

DMRG STUDY OF MANY-BODY LOCALIZATION

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Many-body localization

Many-body localization¹ (MBL) is a dynamical phase transition of an isolated quantum system with finite interaction and quenched disorder.

The signature of MBL is in the highly excited states.

Excited states' entanglement entropies go from volume law to area law.

$$H = - \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i h_i S_i^z, \quad h_i \in [-W, W]$$

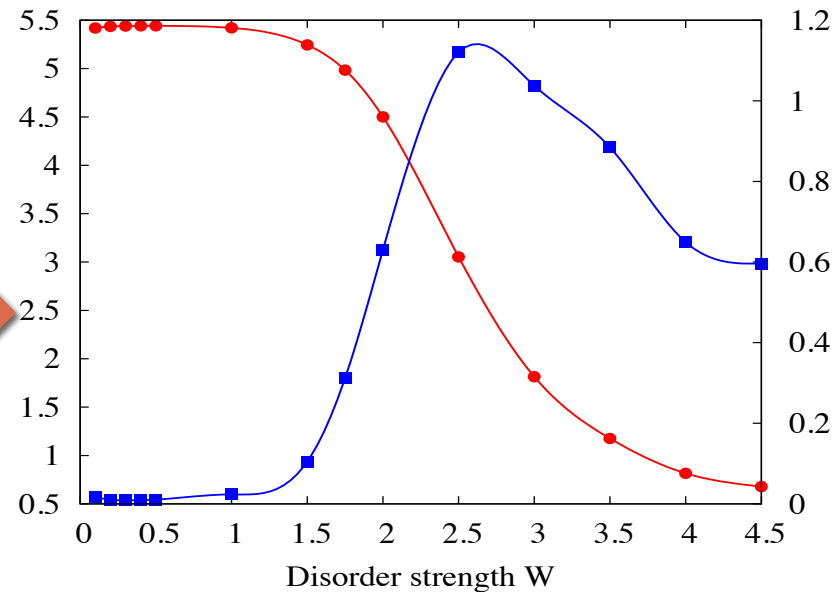
L = 16, exact diagonalization

of disorder realizations > 300

Excited states' energies near 0

Red: mid-bond entanglement entropy (EE)

Blue: standard deviation of mid-bond EE



1. Many good works have been done on this topic following the seminar paper by D. M. Basko, I. L. Aleiner, and B. L. Altshuler, Ann. Phys. 321, 1126 (2006).

To study MBL numerically

We need excited states, usually by doing

1. exact diagonalization (ED): shift-and-invert, ...
2. strong disorder renormalization group for excited states^{1,2}

Our goals:

1. adapt density matrix renormalization group (DMRG) to target excited states
2. produce good matrix product states (MPS), for larger system sizes and better scaling behavior, in the MBL phase (area law region)

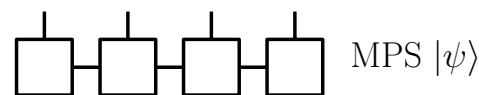
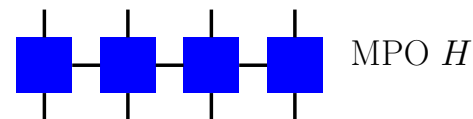
1. *Phys. Rev. X* 4, 011052 (2014), David Pekker, Gil Refael, Ehud Altman, Eugene Demler, and Vadim Oganesyan

2. *arXiv:1412.3117*, Ronen Vosk, David A. Huse, Ehud Altman

Brief introduction of DMRG

DMRG is

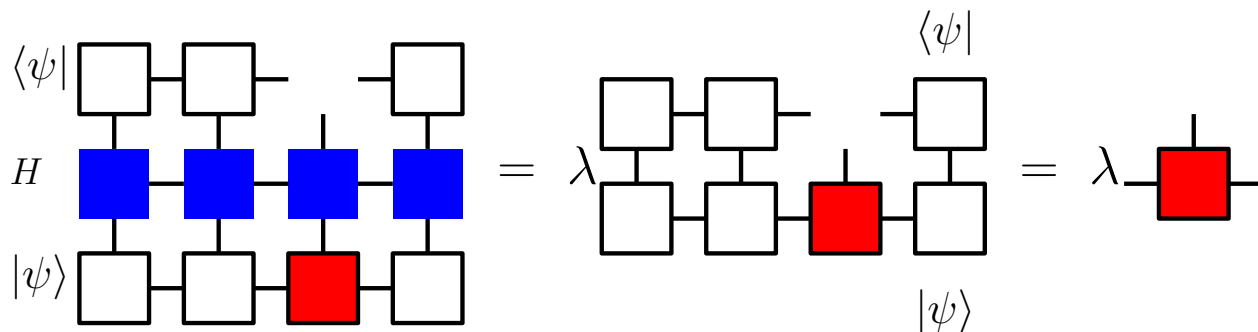
1. a variational ground state algorithm
2. natural in the matrix product state/operator (MPS/MPO) language



$$\frac{\partial}{\partial \psi_i^*} [\langle \psi | H | \psi \rangle - \lambda (\langle \psi | \psi \rangle - 1)] = 0 \quad \rightarrow \quad \frac{\partial}{\partial \psi_i^*} \langle \psi | H | \psi \rangle = \lambda \frac{\partial}{\partial \psi_i^*} \langle \psi | \psi \rangle$$



To optimize the red block, we solve an eigenvalue problem.



