Sign problem in tensor network contraction

Chris (Jielun) Chen

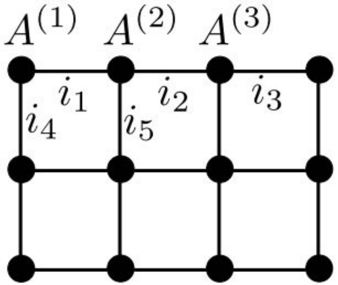
TN weekly meeting 06/17/2024

JC, Jiaqing Jiang, Dominik Hangleiter, Norbert Schuch, arXiv:2404.19023

Jiaqing Jiang, JC, Norbert Schuch, Dominik Hangleiter, in prep

The problem we study

$\mathcal{C} =$



Goal: Contract a 2D (square-lattice) tensor network.

Q:

- Does the complexity of the contraction depend on the sign structure? i.e. whether tensor entries are positive or general (real/complex).

- If yes, when (e.g. fraction of negative/positive) does the contraction become easy/hard?

Our results

- We studied this problem in random tensor networks (i.e. each tensor is drawn from i.i.d. distribution) and identified an entanglement transition point as one increases “positiveness”.

- The transition is surprisingly sharp, from close to maximal entanglement to almost zero entanglement.

- We found that such transition happens before the “sign problem” goes away, in particularly the earlier the larger the bond-dim is, meaning there’s a gap in complexity between TN contraction vs. MC-based contraction.

- We found a mapping from a random PEPS norm into a positive tensor network, providing alternative insights into average-case easiness of PEPS norm contraction [1].

[1] Sofia Gonzalez-Garcia, Shengqi Sang, Timothy H. Hsieh, Sergio Boixo, Guifre Vidal, Andrew C. Potter, Romain Vasseur, Random insights into the complexity of two-dimensional tensor network calculations, Phys. Rev. B 109, 235102 (2024)

Outline

1. Motivations & Evidence of existence of transition
2. Identify the transition point by mapping to stats model
3. Connection to Monte Carlo sampling
4. Map a random PEPS norm into positive TN
5. Other results & Conclusion

Motivation & Evidence: sign problem

In quantum Monte Carlo (QMC) simulations of fermions & frustrated spin systems, there is the infamous "sign problem" which exponentially increases the number of samples needed.

It has often been narrated that tensor networks can circumvent the sign problem, e.g. [1], since by construction TNs do not depend on local basis choices.

> **3.3. Fermions**
>
> An advantage of the TN framework with respect to other numerical methods for quantum many-body problems is the possibility of treating problems with fermionic degrees of freedom, which is of fundamental interest for condensed matter and fundamental physics. Whereas in this case quantum Monte Carlo methods are often obstructed by the sign problem, which causes the cost of convergence to increase exponentially with the system size, TN calculations can indistinctly treat fermionic and spin setups.

[1]

How true is this statement? Lots of details & caveats… but one starting point is to study how the contraction complexity of a tensor network depends on its sign structure!

[1] Mari Carmen Bañuls, Tensor Network Algorithms: a Route Map, Annual Review of Condensed Matter Physics

Motivation & Evidence: Gap from complexity theory

Complexity theory results also suggest there is an intrinsic gap between evaluating sum of exponentially many terms with different sign structure:

General terms	Only positive terms
Average-case #P-hard (counting the number of solutions to an NP problem; believed to be much harder than NP)	Worst-case FBPP^NP (Given an NP oracle, one can count the number of solutions efficiently; polynomially equivalent to NP)

Will this be reflected in random TN contractions? What is the transition point as the TN becomes more positive?

Motivation & Evidence: Observation by Johnnie and Garnet

arXiv > quant-ph > arXiv:2206.07044

Quantum Physics

[Submitted on 14 Jun 2022 (v1), last revised 5 Oct 2023 (this version, v2)]

Hyper-optimized approximate contraction of tensor networks with arbitrary geometry

Johnnie Gray, Garnet Kin-Lic Chan

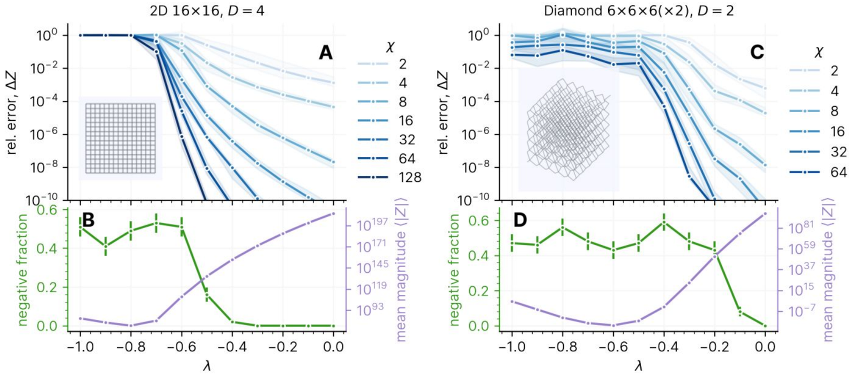


FIG. 17. Hardness transition in approximately contracting tensor networks with random uniform entries $\in [\lambda, 1]$. **A**: relative error, ΔZ, in approximately contracted value of the URand model on the square lattice using the `Greedy` algorithm as a function of λ and χ with $r = 2$. Line and bands show median and interquartile range across 20 instances. **B**: distribution of actual values Z for the square URand model in terms of fraction of negative instances (green, left axis) and average absolute magnitude (purple, right axis). Error bars denote error on mean. **C**: relative error, ΔZ, in approximately contracted value of the URand model on the diamond lattice using the `Greedy` algorithm as a function of λ and χ with $r = 2$. Line and bands show median and interquartile range across 20 instances. **D**: distribution of actual values Z for the diamond URand model in terms of fraction of negative instances (green, left axis) and average absolute magnitude (purple, right axis). Error bars denote error on mean.

Gradually tune entries from uniformly distributed in [-1, 1] to [0, 1].

Observed transition of contraction hardness near [-0.7, 1].

- Is there any significance of their observed number?
- How does this number relate to properties of the tensor network (e.g. bond-dim)?

