Title: Isometric Tensor Network States in Two Dimensions

Speakers: Michael Zaletel

Collection: Quantum Matter: Emergence & Entanglement 3

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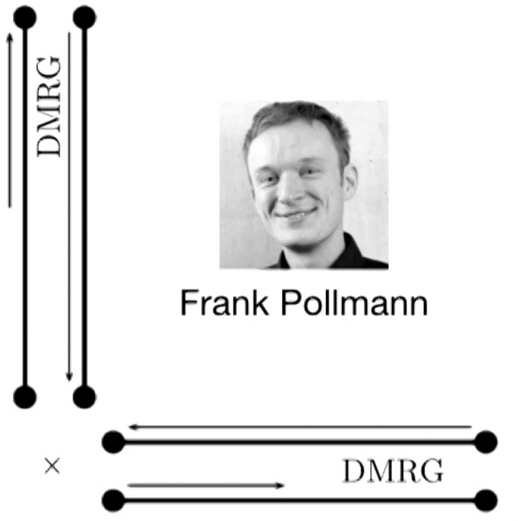
Abstract: We introduce an isometric restriction of the tensor-network ansatz that allows for highly efficient contraction of the network. We consider two concrete applications using this ansatz. First, we show that a matrix-product state representation of a 2D quantum state can be iteratively transformed into an isometric 2D tensor network. Second, we introduce a 2D version of the time-evolving block decimation algorithm (TEBD2) for approximating the ground state of a Hamiltonian as an isometric tensor network, which we demonstrate for the 2D transverse field Ising model.

DMRG^2

arXiv:1902.05100



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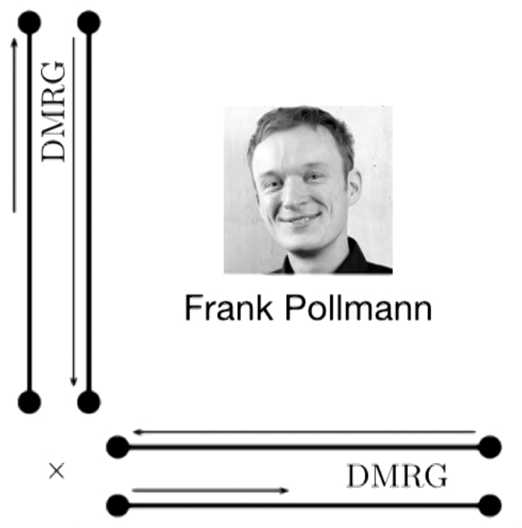
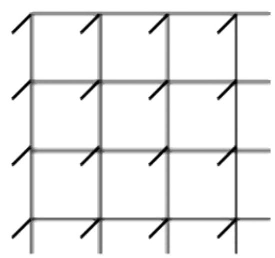
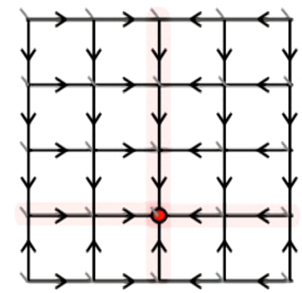


Frank Pollmann

PEPs



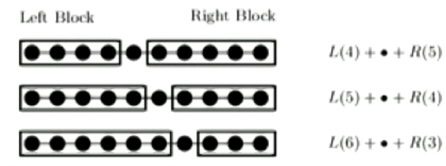
isometric tensor network



Massive leap in notation!

1D: DMRG works really really well for finding ground states!

Density matrix formulation for quantum renormalization groups SR White Physical review letters 69 (19), 2863	5505	1992
Density-matrix algorithms for quantum renormalization groups SR White Physical Review B 48 (14), 10345	3005	1993
Real-time evolution using the density matrix renormalization group SR White, AE Feiguin Physical review letters 93 (7), 076401	989	2004



DMRG finds ground states of Hamiltonians in a time polynomial in system size: for gapped states, effectively linear in L

Unbiased: variants of DMRG provably work for any gapped phase

Easy to get e.g. 12 digit accuracy in observables

Generalizations to time dependence, finite T, etc.

Generalizing it's success to 2D would be great!

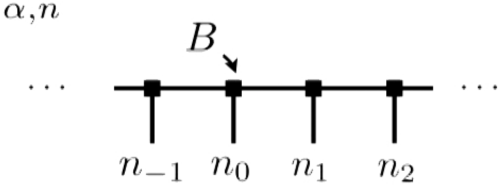
The underlying engine: 1D tensor network ansatz (matrix product state)

[Fannes et al. 1992;
Östlund & Rommer 1995]

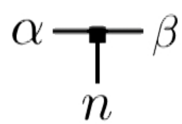
MPS: variational ansatz for spin-chains

$$|\Psi\rangle = \sum_{\alpha,n} \left[\cdots B^{n_1}_{\alpha_1\alpha_2} B^{n_2}_{\alpha_2\alpha_3} \cdots\right] |\cdots n_1 n_2 \cdots\rangle \quad n_i = \uparrow / \downarrow$$

$\Psi_{\cdots n_0 n_1 \cdots} =$



$B^n_{\alpha\beta} =$



$\alpha, \beta \in \{1, 2, \cdots, \text{D}\}$

D = bond dimension / tensor size

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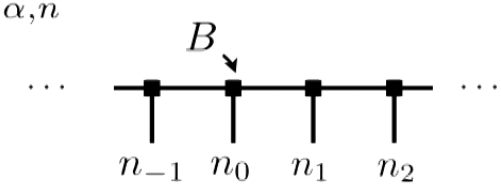

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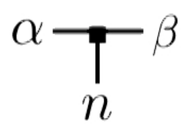


$\alpha, \beta \in \{1, 2, \cdots, \mathrm{D}\}$

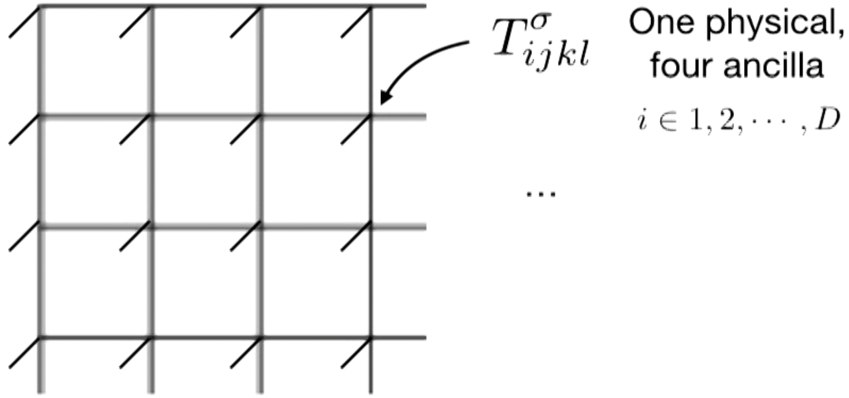
D = bond dimension / tensor size

DMRG is method to variationally minimize energy by sequentially tweaking the "B":

$$E_0 = \min_{\{B\}} \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

2D: TNSs … will eventually work really really well?

(alias "projected entangled pair / PEP")



Theoretical: what phases can be well approximated by PEPs? How does error scale with bond dimension "D"?

Practical: how do we efficiently compute observables and optimize tensors?

[Susanne Richter 1996 (!); Nishino, Okunishi et al. 2001; Verstraete & Cirac 2004;]

Practical: how do we efficiently compute observables and optimize tensors?

Typical object to compute: $E = \min_{\{T\}} \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$

Let's start easy, with the norm:

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

$= \sum_{\{\alpha,\bar{\alpha}\}=1}^{D} T^* T_{\bar{\alpha}_1 \alpha_1} T^* T_{\bar{\alpha}_2 \alpha_2} \cdots$

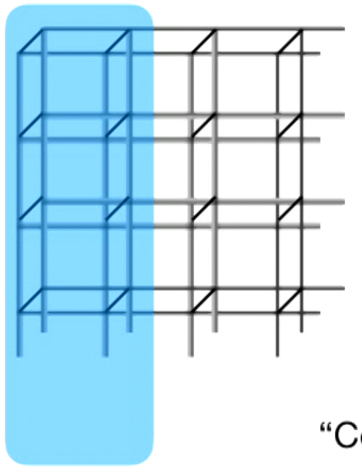
$D^{4 L_x L_y}$ terms, obviously can't be contracted exactly

Need approximation algorithm: *like* computing partition function of 2D classical model

Boundary MPS method

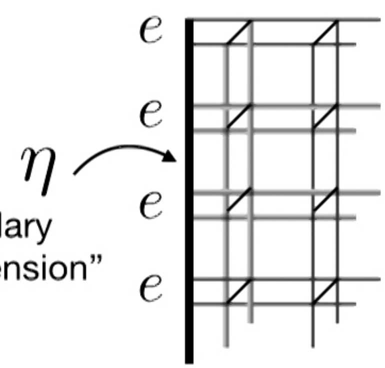
[Verstraete & Cirac 2004; many since;
CTMRG Nishino, Okunishi et al. 2001]

$E_L^{[2]}$



Approximate
boundary
as MPS:

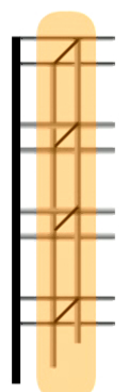
$E_L^{[2]} \approx eee\cdots$



"Boundary
bond dimension"

