motivation

To work with 2D tensor networks

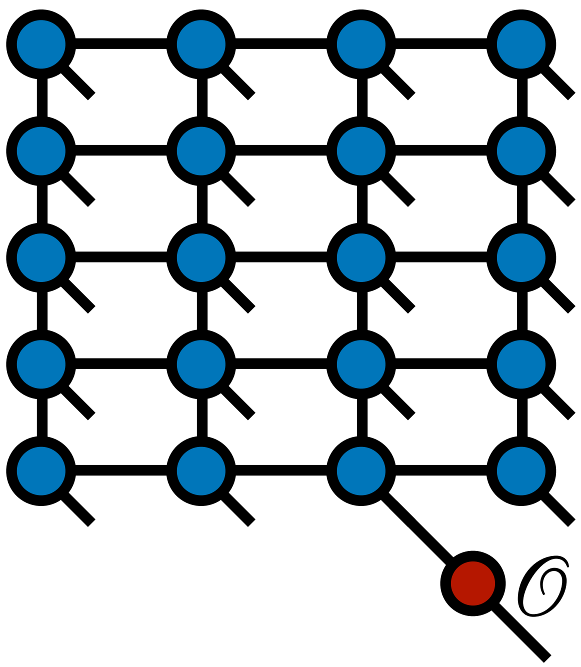


Must be able to **contract** them



Motivation

For example, computing operator expected values



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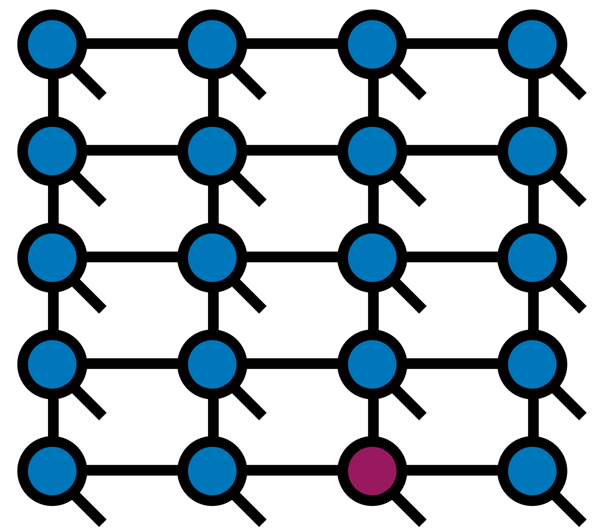
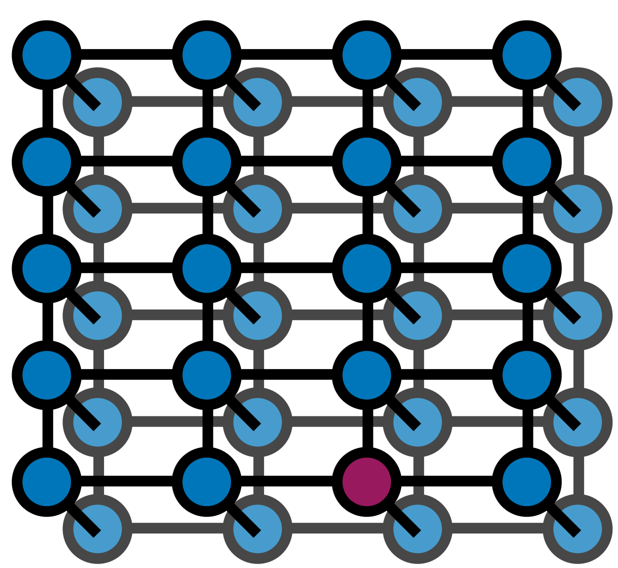


$\langle\psi|\,\mathcal{O}$

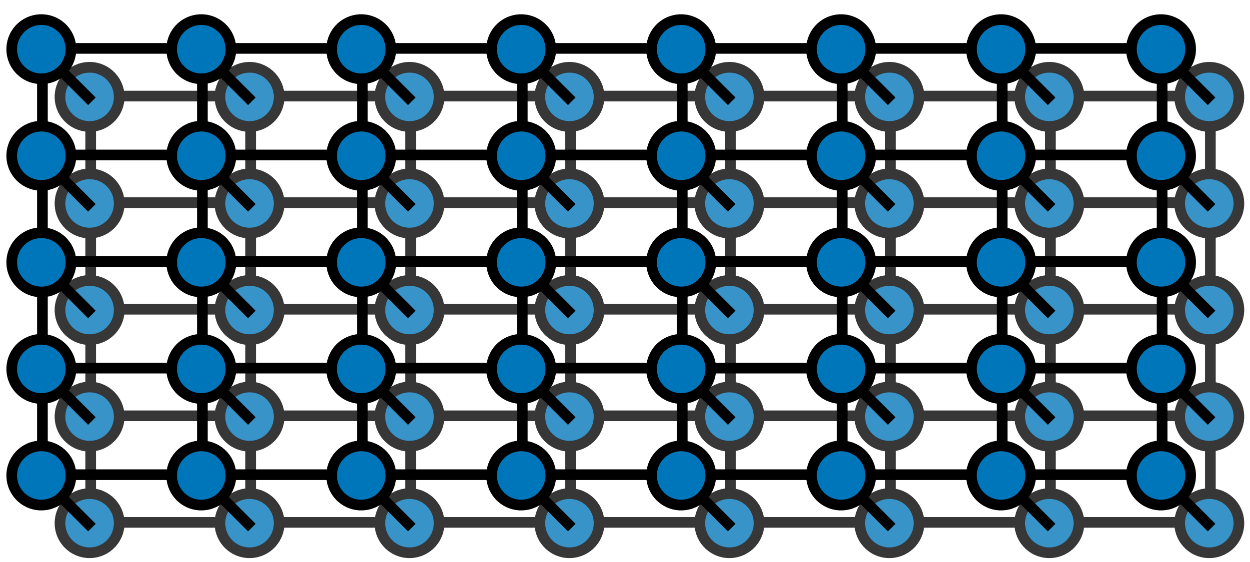
$$\langle\psi|\,\mathcal{O}\,|\psi\rangle =$$



Motivation

However, contracting 2D (3D, etc.) tensor networks exactly is #P-Complete in worst case.

A polynomial time (in system size) to contract any finite bond dimension PEPS would imply P = NP.

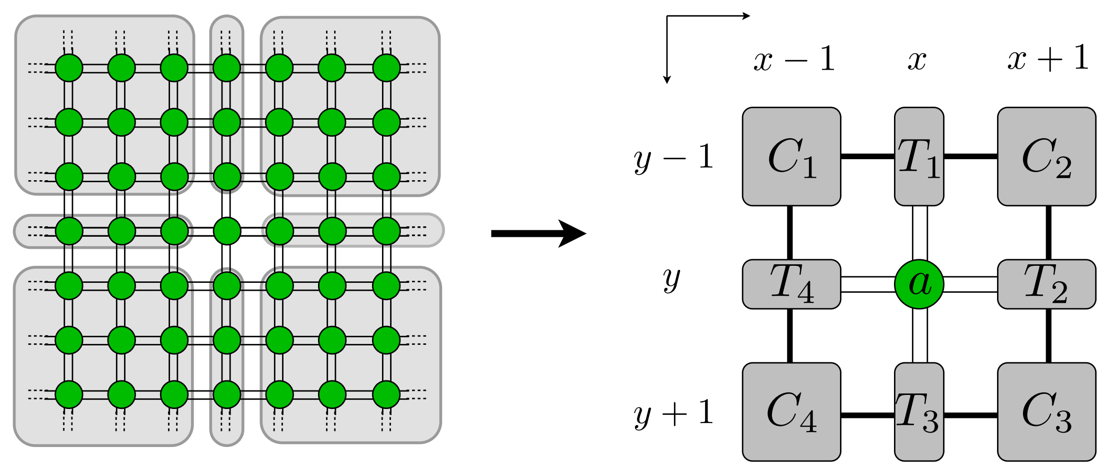


[1] Cirac et al, Phys. Rev. Lett. **98**, 140506 (2007)

Motivation

Highly controlled approximations have been developed for *infinite PEPS* (TNS) optimization [1,2]

$$\langle \Psi | \Psi \rangle =$$



and related works using automatic differentiation [3,4]

[1] Corboz, Phys. Rev. B **94**, 035133 (2016)
[2] Vanderstraeten, Haegeman, Corboz, Verstraete, Phys. Rev. B **94**, 155123 (2016)
[3] Liao, Liu, Wang, Xiang, Phys. Rev. X **9**, 031041 (2019)
[4] Ponsioen, Assaad, Corboz, SciPost Phys. 12, 006 (2022)

Motivation

However, existing 2D tensor network methods are **expensive** and overly-focussed on square lattices

Typical costs: *

- iPEPS optimization – scaling $O(D^{10})$ for square lattice
- VMC optimization – scaling $O(MD^6)$ with M~10,000 the number of samples

Also, 3D lattices seem out of reach

* Liu, Zhai, Peng, Gu, Chan, arxiv:2502.13454

Motivation

Is there *more efficient* method for contracting TNS?

We need to accept larger approximations...

We just need to know how large the approximation is

🧠 "Belief propagation" + extensions gives all three

🧠 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

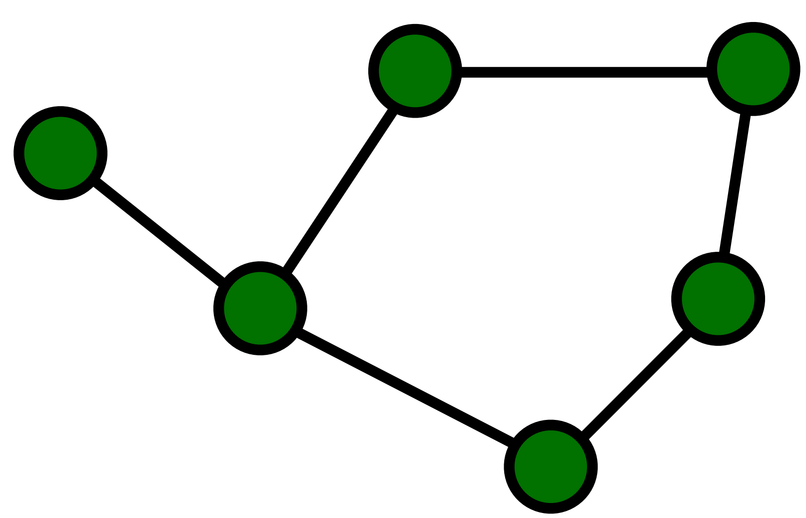
Mezard, Parisi, Virasoro
spin glass physics (1985)