Two ways of adapting DMRG

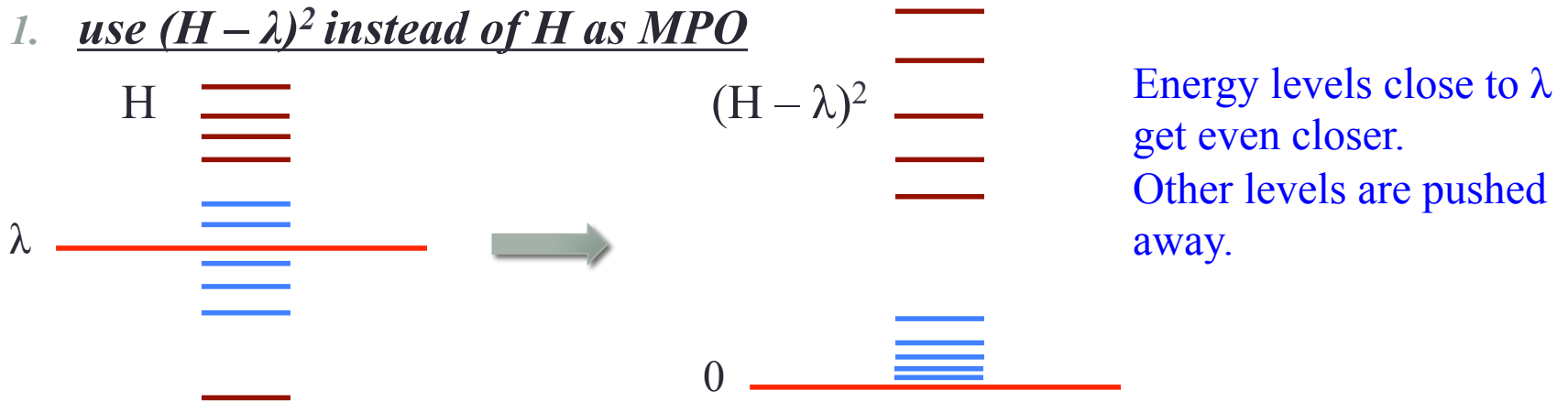
To get excited states whose energies are near λ , we can

1. use $(H - \lambda)^2$ instead of H as MPO
2. optimize MPS with respect to $(H - \lambda)^{-1}$ (like shift-and-invert in ED)

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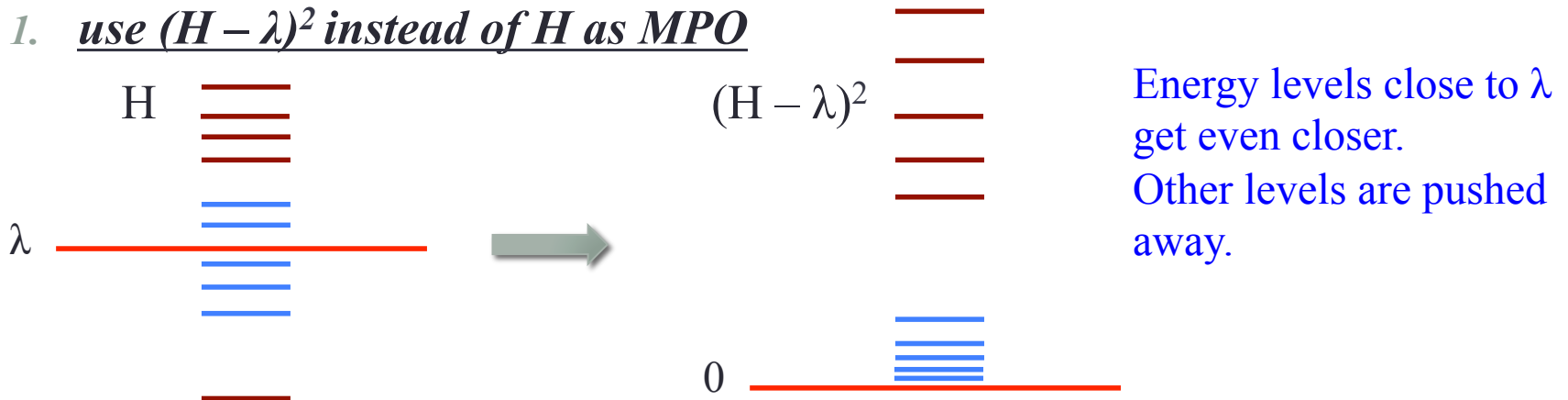


2. optimize MPS with respect to $(H - \lambda)^{-1}$ (like shift-and-invert in ED)

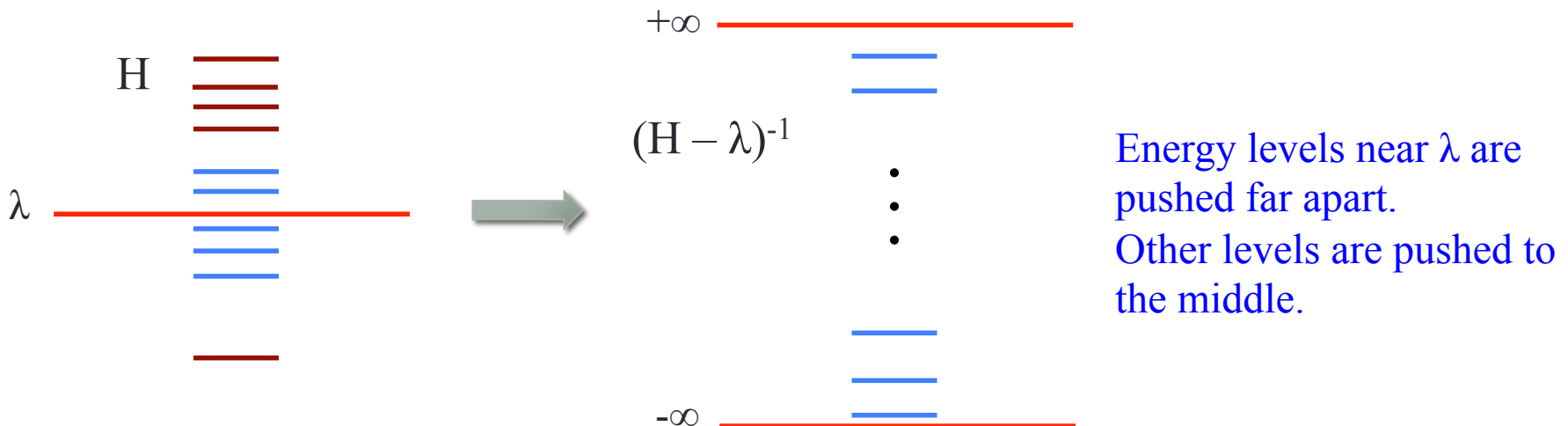
Two ways of adapting DMRG

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Difficulty of using $(H - \lambda)^2$ as MPO

As energy levels near λ cluster together, convergence speed will suffer.