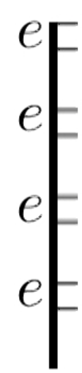
"Column transfer operator"

$$E_L^{[3]} = T^\dagger E_L^{[2]} T =$$



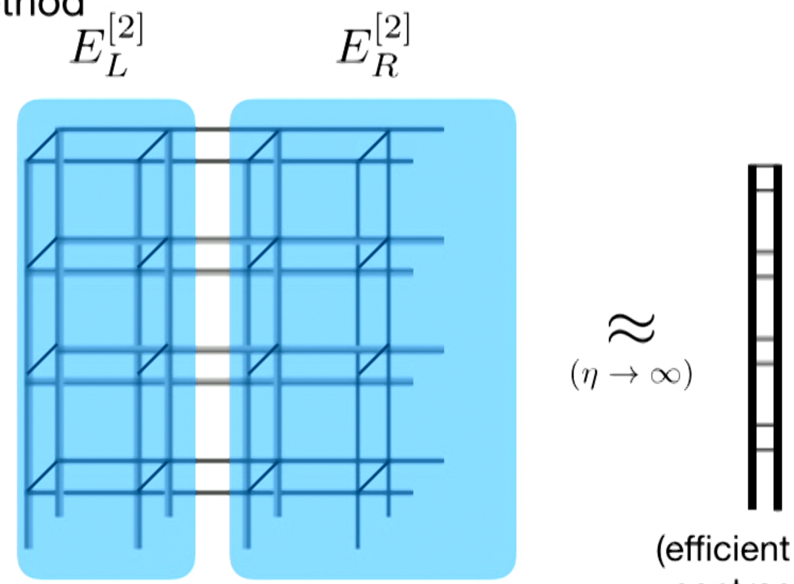
MPS
compression

$\approx$



Boundary MPS method

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



(efficient MPS contraction)

Leading costs:
(VUMPS-based)
[Fishman, et. al. 2018]

$$\mathcal{O}(\eta^3 D^4 + \eta^2 D^6)$$

Empirically it is found $\eta \gg D$ e.g., for 2D Heisenberg model $D = 5, \eta = 100$

Calculating environments is dominant cost of PEPS

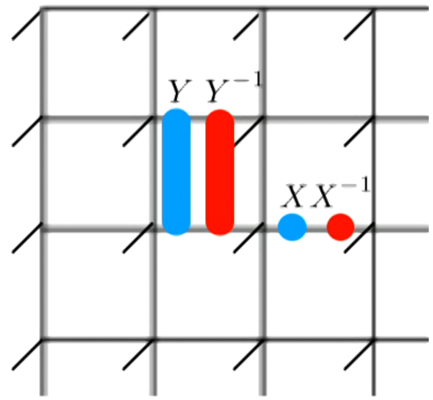
1) **The isometric TNS variational ansatz**

2) Variational power of isoTNS

3) Algorithms: Moses Move, TEBD^2, DMRG^2

Gauge redundancy

The TNS is a many-to-one mapping:
we can insert XX^{-1} into any bond
and absorb into neighboring tensors



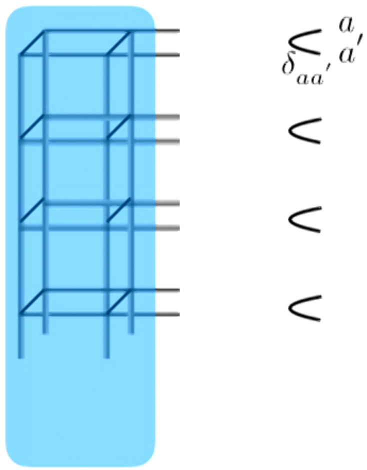
Single-leg transformations don't change bond dimension "D"
But current boundary MPS methods, e.g. VUMPS, *not* invariant under them: will change η

Multi-leg transformations change D; generically increase D,
but up to small error could also *decrease* D

It is natural to try and fix this redundancy by demanding tensors
satisfy some additional conditions, i.e, a "canonical form"

The key property we will try to enforce:

$E_L^{[2]}$ = $\mathbb{1}$



We require environments from E, N, S, W be trivial

This is special property of tensors which *cannot* be achieved by one-leg gauge redundancy; *will change D*

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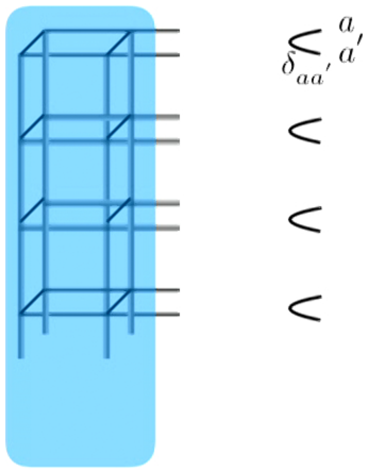

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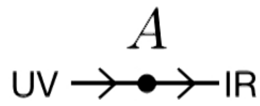
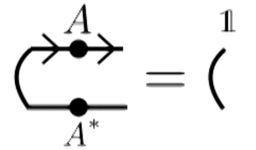
Down with environments!

Review of 1D canonical form

We assign arrows to a matrix if it is *isometry*: a unitary with some columns dropped





$$A^\dagger A = \mathbb{1}_{IR}$$

$$AA^\dagger = P_{UV}, P_{UV}^2 = P_{UV}$$

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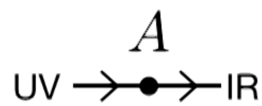

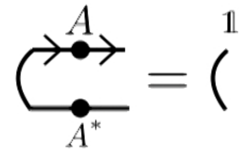

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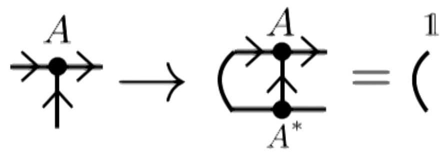
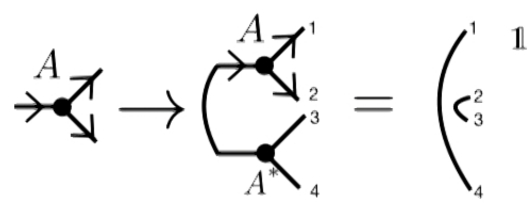
Extends to tensors by grouping in / out legs:





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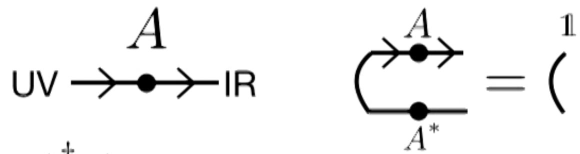

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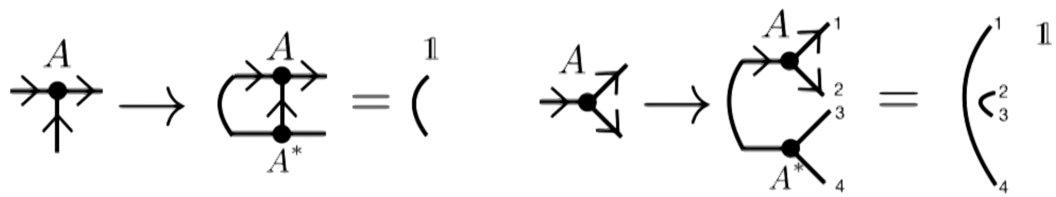
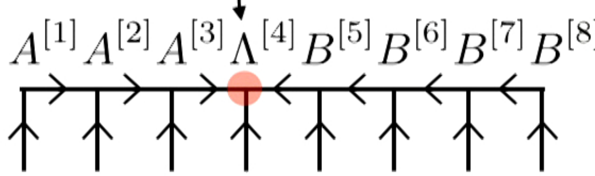


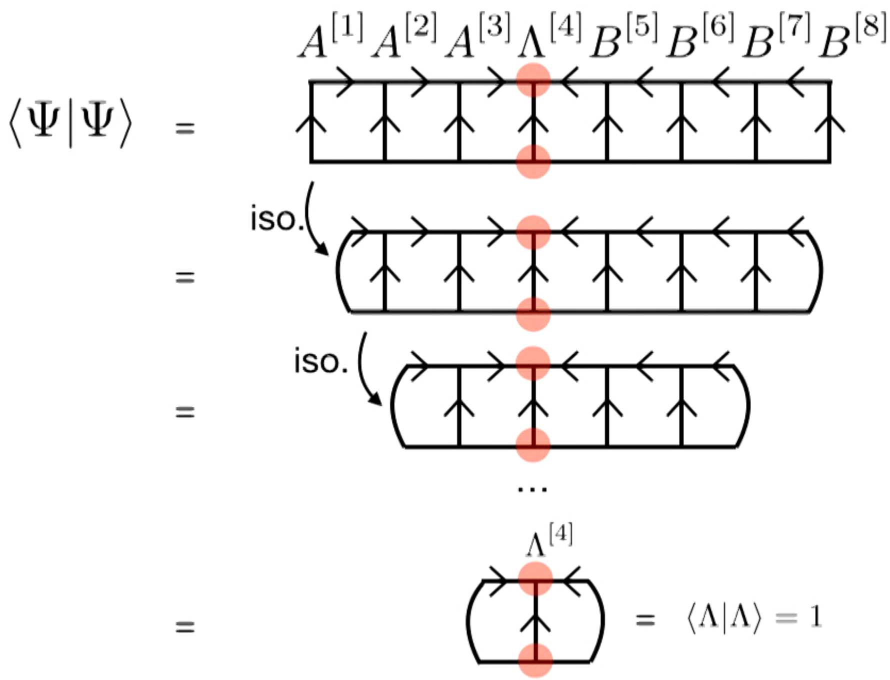
"orthogonality center / one-site wavefunction"



