# Efficient numerical simulations of many-body localized systems

Frank Pollmann

Max Planck Institute for the Physics of Complex Systems

**Vedika Khemani**

J. Ignacio Cirac

S. L. Sondhi

FP, Khemani, Cirac, Sondhi, arxiv:1506.07179
Khemani, FP, Sondhi arXiv:1509.00483

Santa Barbara, Nov. 20 2015

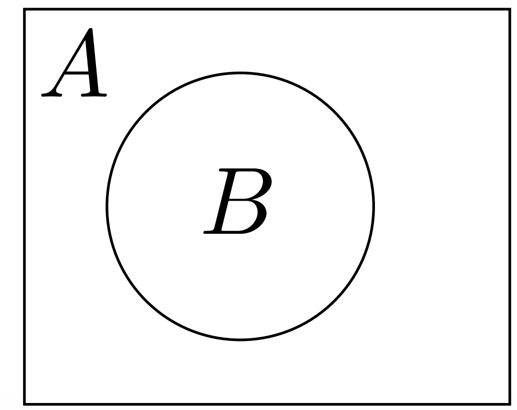
# Many-body localization

$\epsilon > \epsilon_0$

| Extended | Localized |
|---|---|
| ETH | ETH breaks down |
| Volume law | Area law |
| | Local integrals of motion |

disorder


Anderson (1958)
Gornyi, Mirlin, Polyakov (2005)
Basko, Aleiner, Altshuler (2006)
Oganesyan and Huse (2007)
Pal and Huse (2010)
Bardarson, FP, Moore (2012)
Bauer and Nayak (2013)
Huse and Oganesyan (2013)
Serbyn, Papic, Abanin (2013)
**+many more**


$$\rho_B = \mathrm{Tr}_A |\psi\rangle\langle\psi|$$

$$S = -\mathrm{Tr}_B \rho_B \log \rho_B$$

$|\psi_{\tau_1,\tau_2,\ldots,\tau_L}\rangle \quad \tau_j = U^\dagger \sigma_j U$

"p-bits" and "l-bits"

# Many-body localization

- Disordered XXZ model

$$H = J_\perp \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \sum_i h_i S_i^z + J_z \sum_i S_i^z S_{i+1}^z$$

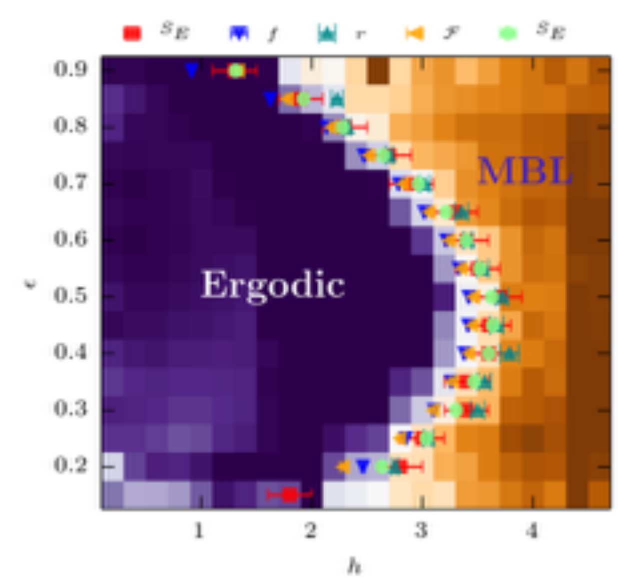
with $h_i \in [-W, W]$

- All single particle states localized for $W \neq 0$

[Anderson '58]

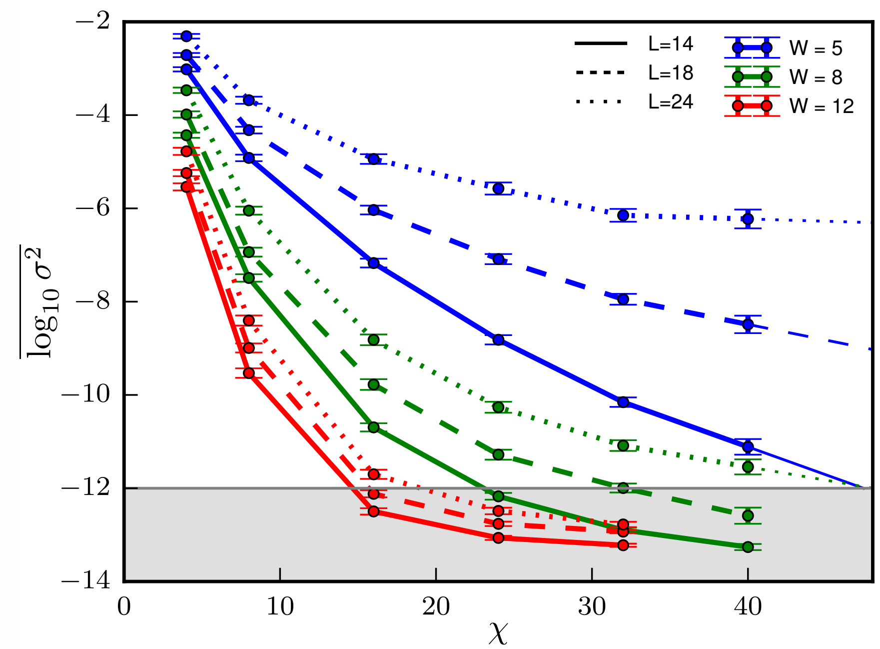
- $J_\perp = J_z = 1$ : fully MBL for $W \gtrsim 3.5$

[Pal & Huse '10, Luitz et al '15]



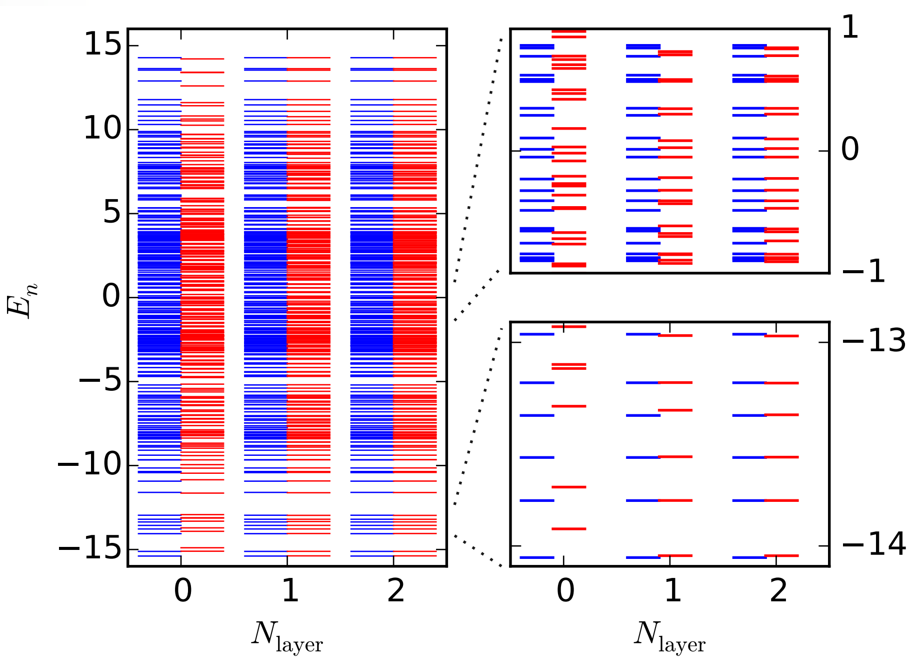
# Overview

(1) Obtaining individual highly excited eigenstates of MBL systems to machine precision accuracy:
**Matrix-product states**




Khemani, FP, Sondhi, arXiv:1509.00483

(2) Variational diagonalization of fully many-body localized Hamiltonians:
**Matrix-product operators**

