Study of Fixed Point Corner Method: Convergence and AD

https://github.com/qiyang-ustc/ADFPCM.jl

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content

- Background
  - The failure of of power method
  - AF Ising in triangle lattice
  - Fermionic system using fPEPS
- FPCM
  - CTMRG v.s. VUMPS
  - Biorthogonal
  - Fixed Point Corner (Transfer) Method
- AD
  - An interesting ignore
- Outlook

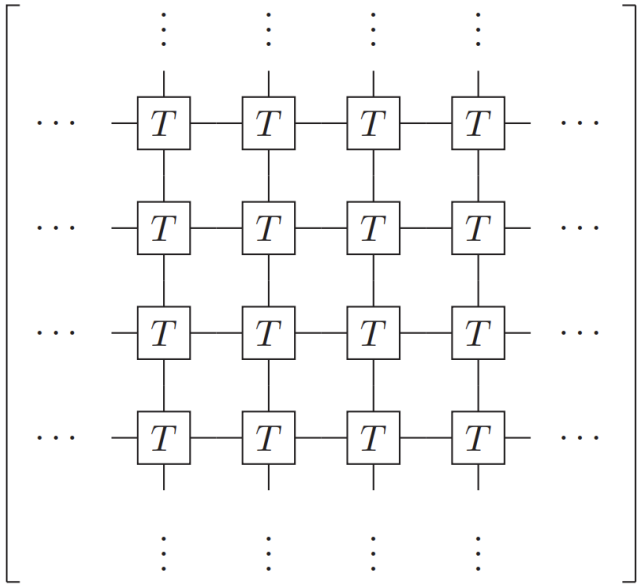
Contraction of 2D infinite tensor network

- Partition function or norm of wave function

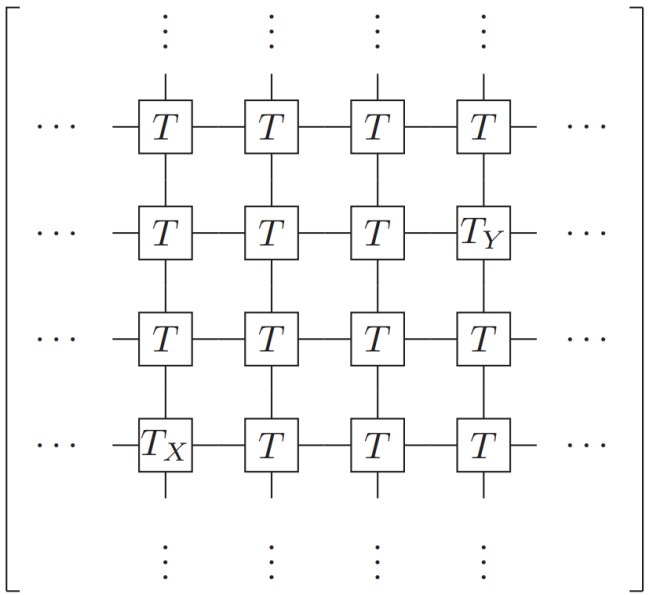
Two ways to contract: RG or boundary

Why boundary?

$\kappa^{MN} \equiv Tr$



$\langle XY \rangle = Tr$

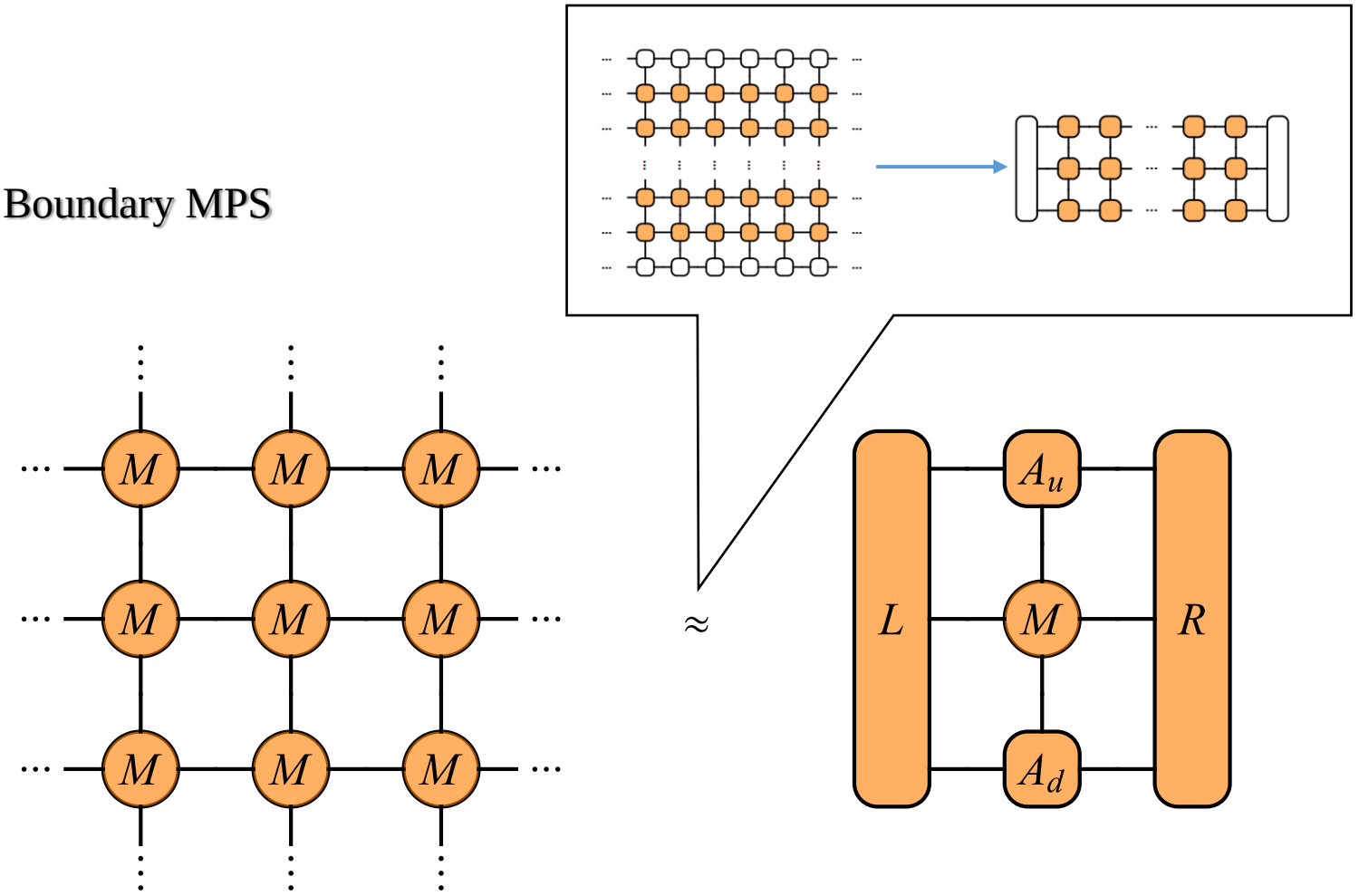


$/\ \kappa^{MN}$

Fishman, PRB 98, 235148 (2018)