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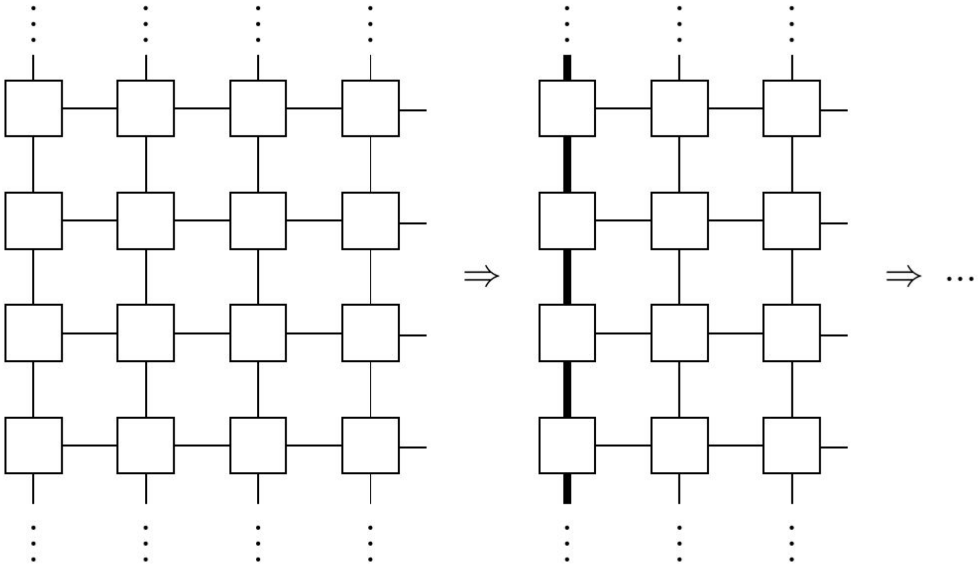
Easy to contract ≈ No entanglement barrier



Contractability is directly related to the bond-dimension required to perform the contraction.

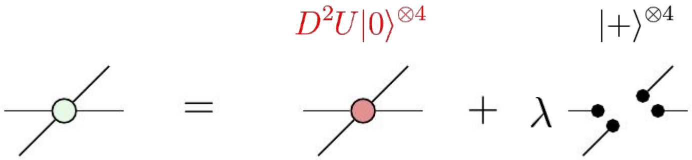
Easy to contract ≈
No entanglement barrier

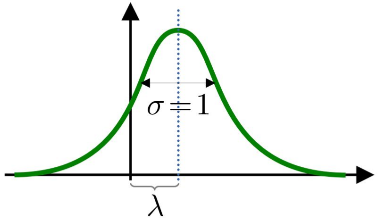
Goal: identify an effective theory to argue that, on average, positivity in a TN implies low entanglement.

Model of random tensor network: Haar-random

Haar-random quantum state i.e. random unitary/orthogonal applied on a fixed state. D^2 makes typical magnitude to be 1.

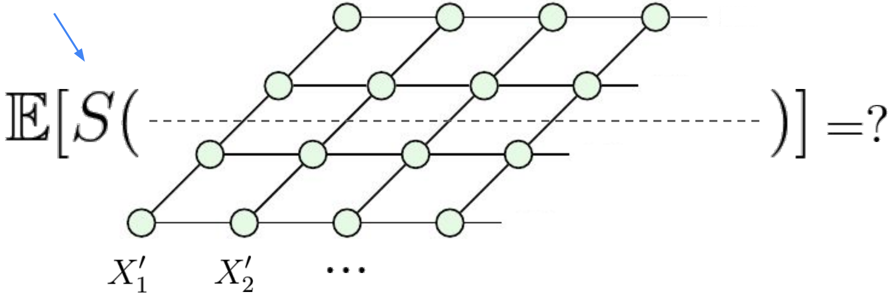
Equivalent to a vector with entries drawn from i.i.d. Gaussian and then normalize it. Converges to Gaussian in limit.





We will consider Rényi-2 entropy for simplicity

Integrating over unitary/orthogonal group



I will show:

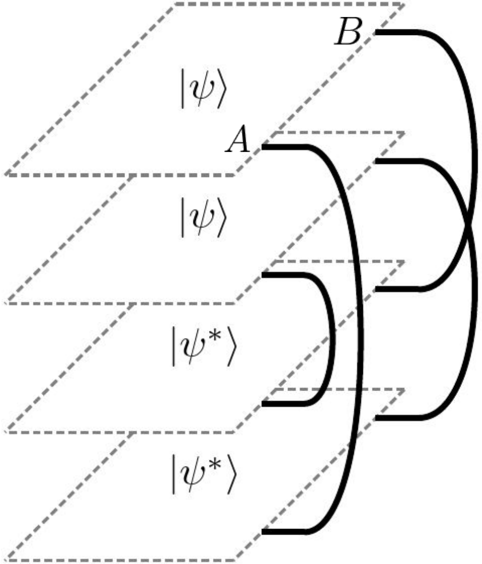
How to map the (average) Rényi-2 entropy to the partition function of a classical stats model.

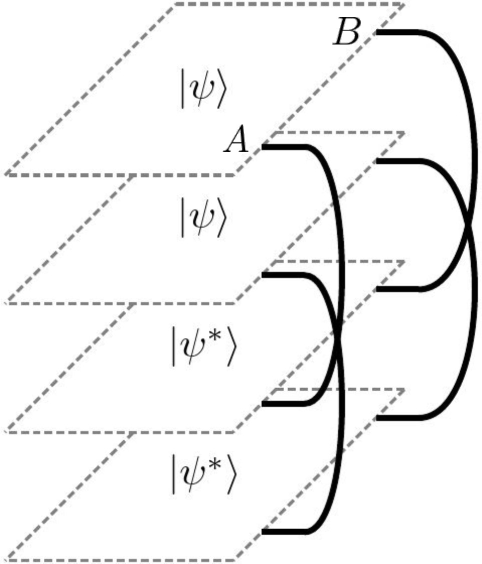
I will use the unitary ensemble as the example.