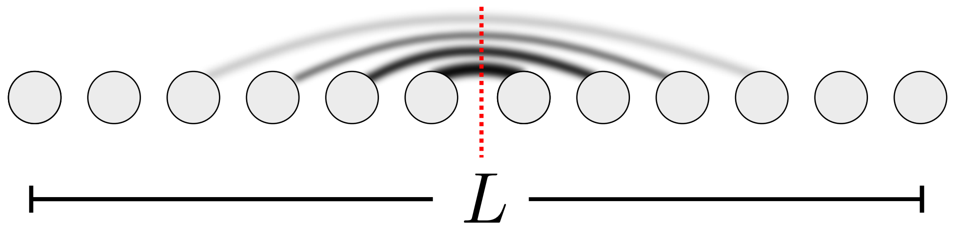


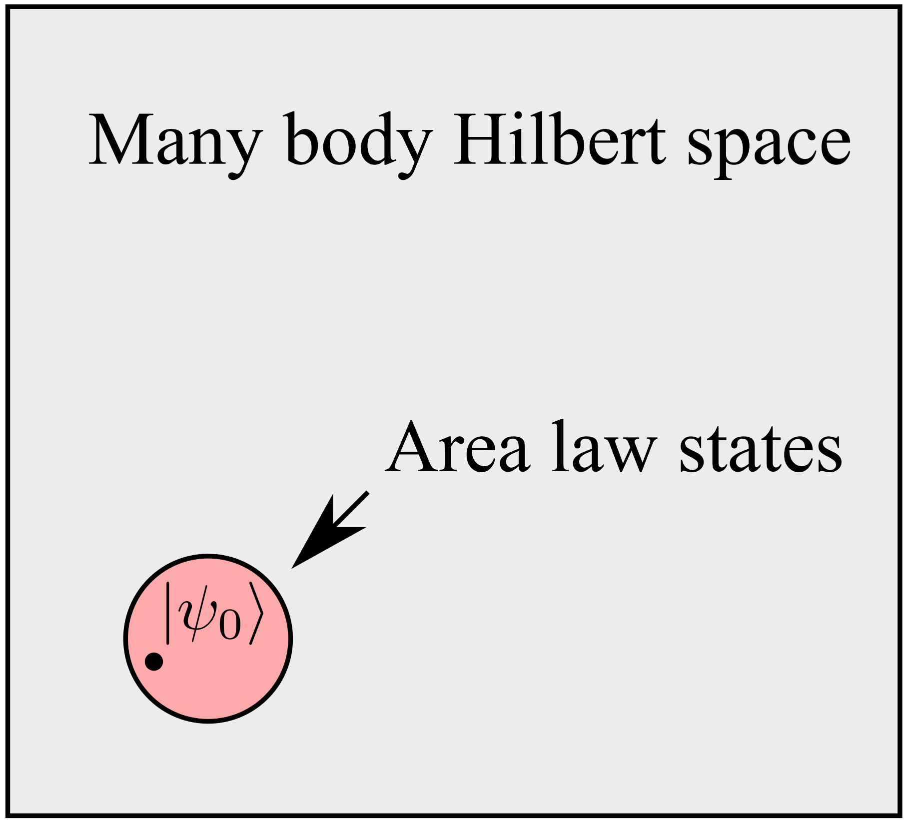

FP, Khemani, Cirac, Sondhi, arxiv:1506.07179

# Entanglement

- Area law for ground states of local (gapped) Hamiltonians in one dimensional systems

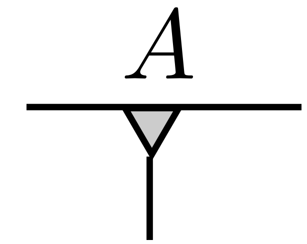
$S(L) = \text{const.}$ [Srednicki '93, Hastings '07]



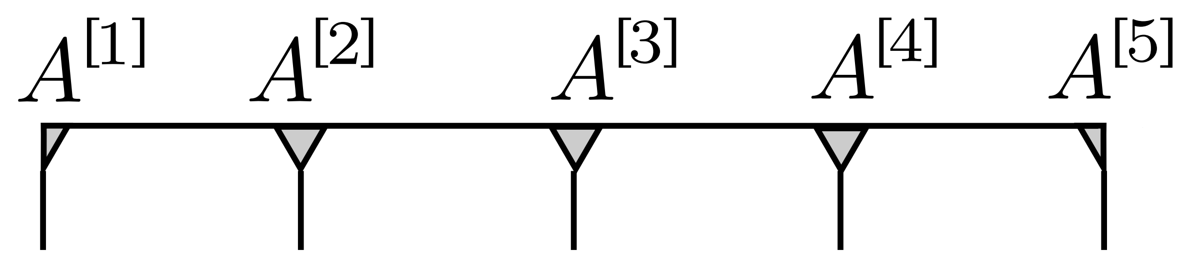

- Efficient representation: Matrix-product states

# Matrix-product states

- **Matrix-product states:** $d^L \to L d \chi^2$ $\qquad A^j_{\alpha\beta} =$ 

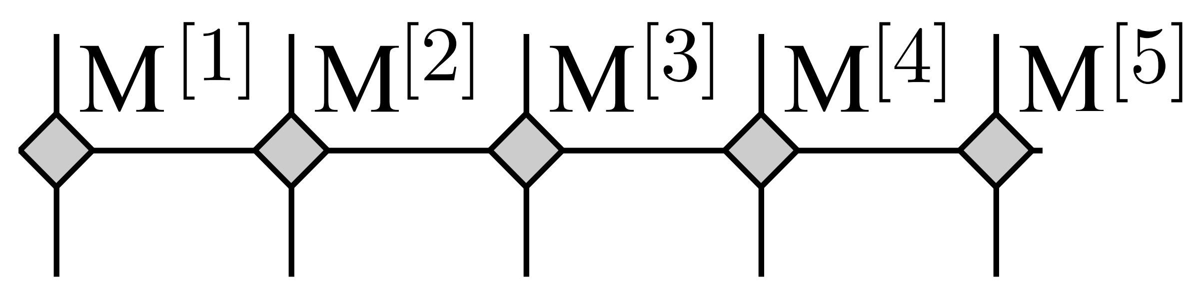

  [M. Fannes et al. 92, Schuch et al '08]

$$\psi_{j_1,j_2,j_3,j_4,j_5} = A^{[1]j_1}_{\alpha} A^{[2]j_2}_{\alpha\beta} A^{[3]j_3}_{\beta\gamma} A^{[4]j_4}_{\gamma\delta} A^{[5]j_5}_{\delta}$$

$=$ 


- **Matrix-product operators** [Verstraete et al '04]

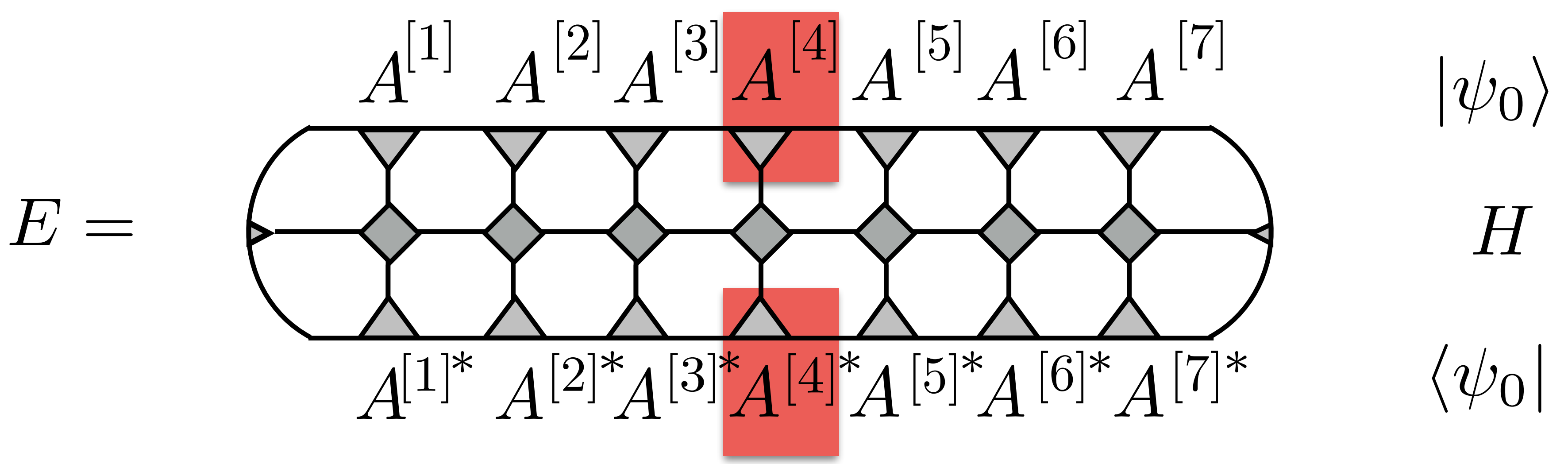
$$O^{j_1',j_2',j_3',j_4',j_5'}_{j_1,j_2,j_3,j_4,j_5} =$$



