A PANOPLY OF NEW (WAVE-FUNCTION BASED) METHODS

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Telluride Conference on Green's Function
August 3, 2016

Finite Temperature Methods

- Variational Finite Temperature
- Finite Temperature FCIQMC
- + attenuating the sign problem (SEMPS; SEWF +)

Excitation Methods (including the ground state)

- A constructive MERA

- SIMPS
- ES-DMRG
- ES-VMC

Goal: Given a Hamiltonian, approximately compute finite temperature properties.

VAFT: Variational Finite Temperature

Other Finite Temperature Approaches:

Path Integral Monte Carlo

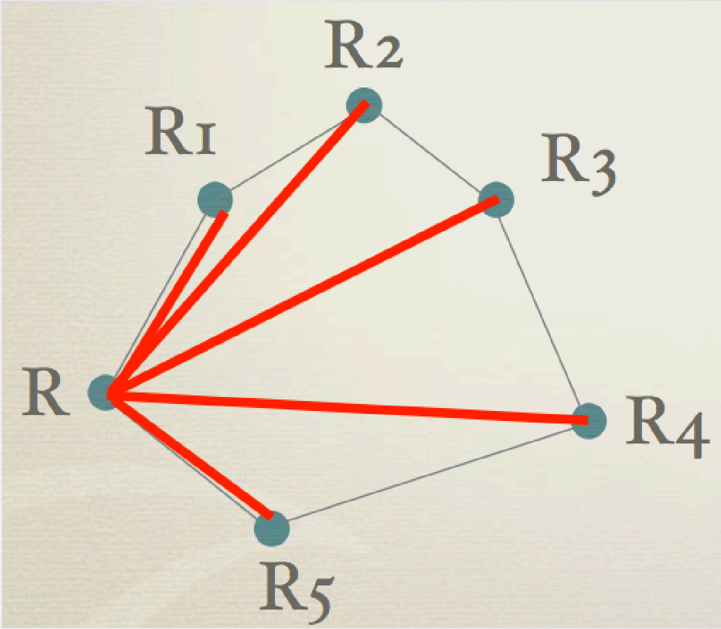
DMRG (METTS/ imaginary time MPO)

Variational Density Matrix

Path Integral Monte Carlo

$$\rho(R,R;\beta) = \rho(R,R_1\beta/n)\underline{\rho(R_1,R_2;\beta/n)}\rho(R_2,R_3;\beta/n)...\rho(R_{n-1},R;\beta/n)$$

Could be negative - Sign Problem



Write low temperature density matrix as convolution of high temperature density matrix.

Fixed node approach: Need a finite temperature density matrix at all $0 \leq \tau \leq \beta$

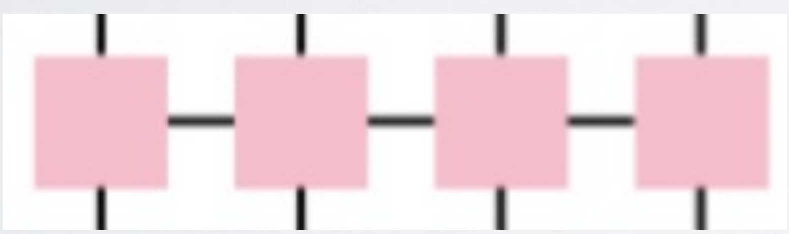
Problem: Sign problem

DMRG approaches

METTS

- Pick R
- Time evolve with MPS to beta/2
- Iterate

Imaginary time evolve MPO



Problem: Stuck in one dimension

Variational Density Matrix

Write out a bunch of density matrices with some parameters

$$\rho(\beta; \vec{\alpha})$$

Choose the parameters $\vec{\alpha}$ with lower free energy?

Problem: How do I write down variational density matrices.

How do I compute their free energy.

Wave-Functions for Finite Temperature (waft)

Path Integral Monte Carlo

Two slices of path integrals.

$$\langle R| \exp[-\beta H/2]|R'\rangle\langle R'| \exp[-\beta H/2]|R\rangle$$

No sign problem..