Contraction: VUMPS

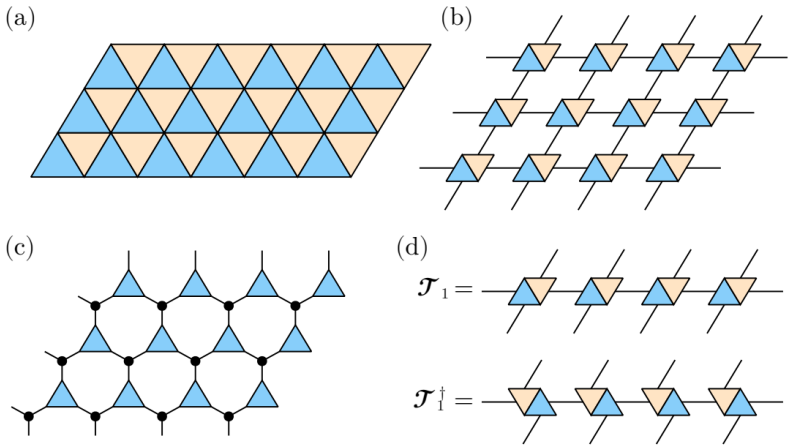
Boundary MPS



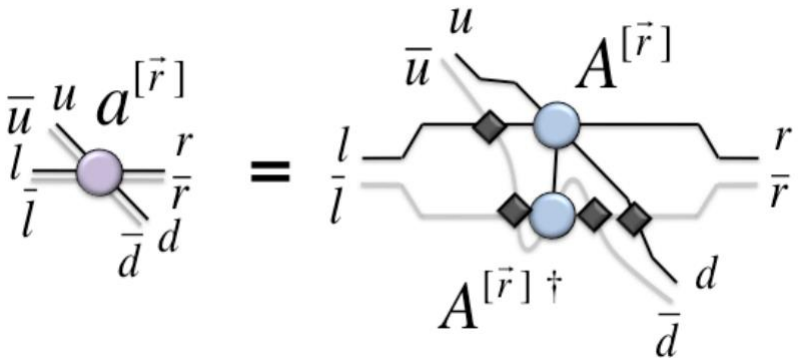
Failure of power method for infinite transfer matrix

- Hermitian→ variational principle
- Non-Hermitian→power method

AF Ising in triangle lattice



fPEPS



$$\frac{\langle\psi_0|T_0|\psi_0\rangle}{\langle\psi_0|\psi_0\rangle}=\frac{\langle\psi_L|\mathcal{T}|\psi_R\rangle}{\langle\psi_L|\psi_R\rangle}\to 0 \qquad \mathcal{T}=\mathcal{P}\mathcal{T}_0\mathcal{P}^{-1}$$

$$|\psi_R\rangle=\mathcal{P}|\psi_0\rangle, \quad |\psi_L\rangle=\mathcal{P}^{-\dagger}|\psi_0\rangle$$

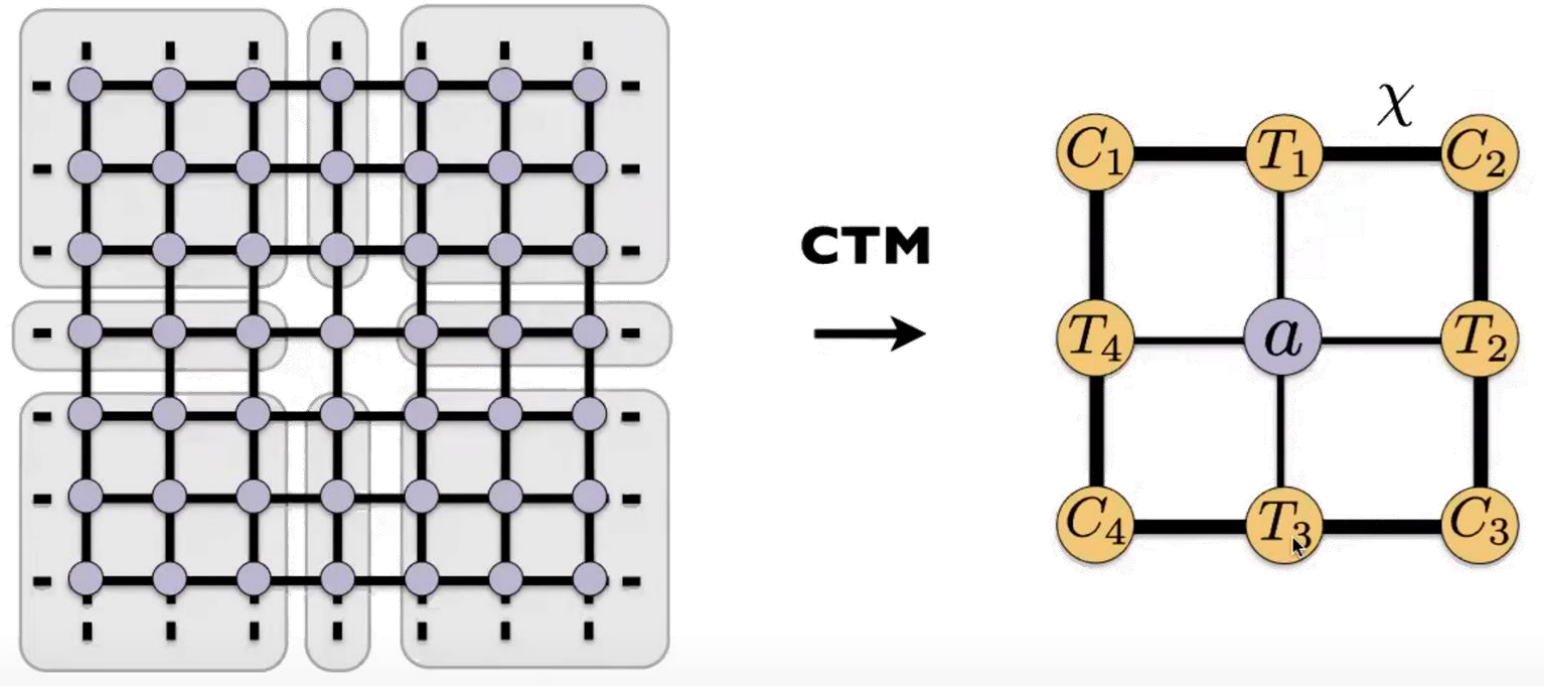
$$\langle\hat{o}\rangle=\frac{\langle\Psi|\hat{o}|\Psi\rangle}{\langle\Psi|\Psi\rangle}\to 0$$