Rényi-2 entropy as tensor network contraction

$$\mathbb{E}\left[-\log(\rho_A^2)\right] \approx -\log\left(\mathbb{E}\left[\frac{Tr\left(Tr_B\left(|\psi\rangle\langle\psi|\right)^2\right)}{|\langle\psi|\psi\rangle|^2}\right]\right)$$

$$\approx -\log\left(\mathbb{E}\left[Tr\left(Tr_B\left(|\psi\rangle\langle\psi|\right)^2\right)\right]\right) + \log\left(\mathbb{E}\left[|\langle\psi|\psi\rangle|^2\right]\right)$$



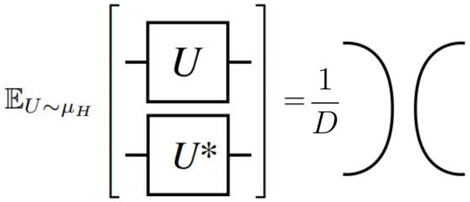


Haar measure & Integrating over unitary

$$\int_{U_d} U_{i_1 j_1}\cdots U_{i_q j_q} U^*_{i'_1 j'_1}\cdots U^*_{i'_q j'_q}\, dU \;=\; \sum_{\sigma,\tau\in S_q} \delta_{i_1 i'_{\sigma(1)}}\cdots\delta_{i_q i'_{\sigma(q)}}\delta_{j_1 j'_{\tau(1)}}\cdots\delta_{j_q j'_{\tau(q)}}\, \underline{Wg(\sigma\tau^{-1}, D)}$$

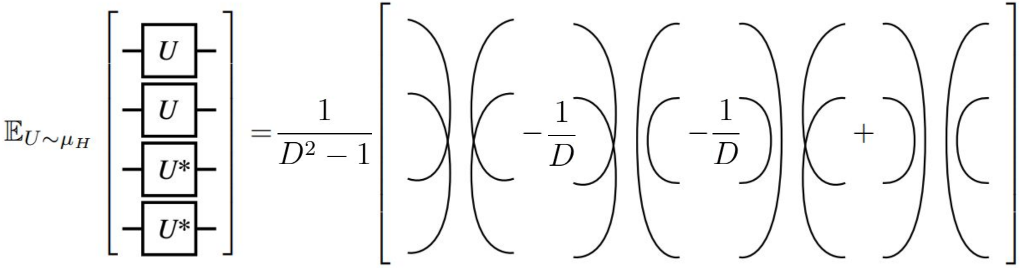
Weingarten Function

$$\mathop{\mathbb{E}}_{U\sim\mu_H}\left[U_{i_1,j_1}U^*_{i_2,j_2}\right] = \frac{1}{D}\delta_{i_1,i_2}\delta_{j_1,j_2}$$



[1]

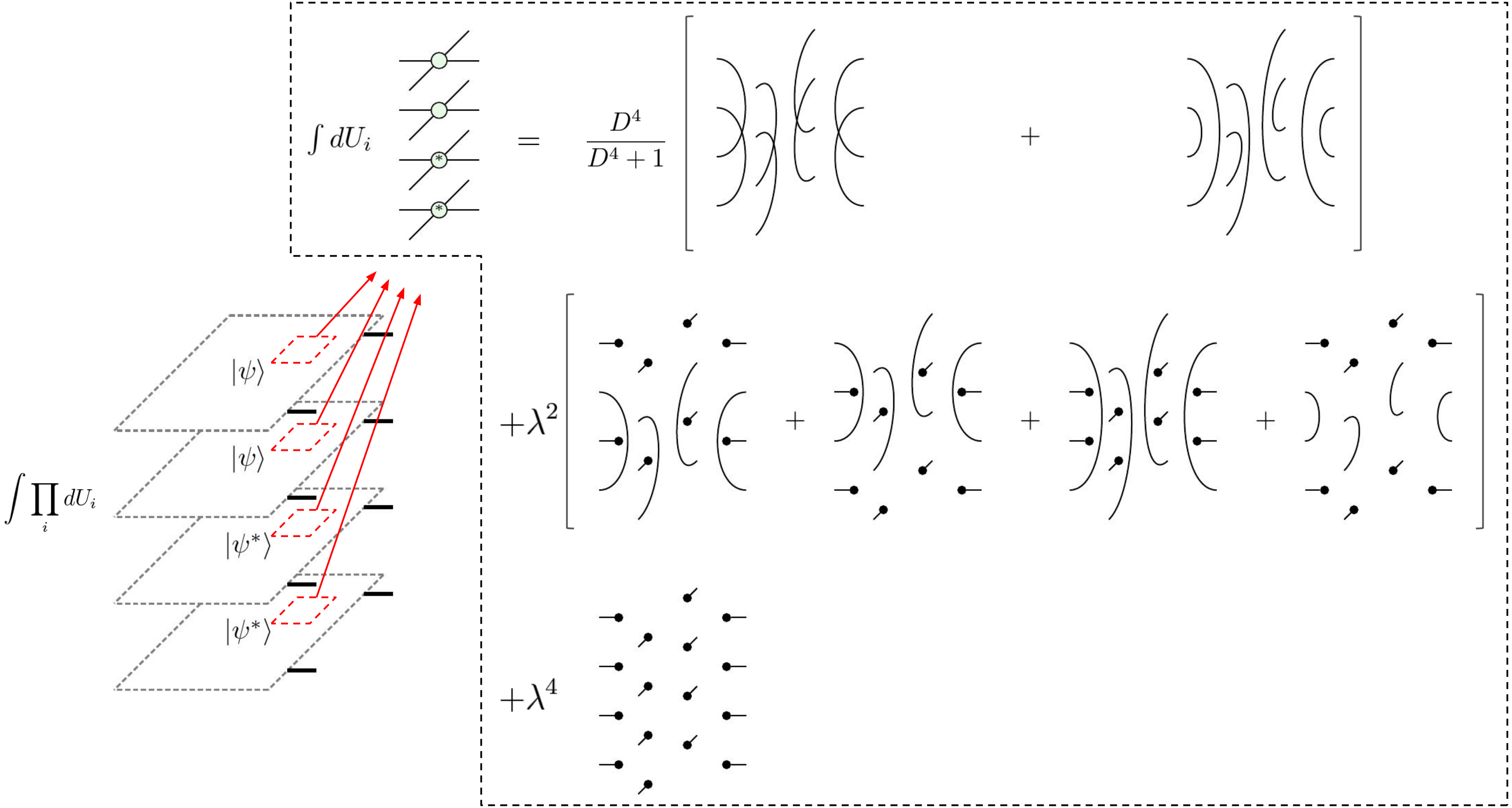
$$\mathop{\mathbb{E}}_{U\sim\mu_H}\left[U_{i_1,j_1}U_{i_2,j_2}U^*_{i_3,j_3}U^*_{i_4,j_4}\right] = \frac{1}{D^2-1}\left[\delta_{i_1,i_3}\delta_{i_2,i_4}\delta_{j_1,j_3}\delta_{j_2,j_4} - \frac{1}{D}\delta_{i_1,i_3}\delta_{i_2,i_4}\delta_{j_1,j_4}\delta_{j_2,j_3}\right] + \frac{1}{D^2-1}\left[-\frac{1}{D}\delta_{i_1,i_4}\delta_{i_2,i_3}\delta_{j_1,j_3}\delta_{j_2,j_4} + \delta_{i_1,i_4}\delta_{i_2,i_3}\delta_{j_1,j_4}\delta_{j_2,j_3}\right]$$