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 via tensor networks

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

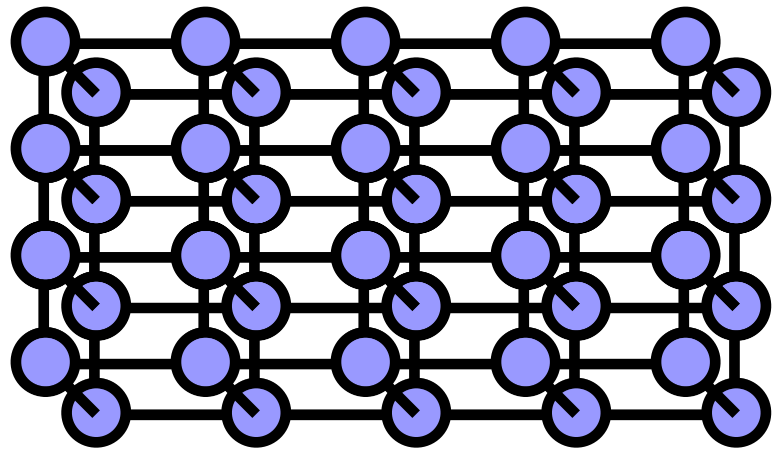
Gauging tensor networks with belief propagation

Joseph Tindall, Matt Fishman

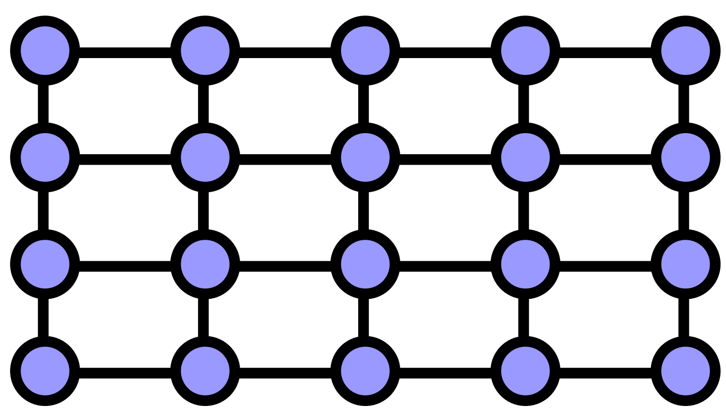
SciPost Phys. 15, 222 (2023) · published 1 December 2023

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)

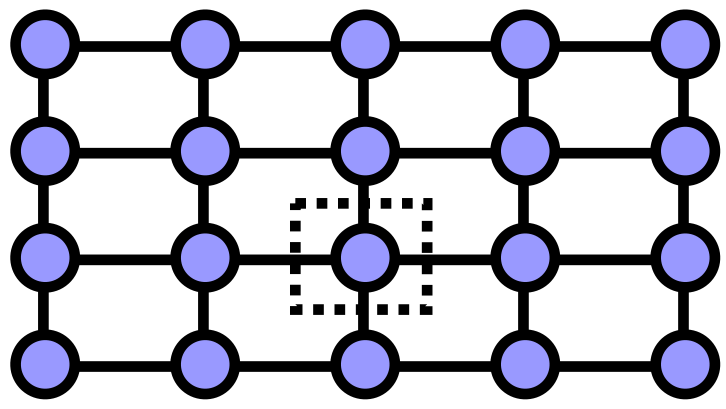
To apply belief propagation to quantum systems, start from "⟨ bra | ket ⟩" network ("norm network")



Top-down view



Ideally compute exact "environment"
Defined as network with one tensor removed



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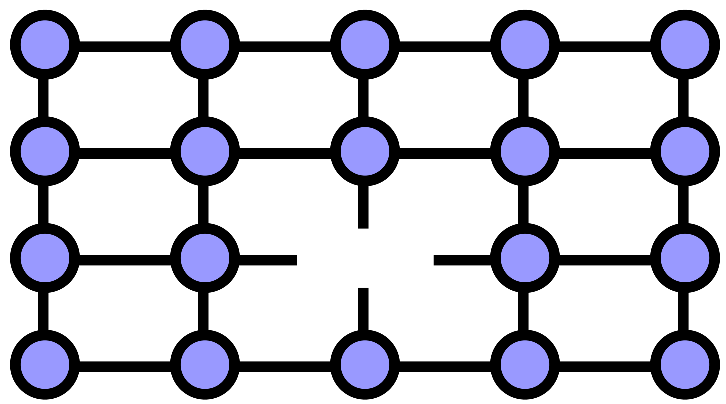

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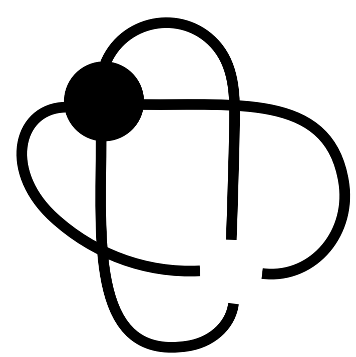

Ideally compute exact "environment"
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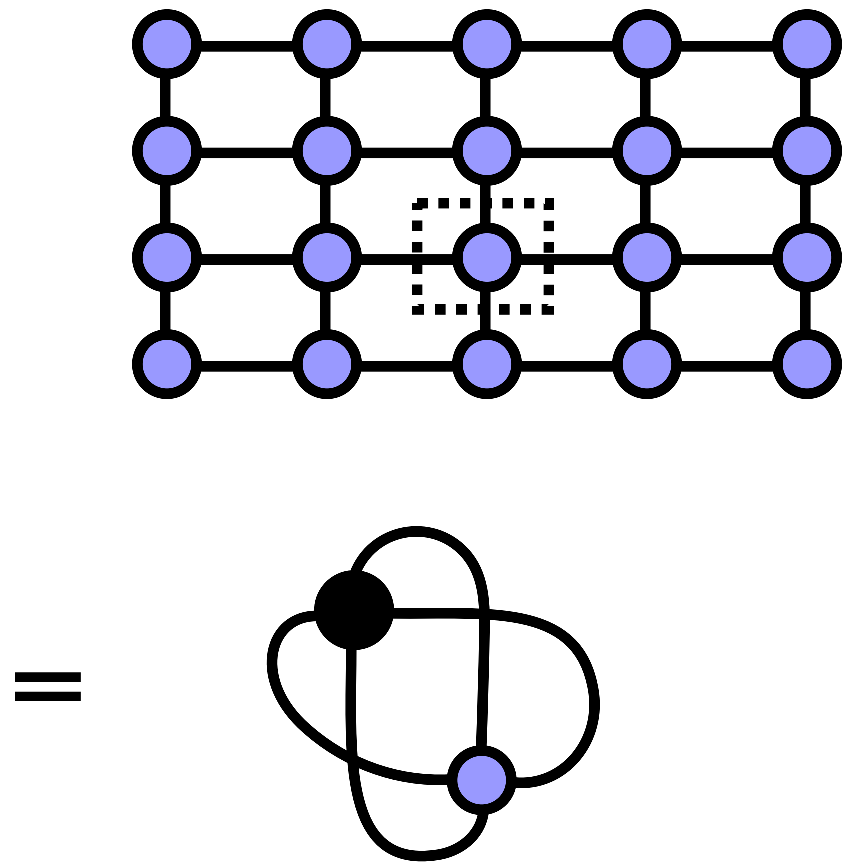
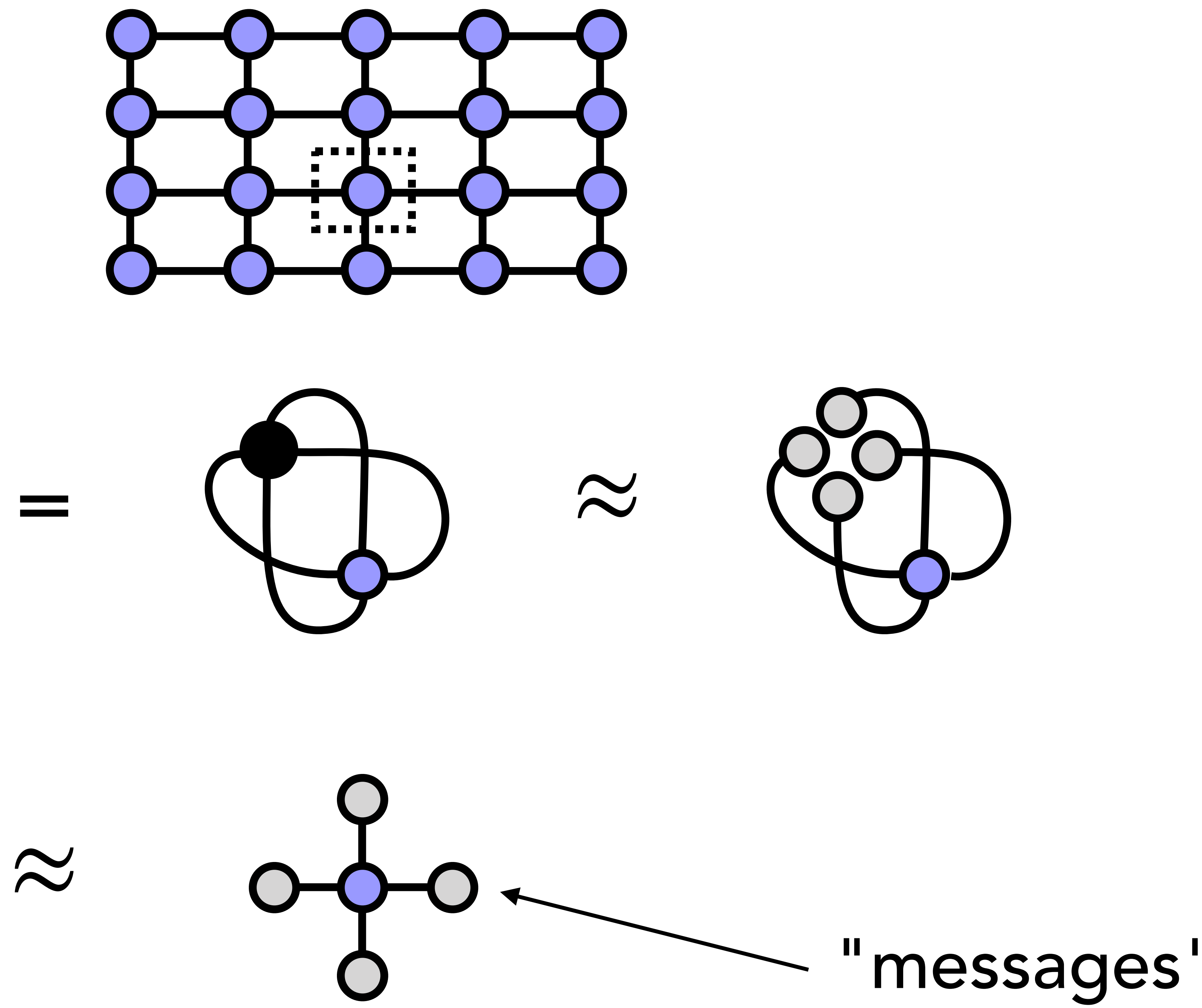
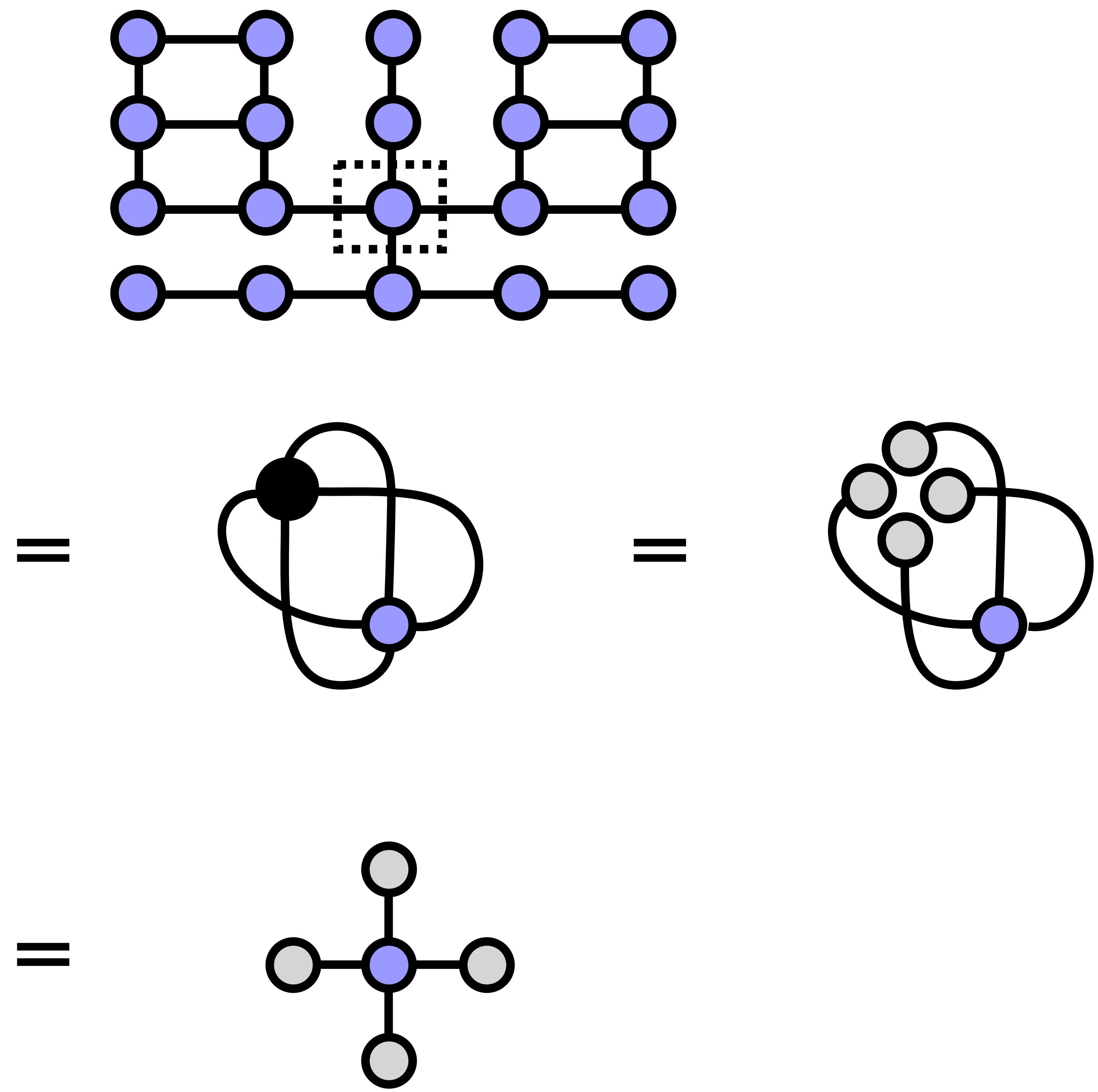