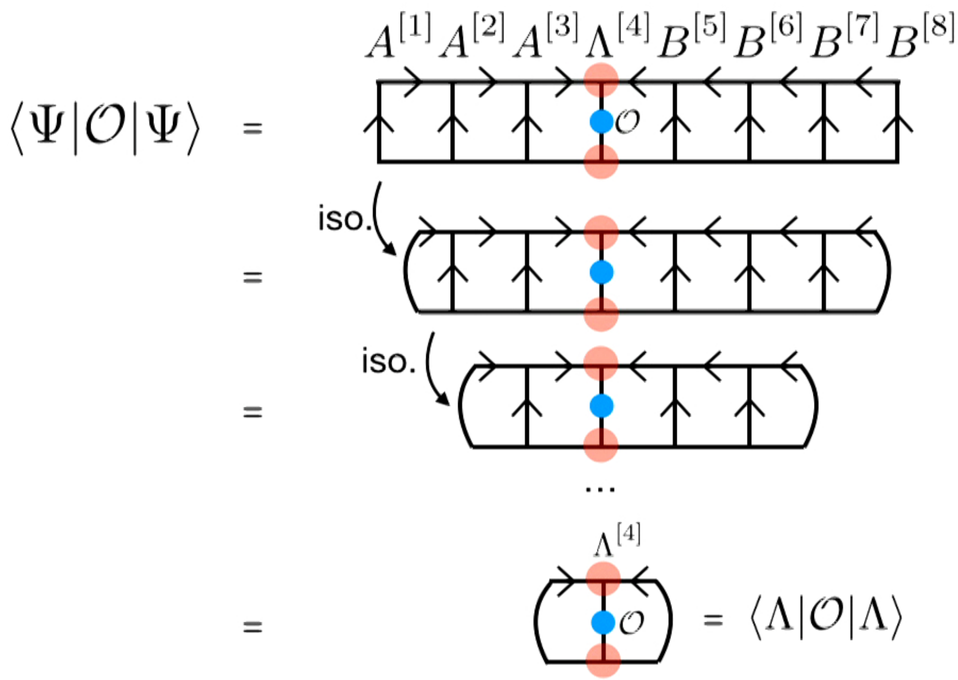
MPS Canonical Form

Any MPS can be brought to canonical form *without increasing* D

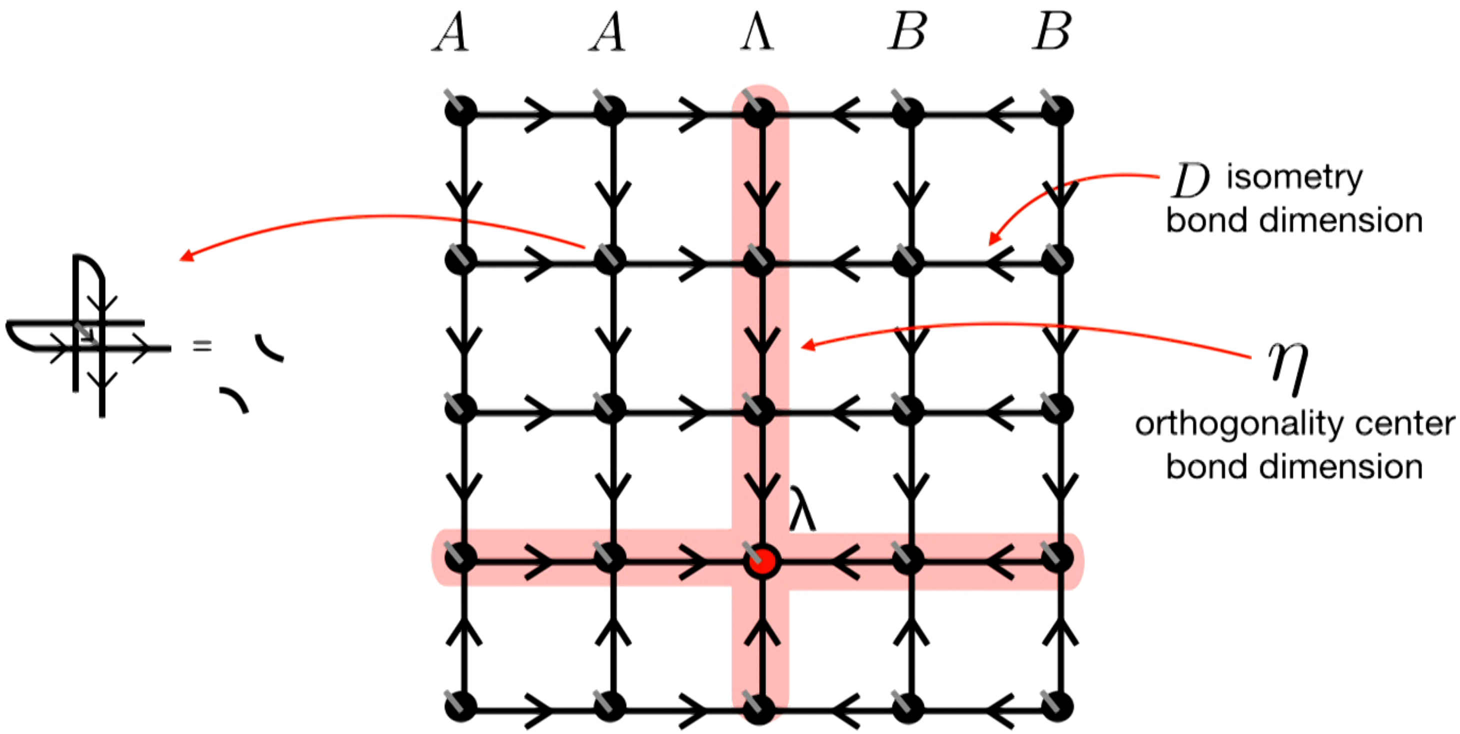
1D Canonical form = trivial environments



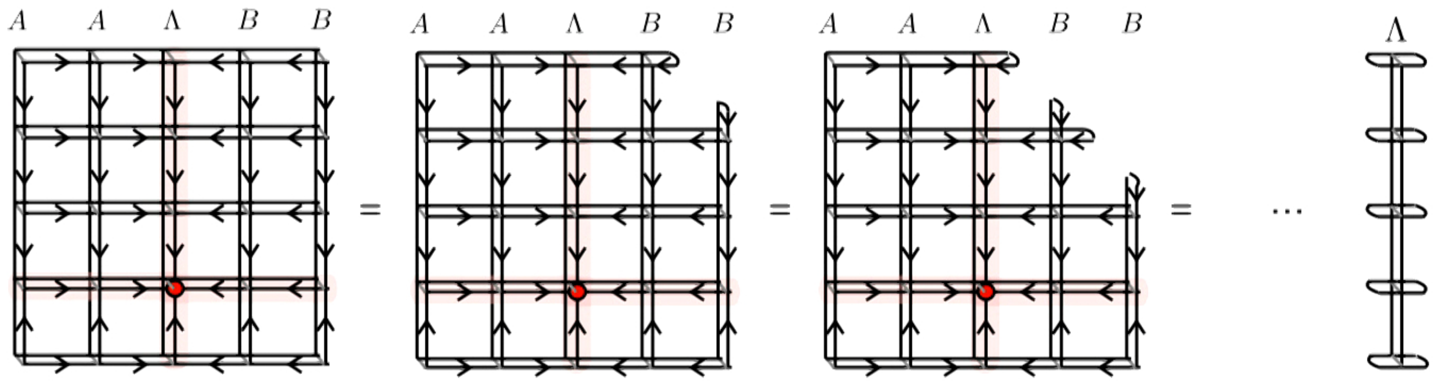
Local observables determined by 1-site wavefunction Λ



2D generalization: “isometric TNS”



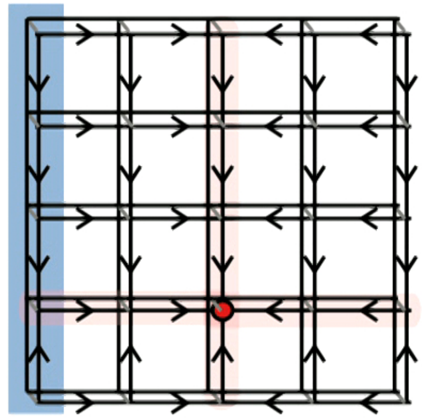
Norm of isoTNS



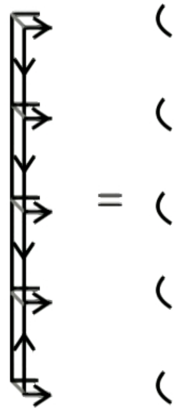
Reduces to norm of 1D Λ, which reduces to norm of 0D λ

Environments of isoTNS

$E_L^{[1]}$

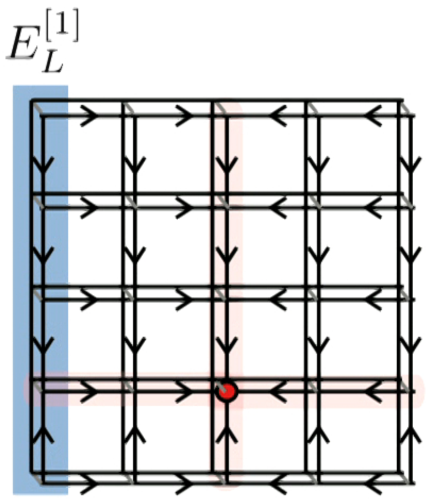


$E_L^{[1]} = \mathbb{1}$



And so on by induction - $E_L^{[2]} = \mathbb{1}, \cdots$
until you hit orthogonality center