[1]

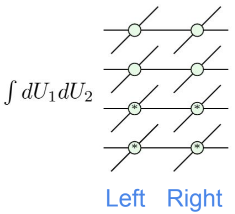
[1] Antonio Anna Mele, Introduction to Haar Measure Tools in Quantum Information: A Beginner's Tutorial, arXiv:2307.08956

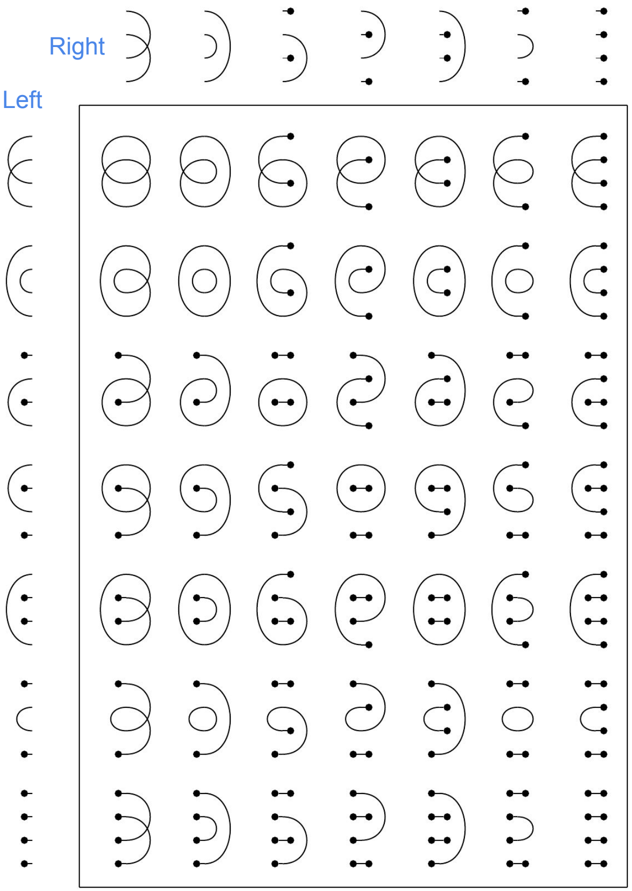
Integrating over local tensors of Rényi-2 TN



Contracting adjacent tensors

Contracting adjacent tensors introduces a scalar depending on the number of loops & lines

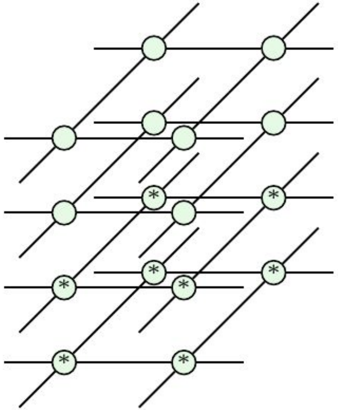




$$
= \begin{bmatrix}
D^2 & D & D^2 & D^2 & D & D & D^2 \\
D & D^2 & D & D & D^2 & D^2 & D^2 \\
D^2 & D & D^3 & D^2 & D^3 & D^2 & D^3 \\
D^2 & D & D^2 & D^3 & D^2 & D^2 & D^3 \\
D & D^2 & D^3 & D^2 & D^3 & D^2 & D^3 \\
D & D^2 & D^2 & D^2 & D^2 & D^3 & D^3 \\
D^2 & D^2 & D^3 & D^3 & D^3 & D^3 & D^4
\end{bmatrix}
$$

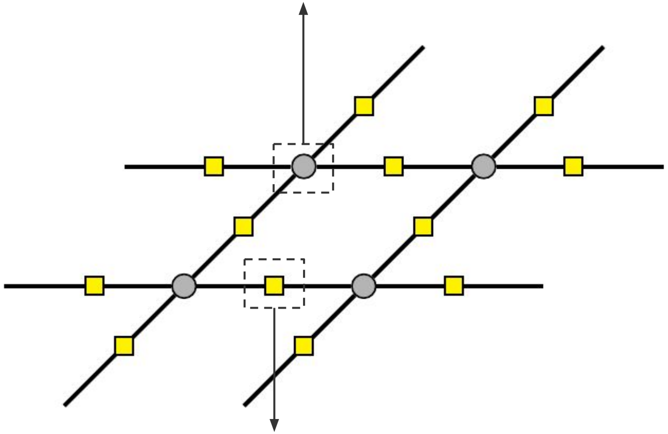
Effective classical stat-mech model

$$\int \prod_i dU_i$$



$$=$$

$$\delta_{ijkl}\begin{bmatrix}\frac{D^4}{D^4+1} & \frac{D^4}{D^4+1} & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^2 & \lambda^4\end{bmatrix}_i$$



$$\begin{bmatrix}
D^2 & D & D^2 & D^2 & D & D & D^2 \\
D & D^2 & D & D & D^2 & D^2 & D^2 \\
D^2 & D & D^3 & D^2 & D^3 & D^2 & D^3 \\
D^2 & D & D^2 & D^3 & D^2 & D^2 & D^3 \\
D & D^2 & D^3 & D^2 & D^3 & D^2 & D^3 \\
D & D^2 & D^2 & D^2 & D^2 & D^3 & D^3 \\
D^2 & D^2 & D^3 & D^3 & D^3 & D^3 & D^4
\end{bmatrix}$$