Just need to get our hands on this many-body density matrix.

METTS (DMRG)

Just do METTS with arbitrary wave-functions (PEPS, Slater-Jastrow, etc.)

Variational Density Matrix

Instead of explicitly writing out the density matrix, let's just sample a purification

WAFT

Input: Variational Manifold of wave-functions

Output: Approximate samples from the many-body density matrix.

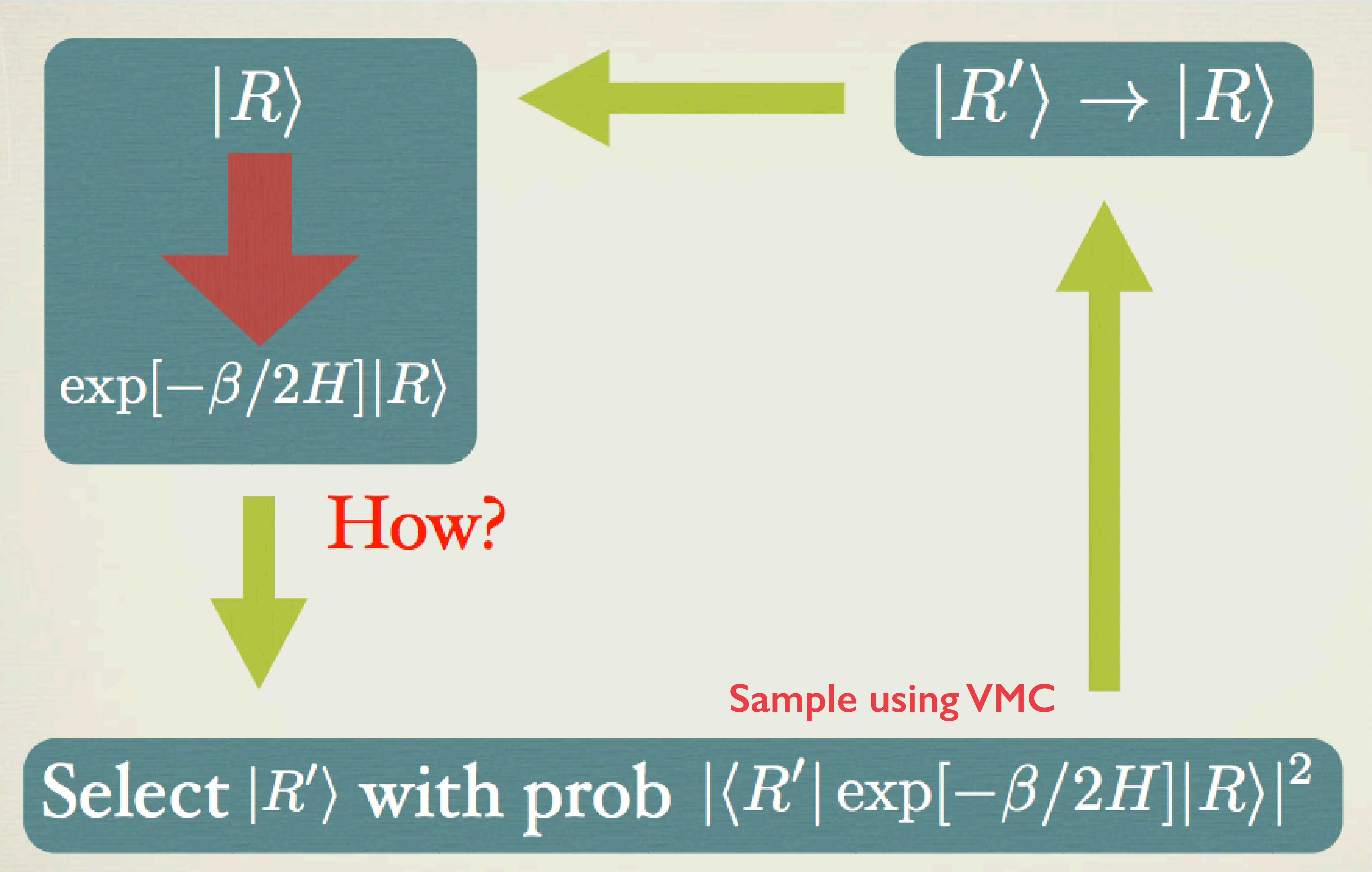
High level approach:

Write down a Markov chain (*not metropolis)* which samples configurations from the many body density matrix.