Wei Tang, arXiv:2311.18733v1, 2023

Corboz, Phys. Rev. B 81, 165104,2010

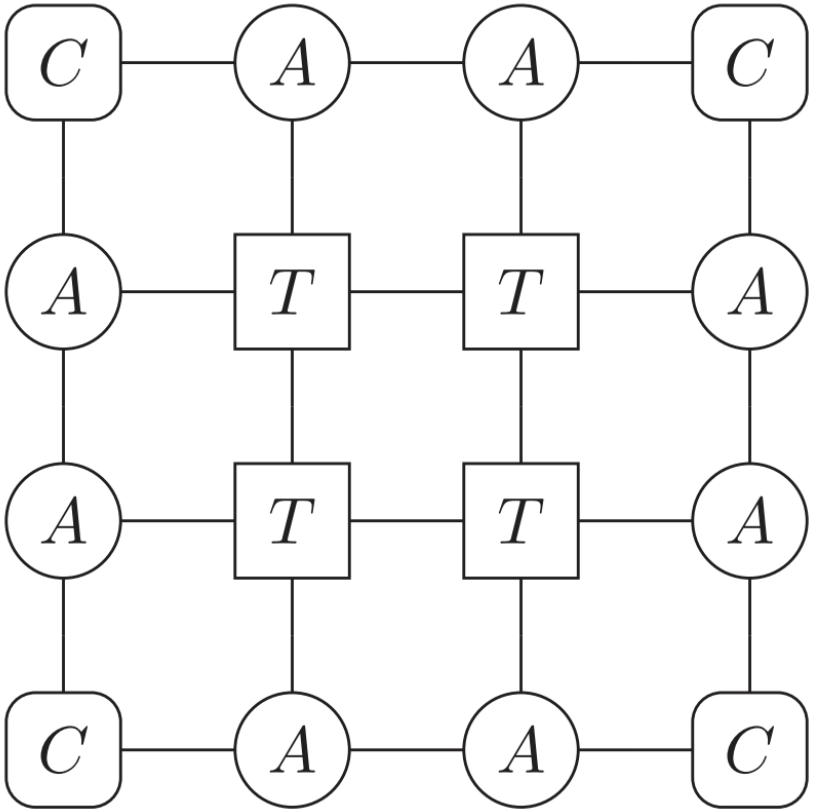
Contraction: CTMRG

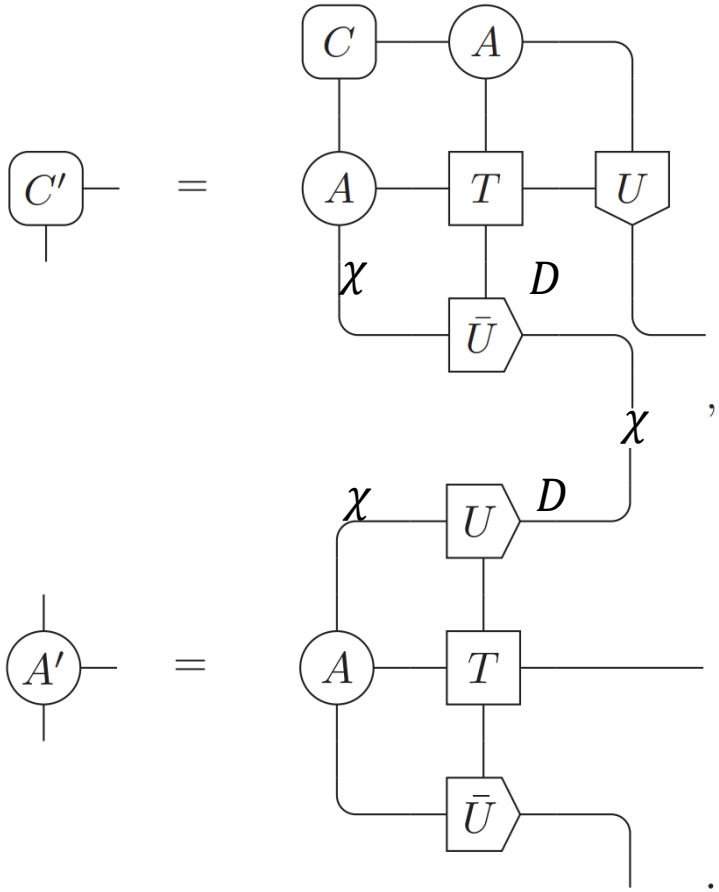
- Corner Transfer environment



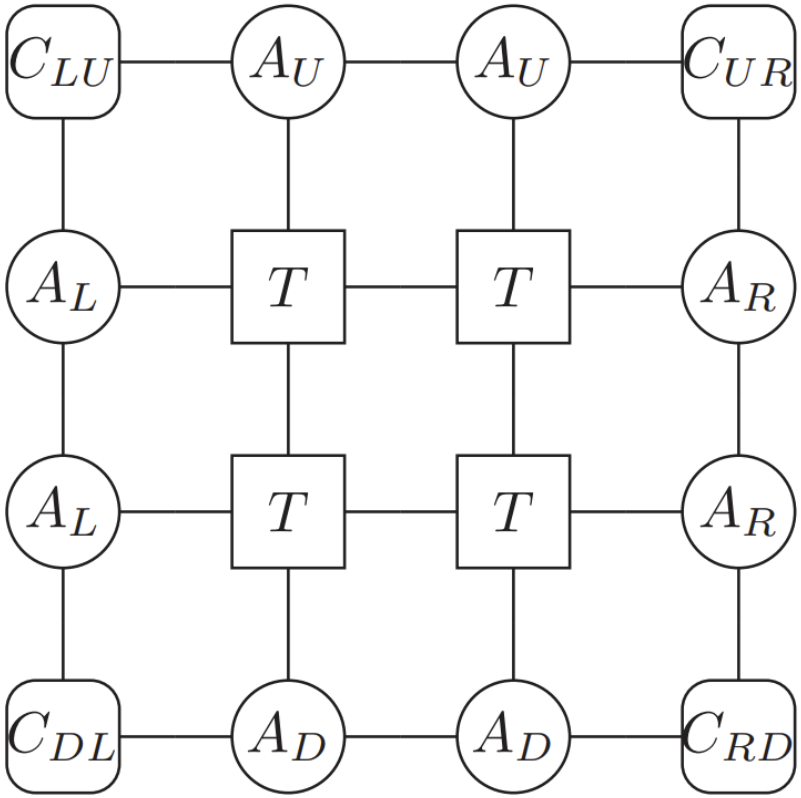
T. Nishino, JPSJ.65.891 (1996)