Small (4-index) environment tensor sufficient to contract whole network, but just as hard to compute

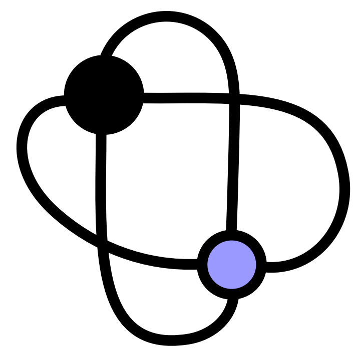
Make seemingly *drastic* approximation



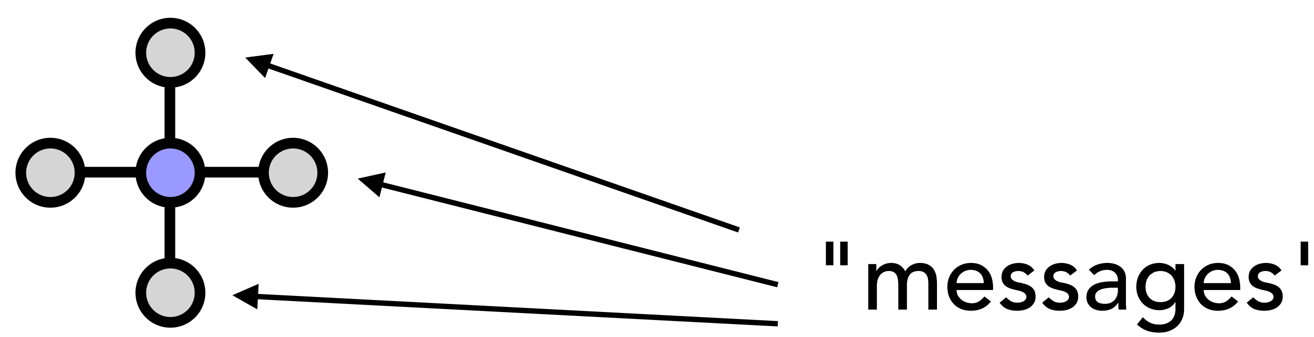
Would be exact if certain loops don't contribute



How to find "messages" in practice?



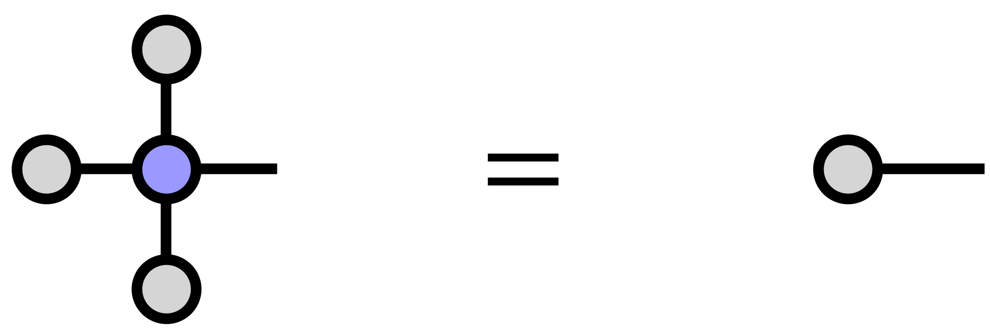
$\approx$



Message Passing

Use "message passing" to converge the messages until self-consistency over all edges of the network

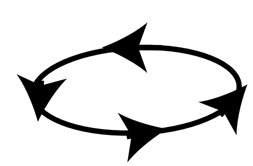
Update rule on edge e



Incoming messages
* Local tensors

Outgoing message

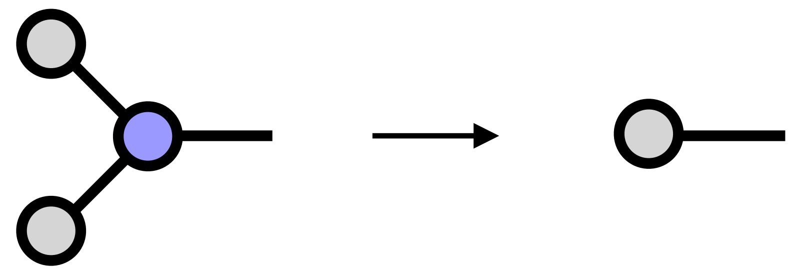
Iterate on all edges until convergence



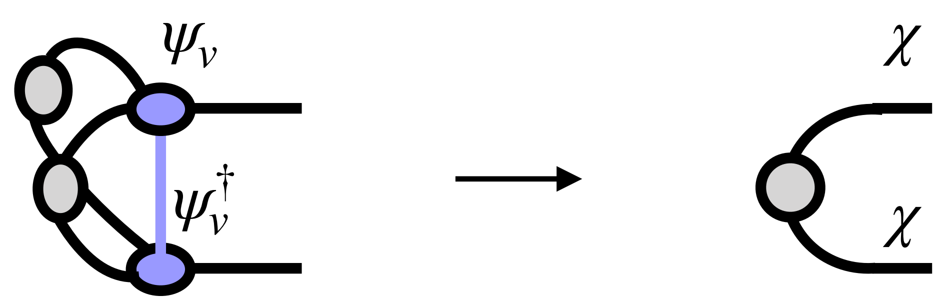
Belief Propagation

Side-on view helpful to understand quantum case. We typically run BP over the norm network $\langle \psi | \psi \rangle$

Top view:



Side view:

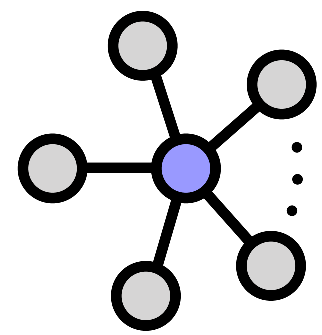


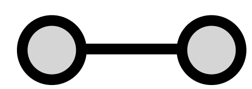
Quantum messages are $\chi \times \chi$ **matrices**, where χ is the bond dimension. They are RDMS in the bond basis

Belief Propagation

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

$$\langle\psi|\psi\rangle \approx \frac{\prod_{\text{vertices}}}{\prod_{\text{edges}}}$$





If the tensor network represents a partition function, this is exactly the Bethe free energy. If $|\psi\rangle$ is a tree tensor network, it is exact.

Belief Propagation

Scaling of quantum belief propagation on the norm $\langle\psi|\psi\rangle$ is

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

where z is the *coordination number* of the lattice, χ the bond dimension, N the number of sites.