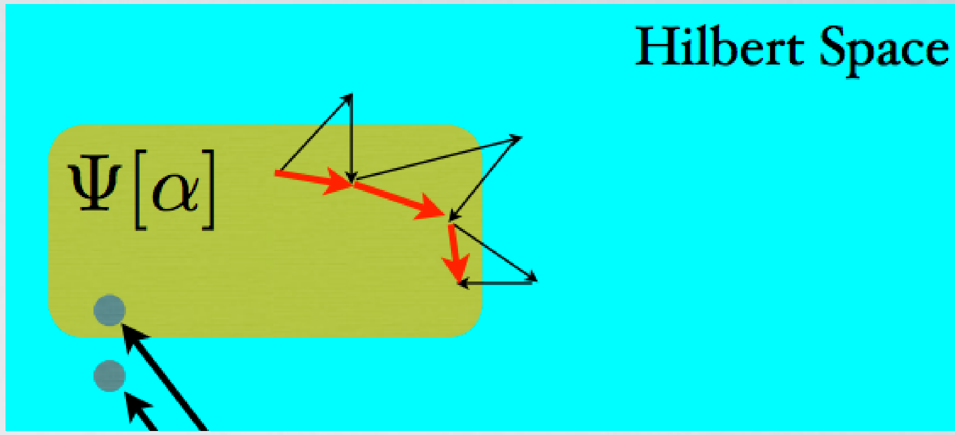
Discover you can't do the Markov chain.

Write down a new Markov chain which hopefully has a stationary distribution close to the actual one.

A Markov chain whose fixed point probability distribution is the diagonal of the finite temperature many-body density matrix.



Imaginary time evolution of arbitrary variational wave-functions



High level approach

$$\exp[-\tau H]\exp[-\tau H]\exp[-\tau H]|R\rangle$$

$$P\exp[-\tau H]P\exp[-\tau H]P\exp[-\tau H]|R\rangle$$

Low level approach: Stochastic reconfiguration

Schrodinger equation in the tangent space of local variational subspace.

Tangent space of $\Psi[\vec{\alpha}]$: $\partial\psi[\vec{\alpha}]/\partial\alpha_0, \partial\psi[\vec{\alpha}]/\partial\alpha_1, \partial\psi[\vec{\alpha}]/\partial\alpha_2, \ldots$

$$H_{ij} \equiv \langle\partial\psi[\alpha_i]|\hat{H}|\partial\psi[\alpha_j]\rangle$$ → Run VMC on $|\Psi[\alpha]\rangle$

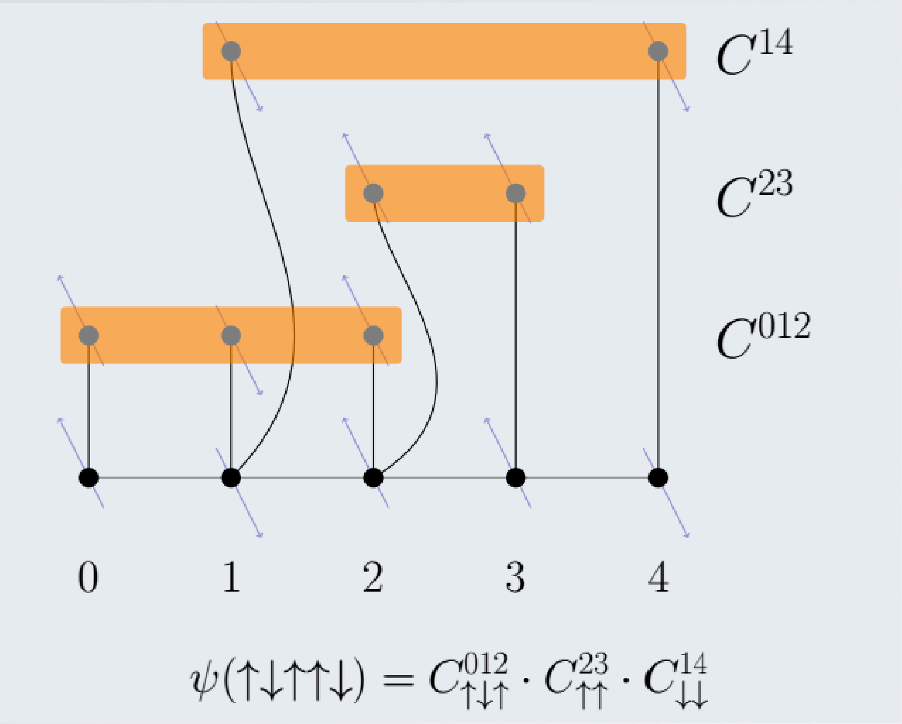
$$S_{ij} \equiv \langle\partial\psi[\alpha_i]|\partial\psi[\alpha_j]\rangle$$ Measure H and S