To illustrate this problem, for $L=12$ spin $\frac{1}{2}$ Heisenberg model,

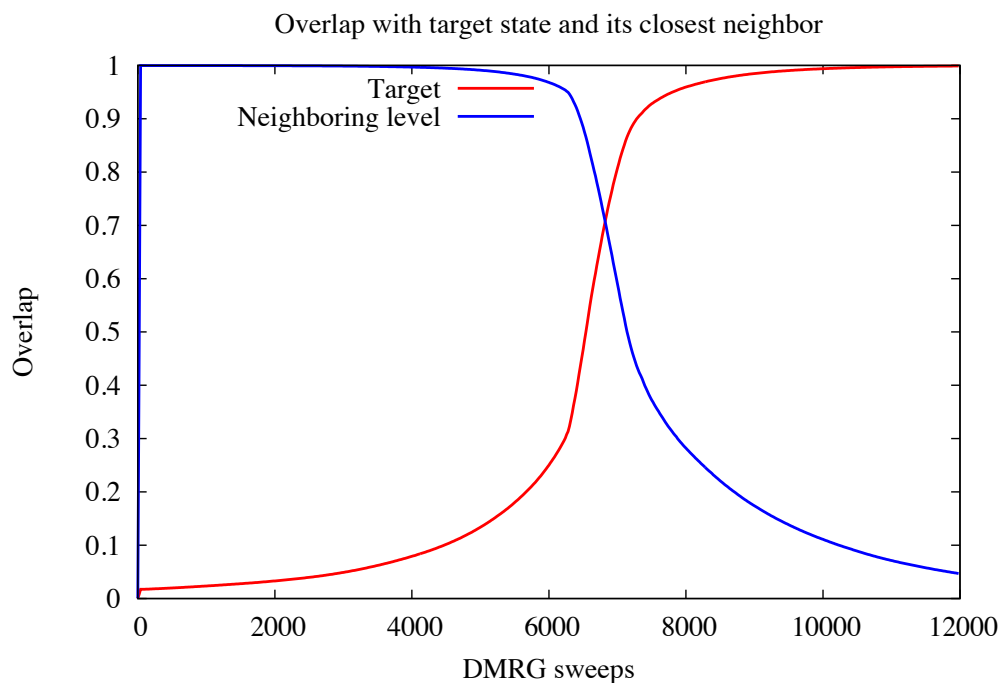
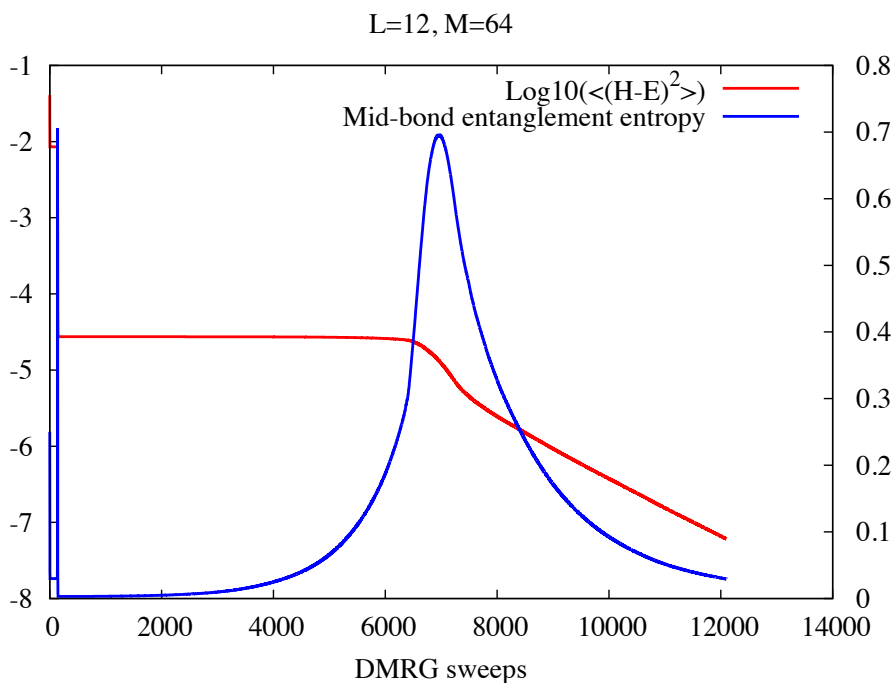
$$H = - \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i h_i S_i^z, \quad h_i \in [0.1 - W, 0.1 + W], \quad W = 5$$

1. We use ED to calculate all energy eigen values/states in advance.
2. Run DMRG with $(H-\lambda)^2$ as MPO. λ sits exactly on an excited state.
3. Check how close $\langle (H-\lambda)^2 \rangle$ is to zero.
4. Check the overlap of the MPS with ED eigenstates whose energies are near λ .