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

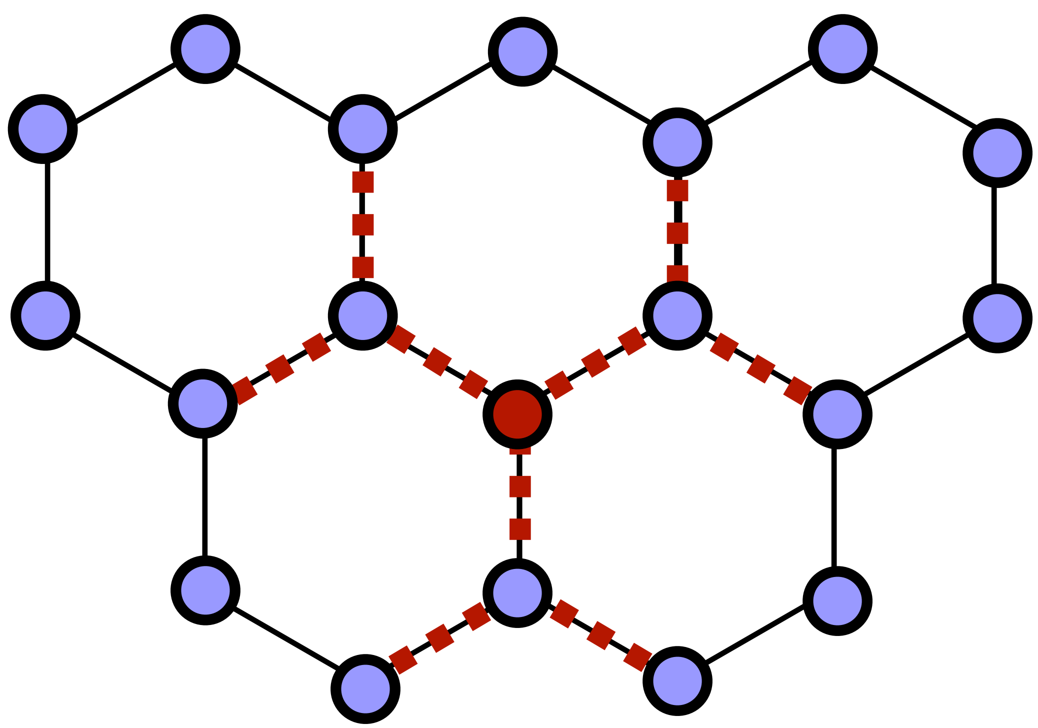
More neighbors (higher z) costs more, but lower bond dimensions usually needed (mean field like)

BP Approximation

Intuitive understanding of BP approximation is viewing its convergence as

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

Correlation length



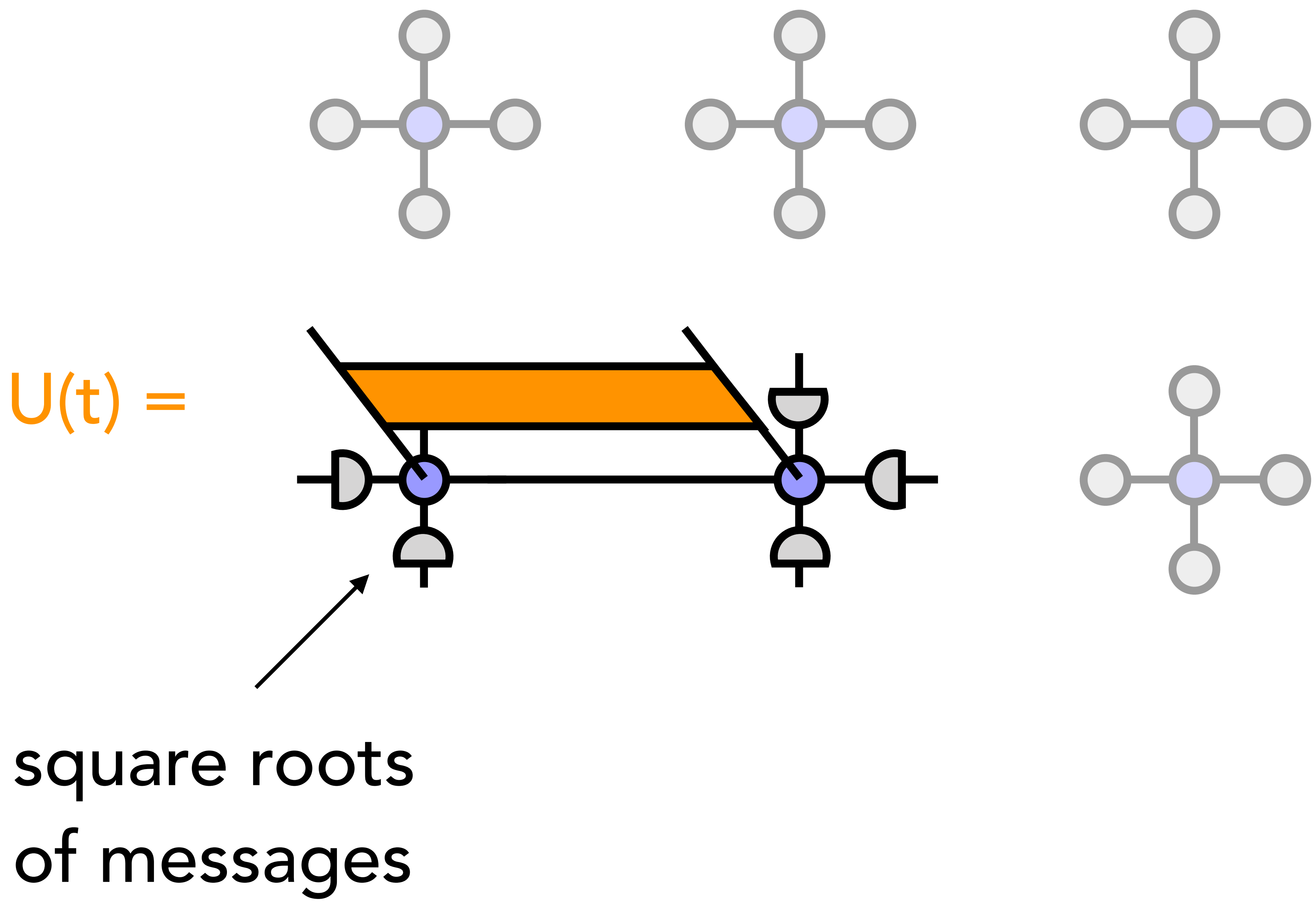
honeycomb lattice

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

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

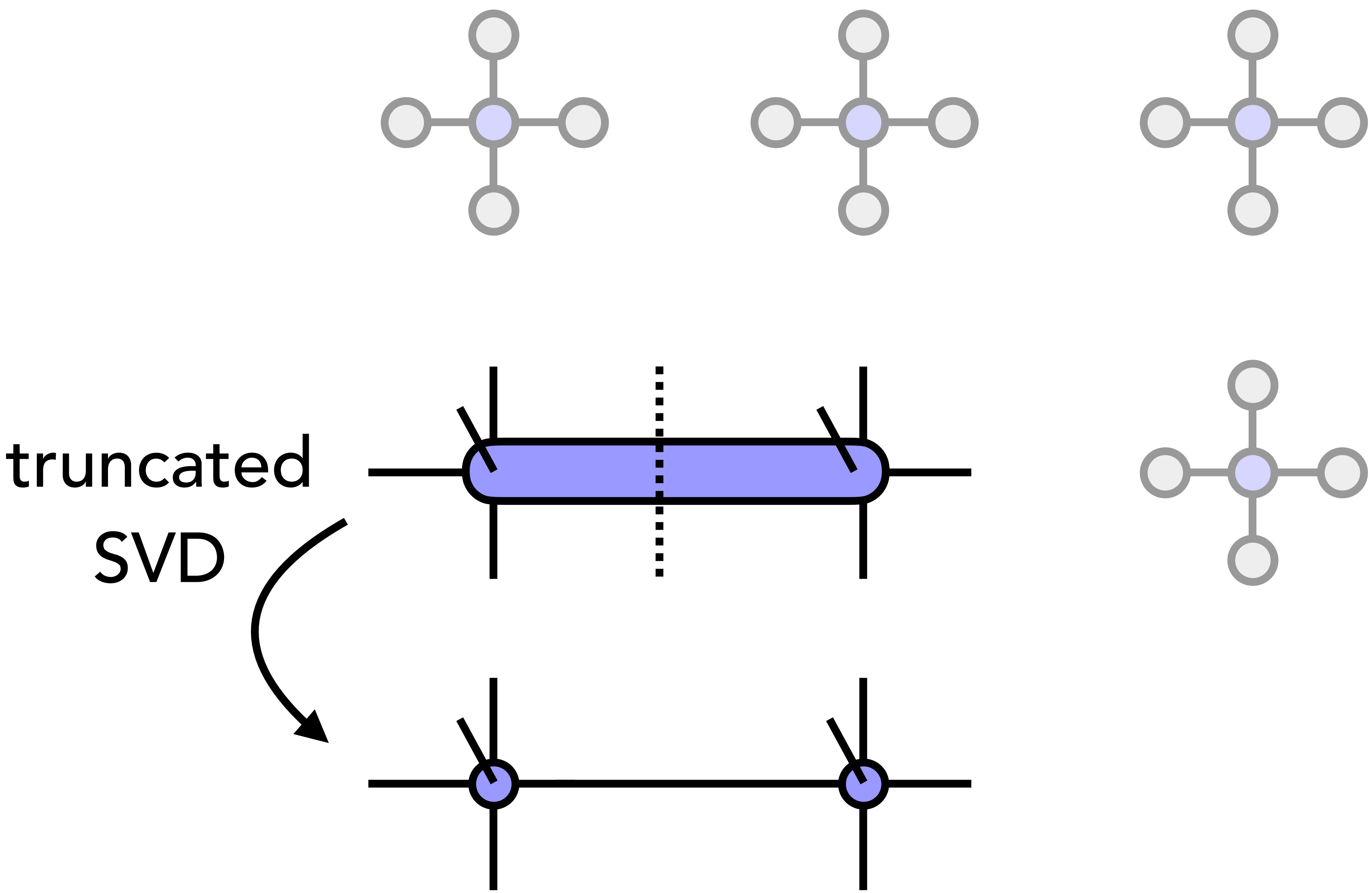
Belief Propagation

Use converged messages to apply gates



Belief Propagation

Messages play important role not so much when we apply the gate, but in order to make the SVD truncation accurate:



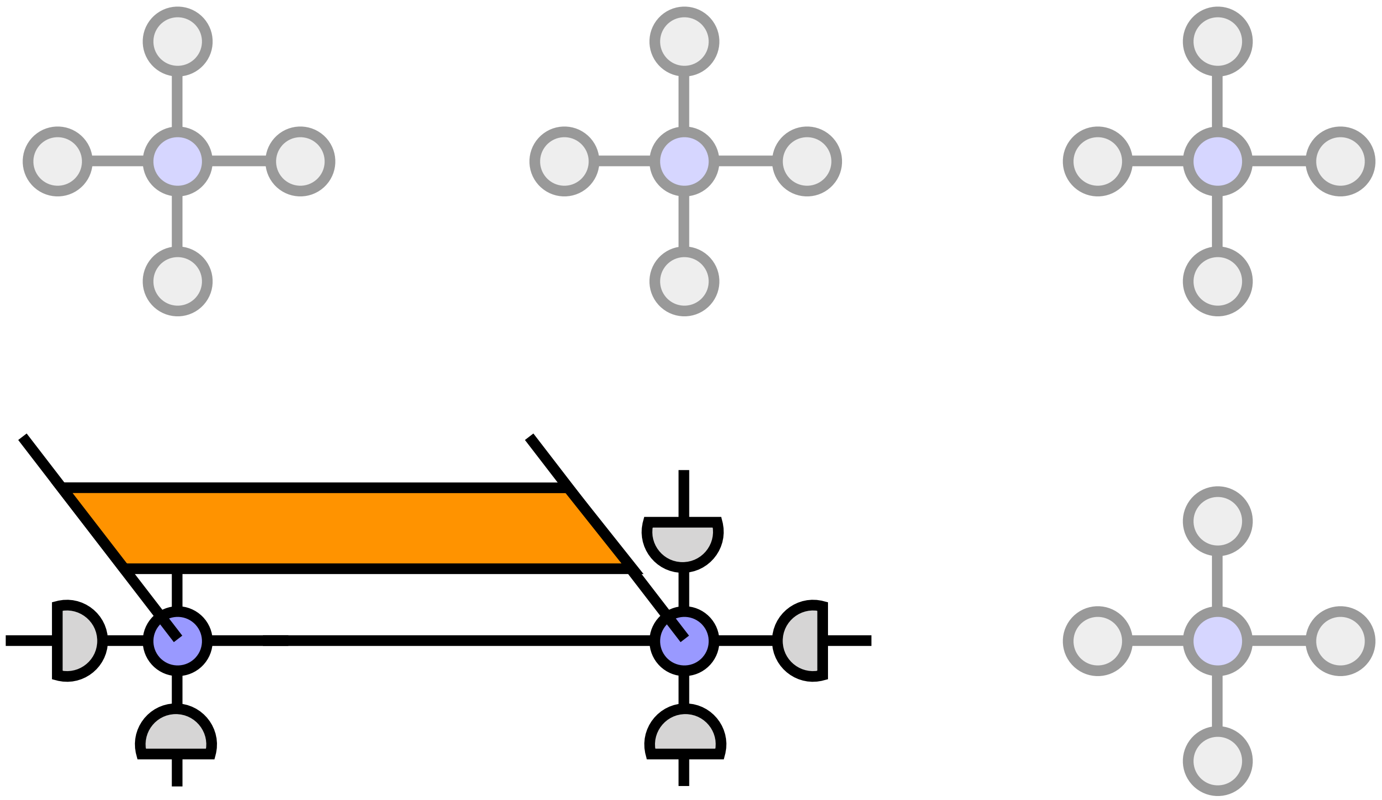
Belief Propagation

Applying gates lets us:

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

2) compute dynamics (real time)

U(t) =



Belief Propagation

For extensive discussion of theory of quantum belief propagation
(relation to gauging, simple update, etc.)

SciPost Phys. 15, 222 (2023)

Gauging tensor networks with belief propagation

Joseph Tindall[*] and Matt Fishman

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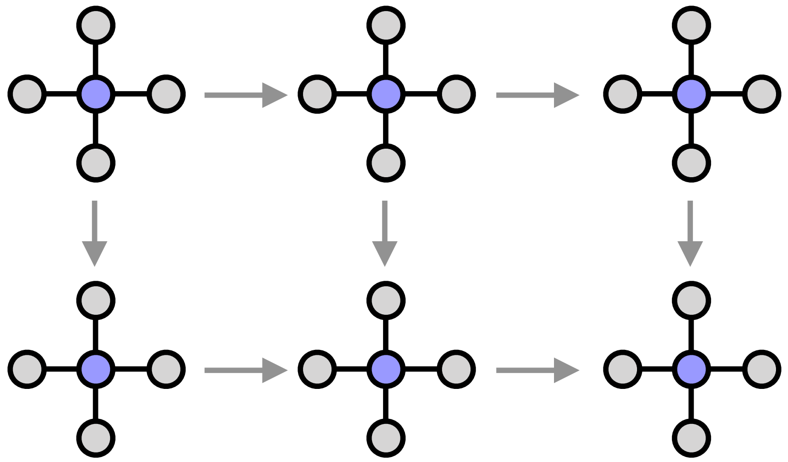
New York, New York 10010, USA

⋆ jtindall@flatironinstitute.org

Joey Tindall

Matt Fishman

Belief Propagation



Benefits of belief propagation:

- if lattice has no loops, fully controlled
- cheap: use large internal bond dimensions χ
- like mean-field theory, but more accurate
- can run dynamics on top
- systematic corrections possible

Applications of Belief Propagation for Quantum Simulation

1) Simulation of quantum utility experiment

Featured in Physics | Open Access

Efficient Tensor Network Simulation of IBM's Eagle Kicked Ising Experiment

Joseph Tindall, Matthew Fishman, E. Miles Stoudenmire, and Dries Sels

PRX Quantum **5**, 010308 – Published 23 January 2024

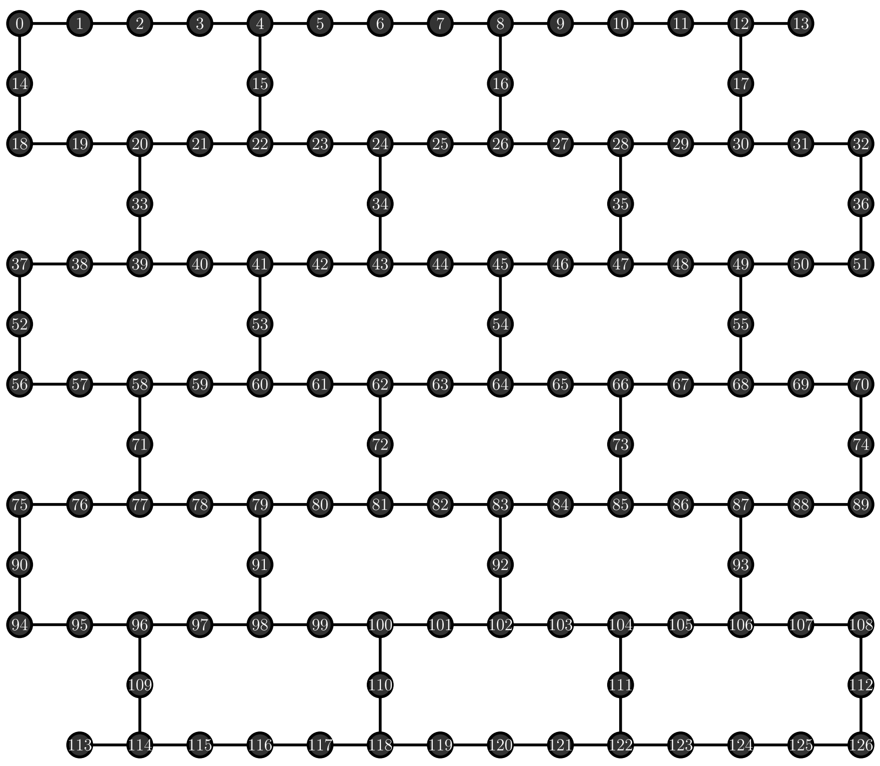
Physics See Research News: A Moving Target for Quantum Advantage

J. Tindall

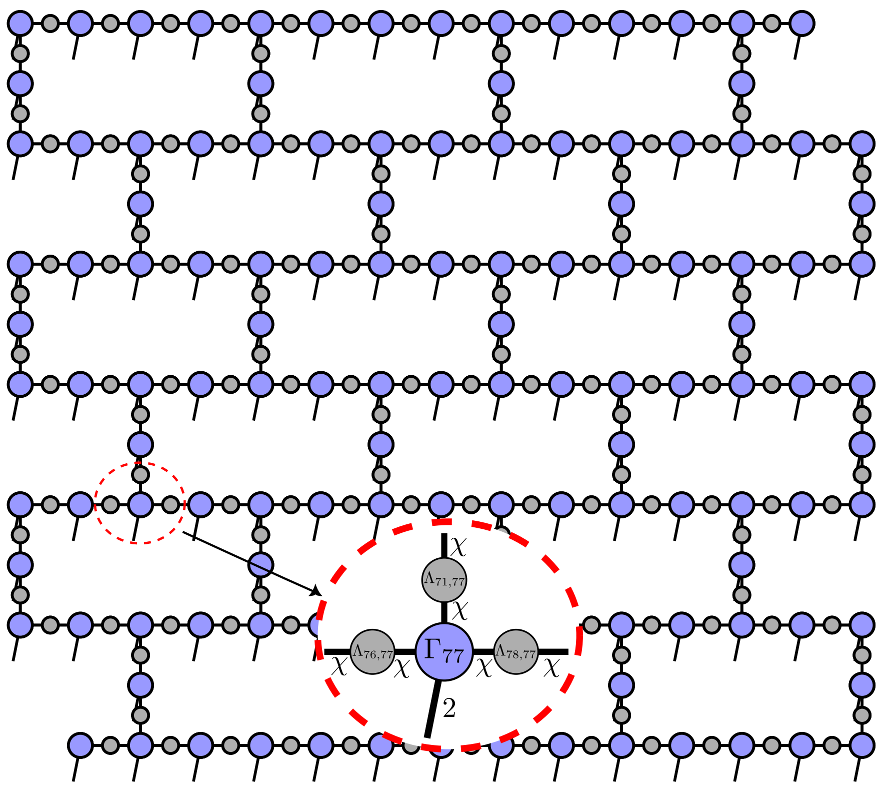
M. Fishman

D. Sels

Eagle Processor 6×3 Heavy − Hex Lattice



Classical Tensor Network Ansatz :