$$(1-\tau H S^{-1})|\Psi[\alpha]\rangle$$

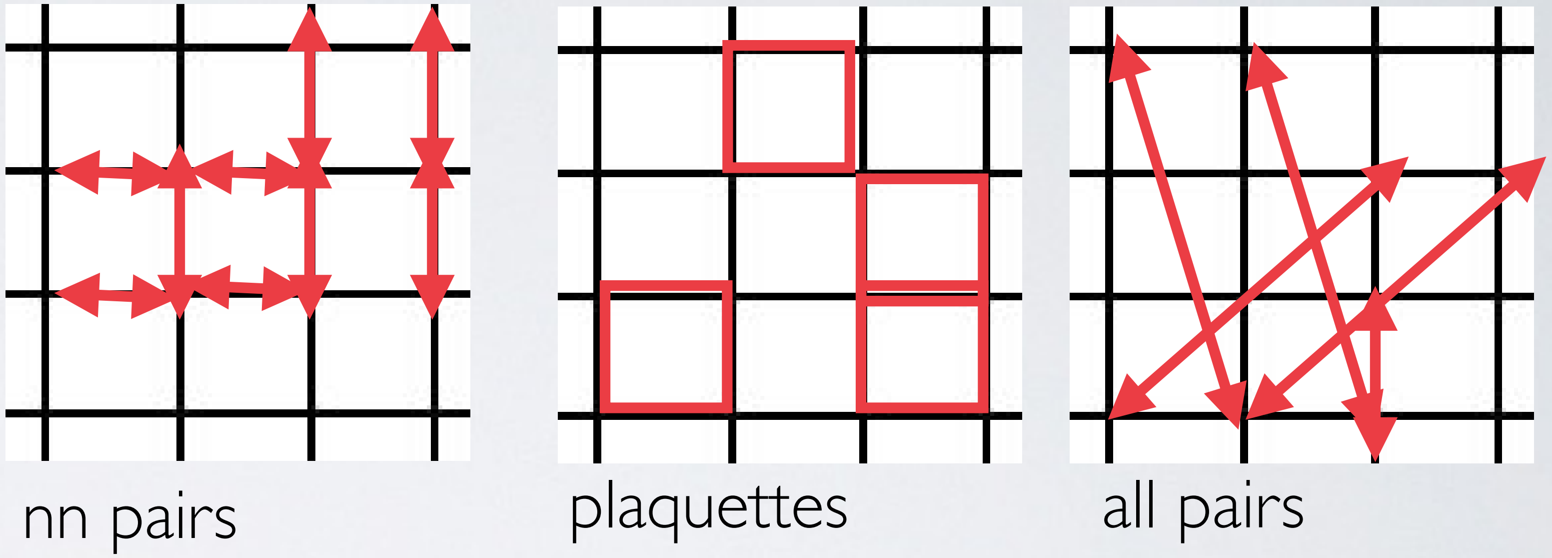
Variational Manifold → Variational Density Matrix