Difficulty of using $(H - \lambda)^2$ as MPO

Key observations:

1. MPS mixes the target state with its neighbor(s)
2. Mixing causes an “entanglement barrier” before convergence

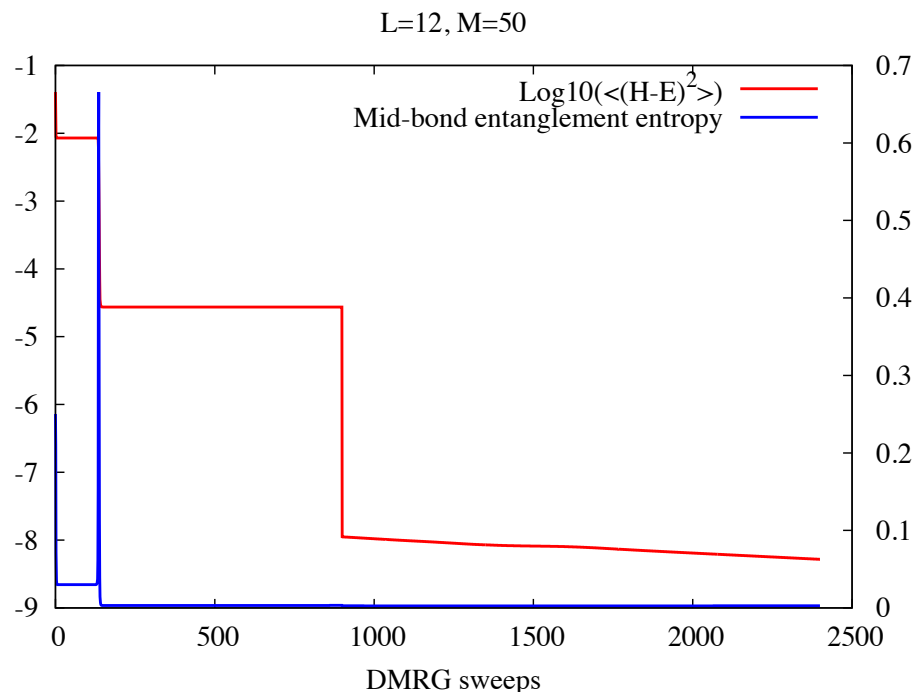


Technique to speed up convergence

During the slow convergence

1. the overlap of the MPS with the target state rises slowly from about 0
2. the overlap with neighbor(s) slowly decreases from about 1
3. subtracting the MPS stored N sweeps ago from the current one will “even up” the “weights” on the target and its neighbors

Subtract out the MPS stored
20 sweeps ago.
This kills the “entanglement
barrier”.



Optimize MPS with respect to $(H - \lambda)^{-1}$

We have implemented a DMRG-like method to construct MPSs that **maximize the magnitude** of $(H - \lambda)^{-1}$, just like shift-and-invert method in ED

As any matrix inverse problem, building $(H - \lambda)^{-1}$ as an MPO is hard

- large bond dimension
- lack of efficient algorithm

To apply $(H - \lambda)^{-1}$ to an MPS, say

$$|\varphi\rangle = (H - \lambda)^{-1}|\psi\rangle, \text{ for a given } |\psi\rangle$$

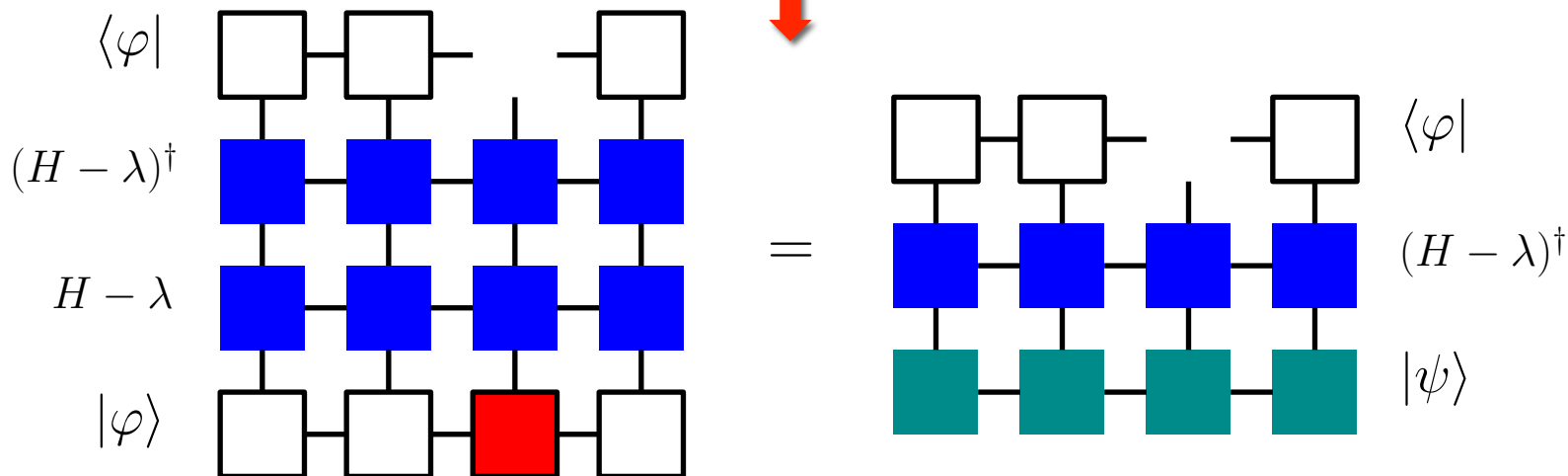
we can try minimize

$$|(H - \lambda)|\varphi\rangle - |\psi\rangle|^2$$

Optimize MPS with respect to $(H - \lambda)^{-1}$

$$\frac{\partial}{\partial \varphi_i^*} |(H - \lambda)|\varphi\rangle - |\psi\rangle|^2 = 0$$

$$\frac{\partial}{\partial \varphi_i^*} \langle \varphi | (H - \lambda)^\dagger (H - \lambda) | \varphi \rangle = \frac{\partial}{\partial \varphi_i^*} \langle \varphi | (H - \lambda)^\dagger | \psi \rangle$$