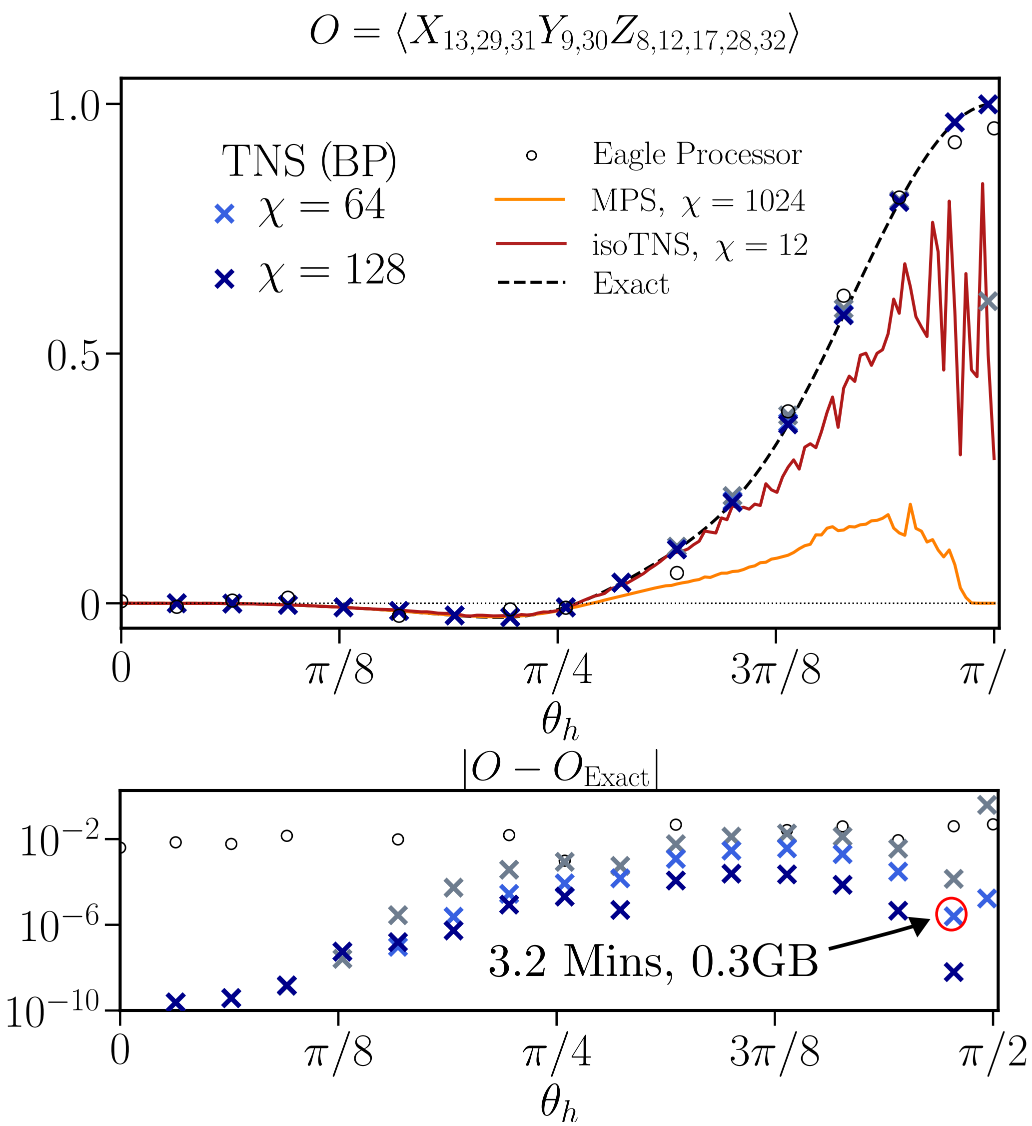


$$U(\theta_h) = \left(\prod_{\langle v,v'\rangle} \exp\left(\mathrm{i}\frac{\pi}{4} Z_v Z_{v'}\right)\right)\left(\prod_{v} \exp\left(-\mathrm{i}\frac{\theta_h}{2} X_v\right)\right)$$

← discretized dynamics

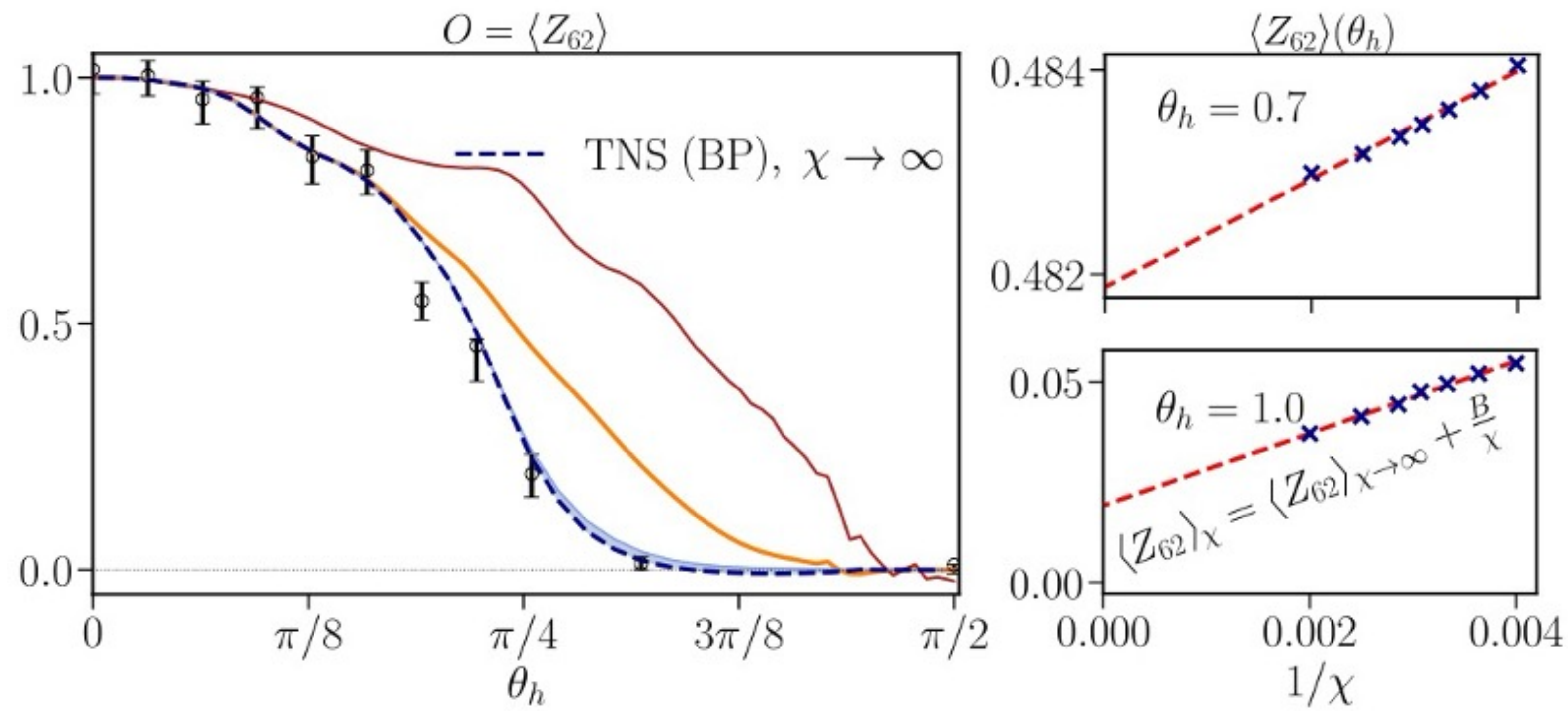
1) Simulation of quantum utility experiment

BP results



Results in verifiable regime

BP results



Results in unverifiable regime

2) Simulation of D-Wave quantum Ising dynamics

Science Current I

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RESEARCH ARTICLE

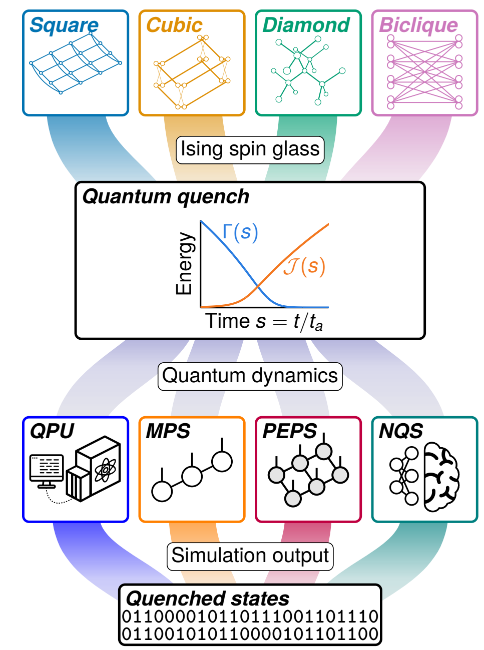
Beyond-classical computation in quantum simulation

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*

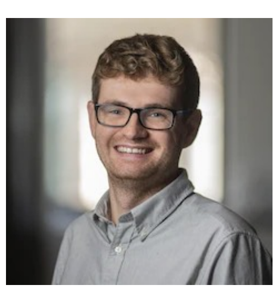


Dynamics of disordered quantum systems with two- and three-dimensional tensor networks

Joseph Tindall,[1] Antonio Francesco Mello,[1,2] Matthew Fishman,[1] E. Miles Stoudenmire,[1] and Dries Sels[1,3]

[1] *Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA*
[2] *International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy*
[3] *Center for Quantum Phenomena, Department of Physics, New York University, 726 Broadway, New York, NY, 10003, USA*

(Dated: March 14, 2025)



Joey Tindall
Flatiron CCQ

Antonio Mello
Flatiron CCQ
SISSA

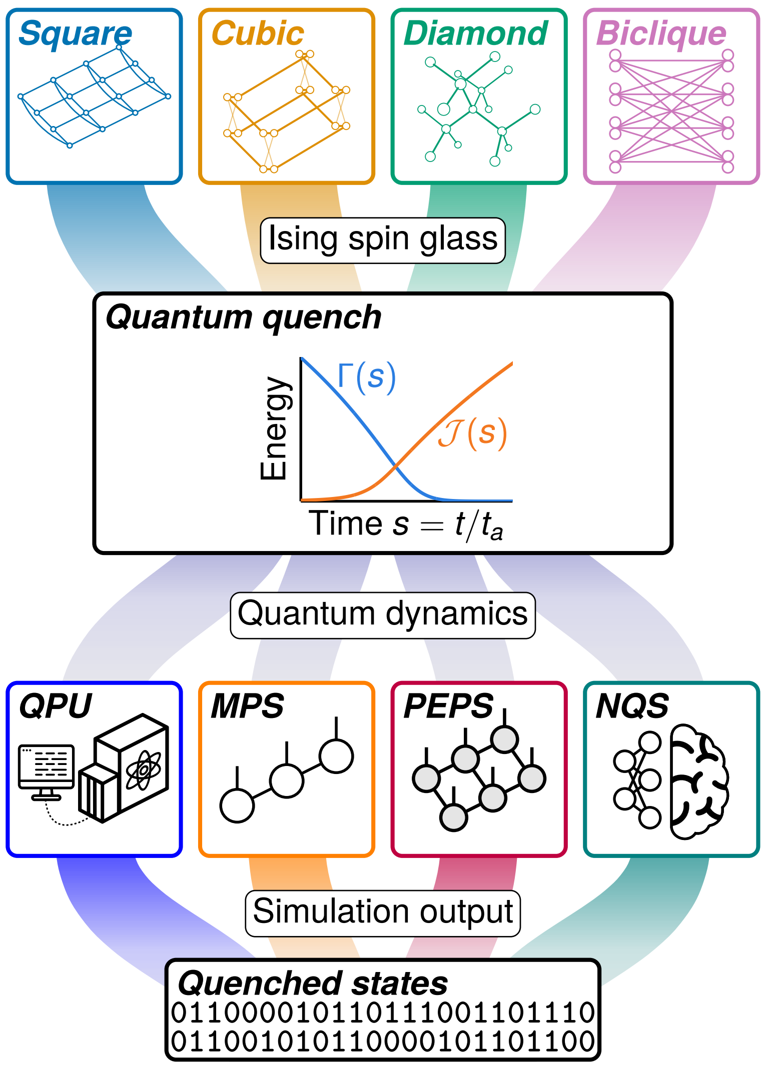
Matt Fishman
Flatiron CCQ

Dries Sels
Flatiron CCQ
New York University

Tindall, Mello et al., "Dynamics of disordered quantum systems...", arxiv:2503.05693

2) Simulation of D-Wave quantum Ising dynamics

What did the experiment compute?