A prototypical variational wave-function:

Huse-Elser States (aka correlated product states, entangled plaquette states, graph tensor networks states, …)



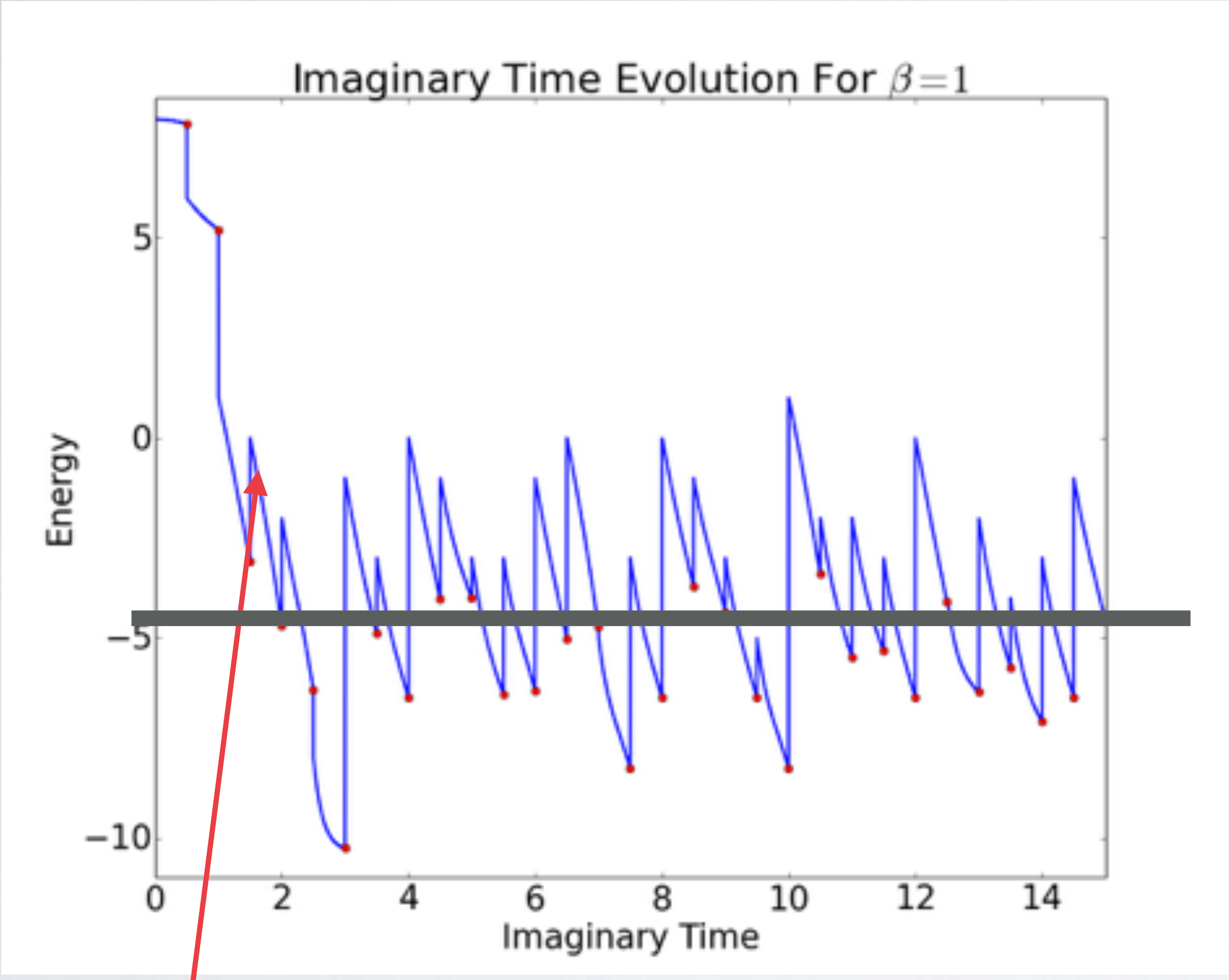
Can choose different patterns.