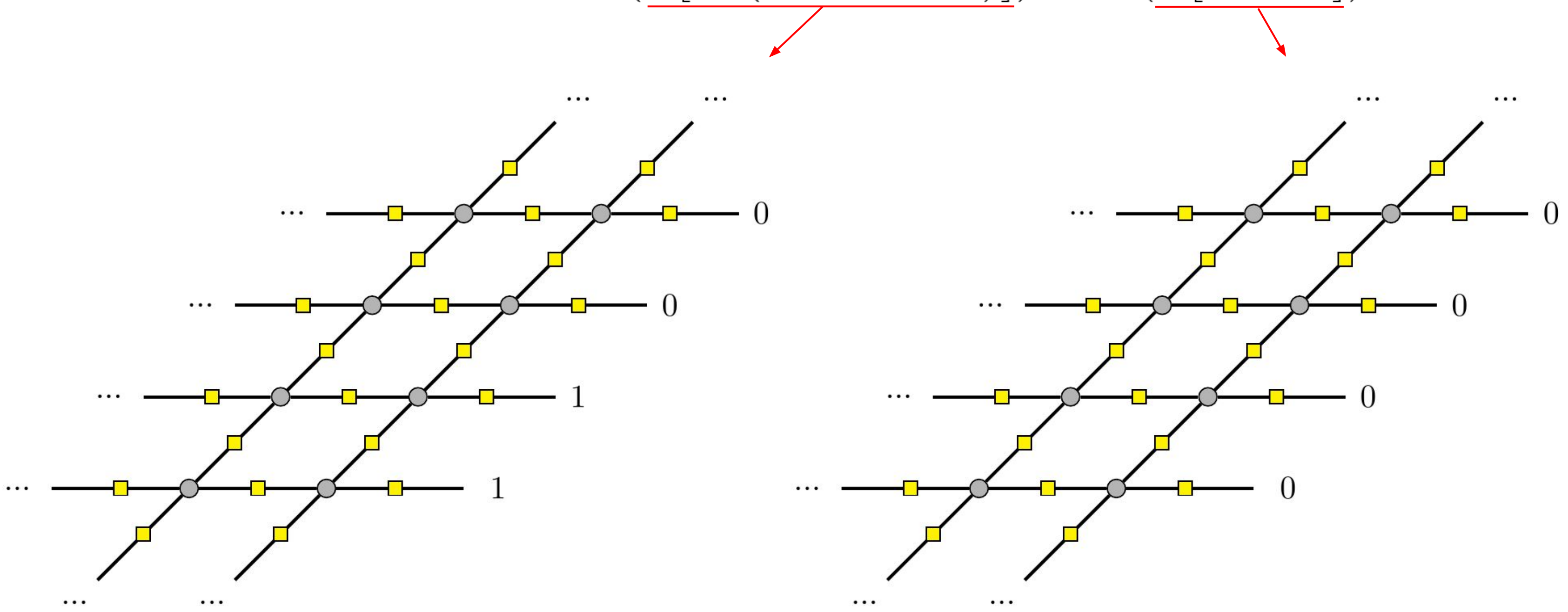
7-level Potts model with external field

$$\sum_{\{\sigma^{(s)}\}} e^{-\sum_s h(\sigma^{(s)})-\sum_{\langle s,s'\rangle} k(\sigma^{(s)},\sigma^{(s')})}$$

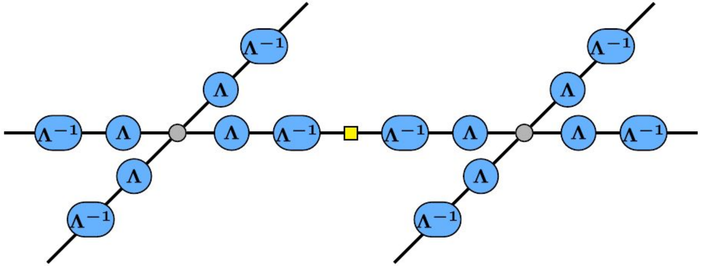
Boundary condition determines denominator & numerator

$$\mathbb{E}\left[-\log(\rho_A^2)\right] \approx -\log\left(\mathbb{E}\left[\frac{Tr\left(Tr_B\left(|\psi\rangle\langle\psi|\right)^2\right)}{|\langle\psi|\psi\rangle|^2}\right]\right)$$

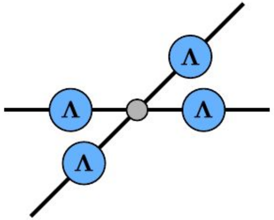
$$\approx -\log\left(\mathbb{E}\left[Tr\left(Tr_B\left(|\psi\rangle\langle\psi|\right)^2\right)\right]\right) + \log\left(\mathbb{E}\left[|\langle\psi|\psi\rangle|^2\right]\right)$$



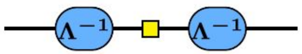
Gauge transform into a ferromagnetic model



$$\Lambda = \begin{pmatrix} D & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & D & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & D^{3/2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & D^{3/2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & D^{3/2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & D^{3/2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & D^2 \end{pmatrix}$$



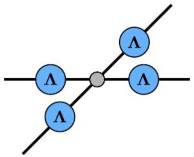
$$= D^4 \delta_{ijkl} \Big[\underbrace{\tfrac{D^4}{D^4+1} \quad \tfrac{D^4}{D^4+1}}_{\approx 1} \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^4\lambda^4 \Big]_i$$



$$= \begin{bmatrix} 1 & 1/D & 1/D^{0.5} & 1/D^{0.5} & 1/D^{1.5} & 1/D^{1.5} & 1/D \\ 1/D & 1 & 1/D^{1.5} & 1/D^{1.5} & 1/D^{0.5} & 1/D^{0.5} & 1/D \\ 1/D^{0.5} & 1/D^{1.5} & 1 & 1/D & 1/D & 1/D & 1/D^{0.5} \\ 1/D^{0.5} & 1/D^{1.5} & 1/D & 1 & 1/D & 1/D & 1/D^{0.5} \\ 1/D^{1.5} & 1/D^{0.5} & 1/D & 1/D & 1 & 1/D & 1/D^{0.5} \\ 1/D^{1.5} & 1/D^{0.5} & 1/D & 1/D & 1/D & 1 & 1/D^{0.5} \\ 1/D & 1/D & 1/D^{0.5} & 1/D^{0.5} & 1/D^{0.5} & 1/D^{0.5} & 1 \end{bmatrix}$$

Becomes ferromagnetic as D → ∞!

Transition point of the effective model

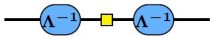


$$= D^4\delta_{ijkl}\left[\frac{D^4}{D^4+1} \quad \frac{D^4}{D^4+1} \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^2\lambda^2 \quad D^4\lambda^4\right]_i$$

$\lambda > 1/D$ → Prefer the latter five configurations → Competition between boundary condition and magnetic field → disorder

$\lambda < 1/D$ → Prefer first two configurations → Mixed boundary condition → domain wall

Transition point $\lambda = 1/D$!