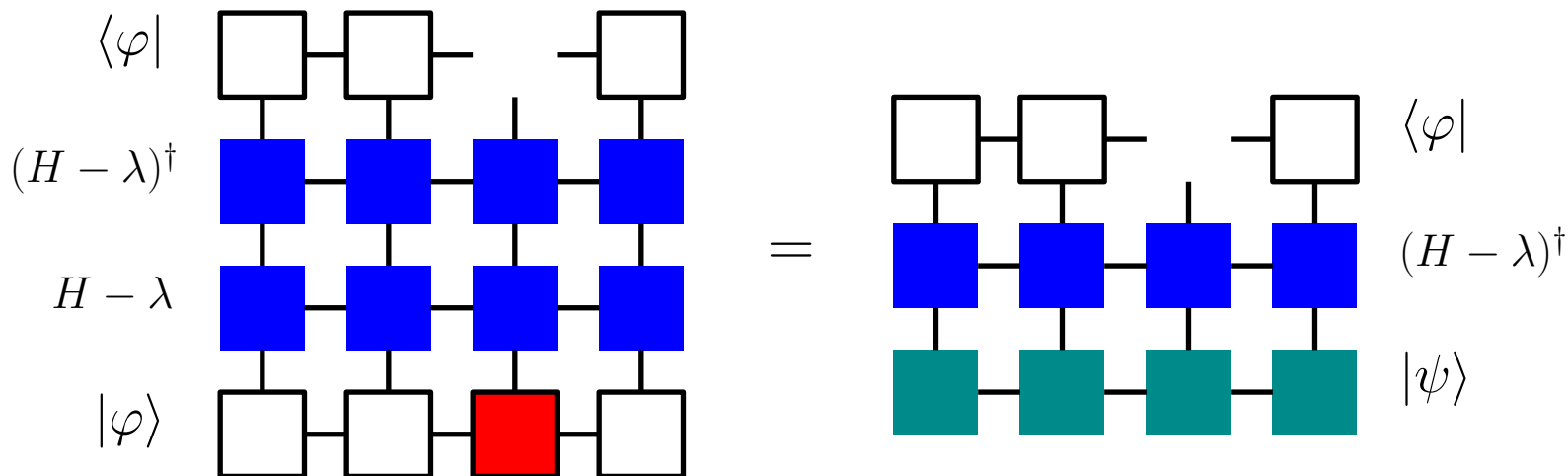


Optimize MPS with respect to $(H - \lambda)^{-1}$

At each step, we solve a *dense positive-definite linear equation problem*, instead of an eigenvalue problem, for the **red block**.

Swapping $|\varphi\rangle$ and $|\psi\rangle$ repeatedly is equivalent to *power method* with matrix $(H - \lambda)^{-1}$ in ED.

We call this inverse-DMRG method.



For best performance

Two methods can be combined:

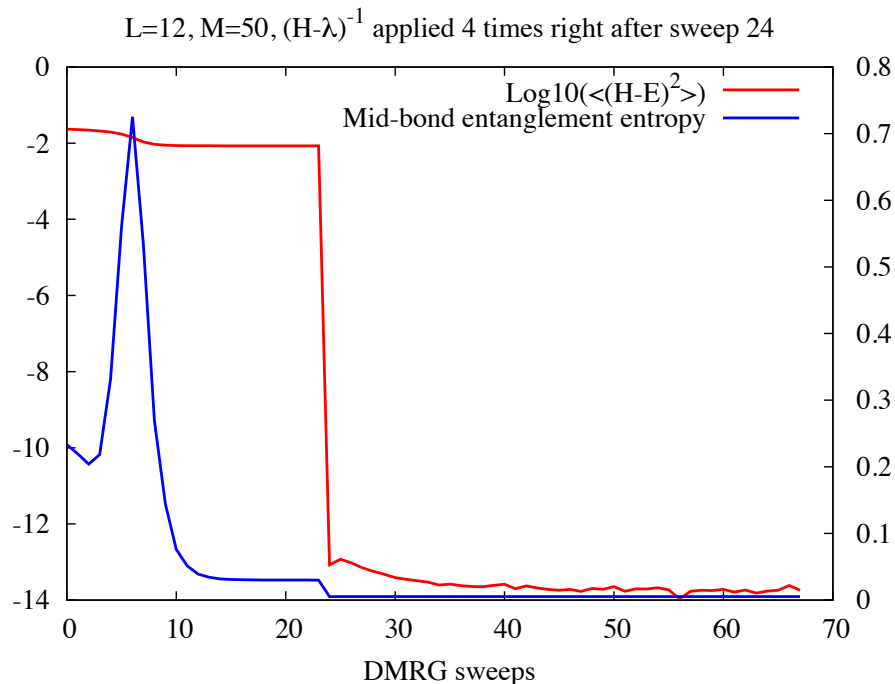
1. DMRG sweeping with $(H - \lambda)^2$ as the MPO quickly removes overlap with levels far away from λ
2. inverse-DMRG method then removes overlap with remaining states, except for the one closest to λ

Implementing conserved quantum number will give significant speedup

1. Dense linear equation solver's cost scales as (problem size)³
2. Problem size at each optimization step is pM^2 (M:bond dimension; p: number of physical degrees of freedom per site)
3. inverse-DMRG scales like p^3M^6

Fast convergence observed

Same $L=12$ Heisenberg model. DMRG sweeping with $(H - \lambda)^2$ as the MPO. inverse-DMRG method used 4 times after the initial 24 DMRG sweepings.