Environments of isoTNS



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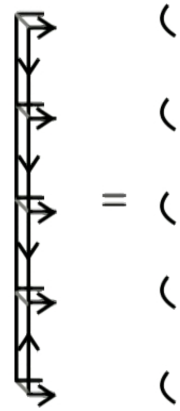

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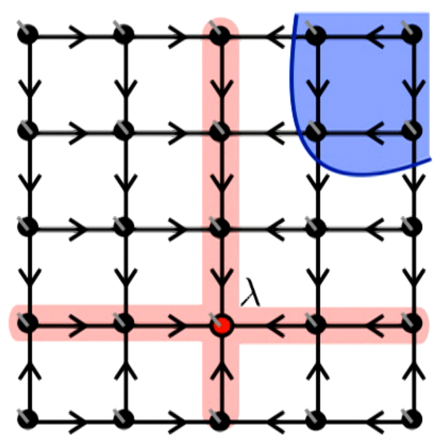
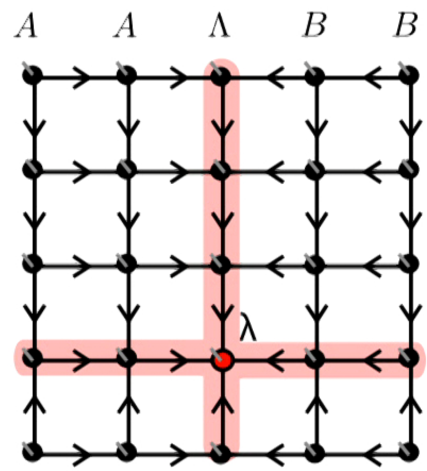


In fact, any boundary which is "space-like," with only *outgoing* arrows, will have a trivial environment

Orthogonality center

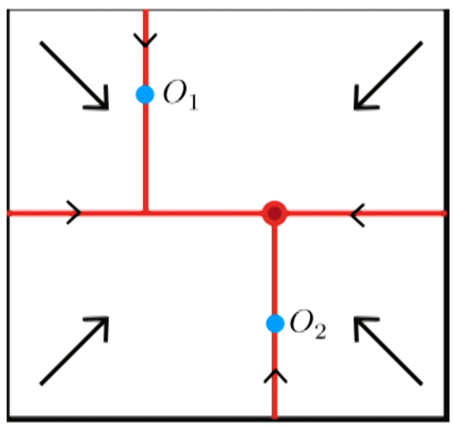


Λ really is the wave-function: the tensors in the surrounding quadrants are an *orthonormal* change of basis (isometry) from physical to ancilla space

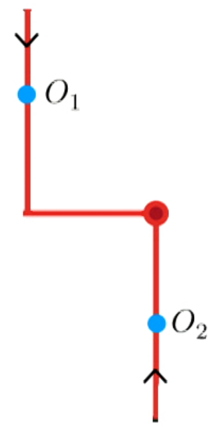
Λ is sufficient to calculate the entanglement spectrum of any combo of quadrants

Efficient two-point functions

$\langle\Psi| O_1 O_2 |\Psi\rangle$ =



= (isometry!)



= 1D MPS (Λ) VEV

Dimensional reduction to 1D MPS VEV = Efficiently computable $\mathcal{O}(\eta^3 D^2)$

Efficient two-point functions

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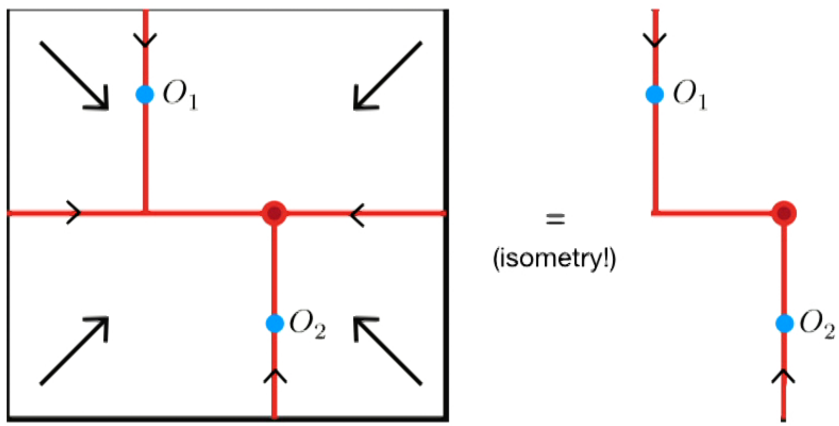


= 1D MPS (Λ) VEV

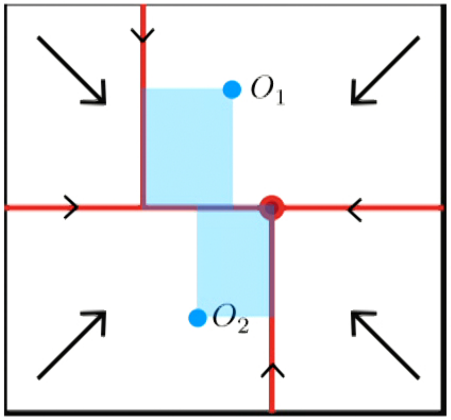
Dimensional reduction to 1D MPS VEV = Efficiently computable $\mathcal{O}(\eta^3 D^2)$

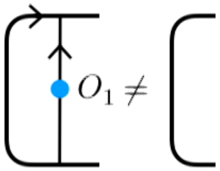
Corollary: *iso-TNS have exponentially decaying correlations*
In contrast, generic TNS can have algebraic correlations (Ising PEPs)
[But: algebraic != 2D CFTs. See A. Läuchli's talk]

Efficient two-point functions

OK, but what if points aren't on Λ ?

$\langle\Psi|\,O_1 O_2\,|\Psi\rangle$ =





O_i will spoil isometry condition in future light cone: they will grow under *dissipative* Heisenberg evolution (quantum channel)

Efficient two-point functions

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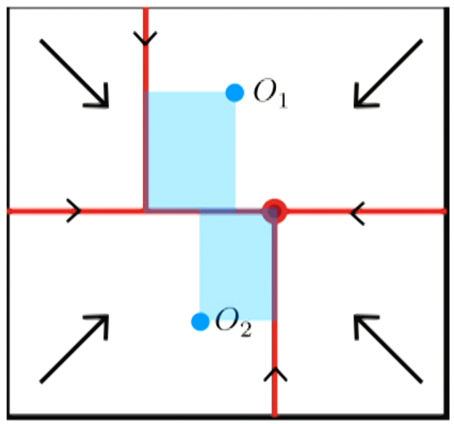
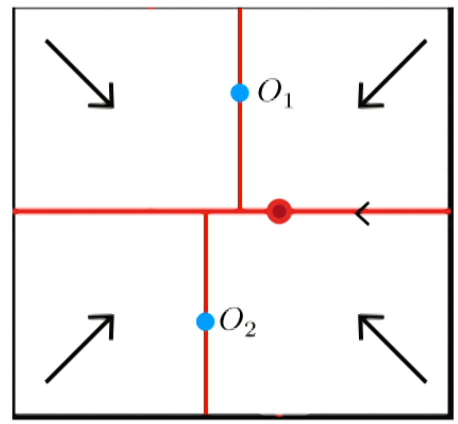
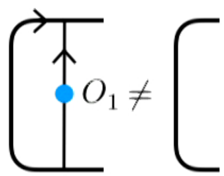


?????
=





We need a way to move Λ around…
I'll return to this! ("MOSES MOVE")

O_i will spoil isometry condition in future light cone:
they will grow under *dissipative* Heisenberg evolution
(quantum channel)

Variational power?

iso-TNS $\subset$ all PEPs

Is it a useful subset?

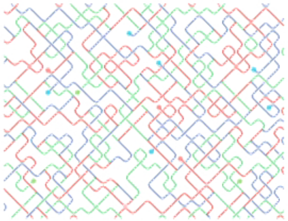
What phases have iso-TNS representation?

What entanglement properties determine convergence behavior?