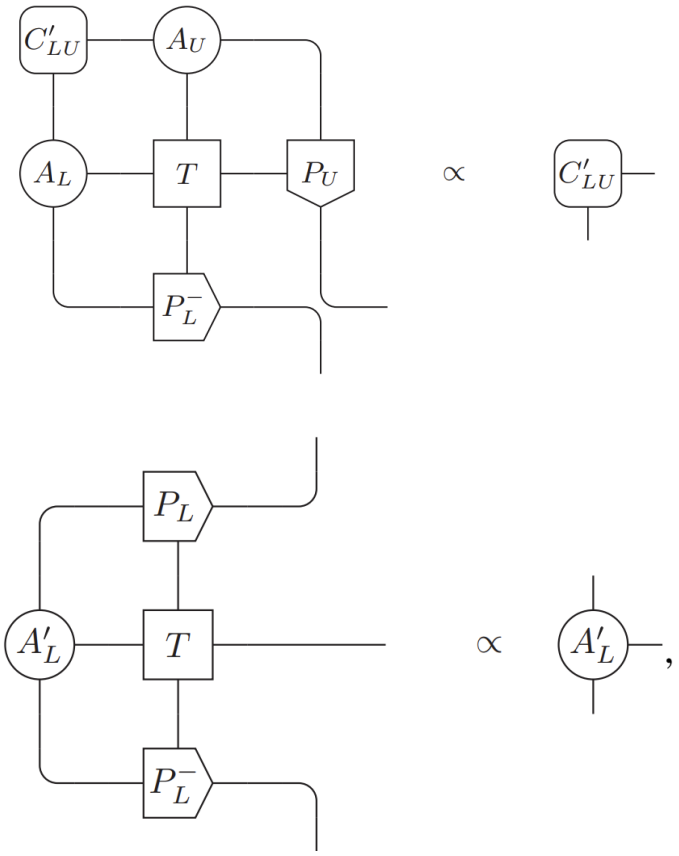
Fixed point of Symmetric CTMRG





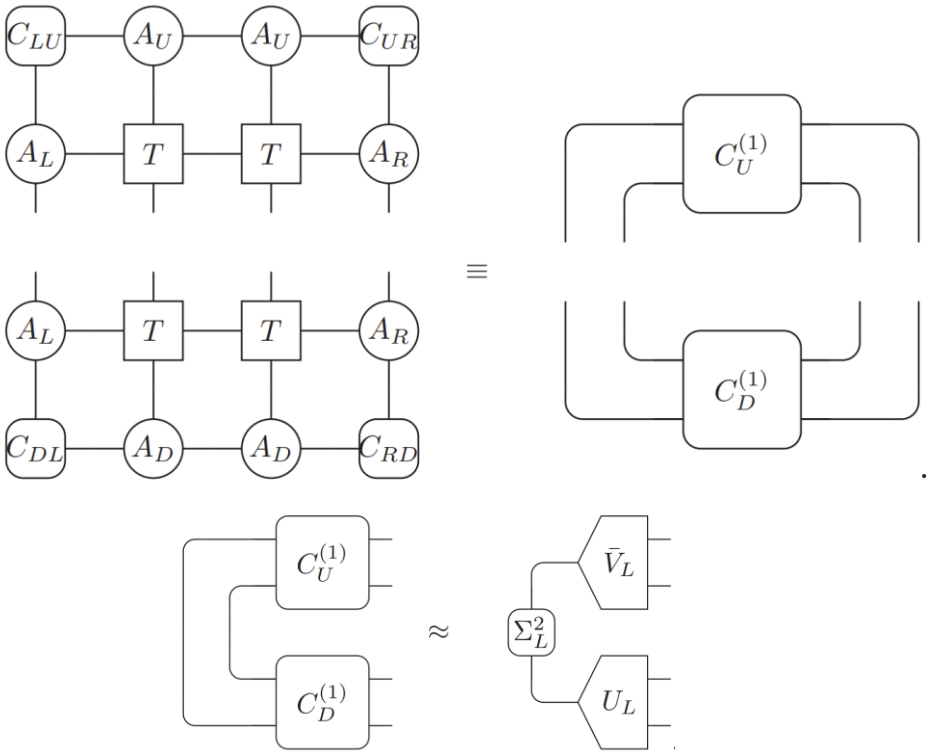
Fixed point of Asymmetric CTMRG

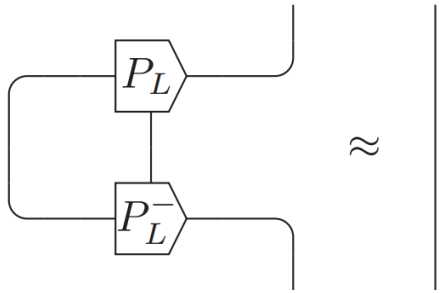




Biorthogonal and Get P

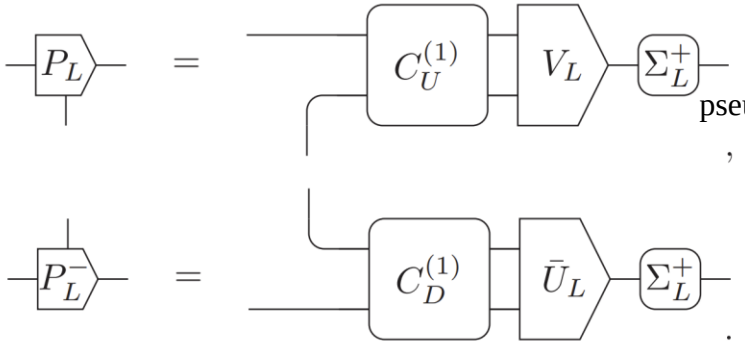
(1)



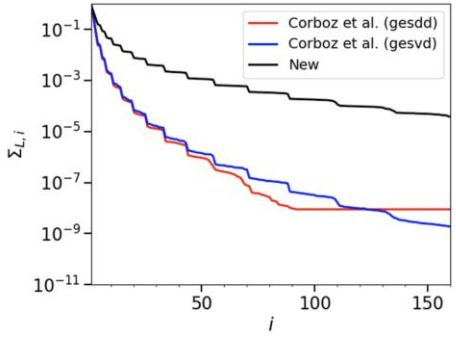


$$\left\langle C_U^{(1)} \middle| C_D^{(1)} \right\rangle \approx 1$$

(2)

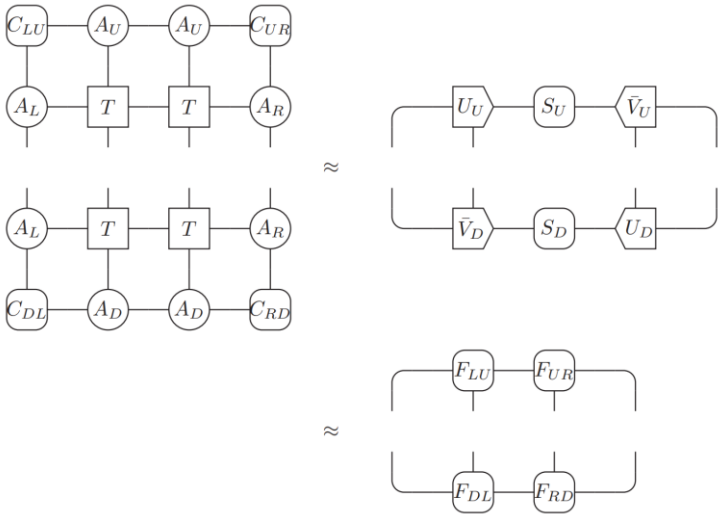


pseudo-inverse

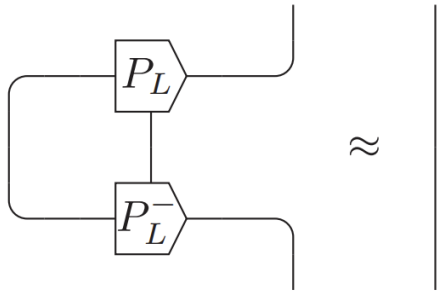


A better method to get P

(1)

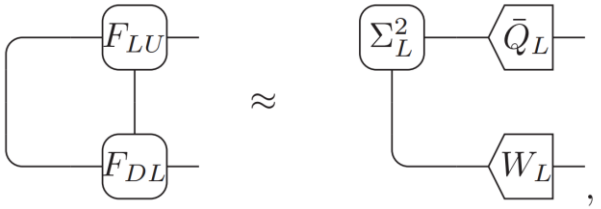


$$F^s_{LU} \equiv U^s_U S^{1/2}_U,\ F^s_{UR} \equiv S^{1/2}_U (V^s_U)^\dagger$$
$$F^s_{RD} \equiv U^s_D S^{1/2}_D \quad F^s_{DL} \equiv S^{1/2}_D (V^s_D)^\dagger$$

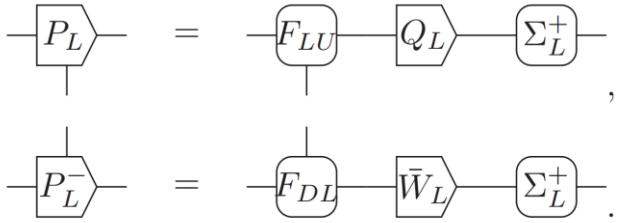


$$\left\langle C_U^{(1)} \middle| C_D^{(1)} \right\rangle \approx 1$$

(2)

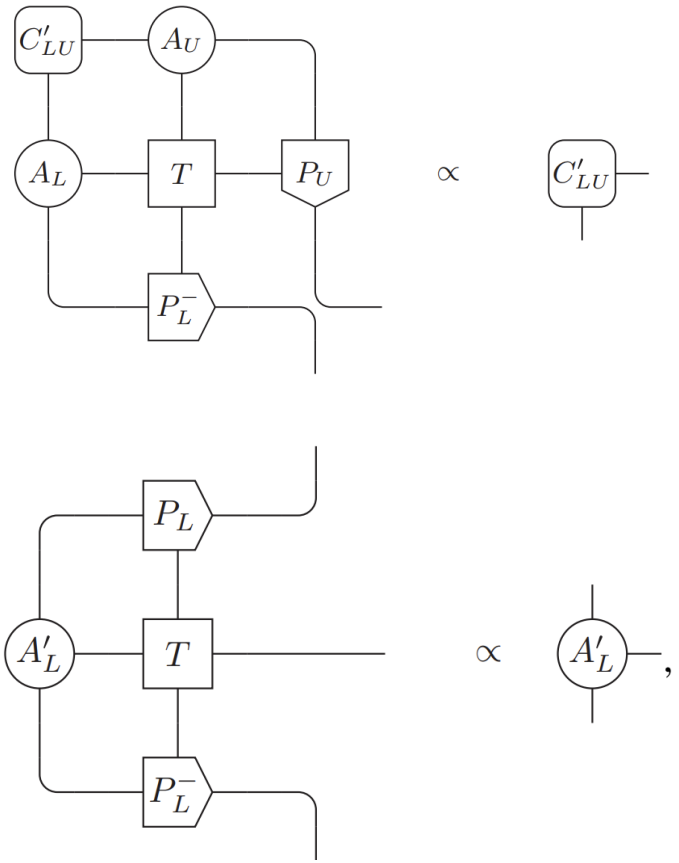


(3)