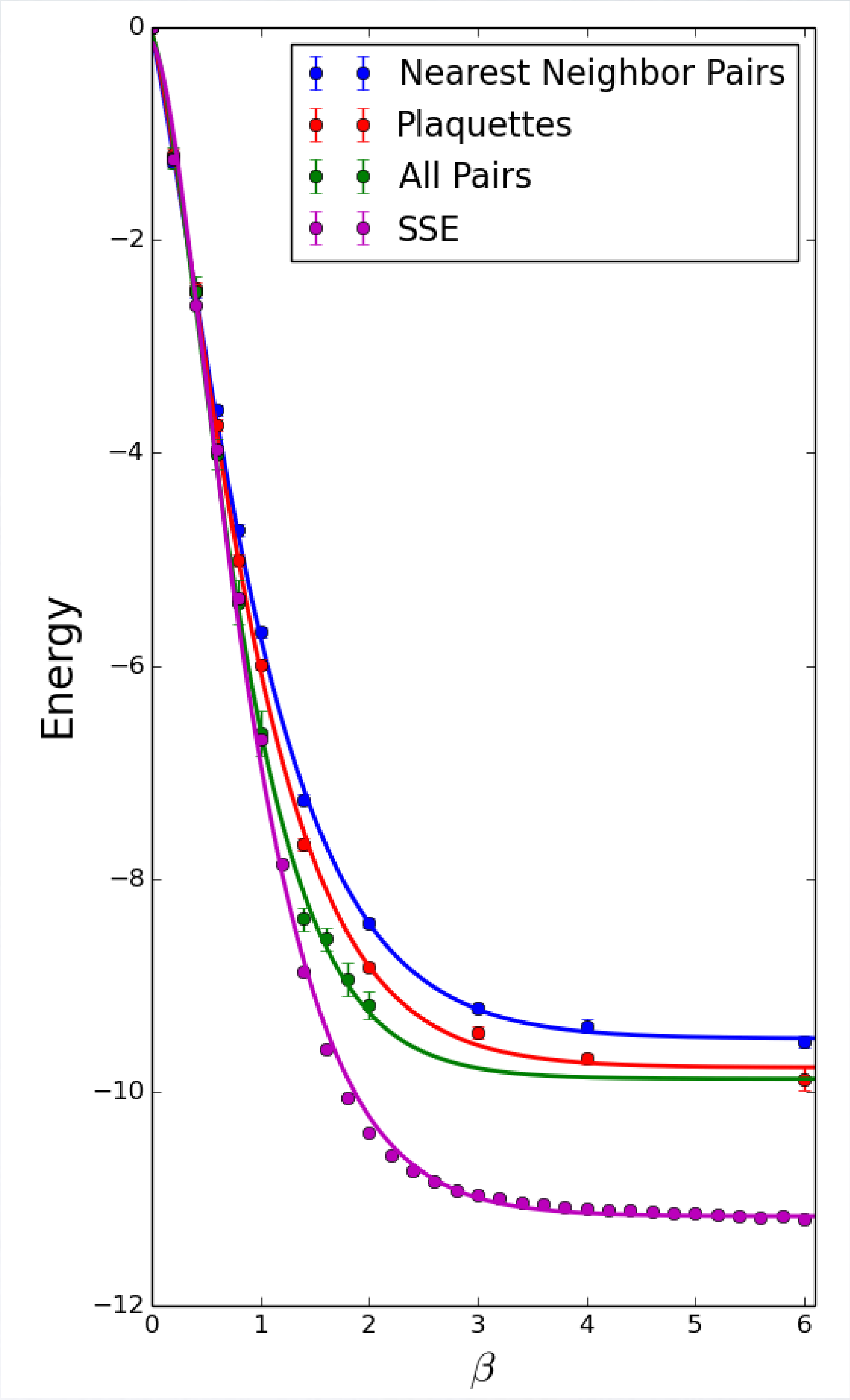
A prototypical Hamiltonian: **Heisenberg Model**