# Finding ground states

- Efficient variational optimization of $\{A^j_{\alpha\beta}\}$ :
  **Density matrix renormalization group** (DMRG) [White '92]

- Find the **ground state** iteratively

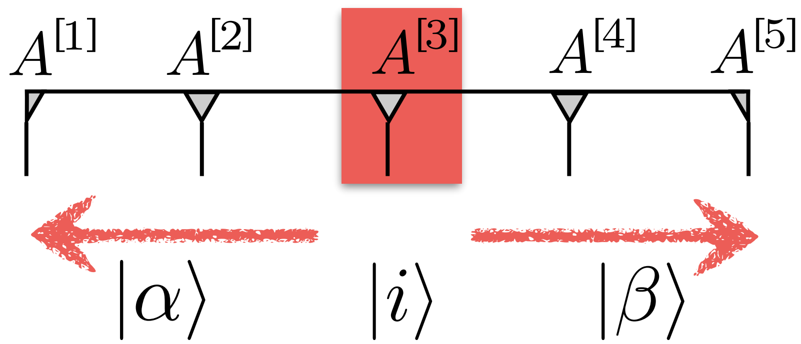



by locally minimizing energy of $H_{\alpha i\beta;\alpha' i'\beta'}$ (e.g., Lanczos)

# Finding excited states

- DMRG-X algorithm
  1. Initiate MPS $|\psi\rangle$ (close to "l-bit" state)
  2. Diagonalize $H_{\alpha i \beta;\alpha' i' \beta'}$ at $m$:
     $H|\tilde{\psi}_n\rangle = E_n|\tilde{\psi}_n\rangle$
  3. Pick eigenstate that has largest overlap with $|\psi\rangle$: $A^{[m]i}_{\alpha\beta} \rightarrow \tilde{A}^{[m]i}_{\alpha\beta}$
  4. Move to site $m+1$

$$|\psi\rangle = |\sigma_1^z\rangle|\sigma_2^z\rangle\ldots|\sigma_L^z\rangle$$




- No individual update step of the MPS matrices results in a global spatial reorganization $|\psi_{\tau_1,\tau_2,\ldots,\tau_L}\rangle$

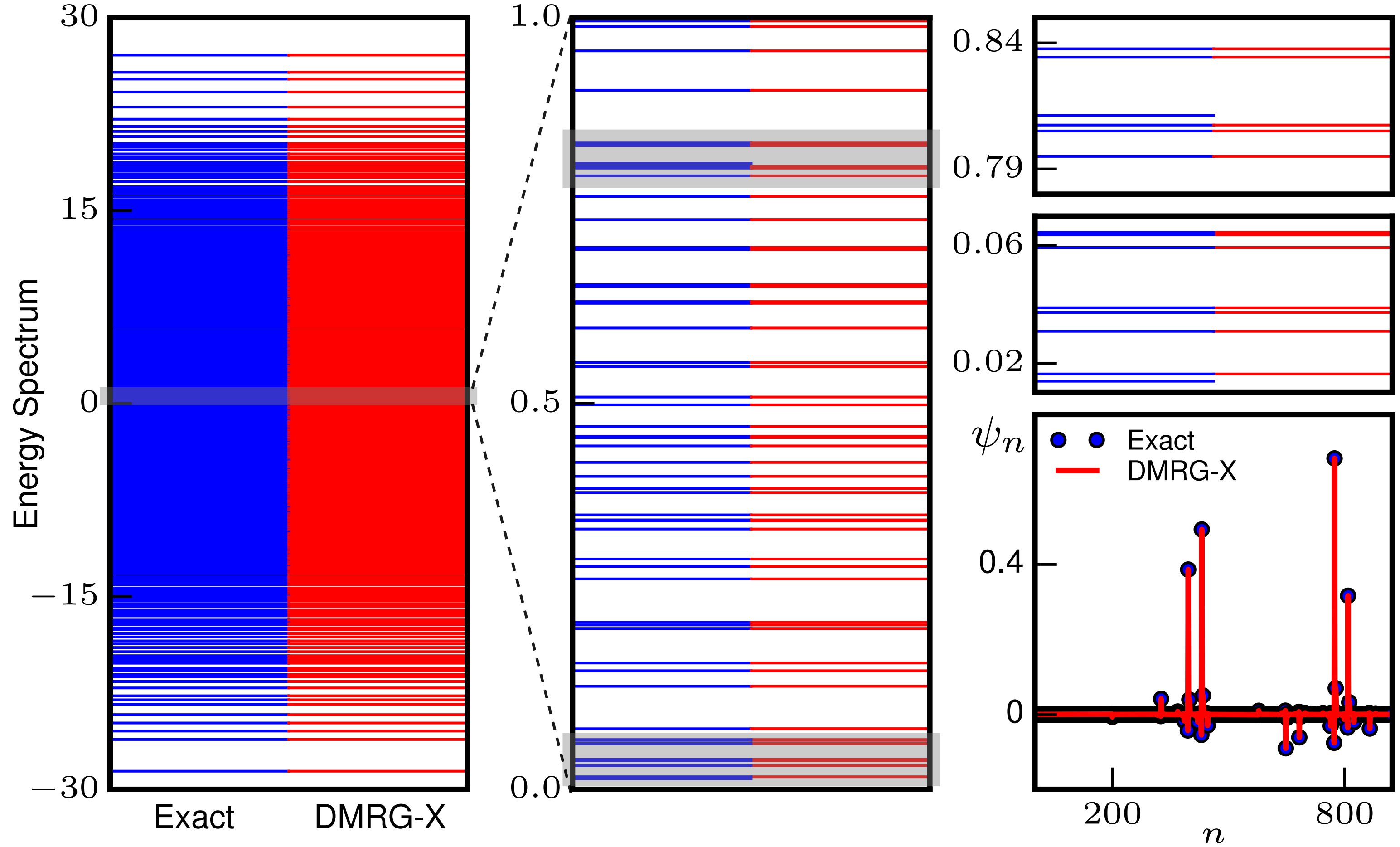
see also: Yu, Pekker, Clark , arXiv:1509.01244
S. P. Lim, D. N. Sheng, arXiv:1510.08145
D. M. Kennes, C. Karrasch, arXiv:1511.02205