MBL Data using $(H - \lambda)^2$ as MPO

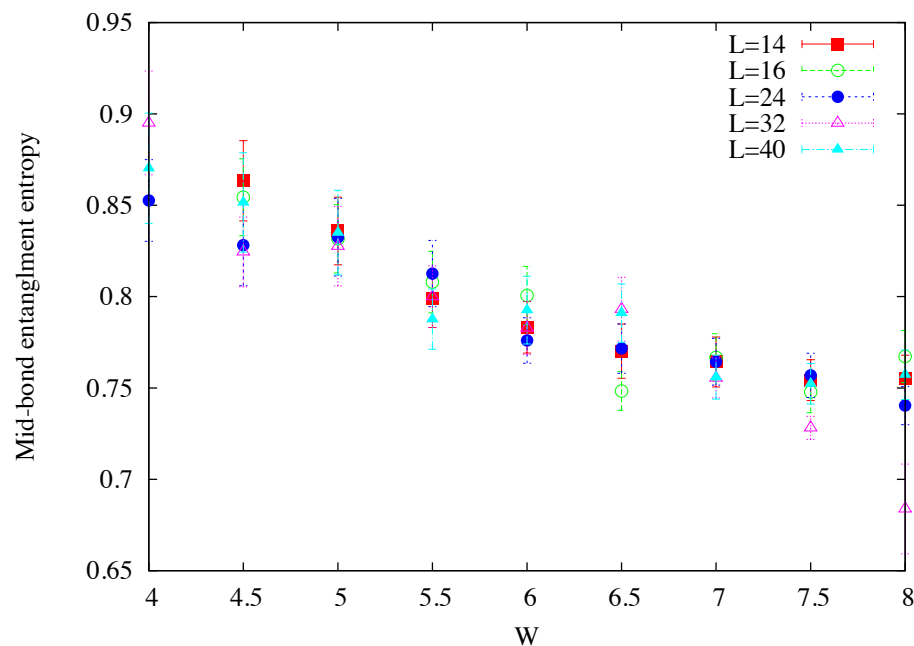
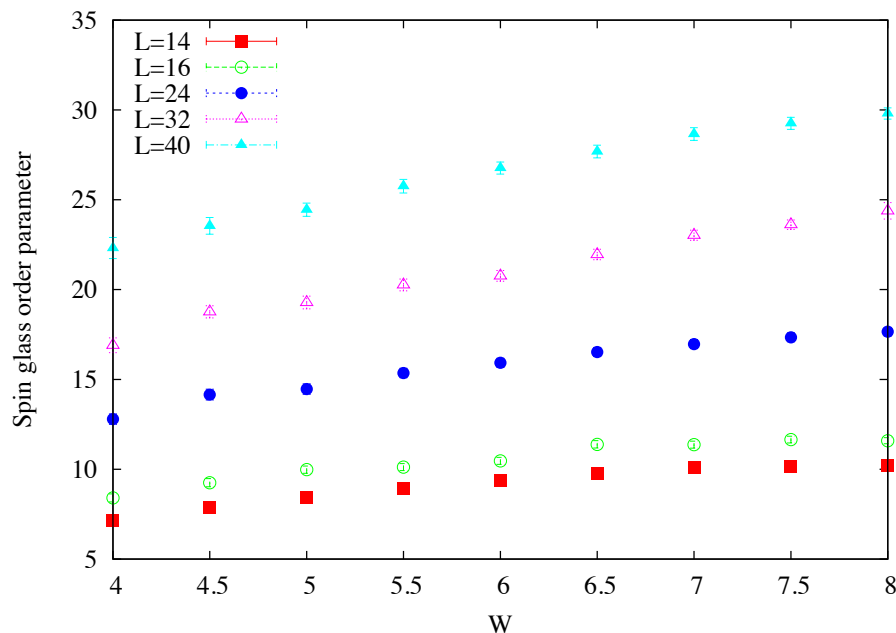
$$H = - \sum_i J_i \sigma_i^z \sigma_{i+1}^z + 0.3 \sum_i \sigma_i^z \sigma_{i+2}^z + 0.6 \sum_i \sigma_i^x, \quad J_i \in [1 - W, 1 + W]$$

- Disordered random transverse Ising chain with NNN interaction
- We have data of system sizes $L=14, 16, 24, 32, 40$
- For $L=14, 16, 24$, most MPSs produced have energy standard deviations below 10^{-5} (**estimation of inter-level spacing**).
- For $L=32, 40$, hard to get MPSs whose energy standard deviations are below 10^{-8} and 10^{-10} (**estimations of inter-level spacing**).

MBL Data using $(H - \lambda)^2$ as MPO

$$H = - \sum_i J_i \sigma_i^z \sigma_{i+1}^z + 0.3 \sum_i \sigma_i^z \sigma_{i+2}^z + 0.6 \sum_i \sigma_i^x, \quad J_i \in [1 - W, 1 + W]$$

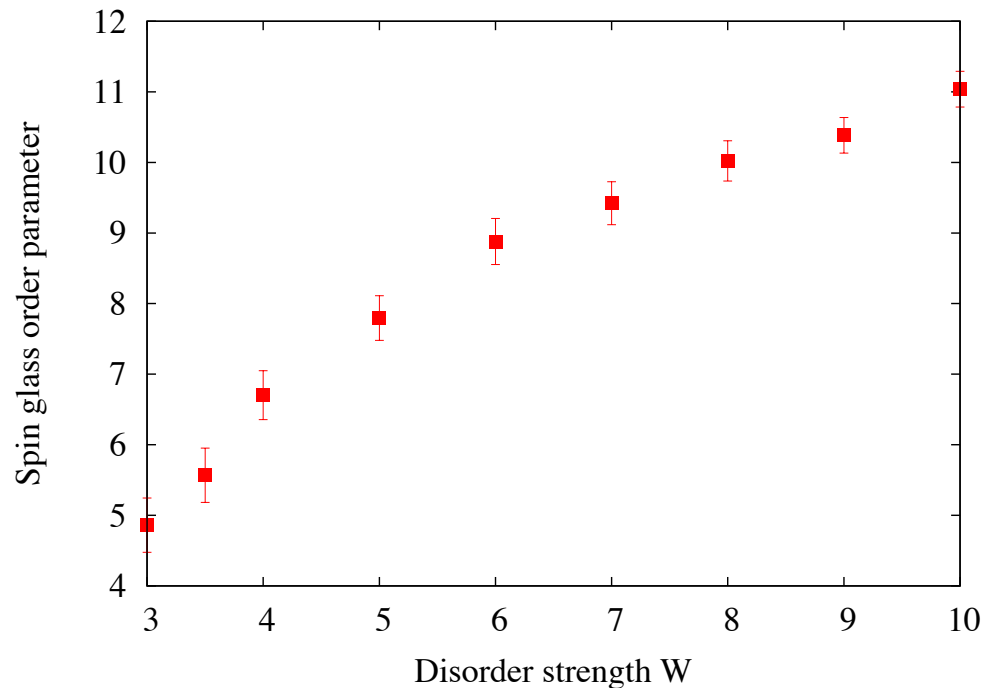
- All data points included here have energy standard deviations below 10^{-5}



MBL Data using inverse-DMRG

L=14 disordered random transverse Ising chain with NNN interaction.
Larger sizes computation under progress.