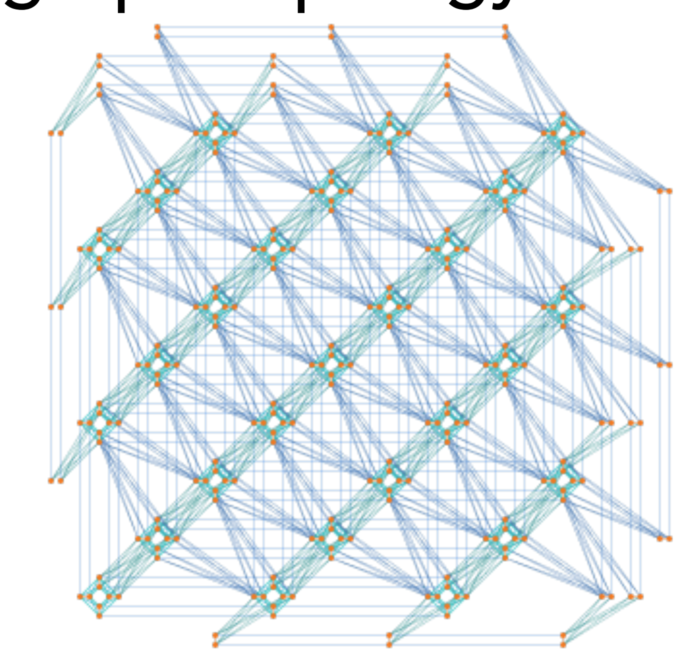


We consider a time-dependent Hamiltonian that interpolates between a driving Hamiltonian $\mathcal{H}_D$ and a classical Ising problem Hamiltonian $\mathcal{H}_P$:

$$\mathcal{H}(t) = \Gamma(t/t_a)\mathcal{H}_D + \mathcal{J}(t/t_a)\mathcal{H}_P, \tag{1}$$

$$\mathcal{H}_D = -\sum_i \sigma_i^x, \qquad \mathcal{H}_P = \sum_{i<j} J_{ij}\sigma_i^z\sigma_j^z, \tag{2}$$

Hardware: SQUIDs (quantum Ising spins) on "Pegasus" graph topology



Goal: compute **post-quench correlations**

$$c_{ij} = \langle \sigma_i^z \sigma_j^z \rangle \qquad \epsilon_c = \left(\frac{\sum_{i,j}(c_{ij} - \tilde{c}_{ij})^2}{\sum_{i,j}\tilde{c}_{ij}^2} \right)^{1/2}$$

King, et al. "Beyond-classical computation in quantum simulation." *Science* (2025)

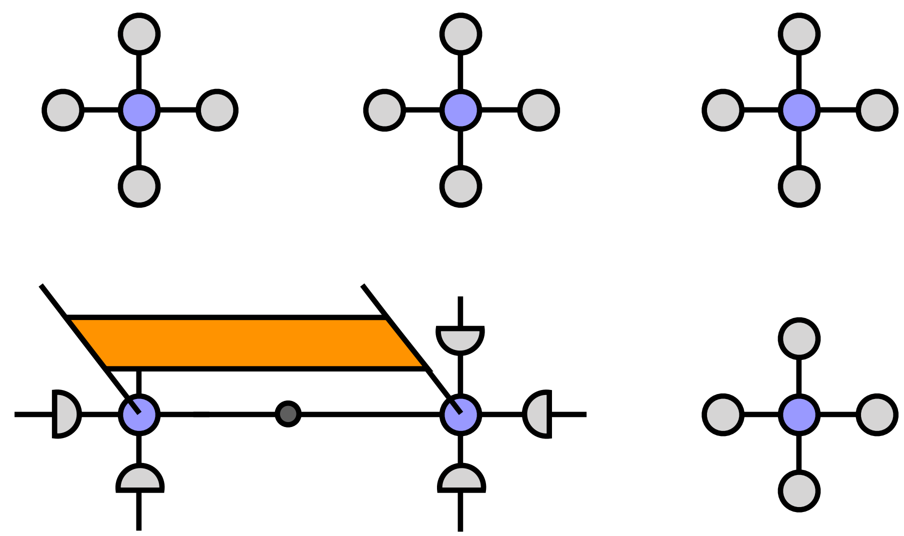
Tensor BP for Annealing

Our approach to simulate:

1. Time evolution at BP level

(allowing bonds to grow large, cheaply)

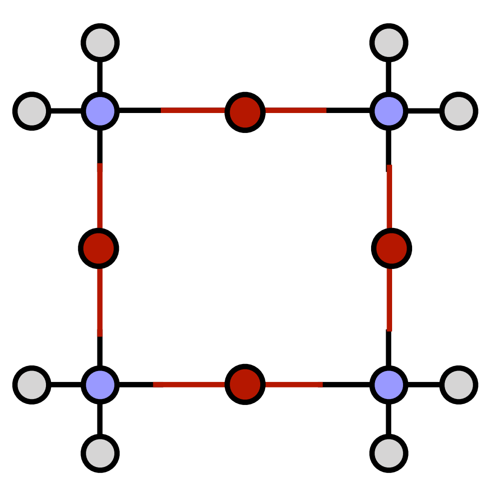
U(t) =



2. Corrected calculation of correlators

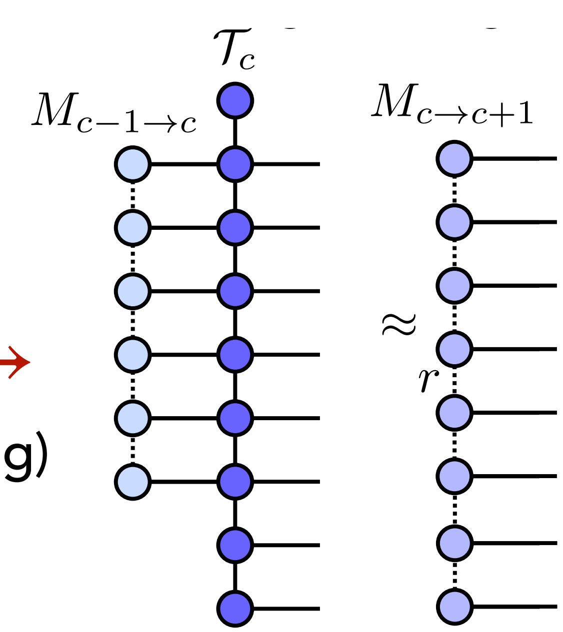
(truncate bonds before this step)

loop correction →



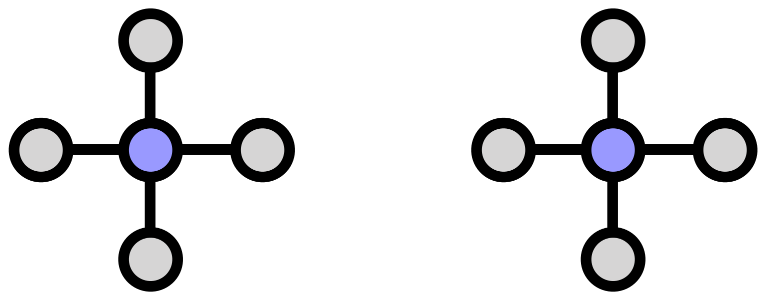
Boundary MPS →

(2D MPS Message Passing)

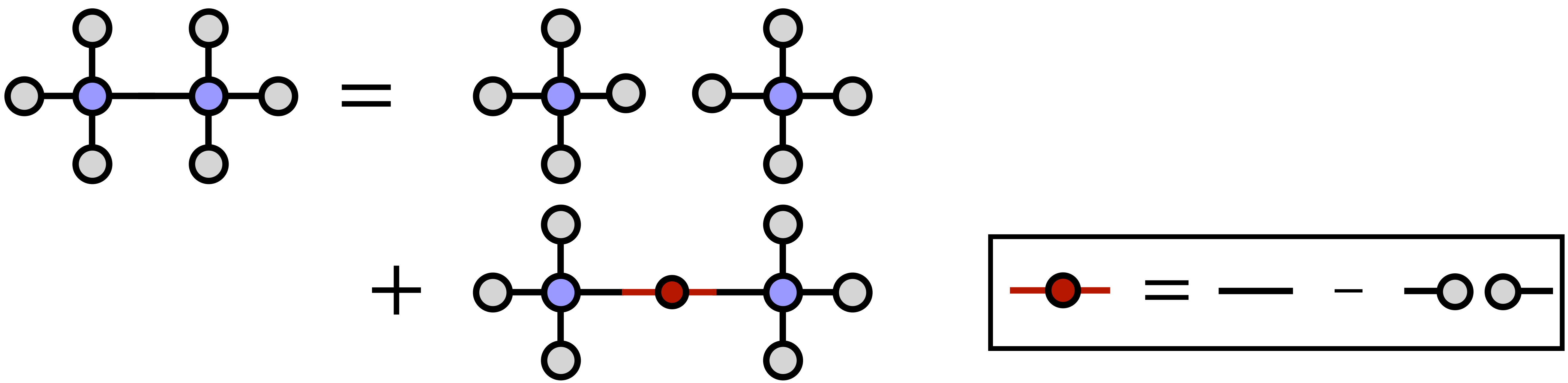


Loop Corrections – What are They?