Khemani, FP, Sondhi arXiv:1509.00483

# DMRG-X: Results

- Finding eigenstates starting from different product states

$L = 12,\ W = 8$

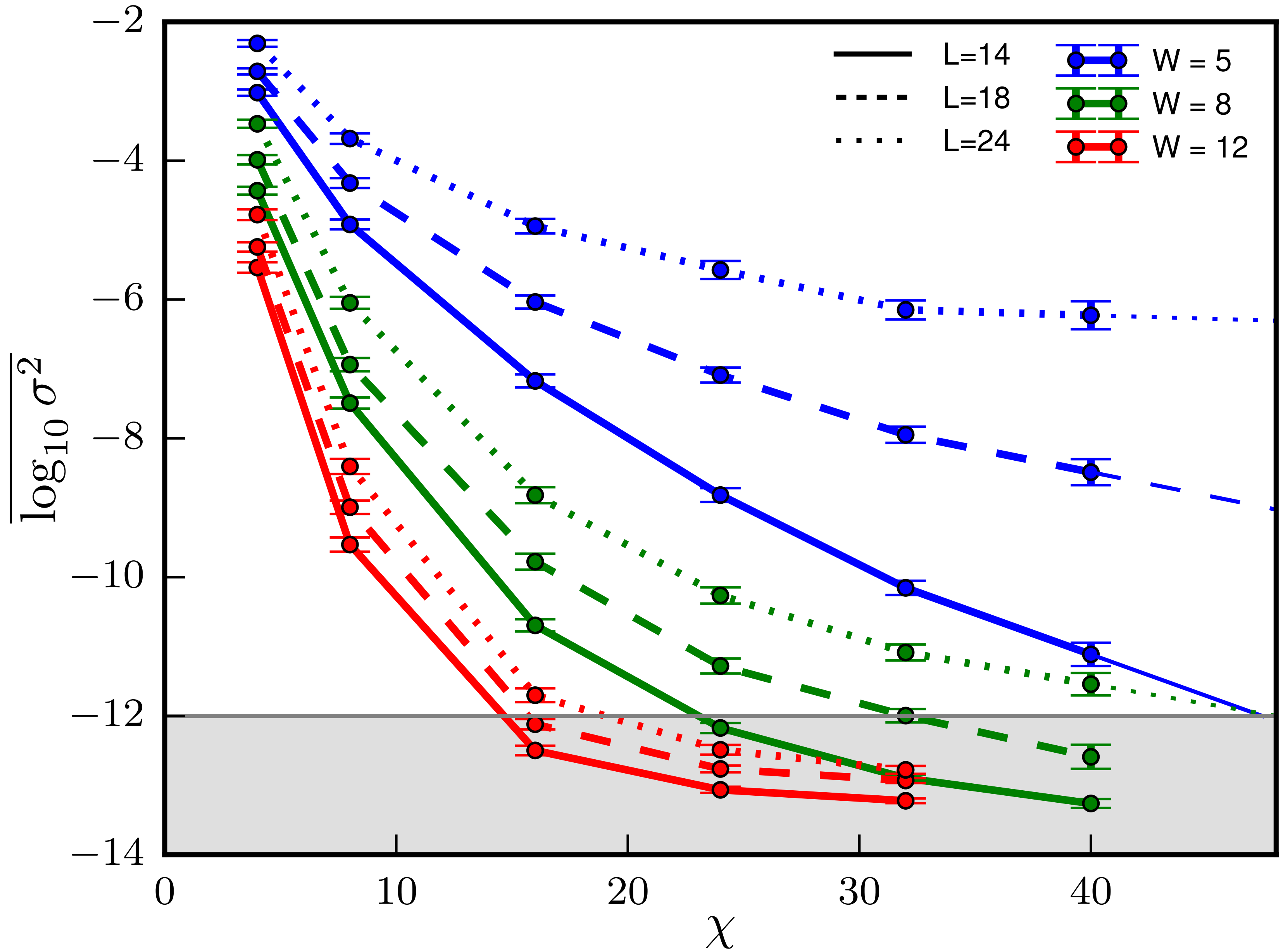



- **Algorithm finds resonances!**

Khemani, FP, Sondhi arXiv:1509.00483

# DMRG-X: Results

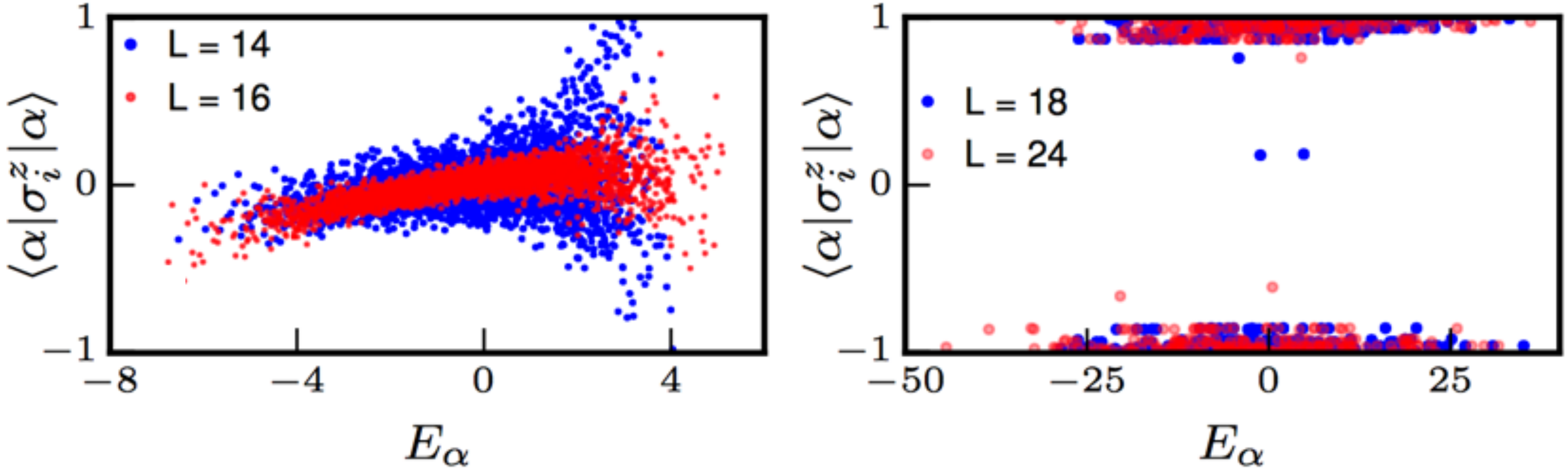
- Convergence criteria: **Energy variance**




Khemani, FP, Sondhi arXiv:1509.00483

# DMRG-X: Results

- Violation of ETH in the MBL phase




Khemani, FP, Sondhi arXiv:1509.00483

# Overview

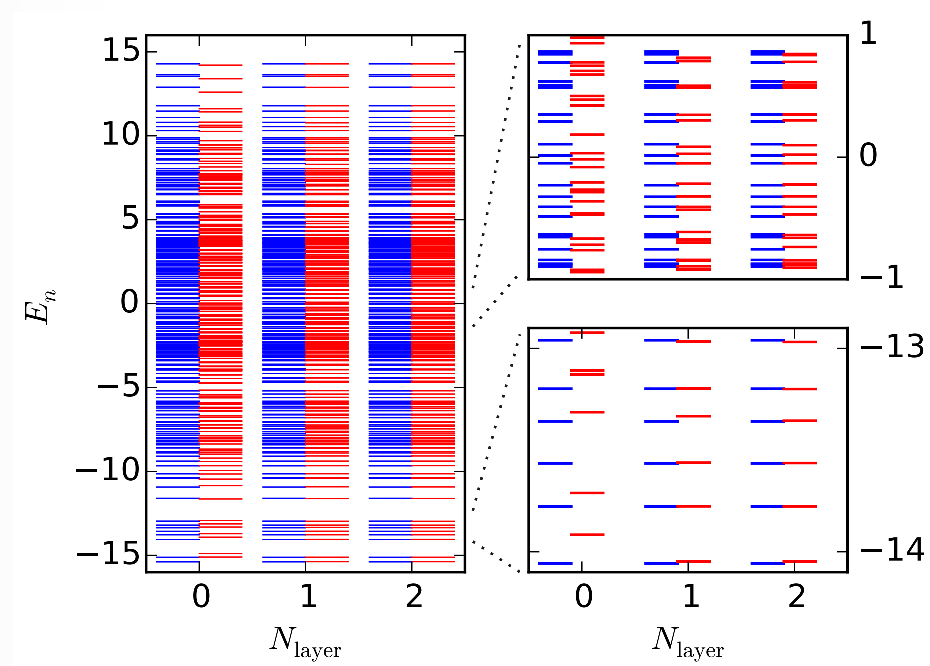
(1) Obtaining individual highly excited eigenstates of MBL systems to machine precision accuracy:
Matrix-product states