All data points included here have energy standard deviations below 10^{-5}



Conclusion and Future work

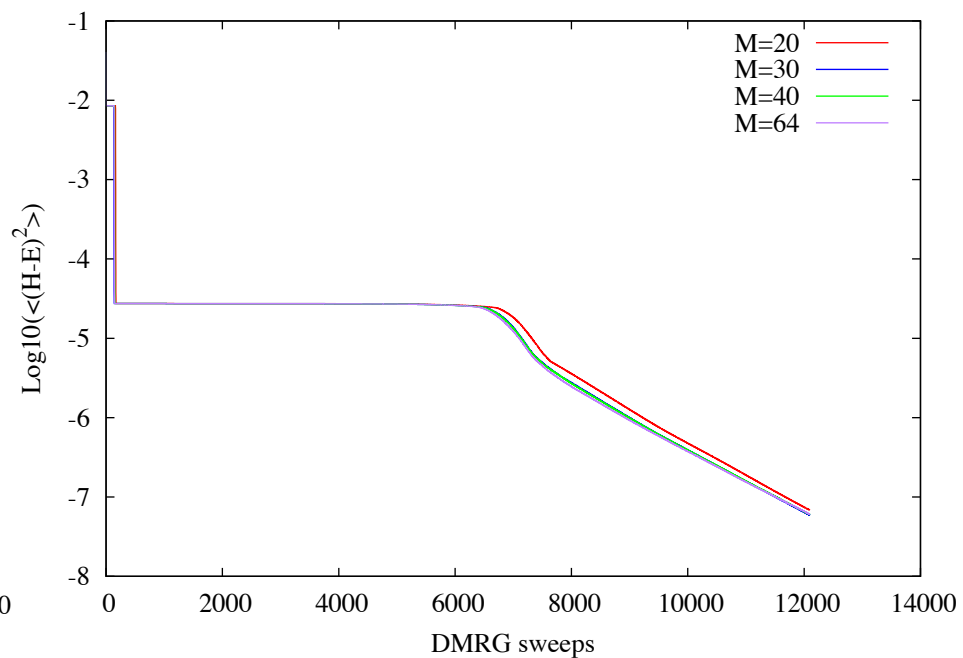
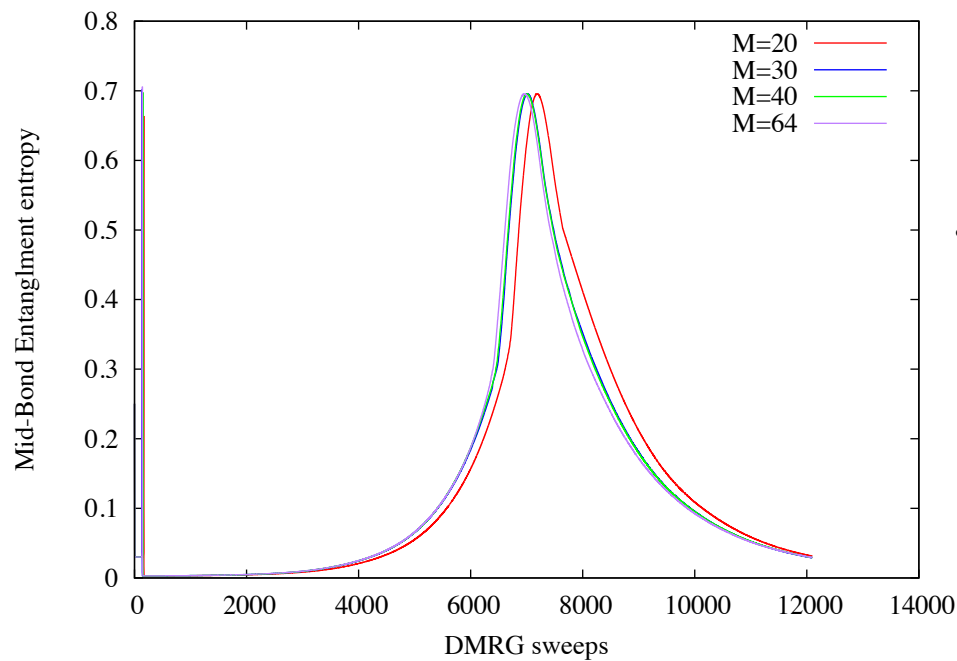
- DMRG sweeping with $(H - \lambda)^2$ tends to get stuck due to “entanglement barrier” when mixing multiple eigenstates
- Combining DMRG sweeping with $(H - \lambda)^2$ with inverse-DMRG has the best performance on targeting excited states

- Produce better scaling data describing physics in MBL phase
- Seek other usage of inverse-DMRG method, like adapting Arnoldi or Lanczos algorithm into MPS language

Thank you!

Difficulty of using $(H - \lambda)^2$ as MPO

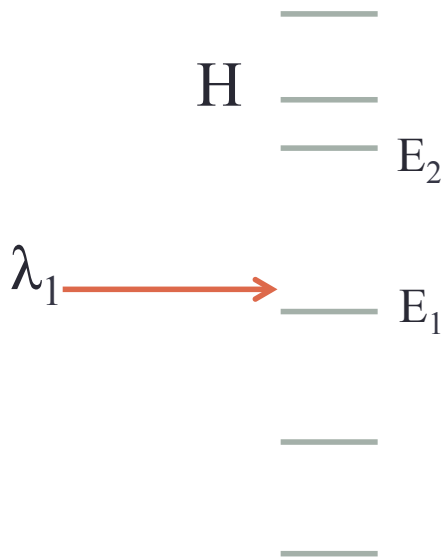
- Tuning bond dimensions does not change the behavior qualitatively



Difficulty of using $(H - \lambda)^2$ as MPO

Sweeping with $(H - \lambda)^2$ where λ does NOT sit exactly on an energy level calculated by ED in advance.