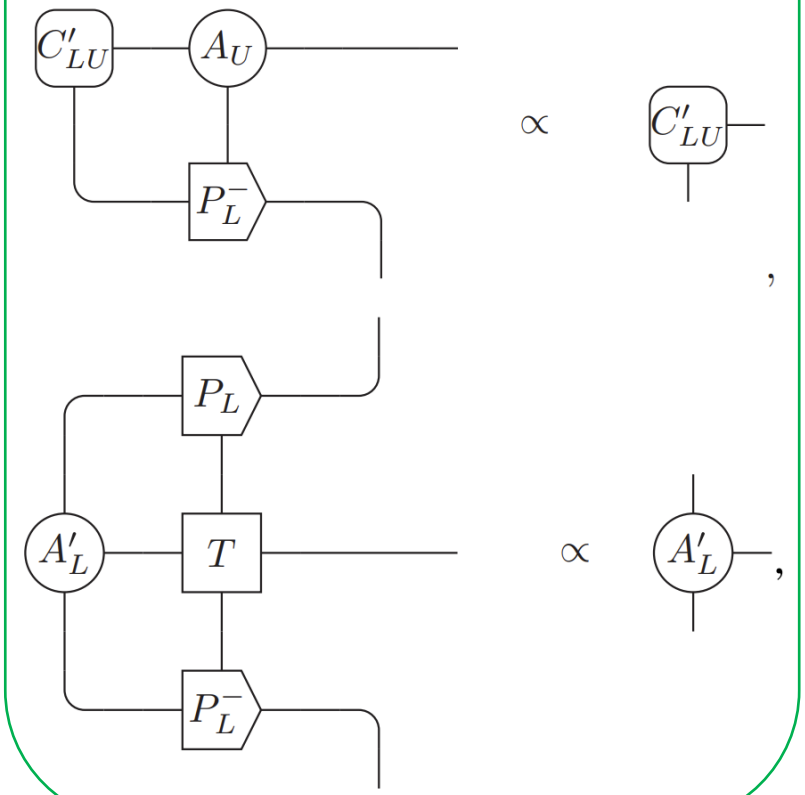


Fixed Point Corner Method

General CTM

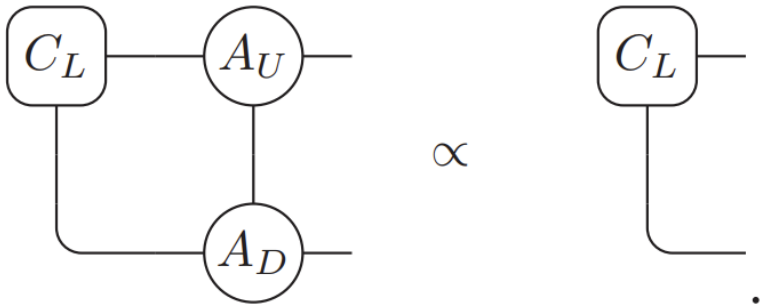


FP CTM



Biorthogonal and Get P

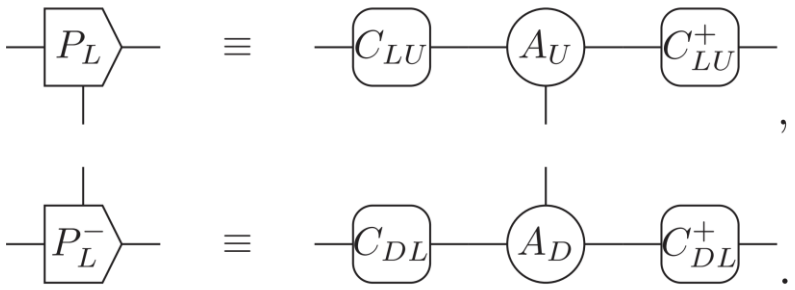
(1)

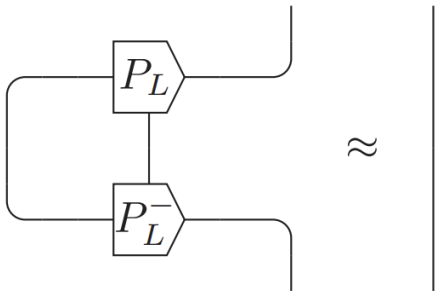


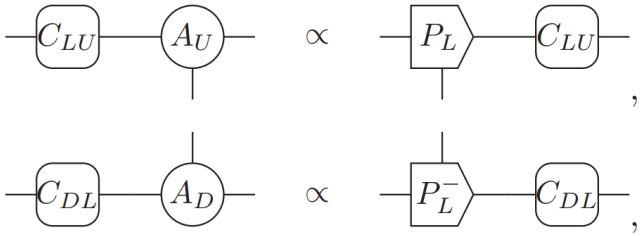
$$C_L = U_L \Sigma_L^2 V_L^\dagger$$

$$C_{LU} \equiv \Sigma_L V_L^\dagger \quad C_{DL} \equiv U_L \Sigma_L$$

(2)