Khemani, FP, Sondhi, arXiv:1509.00483




(2) Variational diagonalization of fully many-body localized Hamiltonians:
Matrix-product operators

FP, Khemani, Cirac, Sondhi, arxiv:1506.07179



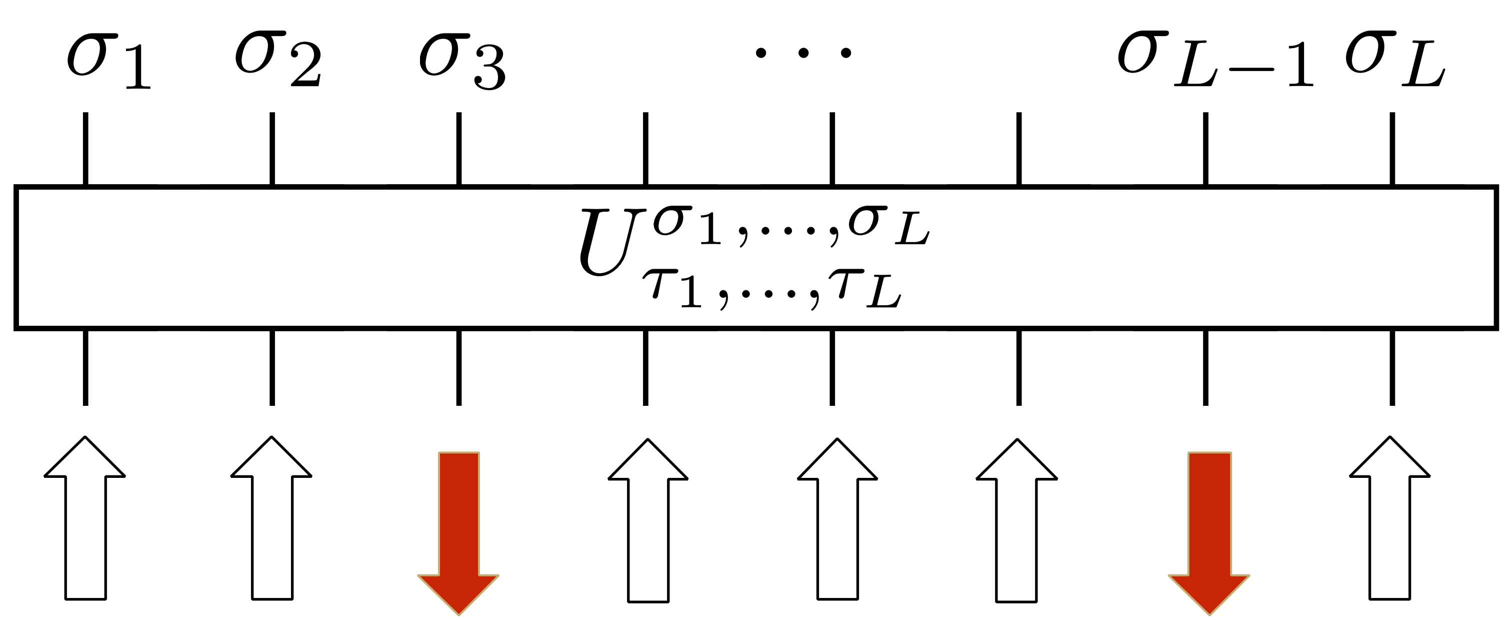
# Quasi local integrals of motion

- Many-body localization: **"p-bits"** ($\sigma$) and **"l-bits"** ($\tau$):

$$\tau_j = U^\dagger \sigma_j U$$ [Huse & Oganesyan '13, Serbyn, Papic, Abanin '13]