Variational power: at least SRE and non-chiral topo. order

1) All string net states can be exactly put in iso-TNS form

Folklore: any gapped 2D phase with “gappable” edges (e.g., non-chiral) has string net representative



[Levin & Wen, PRB 2004]

2) If $|\Phi\rangle$ is iso-TNS, and U is finite-depth circuit, then $U|\Phi\rangle$ has exact iso-TNS form

Variational power: at least SRE and non-chiral topo. order

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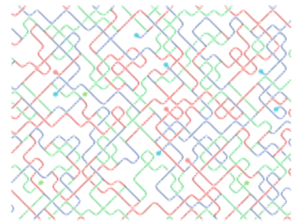
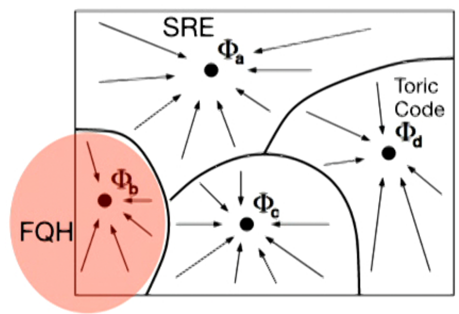


[Levin & Wen, PRB 2004]

2) If $|\Phi\rangle$ is iso-TNS, and U is finite-depth circuit, then $U|\Phi\rangle$ has exact iso-TNS form

1+2): roughly speaking - all 2D gapped *phases* with gappable edges have iso-TNS form

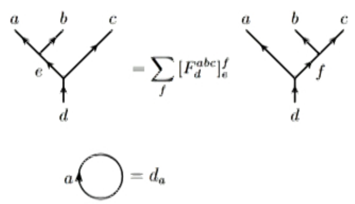


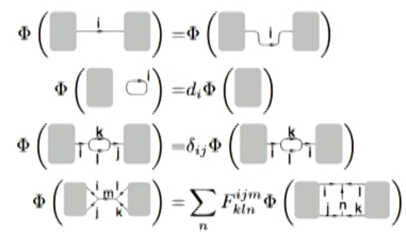
(However - does not estimate error to *approximate* state with given bond dimension)

All string net states can be exactly put in iso-TNS form

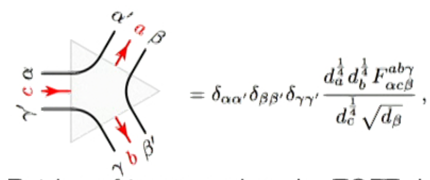
Tensor network representation of string nets known

Data from TQFT → String-net construction → TNS representation





[Levin & Wen, PRB 2004]

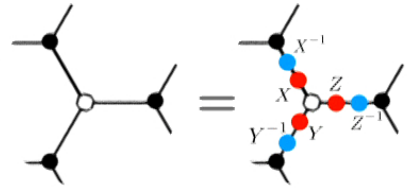


Entries of tensors given by TQFT data

[Buerschaper et al. 2008; Gu et al. 2008; Williamson et al. 2017]

All string net states can be exactly put in iso-TNS form

Tensors can be massaged with gauge transformations:



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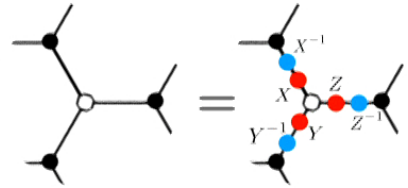

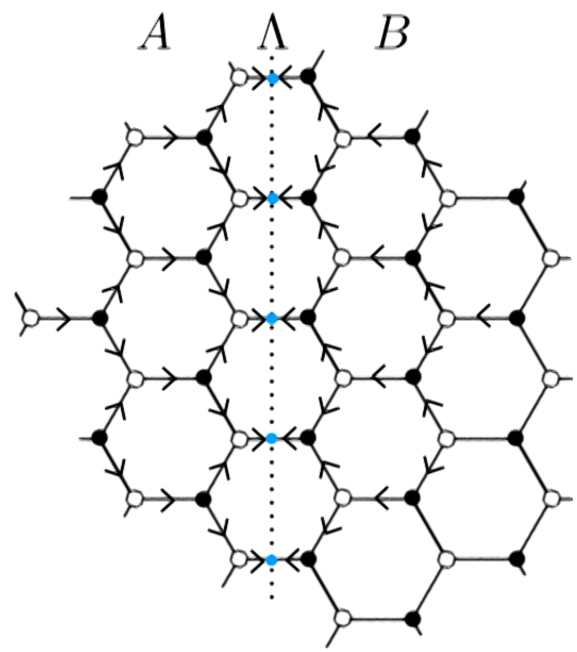

Choosing X, Y, Z related to d_a and using the unitarity properties of F-matrices

$$\left[F_d^{abc}\right]\left[F_d^{abc}\right]^\dagger = \mathbb{1} = \left[F_{cd}^{ab}\right]\left[F_{cd}^{ab}\right]^\dagger$$

+ some other TQFT relations, can be made isometric tensor-by-tensor

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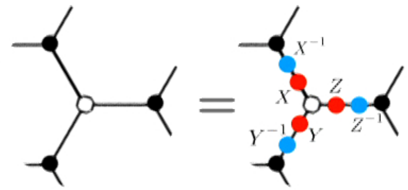

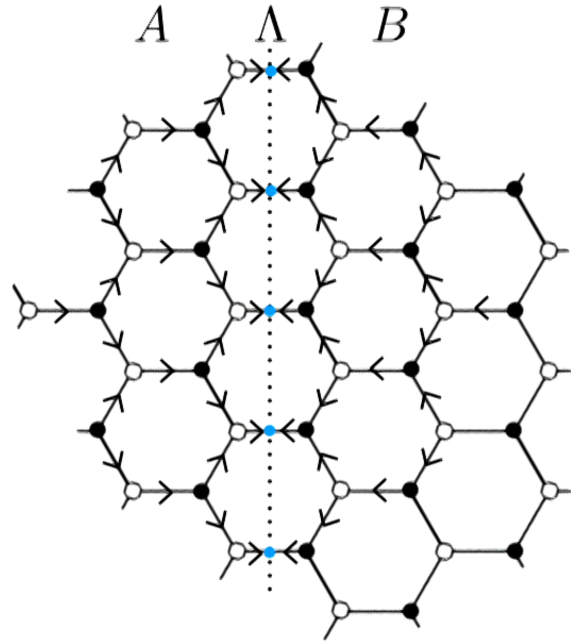

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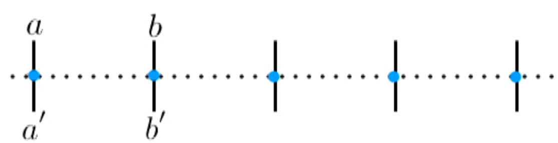
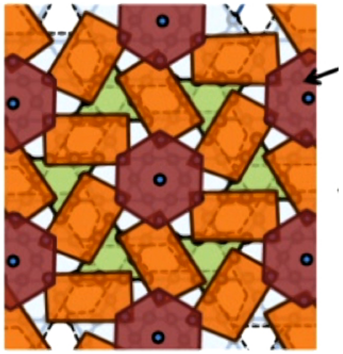
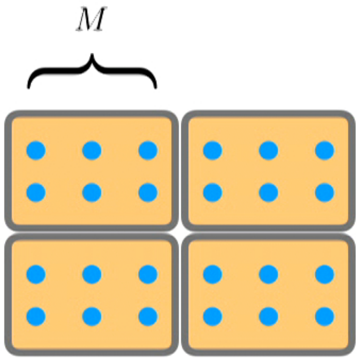
$\Lambda =$  $= \cdots d_a \delta_{aa'}\ d_b \delta_{bb'} \cdots$

Orthogonality center is tensor-product of quantum dimensions; produces correct entanglement spectrum etc.

If $|\Phi\rangle$ is iso-TNS, and U is finite-depth circuit, then $U|\Phi\rangle$ has exact iso-TNS form

$U =$ 

$U_M =$ 

Sufficient to bound growth in bond dimension D for one parallel circuit

1) Course-graining move

2) Onsite-unitary move (preserves iso-TNS)

3) Fine-graining move

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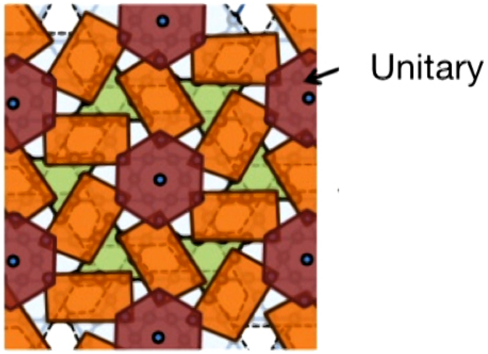
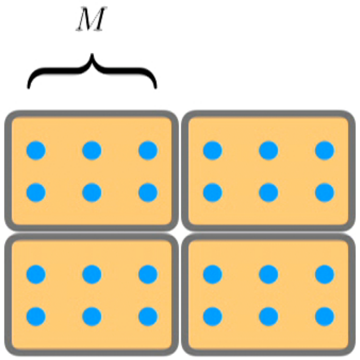
$U =$ 

$U_M =$ 

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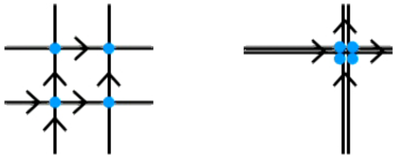
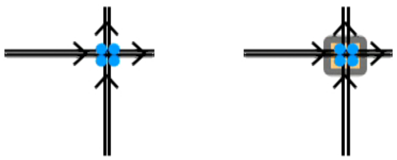


2) Onsite-unitary move (preserves iso-TNS)



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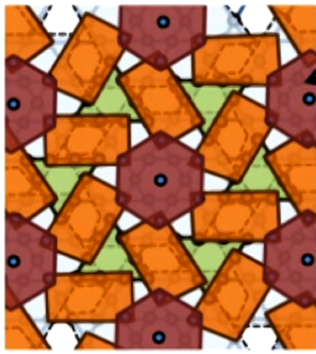
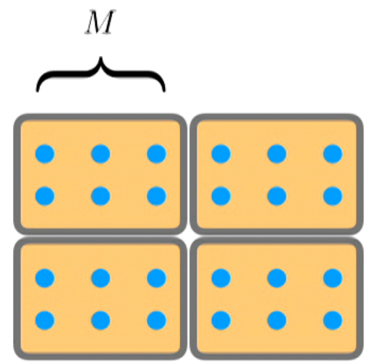


Unitary

$U_M =$



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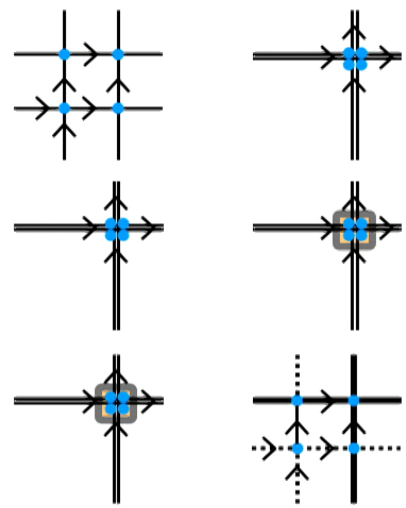

Bad / stupid bound, but establishes principle: $D \to D^M d^{M^2/2}$

spin size

Variational power: future questions

Let $|\psi\rangle$ be target state and $|\psi_D\rangle$ a rank-D isoTNS approximation. What entanglement properties of $|\psi\rangle$ are sufficient to bound the error $||\psi\rangle - |\psi_D\rangle|^2$?