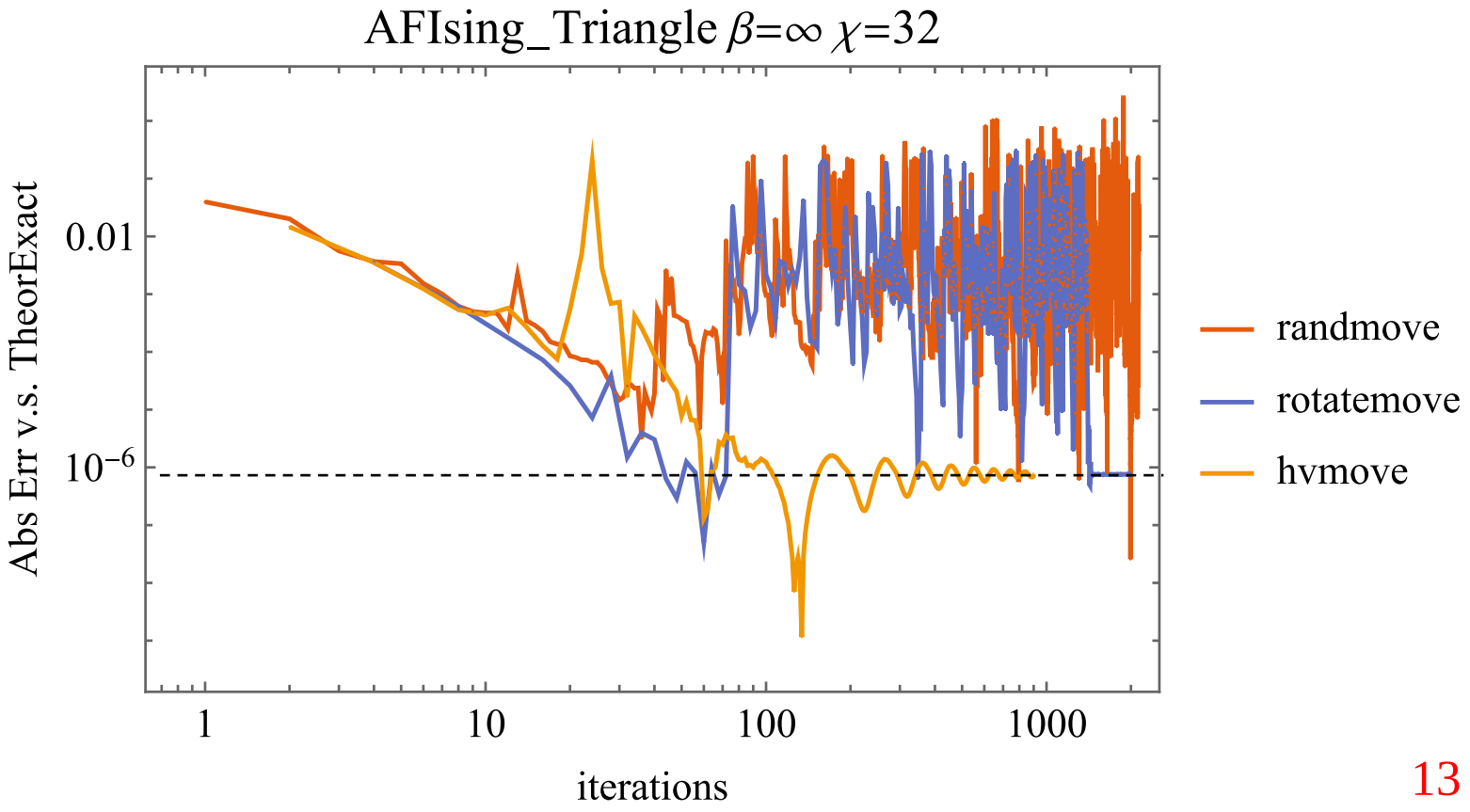




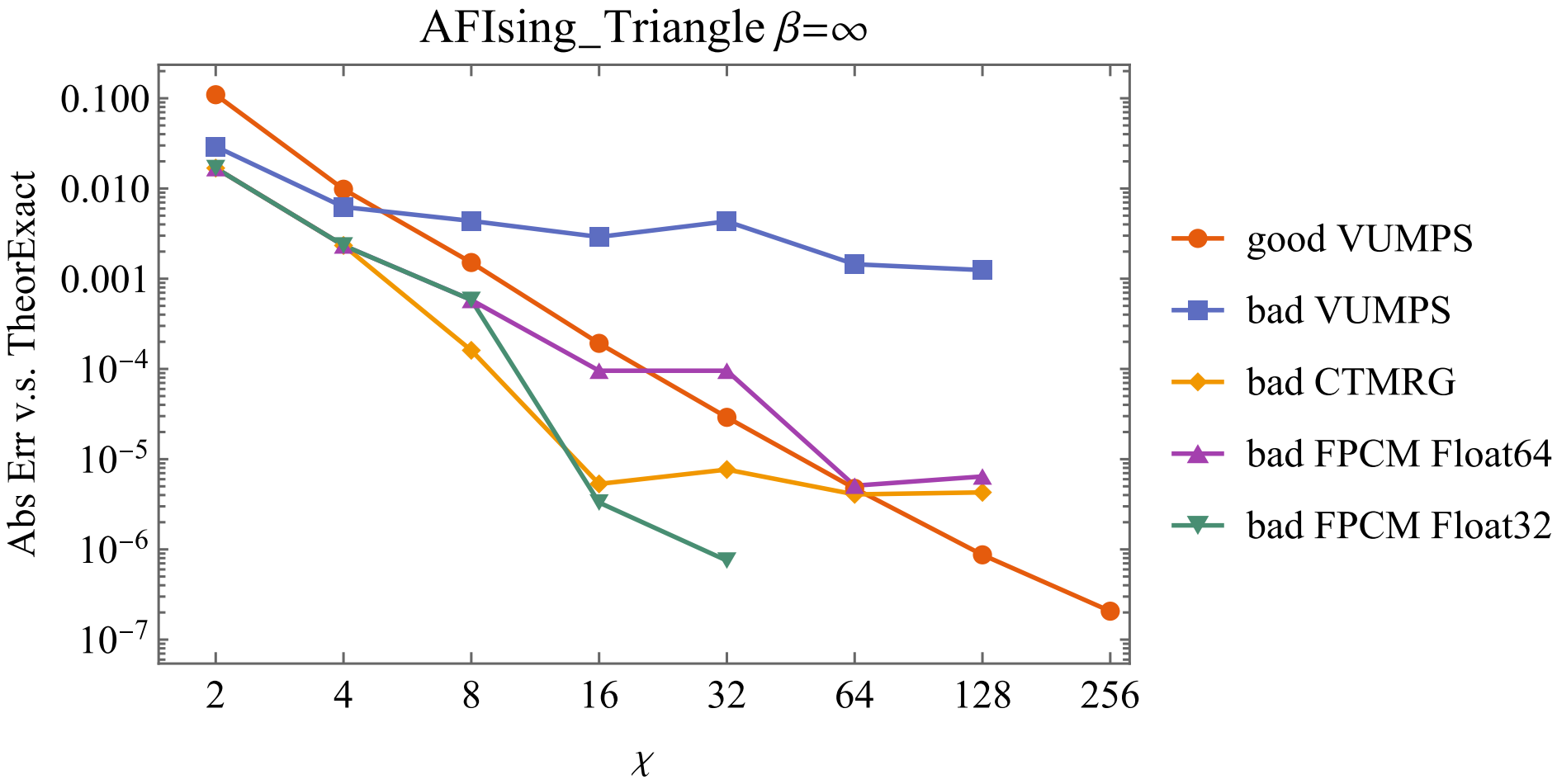
$$\langle A_U | A_D \rangle \approx 1$$

Different move

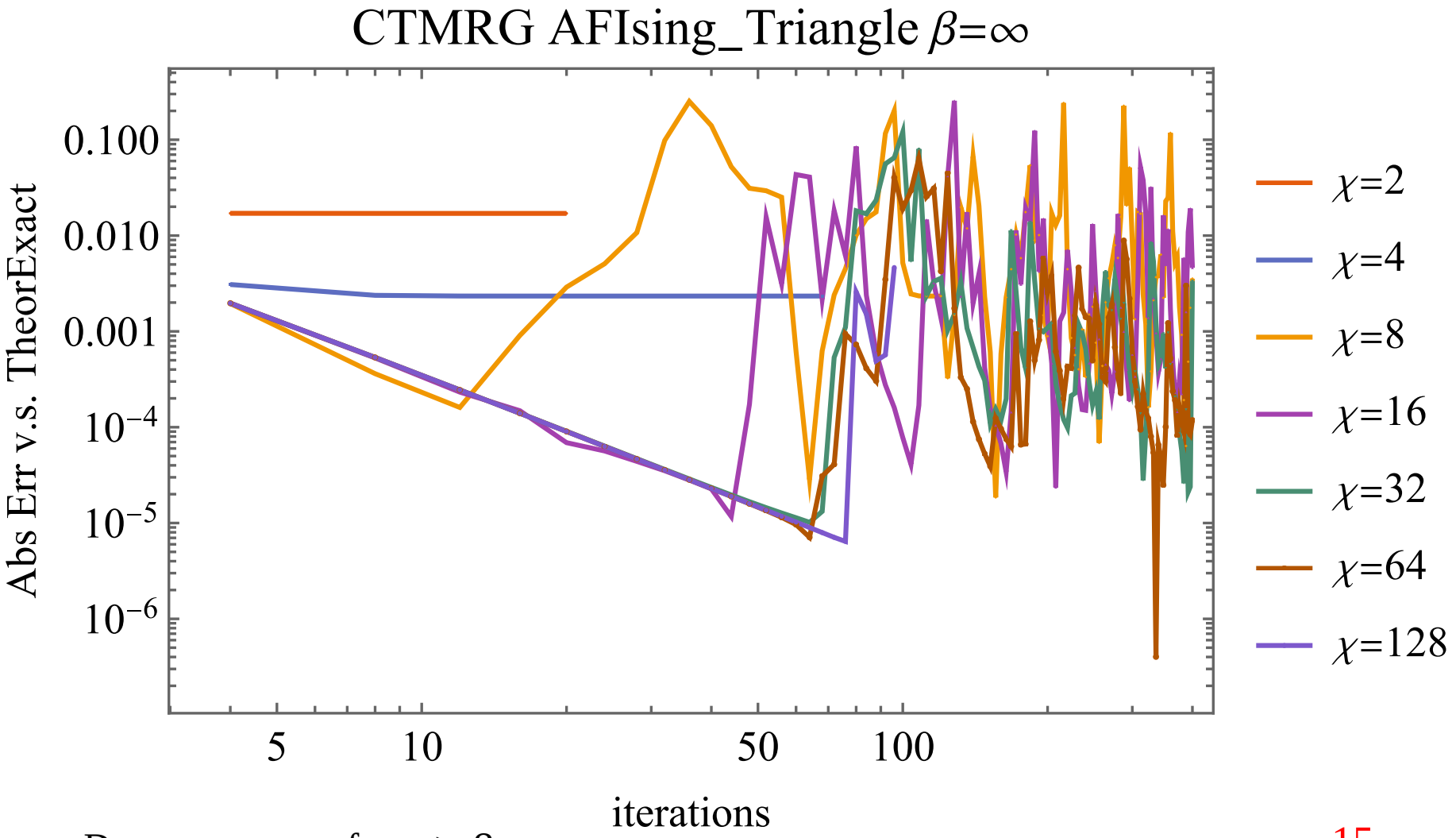
- In practice, we do not find that the ordering makes a noticeable difference in the performance of the algorithm.