$$|\psi_{\tau_1,\tau_2,\ldots,\tau_L}\rangle =$$

$$|\tau_1,\tau_2,\ldots,\tau_L\rangle =$$

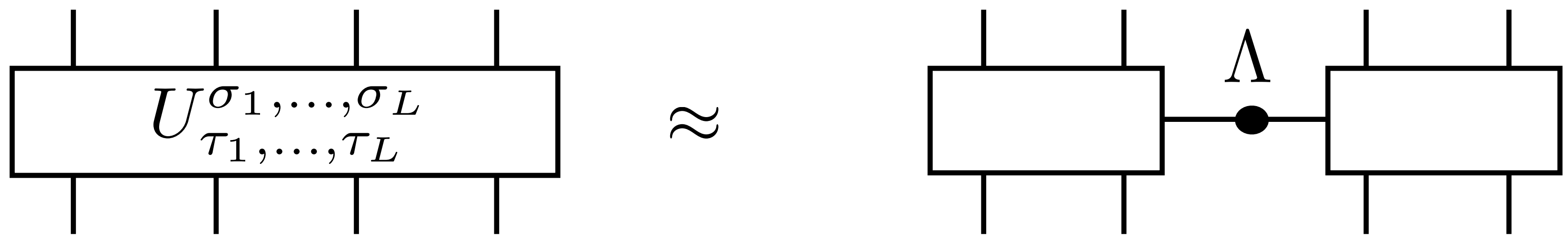


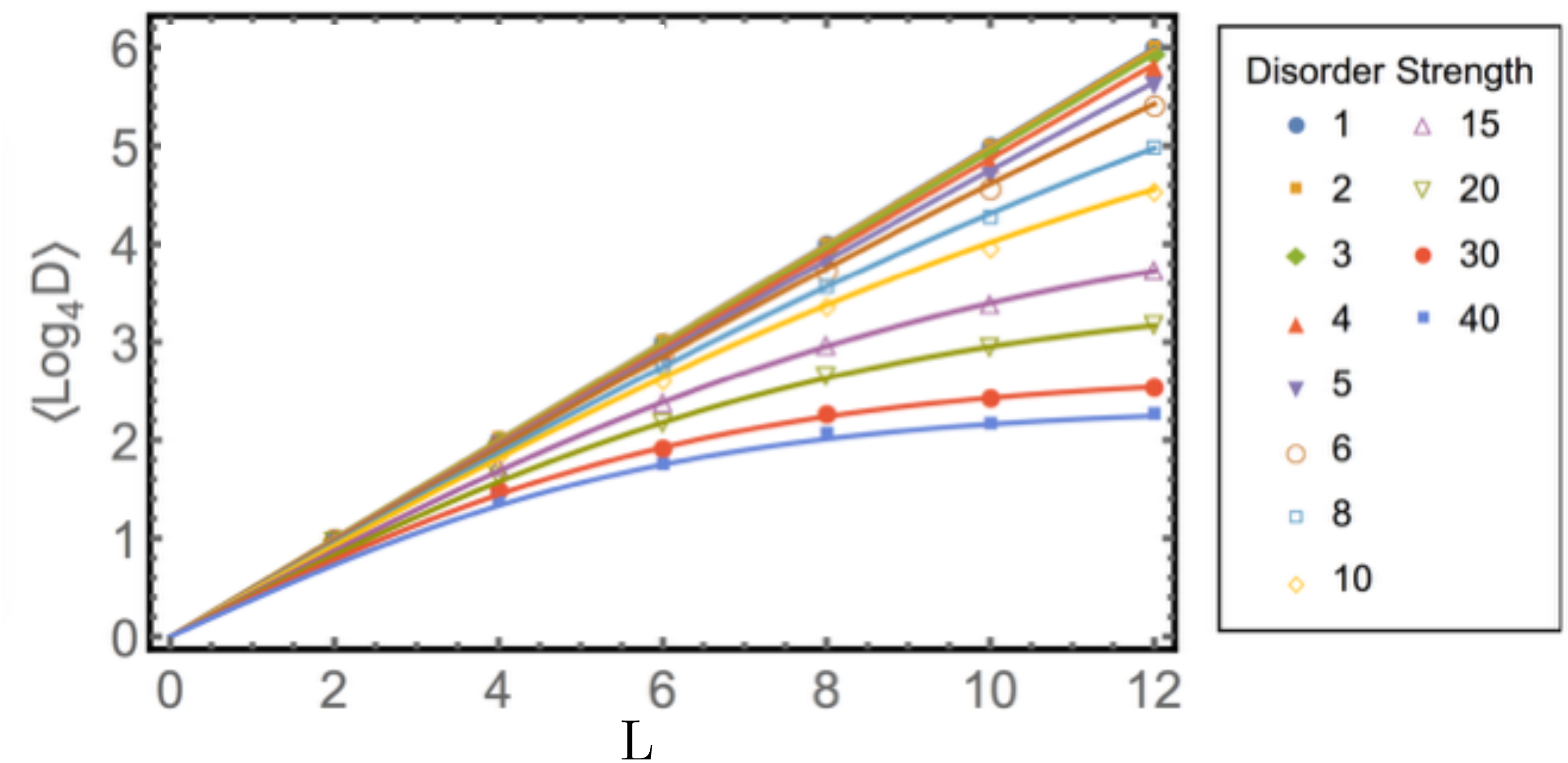

- All $2^L$ many-body eigenstates given by a **"quasi local"** unitary

➡ Efficient representation as **matrix-product operator** ???

# Quasi local integrals of motion

- Compression using exact diagonalization (ED) [Pekker & Clark '14]

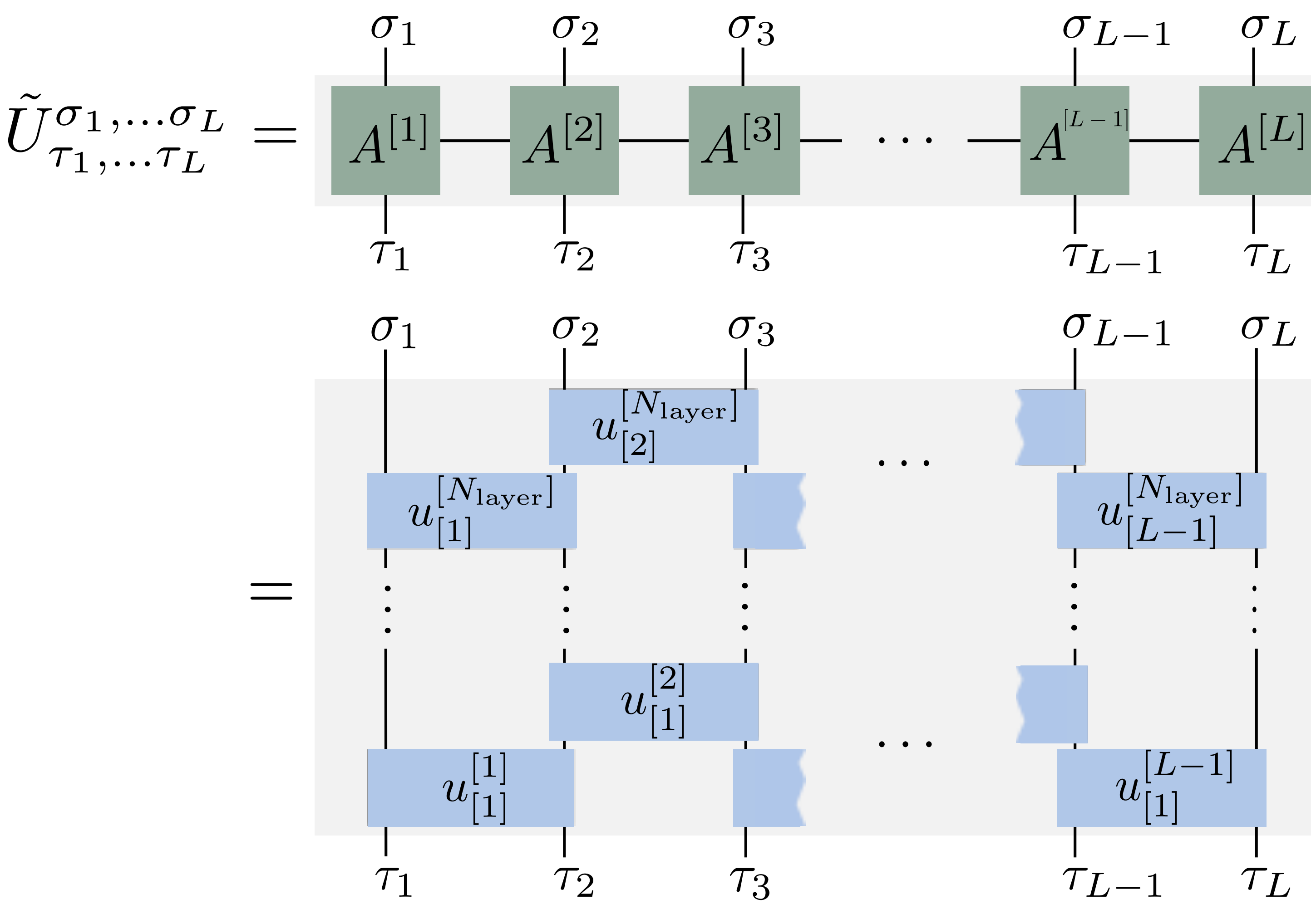



- ED exponential in size! Gauge of $U^{\sigma_1,\ldots,\sigma_L}_{\tau_1,\ldots,\tau_L}$? Unitarity?

# Variational unitary MPO ansatz

- Finite depth local unitary network (VUMPO):



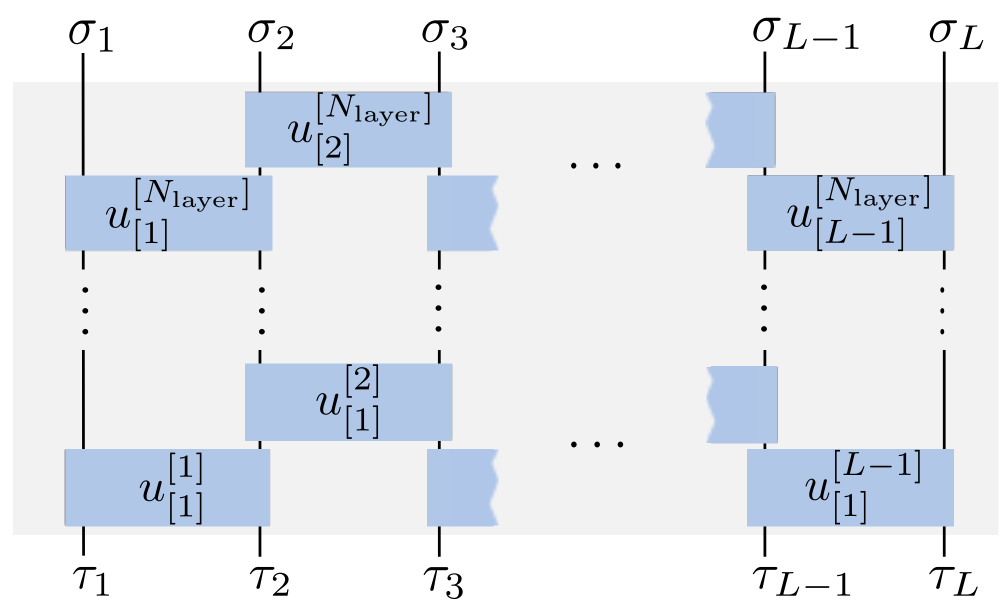

Different unitary networks possible…

- Variationally minimize the **variance of the energy**

FP, Khemani, Cirac, Sondhi, arXiv:1506.07179

# Variational unitary MPO ansatz

- VUMPO algorithm
  1. Initiate random unitaries
  2. Locally minimize cost function (e.g., CG)




$$f(\{u_{[i]}^{[j]}\}) = \sum_{\{\boldsymbol{\tau}\}} \langle \psi_{\boldsymbol{\tau}} | H^2 | \psi_{\boldsymbol{\tau}} \rangle - \langle \psi_{\boldsymbol{\tau}} | H | \psi_{\boldsymbol{\tau}} \rangle^2 \geq 0$$