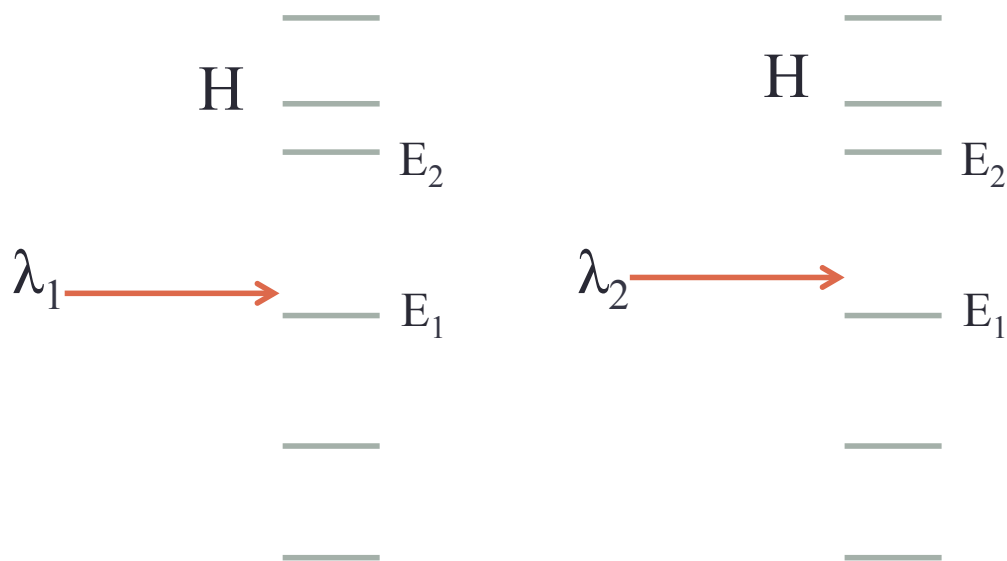
$$\lambda_1 = E_1 + 0.1 (E_2 - E_1)$$



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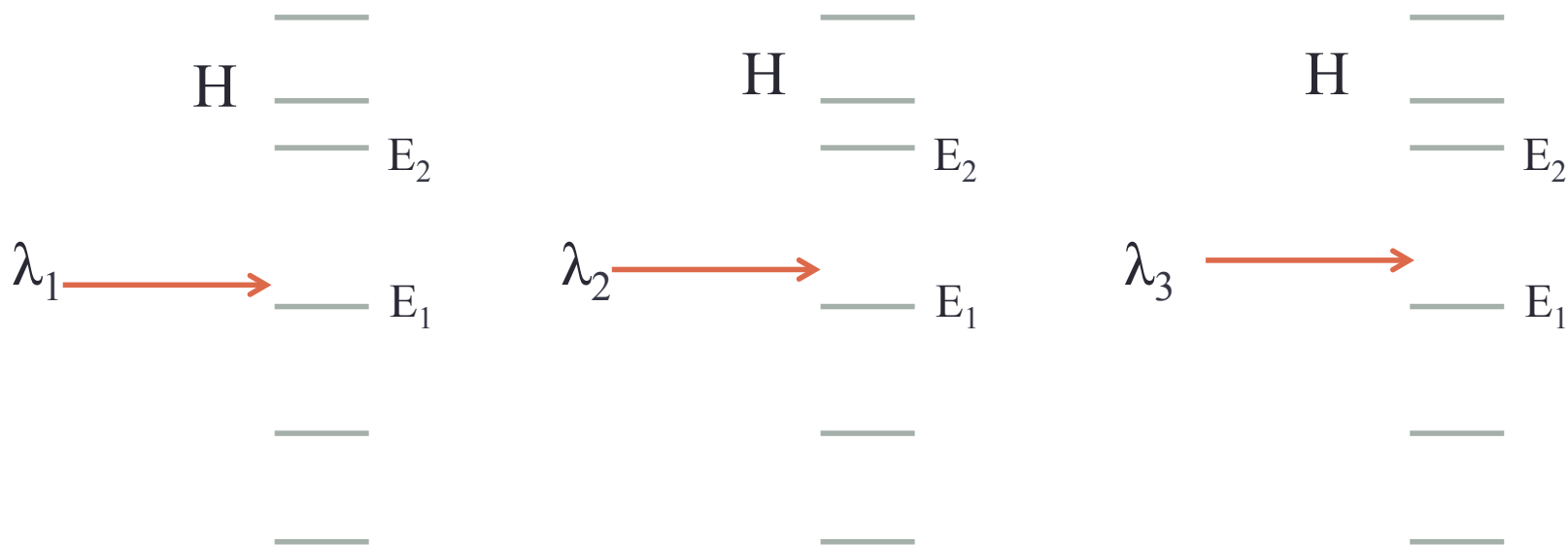
$$\lambda_1 = E_1 + 0.1 (E_2 - E_1), \quad \lambda_2 = E_1 + 0.2 (E_2 - E_1)$$



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Sweeping with $(H - \lambda)^2$ where λ does NOT sit exactly on an energy level calculated by ED in advance.

$$\lambda_1 = E_1 + 0.1 (E_2 - E_1), \quad \lambda_2 = E_1 + 0.2 (E_2 - E_1), \quad \lambda_3 = E_1 + 0.3 (E_2 - E_1)$$



Difficulty of using $(H - \lambda)^2$ as MPO

Sweeping with $(H - \lambda)^2$ where λ sits not exactly on an energy level calculated by ED in advance.