AFIsing results



CTMRG result for AFIsing

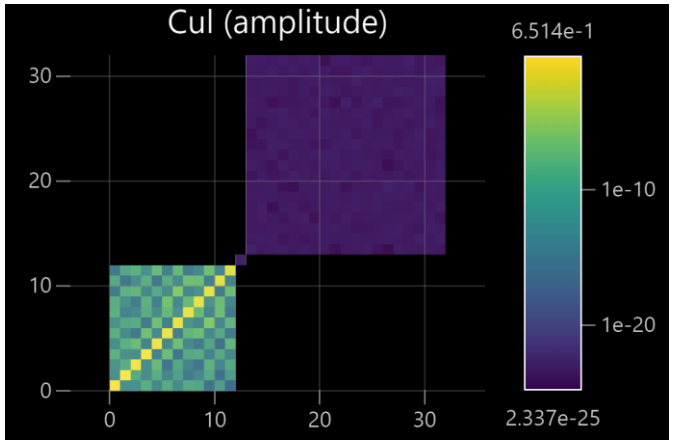


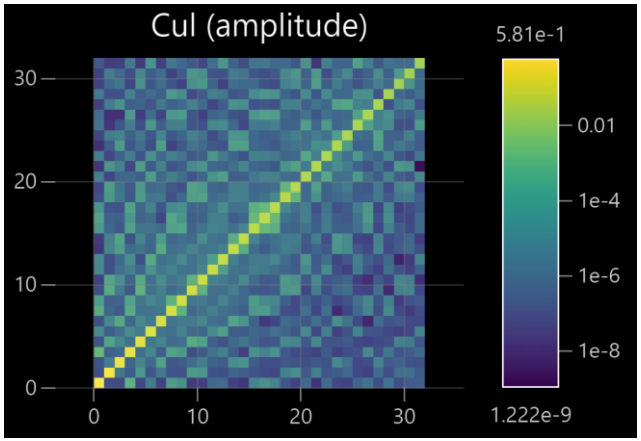
Do not converge for $\chi > 8$

Spectrum of C

- FPCM $\chi = 32$

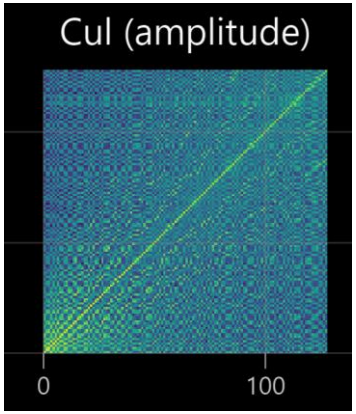
When get P using ComplexF64 or ComplexF32



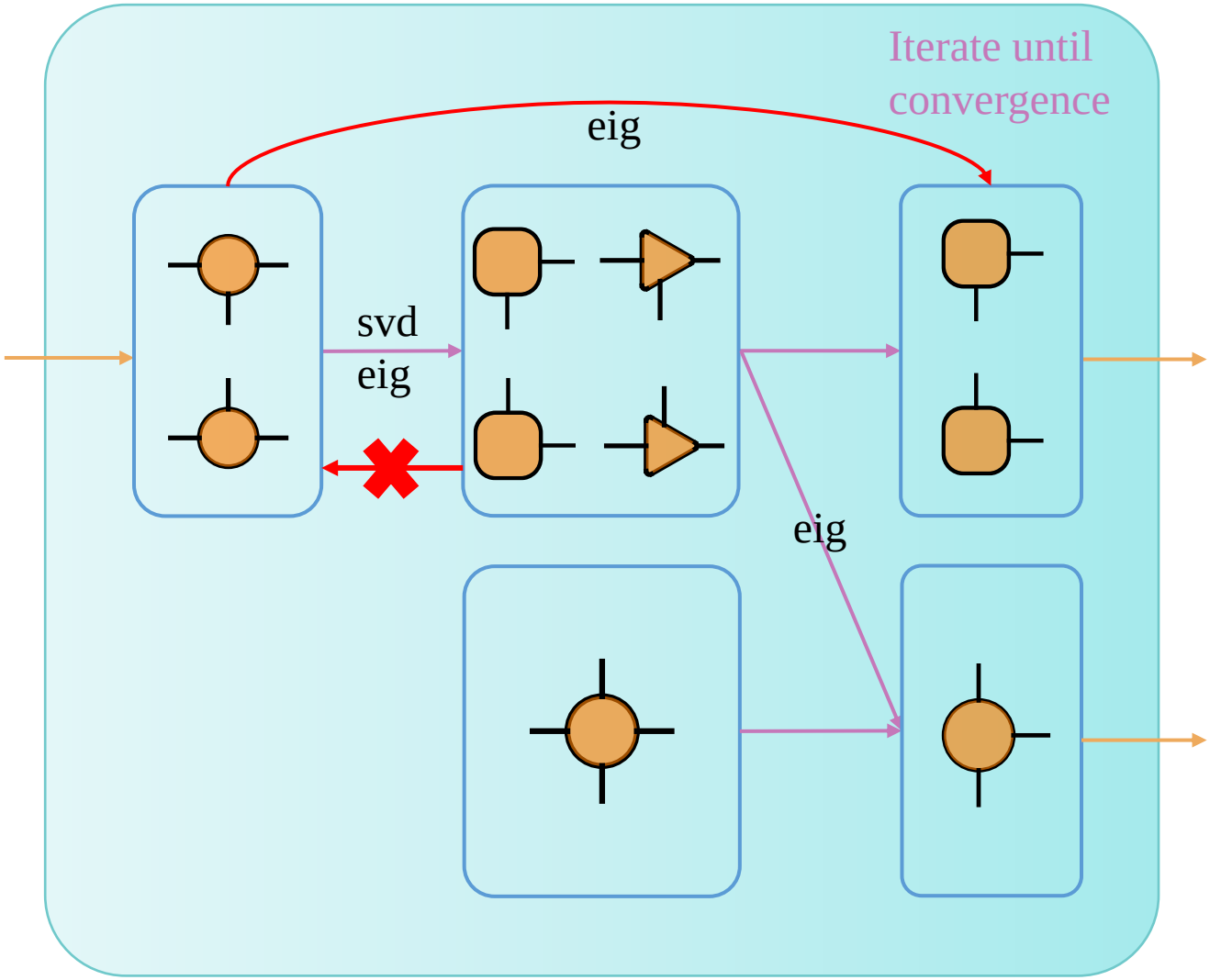


Get stuck/collapse to small χ

- CTMRG $\chi = 128$
  - The effective Block will increase during iterating!
  - But it is not stable when iterating more