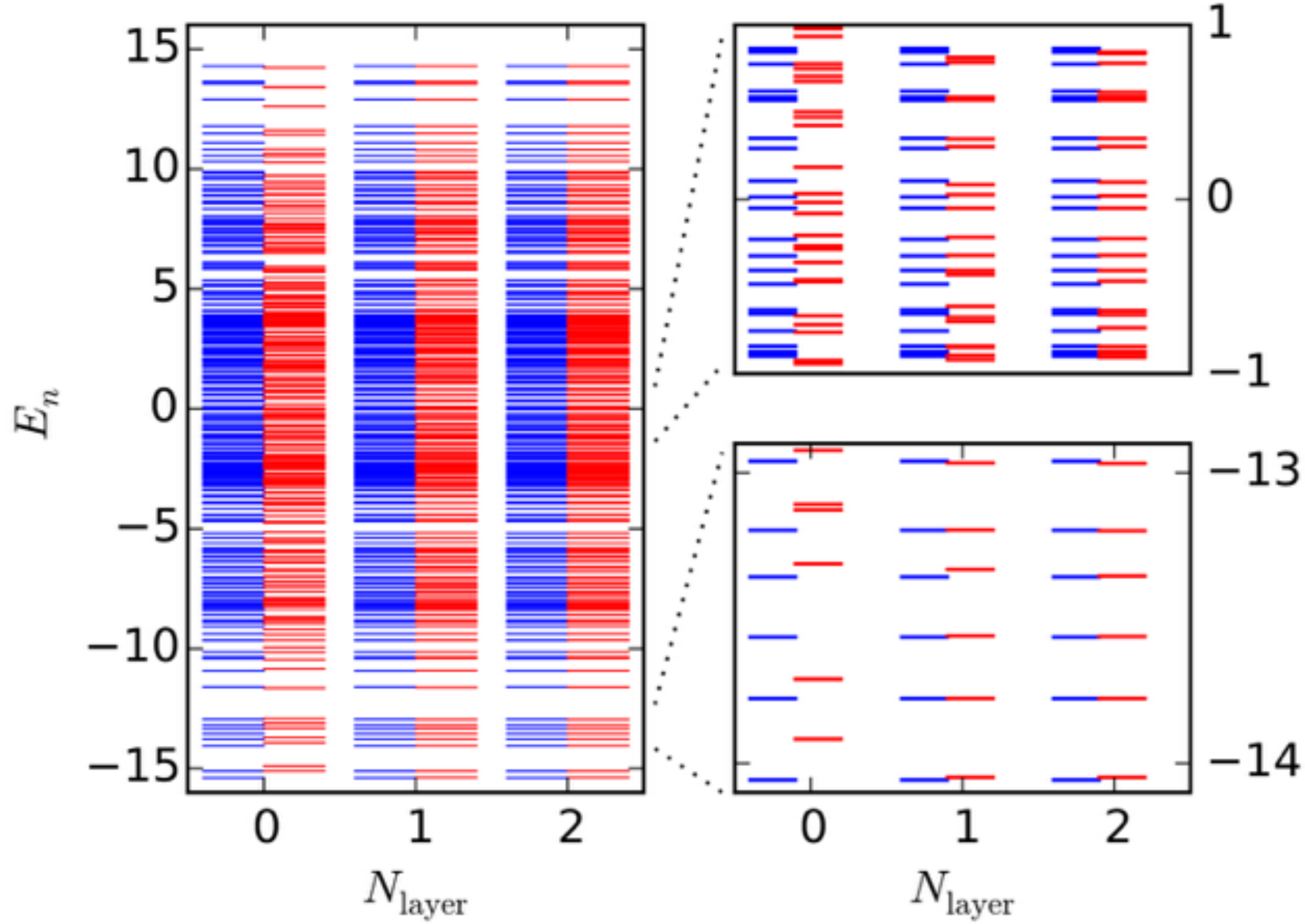
  3. Move to next bond

- Scaling: Linear in $L$ and exponential in $N_{\mathrm{Layer}}$
- Ansatz preserves unitarity and locality at all times!

FP, Khemani, Cirac, Sondhi, arXiv:1506.07179

# Variational unitary MPO ansatz: Result

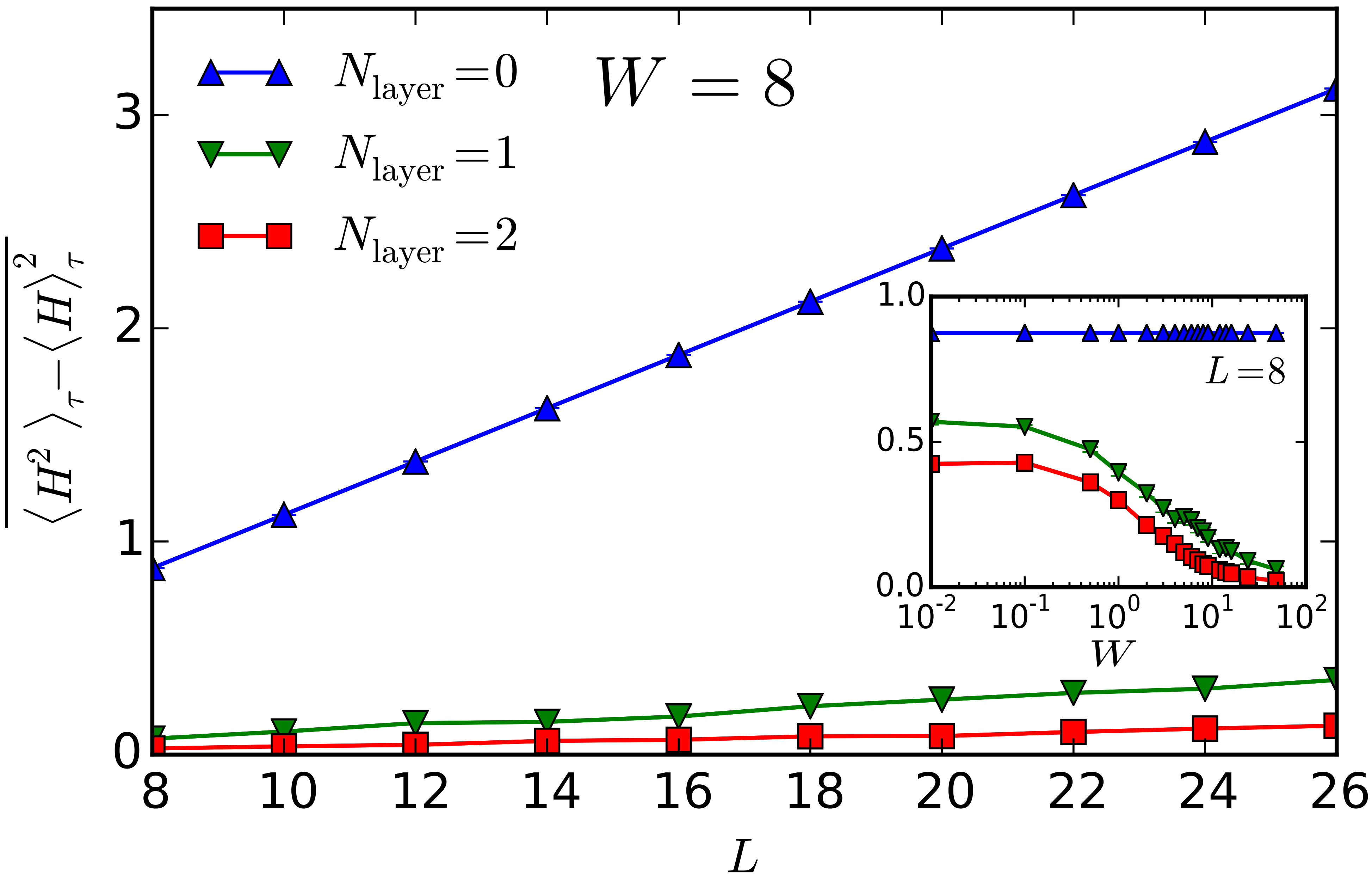
- Deep in localized phase with $W = 8$ and $L = 8$:




FP, Khemani, Cirac, Sondhi, arXiv:1506.07179

# Variational unitary MPO ansatz: Result

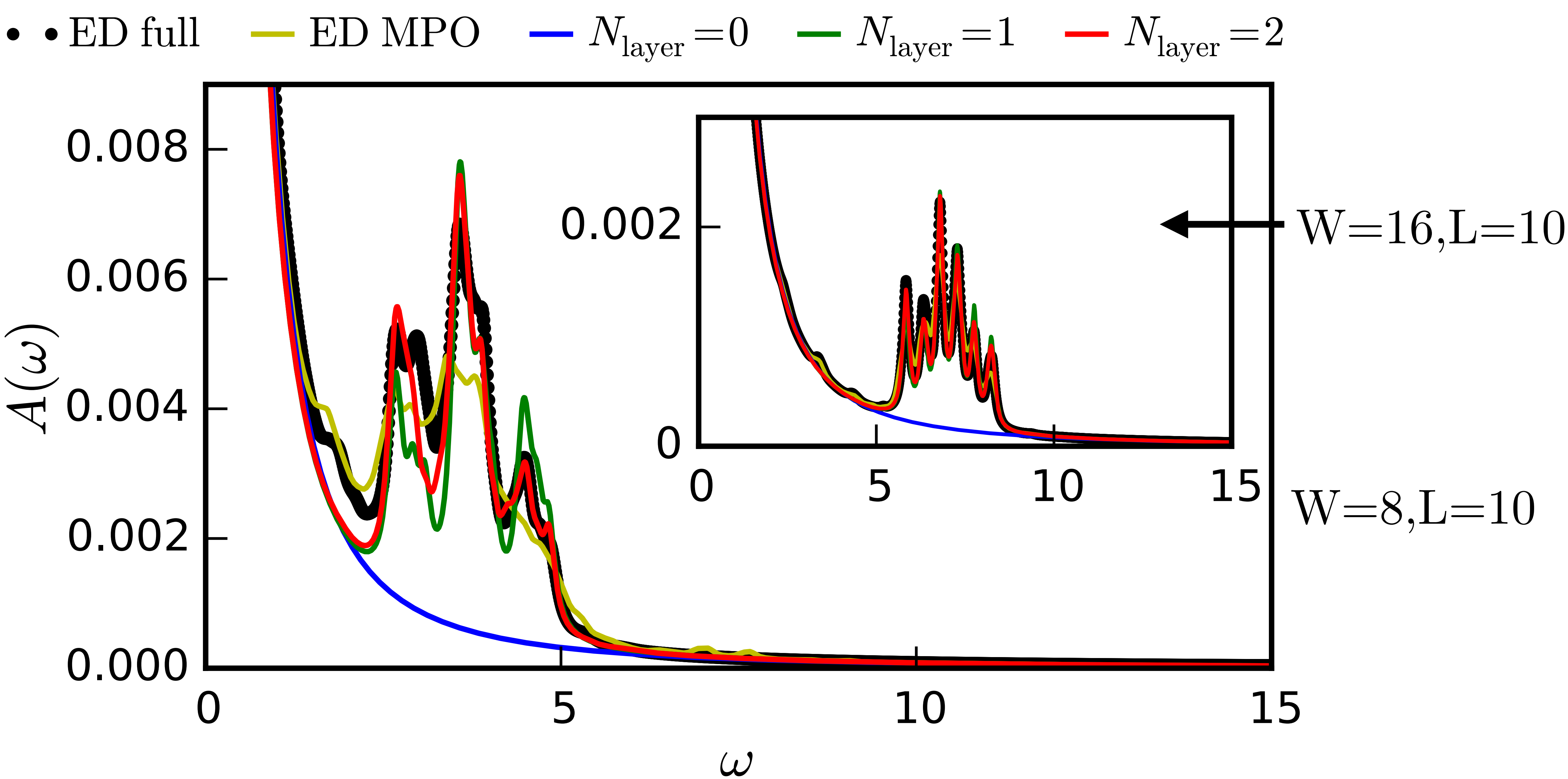
- Linear scaling of the mean variance: **Constant error density**




FP, Khemani, Cirac, Sondhi, arXiv:1506.07179

# Variational unitary MPO ansatz: Result

- Spectral function: $A(\omega) = \frac{1}{2^L} \sum_{\{\boldsymbol{\tau_1}\},\{\boldsymbol{\tau_2}\}} |\langle \boldsymbol{\tau_1} | S^z_{L/2} | \boldsymbol{\tau_2} \rangle|^2 \delta(\omega - E_{\boldsymbol{\tau_1}} + E_{\boldsymbol{\tau_2}})$

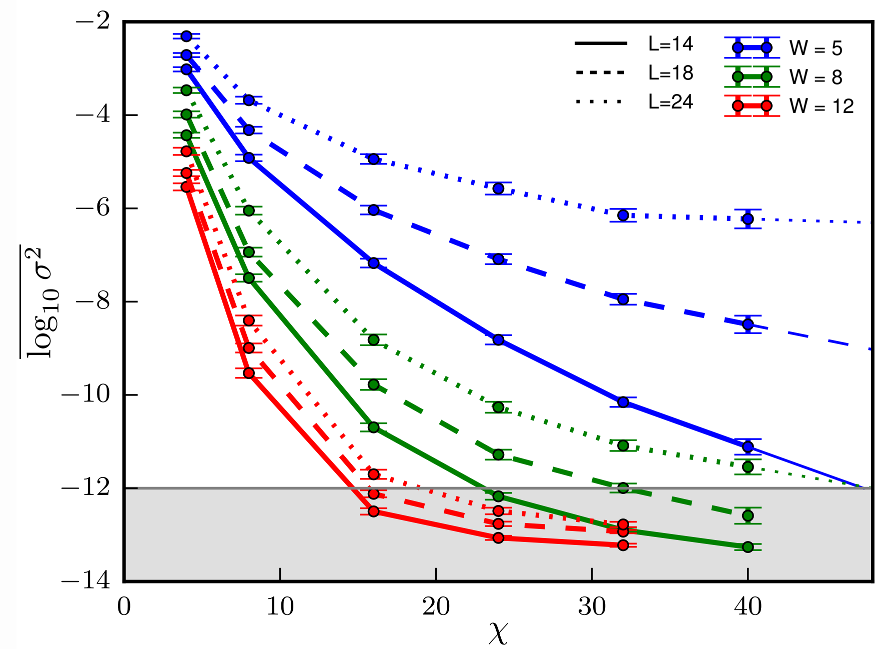



FP, Khemani, Cirac, Sondhi, arXiv:1506.07179

# Summary

(1) Obtaining individual highly excited eigenstates of MBL systems to machine precision accuracy:
**Matrix-product states**

Khemani, FP, Sondhi, arXiv:1509.00483




(2) Variational diagonalization of fully many-body localized Hamiltonians:
**Matrix-product operators**

FP, Khemani, Cirac, Sondhi, arxiv:1506.07179