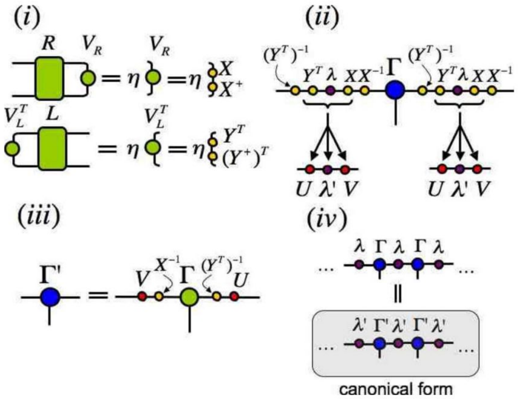
$$= \begin{bmatrix} 1 & 1/D & 1/D^{0.5} & 1/D^{0.5} & 1/D^{1.5} & 1/D^{1.5} & 1/D \\ 1/D & 1 & 1/D^{1.5} & 1/D^{1.5} & 1/D^{0.5} & 1/D^{0.5} & 1/D \\ 1/D^{0.5} & 1/D^{1.5} & 1 & 1/D & 1/D & 1/D & 1/D^{0.5} \\ 1/D^{0.5} & 1/D^{1.5} & 1/D & 1 & 1/D & 1/D & 1/D^{0.5} \\ 1/D^{1.5} & 1/D^{0.5} & 1/D & 1/D & 1 & 1/D & 1/D^{0.5} \\ 1/D^{1.5} & 1/D^{0.5} & 1/D & 1/D & 1/D & 1 & 1/D^{0.5} \\ 1/D & 1/D & 1/D^{0.5} & 1/D^{0.5} & 1/D^{0.5} & 1/D^{0.5} & 1 \end{bmatrix}$$

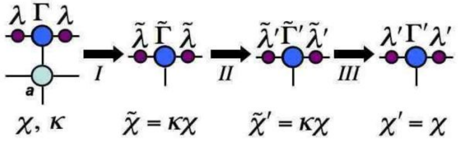
→ Tend to be ferromagnetic (spins aligned)

iMPS simulation of the effective model

iMPS - iMPO algorithm

Roman Orus and Guifre Vidal, The iTEBD algorithm beyond unitary evolution, Phys. Rev. B 78, 155117 (2008)

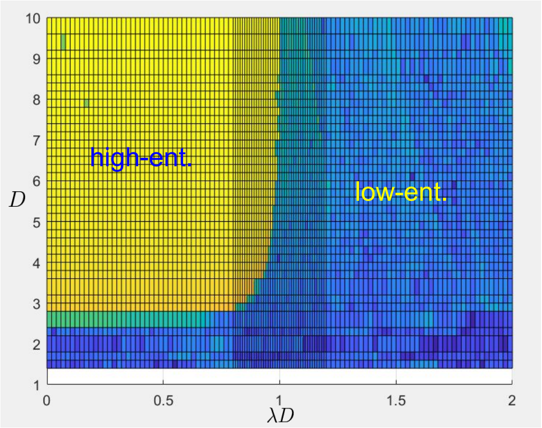




Overlap between left/right dominant eigenvectors of fixed-point iMPS

$$\left|\frac{\langle l_1|\lambda|r_0\rangle}{\langle l_0|\lambda|r_0\rangle}\right|$$

$$|r_i\rangle = \mathrm{v}^r_{\max}(\Gamma_i\lambda)$$
$$\langle l_i| = \mathrm{v}^l_{\max}(\lambda\Gamma_i)$$

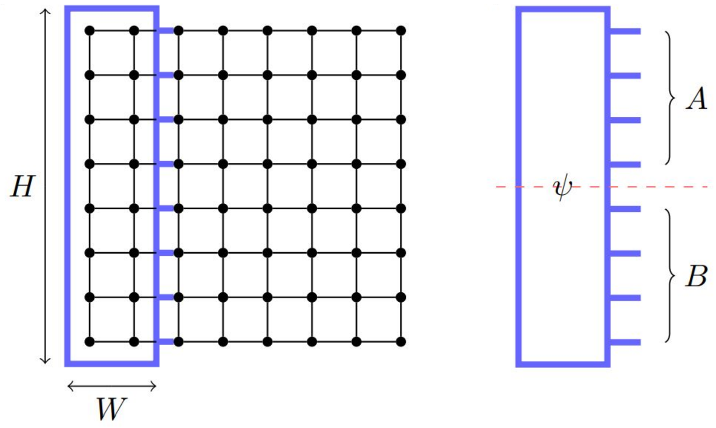


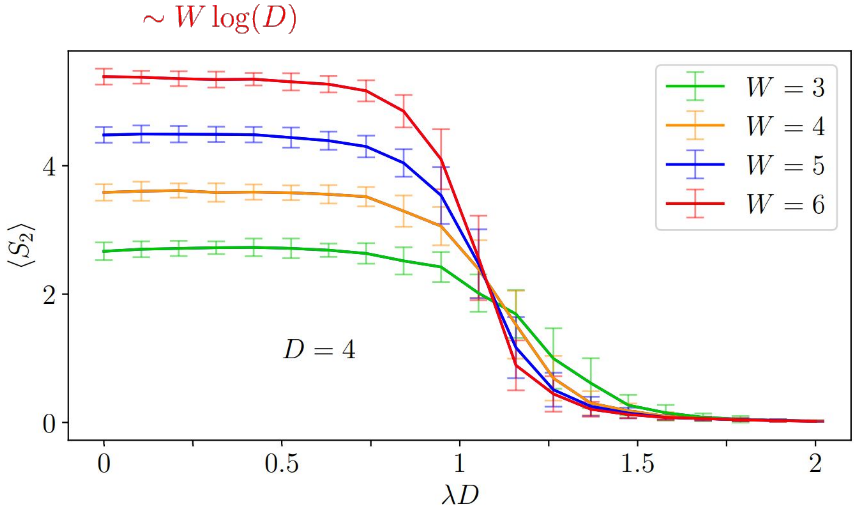
λ = 0 case also relates to previous results:

[1] Romain Vasseur, Andrew C. Potter, Yi-Zhuang You, Andreas W. W. Ludwig, Entanglement Transitions from Holographic Random Tensor Networks, Phys. Rev. B 100, 134203 (2019)
[2] Ryan Levy, Bryan K. Clark, Entanglement Entropy Transitions with Random Tensor Networks, arXiv:2108.02225

Finite-size simulation

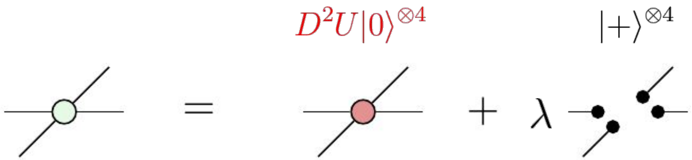
We observed the same transition in finite-size simulation. We choose H >> W so the entropy saturates (H = 4W in our simulation).





Is it because of rank-one instead of positivity?