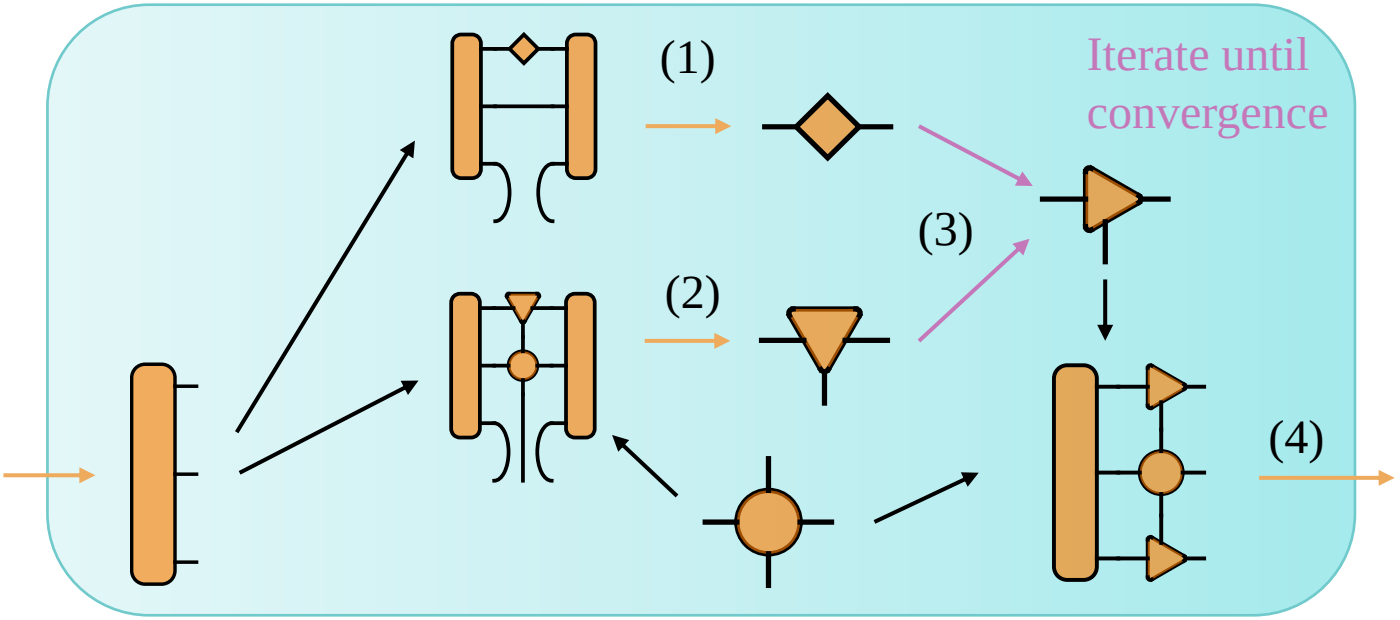


An interesting ignore for AD



Without svd the backward AD is stable

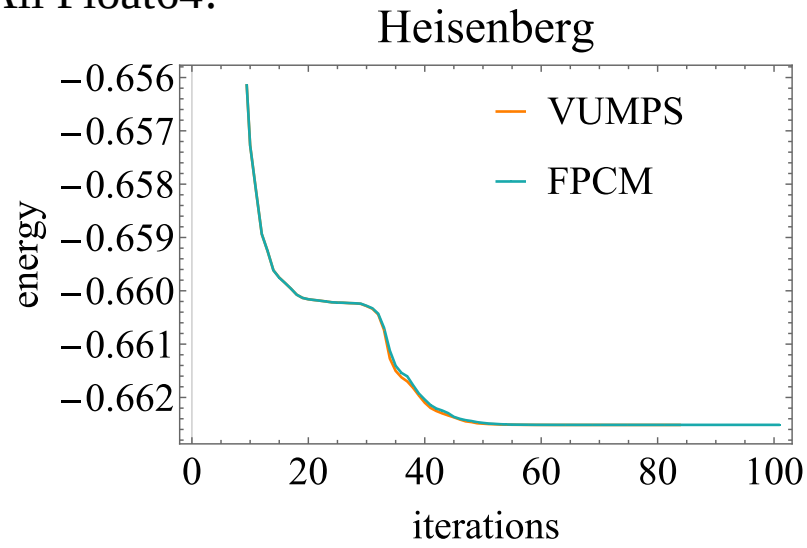
VUMPS steps

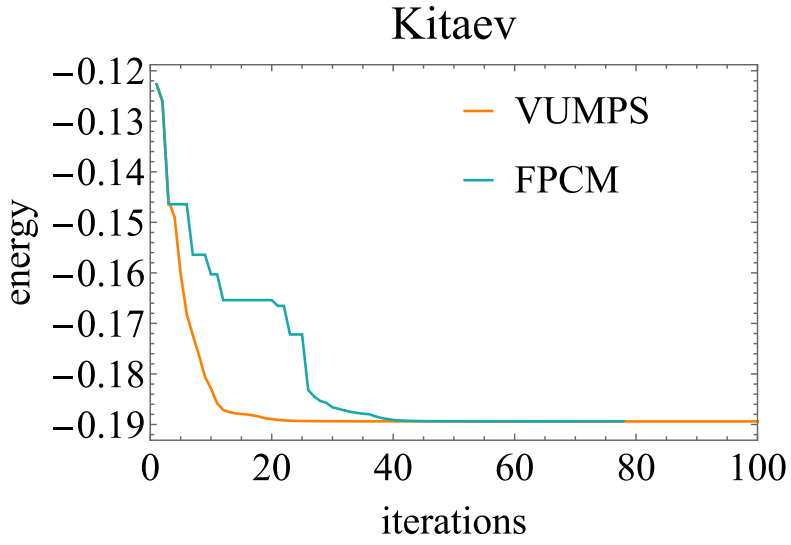


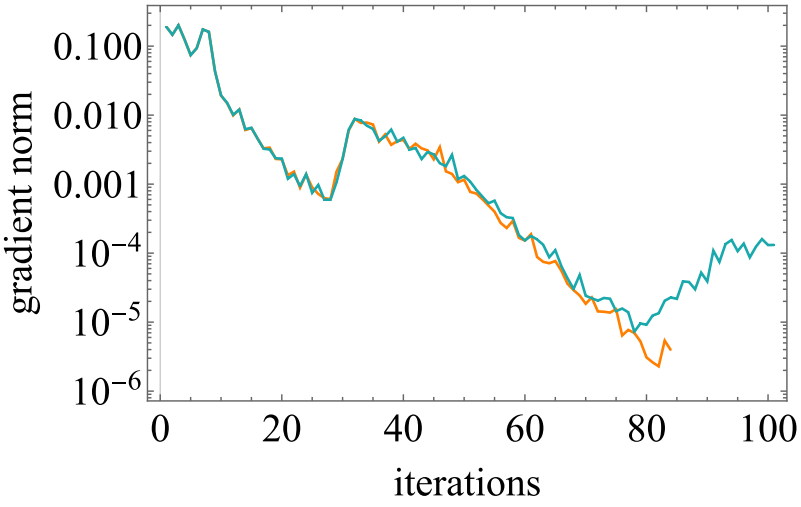
Same thing to get left environment!

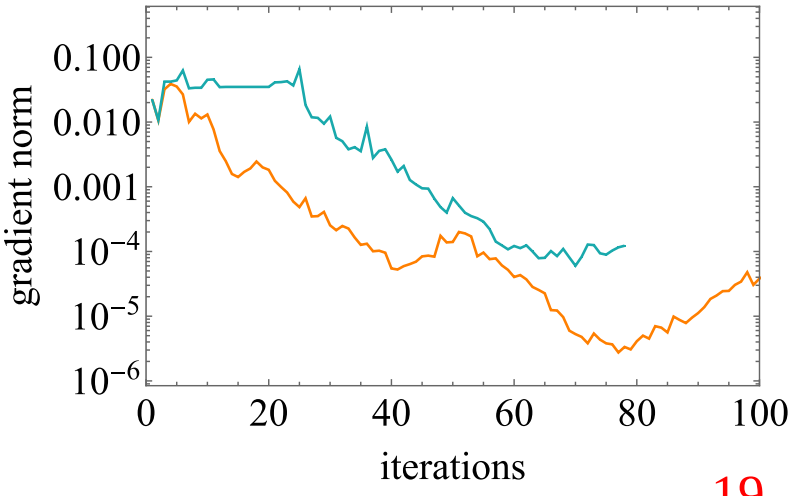
AD optimize iPEPS for spin system

All Float64!









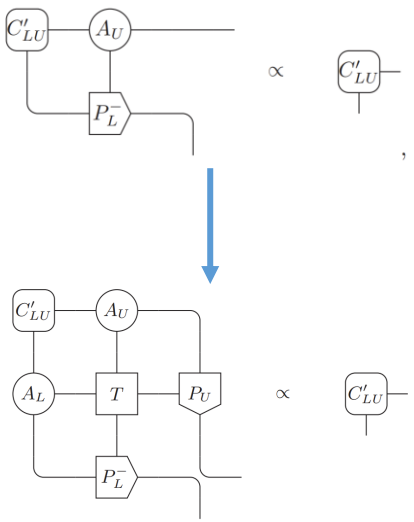
AD optimize fPEPS for fermionic system

- With Z2 symmetry the FPCM environment prefers to get Hermitian transfer matrix
  - Spectrum of C collapses to $\chi = 1$
- With dense tensor, the norm of wave function is quite small$\sim 10^{-6}$
  - The “sign problem” in fPEPS may be intrinsic

Outlook

- Better Biorthogonal method form Yu-Kun Huang

Biorthonormal matrix-product-state analysis for the non-Hermitian transfer-matrix renormalization group in the thermodynamic limit



- CTM fixed point?
- ComplexF128? Deal with generic svd/Krylov
- Biorthogonal method for VUMPS?

Thank you for listening!

Q&A?