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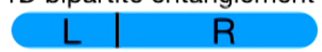
1D: the Renyi Entropy $S^{(n)}$. If 1D bipartite entanglement is bounded by $S^{(n)}$,



$$||\psi\rangle - |\psi_D\rangle|^2/L \leq \left(\frac{1-n}{D}\right)^{\frac{1-n}{n}} e^{\frac{1-n}{n}S^{(n)}}, \quad n < 1$$

[Verstraete & Cirac, 2005]

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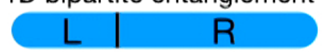

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[Verstraete & Cirac, 2005]

Establishes linear-L difficulty for area-law phases and poly(L) for CFTs

2D: bipartite entanglement certainly won't be enough! [Ge & Eisert, 2016]

Hierarchy (?) of area-law states: gapped, non-chiral < gapped, chiral < gapless CFT < ground states < area law < ….

What are entanglement distinctions between area-law phases, and how do they lead to different TNS accuracy?

Extremely difficult question for generic PEPs, but the isometry condition may make iso-TNS much more tractable to analyze

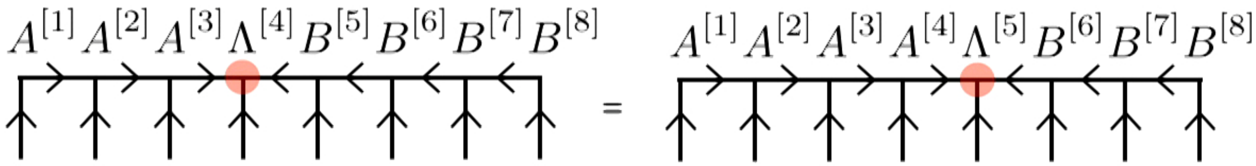
1) The isometric TNS variational ansatz

2) Variational power of isoTNS

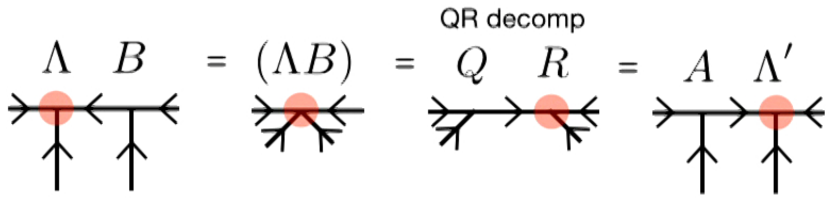
3) **Algorithms**: Moses Move, TEBD^2, DMRG^2

How do we move the orthogonality center?

For 1D MPS:



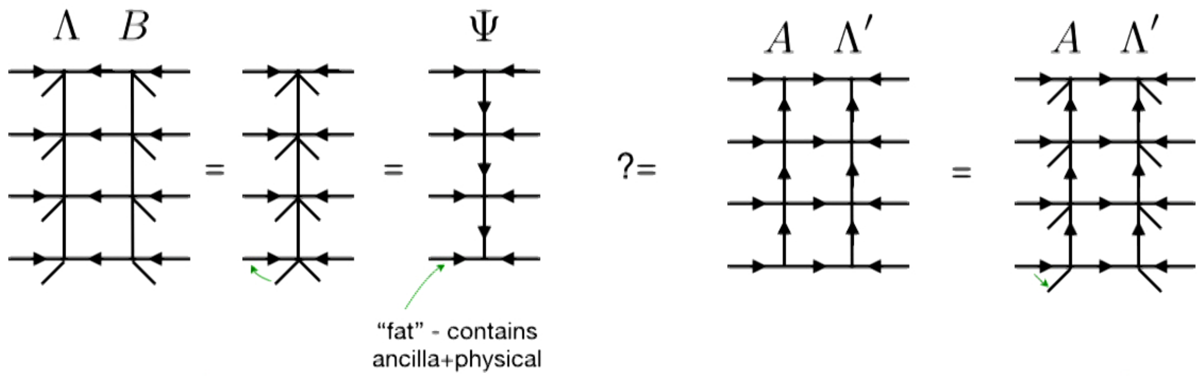
Done locally:



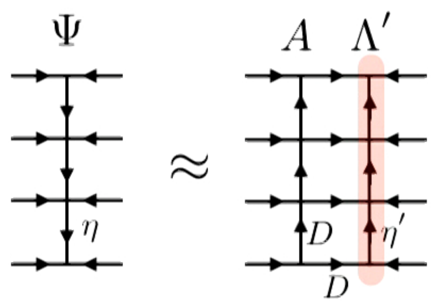
Any orthogonal decomposition of a matrix will do: $(\Lambda B) = QR = U(sV) = \cdots$

We can use this (unitary) ambiguity to fix various properties of Λ'

First group columns
together into a can. MPS Ψ



Moses Move



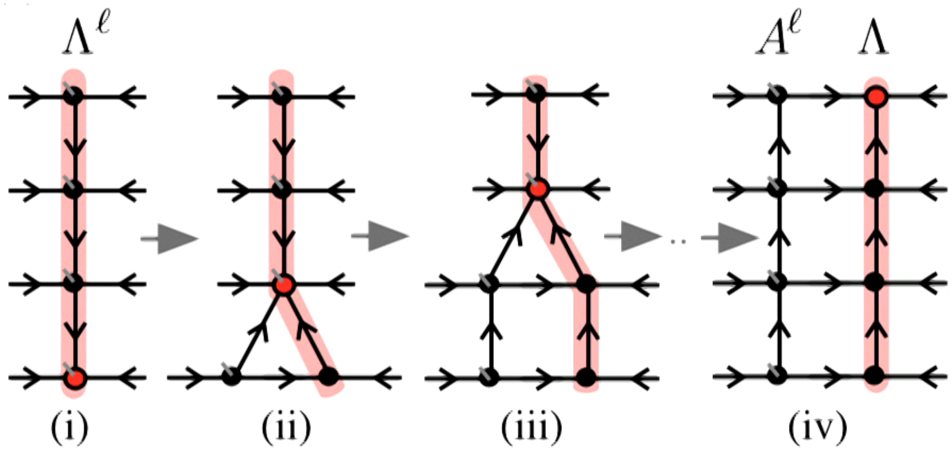
$$A^{\dagger}\Psi = \Lambda'$$

We choose A
so that entanglement
of Λ' is minimal

Caveat: unless $\eta' = D\eta$, MM is approximate, so eventually make small errors

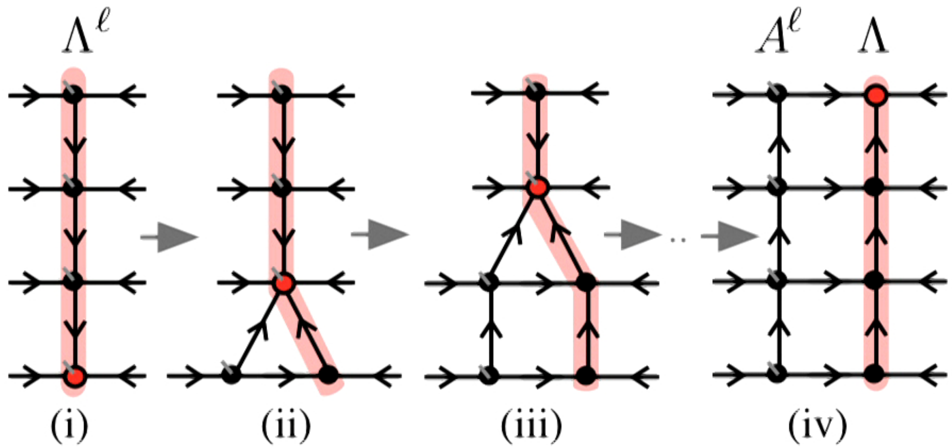
Moses Move

[Thanks to R. Mong
for name!]