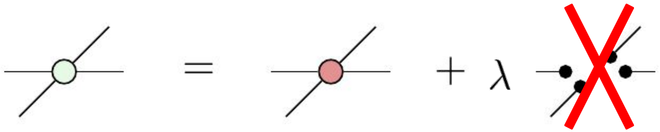
Recall our model of random tensors:



A natural question to ask is whether the second component being rank-one (i.e. percolation types of arguments) is the main reason for the complexity transition.

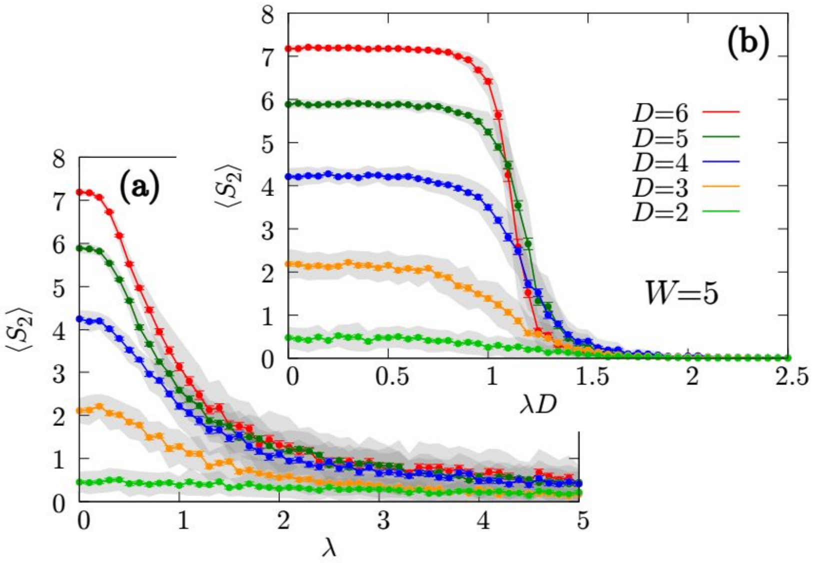
That is, what is the role of “positivity”?

Is it because of rank-one instead of positivity?



(a) random rank-one (but not positive)

(b) random positive (but not rank-one)



The “positivity” part is important to observe the transition!

Or in other words, the rank-one states need to be “aligned”.

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Sign problem in quantum monte carlo sampling

$$\langle O\rangle = \frac{1}{Z}\mathrm{Tr}[Oe^{-\beta H}] = \frac{1}{Z}\mathrm{Tr}[O(e^{-\beta H/M})^M]$$
$$= \frac{1}{Z}\sum_{\{x_i\}}\langle x_0|O|x_1\rangle\langle x_1|e^{-\beta H/M}|x_2\rangle\langle x_2|...|x_M\rangle\langle x_M|e^{-\beta H/M}|x_0\rangle$$
$$= \frac{1}{Z}\sum_x O(x)T(x)$$

$T(x) = \mathrm{sign}(T(x))|T(x)|$

$\langle\mathrm{sign}\rangle = \frac{\sum_x T(x)}{\sum_x |T(x)|} = e^{-\beta N\Delta f}$

$T(x) \geq 0$

sample $x_i^* \sim \frac{T(x)}{\sum_x T(x)}$

estimate by $\frac{1}{K}\sum_{i=1}^{K} O(x_i^*)$

error $\sim \frac{1}{\sqrt{K}}$

$T(x)$ positive/negative

sample $x_i^* \sim \frac{|T(x)|}{\sum_x |T(x)|}$

estimate by $\frac{1}{K}\frac{1}{\langle\mathrm{sign}\rangle}\sum_{i=1}^{K} O(x_i^*)\mathrm{sign}(T(x_i^*))$

error $\sim \frac{e^{\beta N\Delta f}}{\sqrt{K}}$

“sign problem”: exponential dependence on N caused by $\langle\mathrm{sign}\rangle$

Sign problem of random TN

Sign problem only starts to disappear when $\lambda \gtrsim 1$

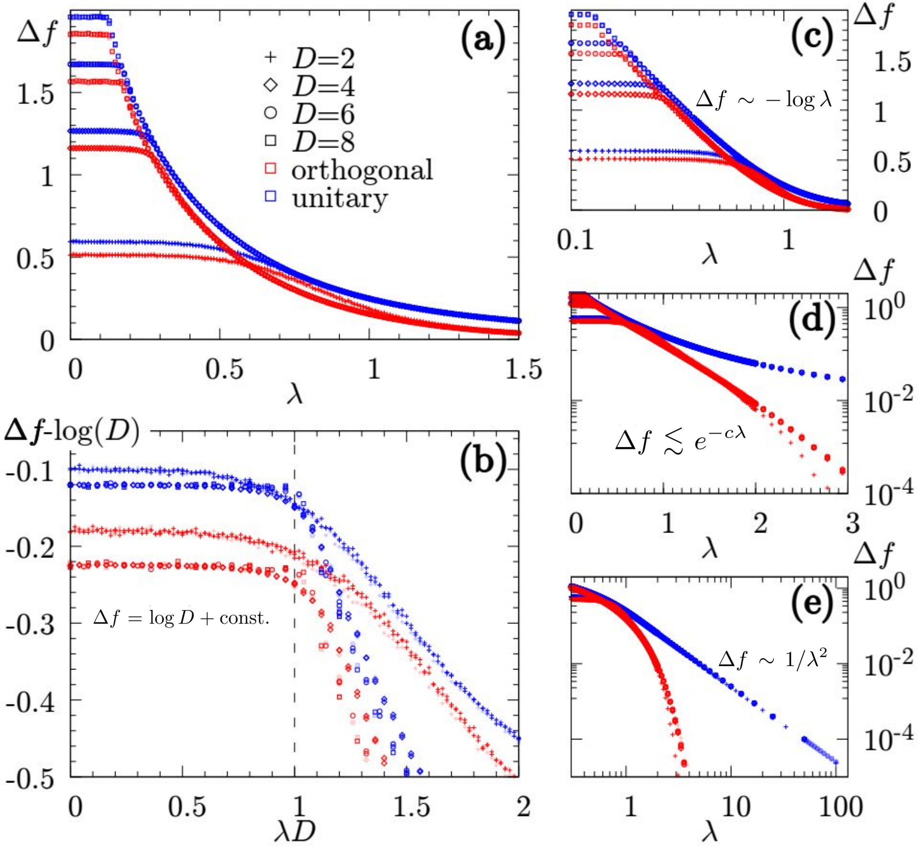
"Sign problem" in TN: $e^{-\Delta f\, N} := \dfrac{\sum_{\boldsymbol{x}} T(\boldsymbol{x})}{\sum_{\boldsymbol{x}} |T(\boldsymbol{x})|}$