Messages "cut" the original network:



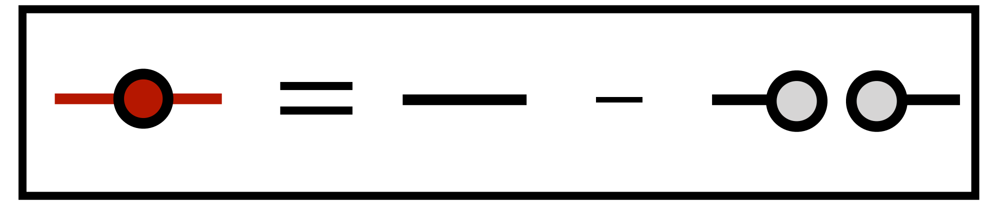
Missing contributions from orthogonal "message space":



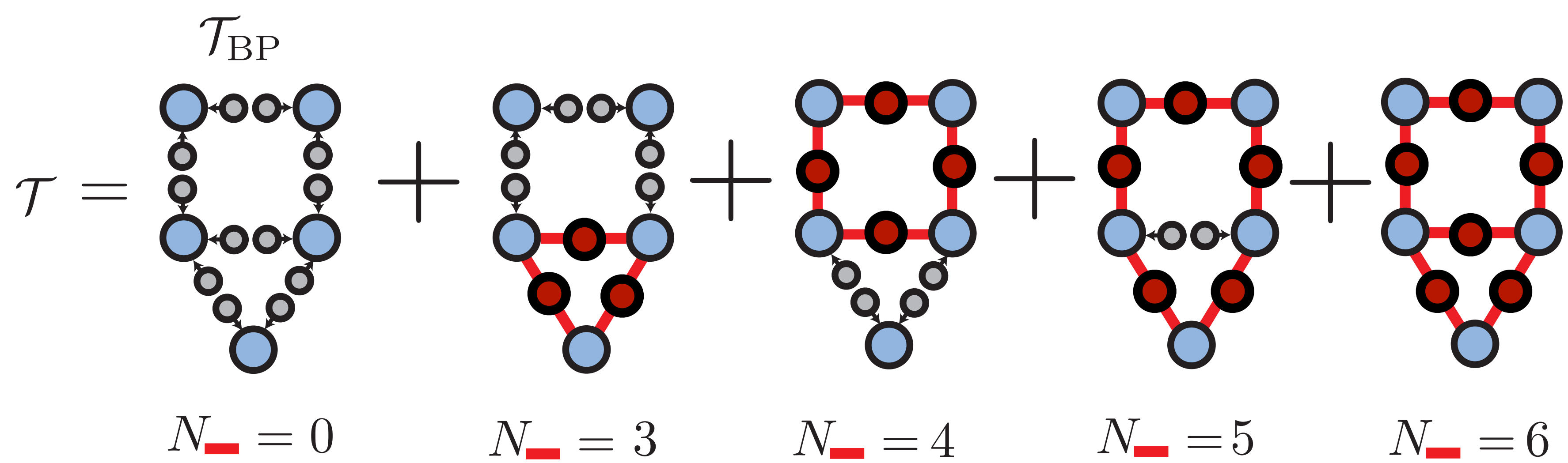
Only closed loops give non-zero correction

Glen Evenbly, et al., "Loop Series Expansions for Tensor Networks", arxiv: 2409.03108

Loop Corrections – What are They?



Only closed loops give non-zero correction



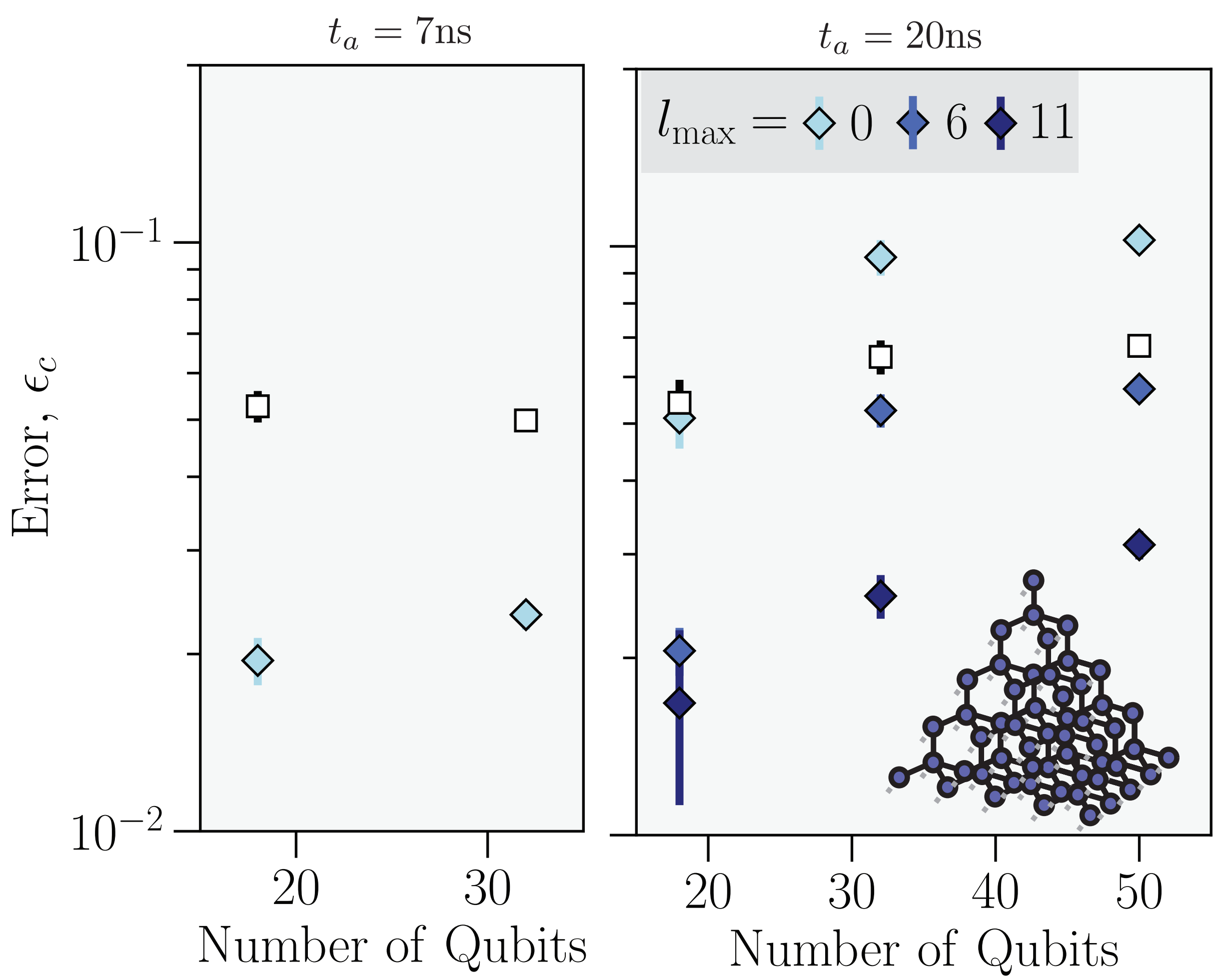
Like a Feynman diagram expansion but controlled by correlation length

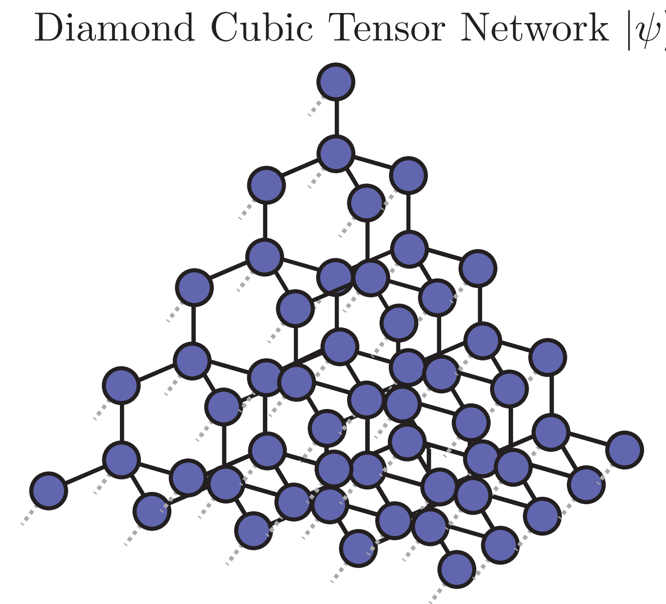
Glen Evenbly, et al., "Loop Series Expansions for Tensor Networks", arxiv: 2409.03108
Tindall, Mello, et al., "Dynamics of disordered quantum systems...", arxiv:2503.05693
Siddhant Midha and Yifan F. Zhang, “Beyond Belief Propagation…. “arXiv: 2510.02290
J. Gray et al, “Tensor Network Loop Cluster Expansions…..” arXiv: 2510.05647

Annealing Simulation Results

Can compute 3D quantum dynamics with these tools

Correlator errors:





Quantum annealer

Loop corrected BP method

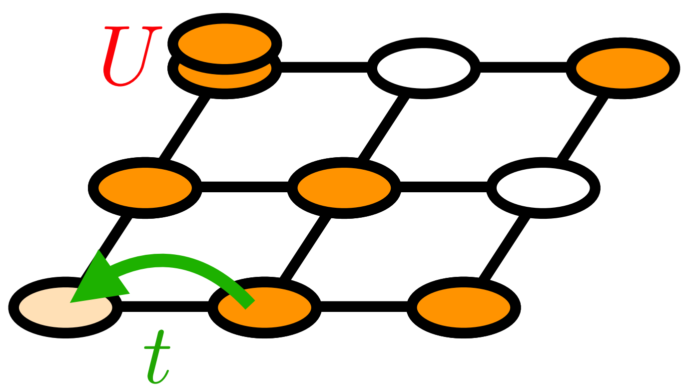
Competitive with quantum annealer results, using scalable methods

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

Future Directions & Open Questions

<u>What is the limit?</u>

Can we simulate dynamics of strongly-correlated electrons in 2D and 3D?



$$\hat{H} = -\, t \sum_{ij} (\hat{c}_i^\dagger \hat{c}_j + \hat{c}_j^\dagger \hat{c}_j) + U \sum_j \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}$$

Can novel dynamics approaches (space + time) "influence functional [1]" bring long time dynamics into reach?

[1] Park, Gray, Chan, arxiv:2504.07344

Summary

Newly efficient methods for 2D and 3D tensor networks are being developed based on message passing

Actually easier in high dimensions (more neighbors)

Opportunities to study quantum dynamics in higher dimensions

Now we are going to work with our own BP + PEPS Code using ITensors.jl and NamedGraphs.jl