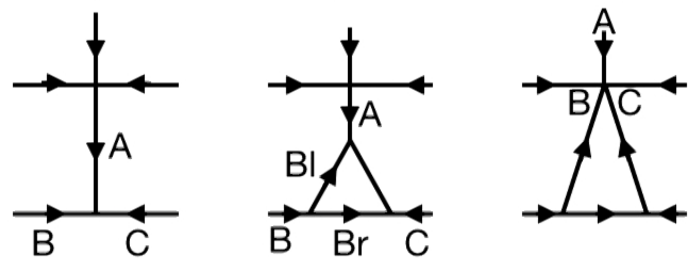


Let me unpack this…

Moses Move



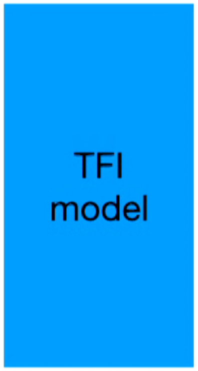
(i) to (ii):



Testing the Moses Move: MPS to isoTNS

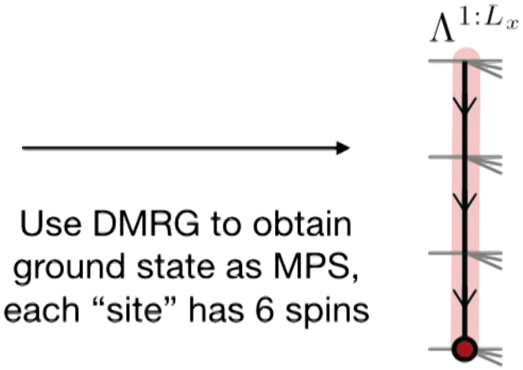
Suppose we are *given* a 2D wavefunction :
can we uses MM to iteratively put it in isoTNS form?

Ly = 20



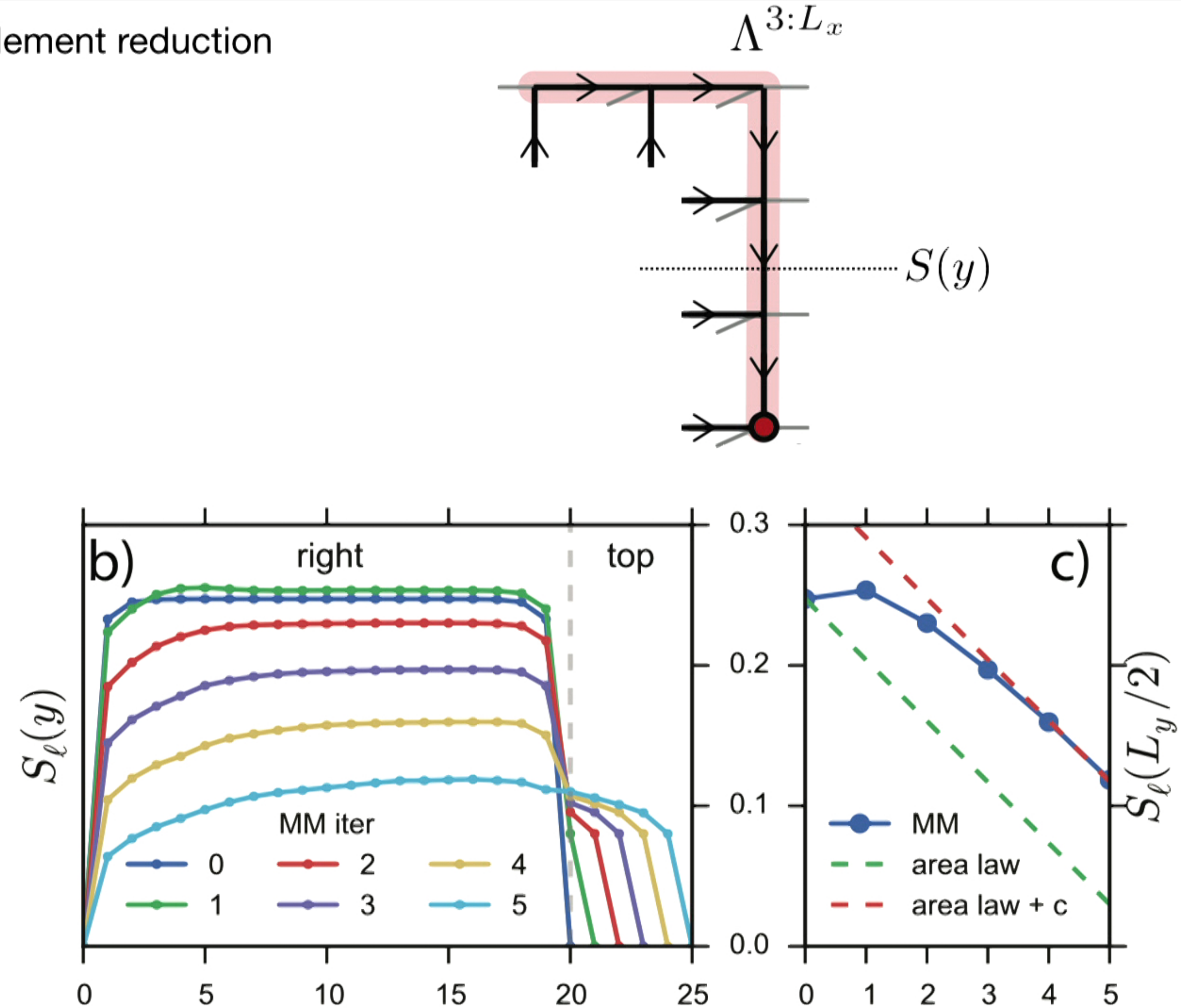
Lx = 6

Use DMRG to obtain
ground state as MPS,
each “site” has 6 spins



(I want to separate out *finding* ground state
from *representing* ground state)

Entanglement reduction



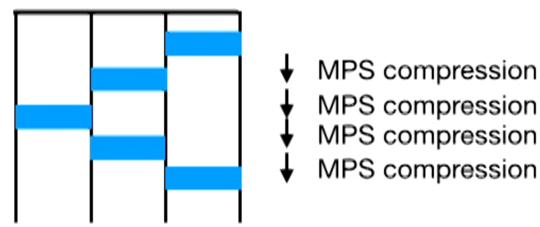
TEBD^2

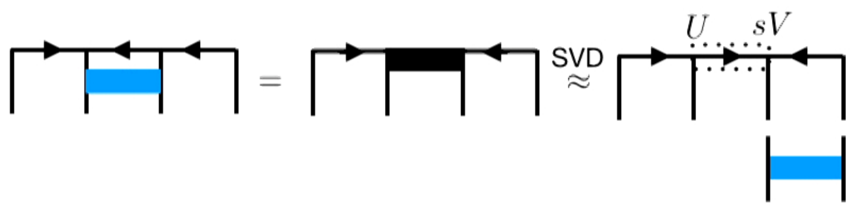
First review:

TEBD^1

[Vidal 2003]

$$e^{-tH}|0\rangle = \prod_j e^{-\Delta t H_j}|0\rangle$$





Orthogonality center sweeps back & forth with trotterization, ensuring local SVD truncation is globally optimal

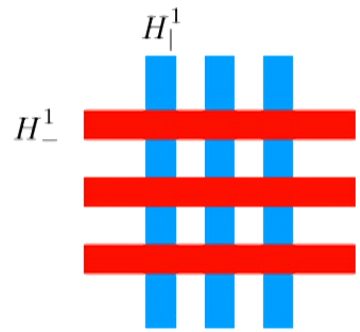
TEBD^2 Trotterization

$$H = \sum_c H_{|}^{c} + \sum_r H_{-}^{r}$$

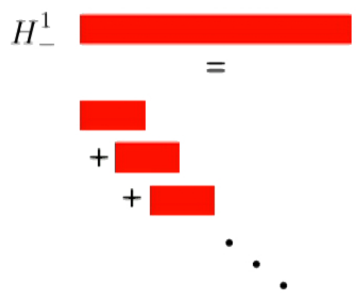
$$H_{|}^{c} = \sum_r h_{|}^{c,r}$$

$$H_{-}^{r} = \sum_c h_{-}^{c,r}$$

Split into columns & rows
(assume nearest-neighbor H)



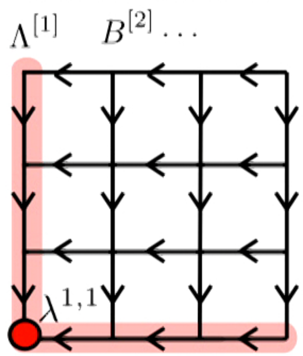
Each column / row has own
1D trotterization



$$\cdots \prod_r e^{-dt H_{-}^{r}} \prod_c e^{-dt H_{|}^{c}} |0\rangle$$

TEBD^2

Start in this form:



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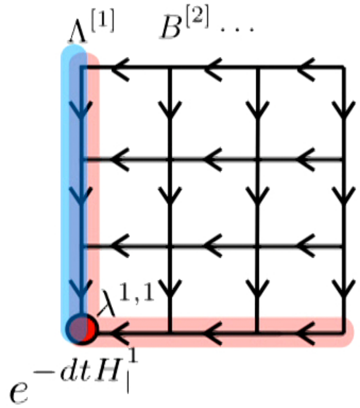
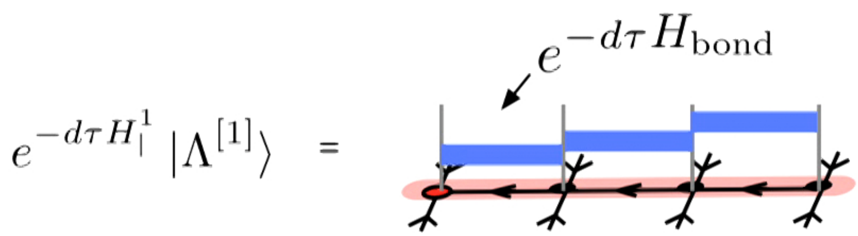


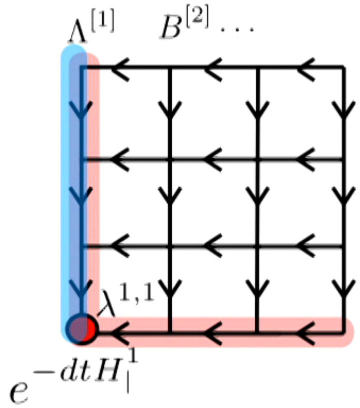
Now apply $e^{-dtH_{|}^{1}}$ by *literally* calling 1D TEBD on $\Lambda^{[1]}$



No environments, "full update," or other complications.