$\exp(2\Delta f N)$ samples needed to overcome the sign problem.

$$\lambda \lesssim \frac{1}{D} \quad : \qquad \Delta f = \log D + \text{const.}$$

$$\frac{1}{D} \lesssim \lambda \lesssim 1 : \qquad \Delta f \sim -\log \lambda$$

$$1 \lesssim \lambda : \begin{cases} \Delta f \lesssim e^{-c\lambda} & \text{orthogonal} \\ \Delta f \sim 1/\lambda^2 & \text{unitary} \end{cases}$$

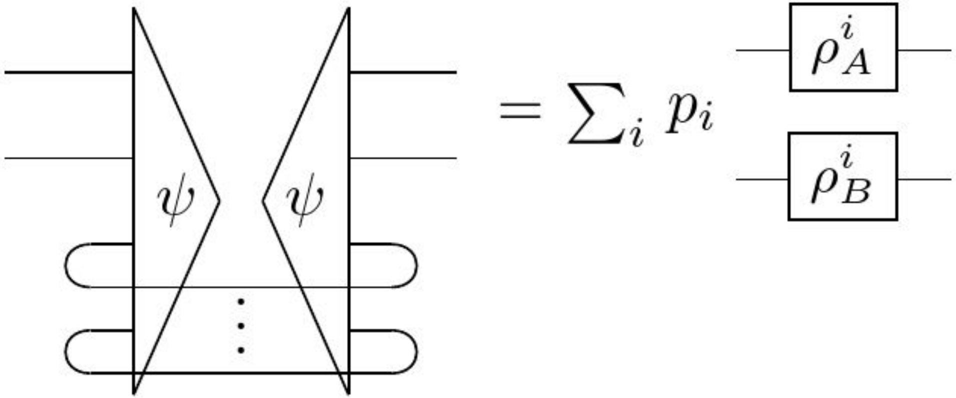


Outline

1. Motivations & Evidence of existence of transition
2. Identify the transition point by mapping to stats model
3. Connection to Monte Carlo sampling
4. Map a random PEPS norm into positive TN
5. Other results & Conclusion

Map a random PEPS norm into a positive TN

If one traces out a large subsystem of a Haar random state, the remaining density matrix is very likely to be highly noisy (very close to identity) [1], which means they are separable [2].



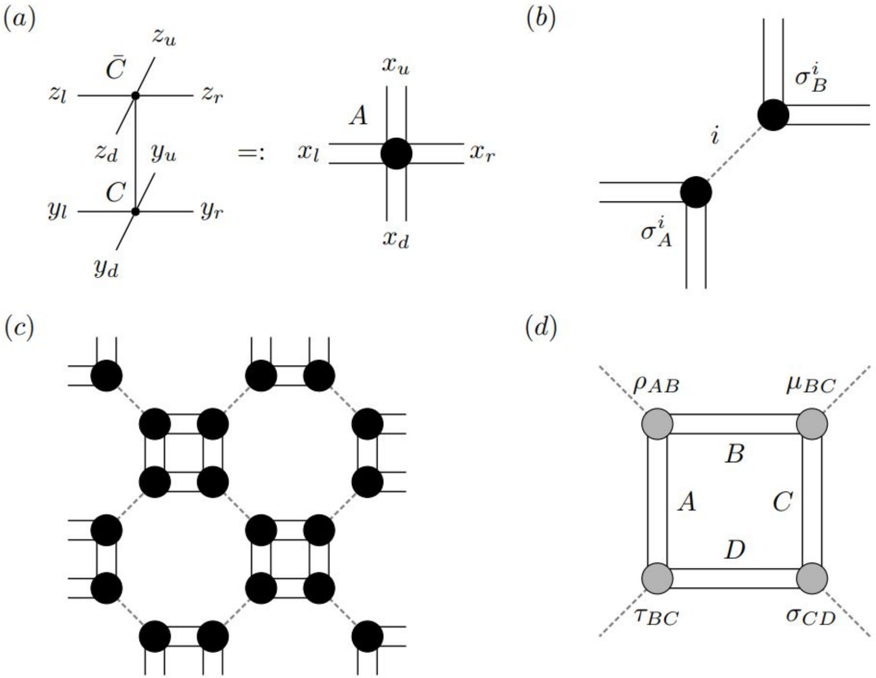
[1] Patrick Hayden, Debbie W. Leung, Andreas Winter, Aspects of generic entanglement, Commun. Math. Phys. 265, 95–117 (2006)
[2] S. L. Braunstein, C. M. Caves, R. Jozsa, N. Linden, S. Popescu, and R. Schack, Separability of Very Noisy Mixed States and Implications for NMR Quantum Computing, Phys. Rev. Lett. 83, 1054–1057 (1999)

Map a random PEPS norm into a positive TN

For a PEPS with Haar-random tensors with large enough physical dimension, one can do such decomposition in a TNR-like way, as in (c), and regroup tensors as in (d).

This maps it into a new TN with entries being the trace of product of PSD matrices, which are always positive.

This gives alternative insights into average-case easiness of PEPS norm contraction [1].



[1] Sofia Gonzalez-Garcia, Shengqi Sang, Timothy H. Hsieh, Sergio Boixo, Guifre Vidal, Andrew C. Potter, Romain Vasseur, Random insights into the complexity of two-dimensional tensor network calculations, Phys. Rev. B 109, 235102 (2024)

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Complexity of positive TNs (in progress)

I will share two most interesting results:

1. For $\lambda \gtrsim 1/D$ and $D \geq n/(c\ln(n))$, there is a quasi-polynomial ($poly(n^{\ln^5 n})$) time algorithm to approximate the random TN's contracted value with high probability, up to $1/poly(n)$ multiplicative error. No reference to entanglement is made in the algorithm.

2. Contracting an arbitrary TN with additive error bounded by the product of 2-norm of each tensor is BQP-complete.

   Contracting a positive TN with additive error bounded by the product of 1-norm of each tensor is BPP-complete.

Itai Arad, Zeph Landau, Quantum computation and the evaluation of tensor networks, arXiv:0805.0040

Summary

- We found a sharp transition from high-entangled phase to low-entangled phase when the TN becomes positive, where the transition point is inversely proportional to the bond-dim.

- On contrast, the sign problem in TN disappears only gradually as the positiveness increases.

- The transition is a extremely strong concentration of measurement effect. How to understand this better?

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