TEBD^2

Start in this form:



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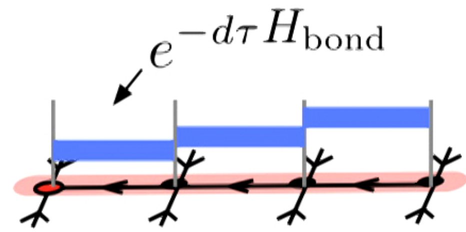
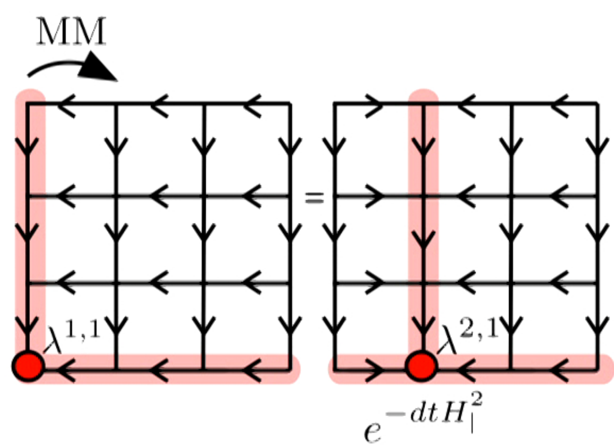
$e^{-d\tau H_{|}^{1}}\,|\Lambda^{[1]}\rangle$ =



No environments, “full update,” or other complications.

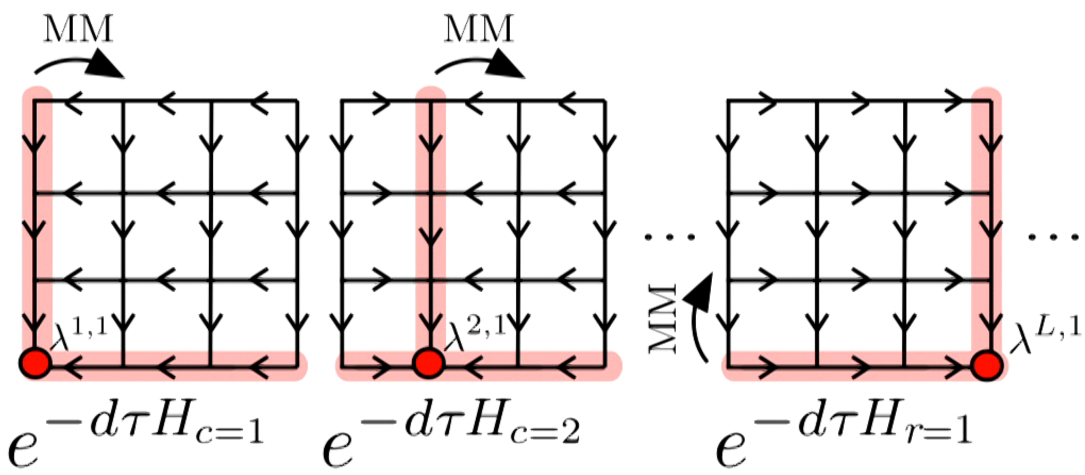
Then MM over ortho-center, and apply $e^{-dtH_{|}^{2}}$



etc.

TEBD^2

After columns, tilt head 90° and apply rows:

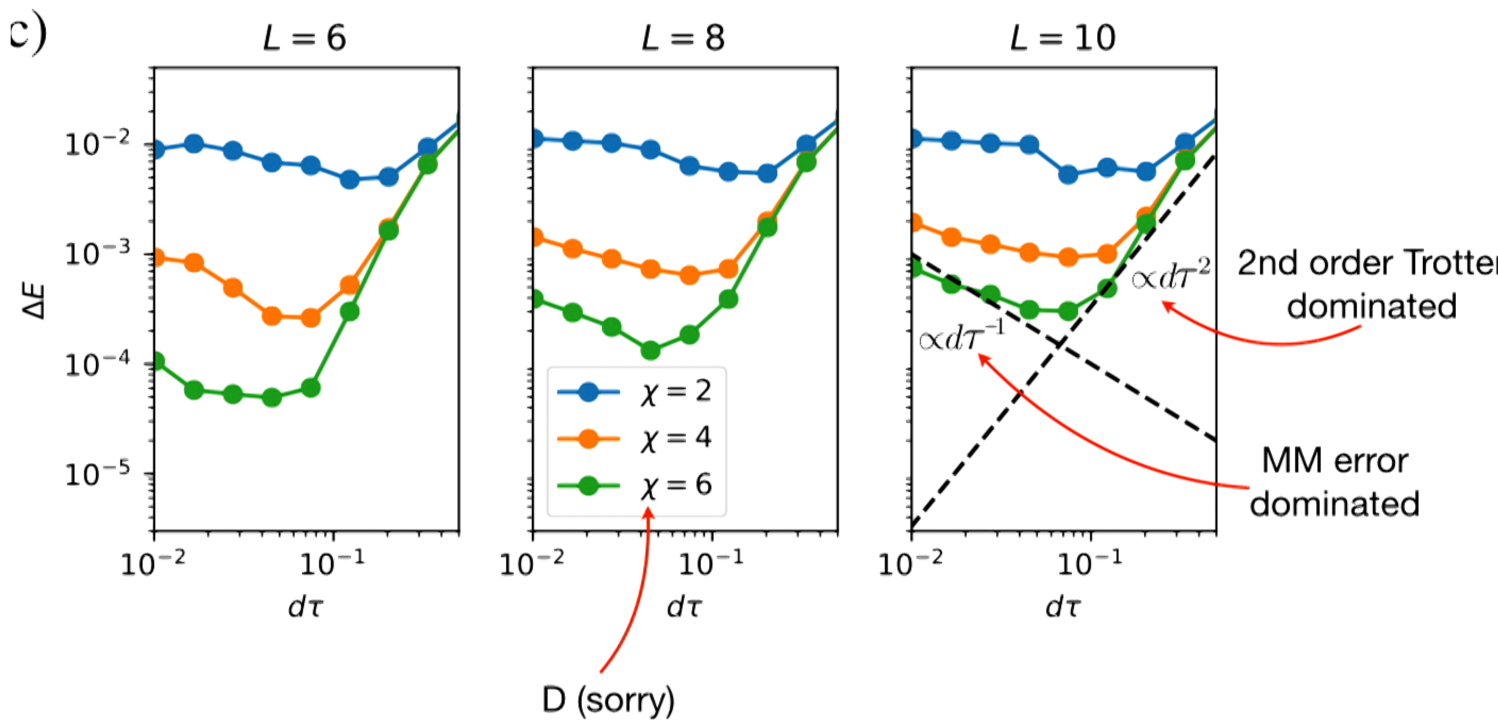


COST:

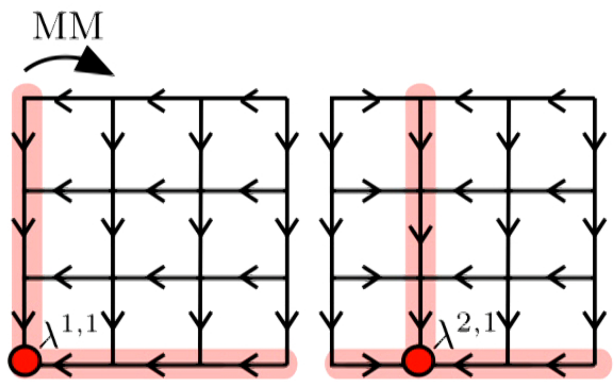
isoTNS TEBD^2: $\mathcal{O}(\eta^3 D^3 + D^6)$

TNS Full-update w/ boundary MPS: $\mathcal{O}(\eta^3 D^4 + \eta^2 D^6 + D^{12})$

Error in TFI energy (g = 3.5)



DMRG^2



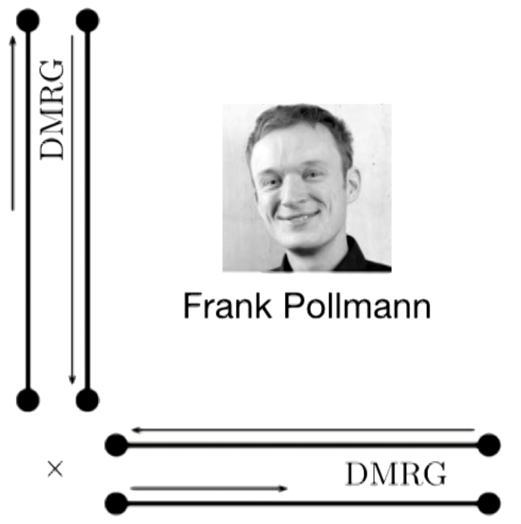
Call 1D DMRG for each column (“inner sweep”)
sweep left / right between columns using MM (“outer sweep”)

$$\mathrm{DMRG}^2 = \mathrm{DMRG} \otimes \mathrm{DMRG}$$

Trickier to implement than TEBD because
need Hamiltonian terms… but testing now

Thanks!

arXiv:1902.05100



Frank Pollmann