$$H = \sum_{\langle ij \rangle} \sigma_i \cdot \sigma_j$$

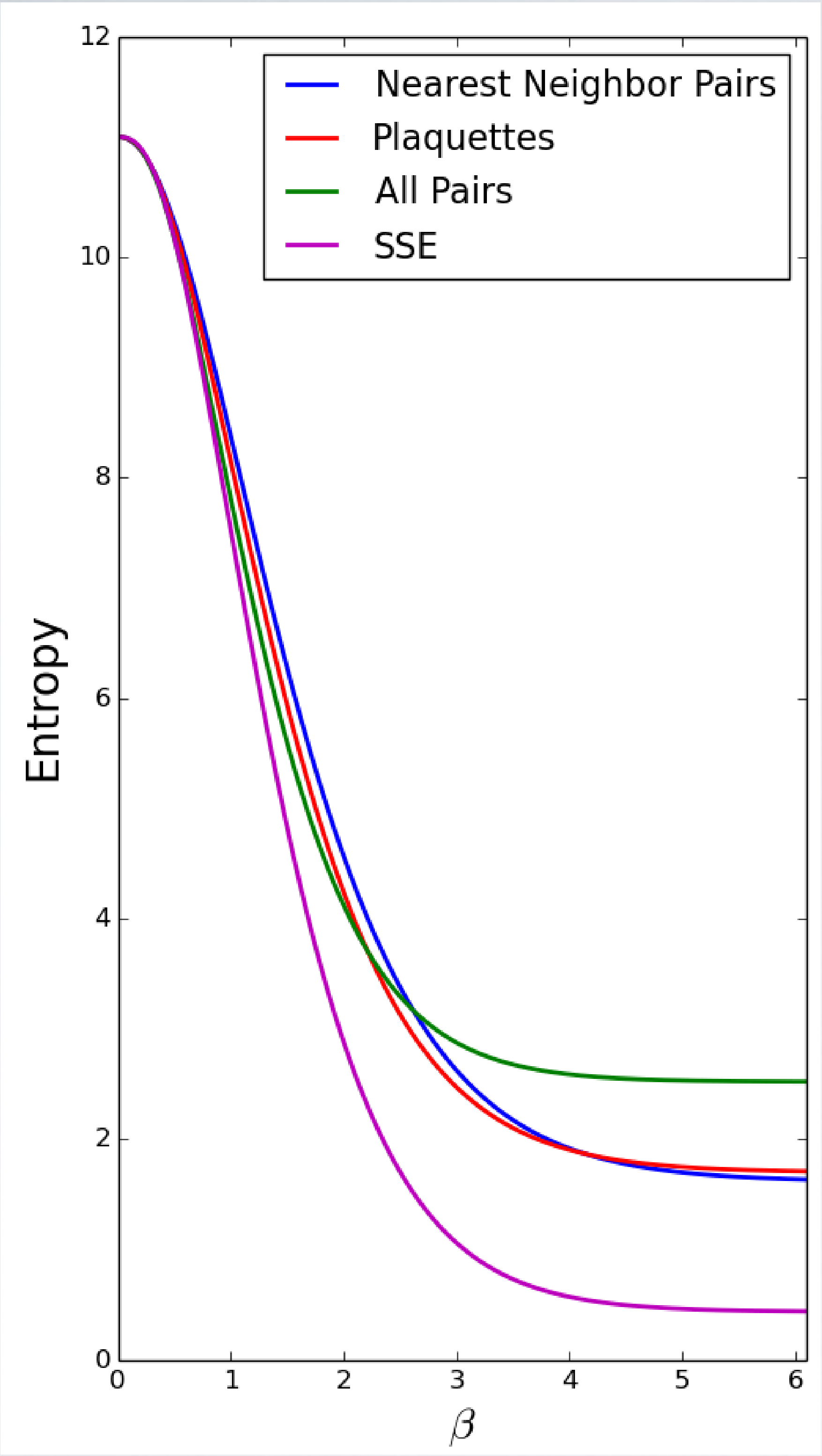
On a bipartite lattice can do exactly with SSE to compare new method against.

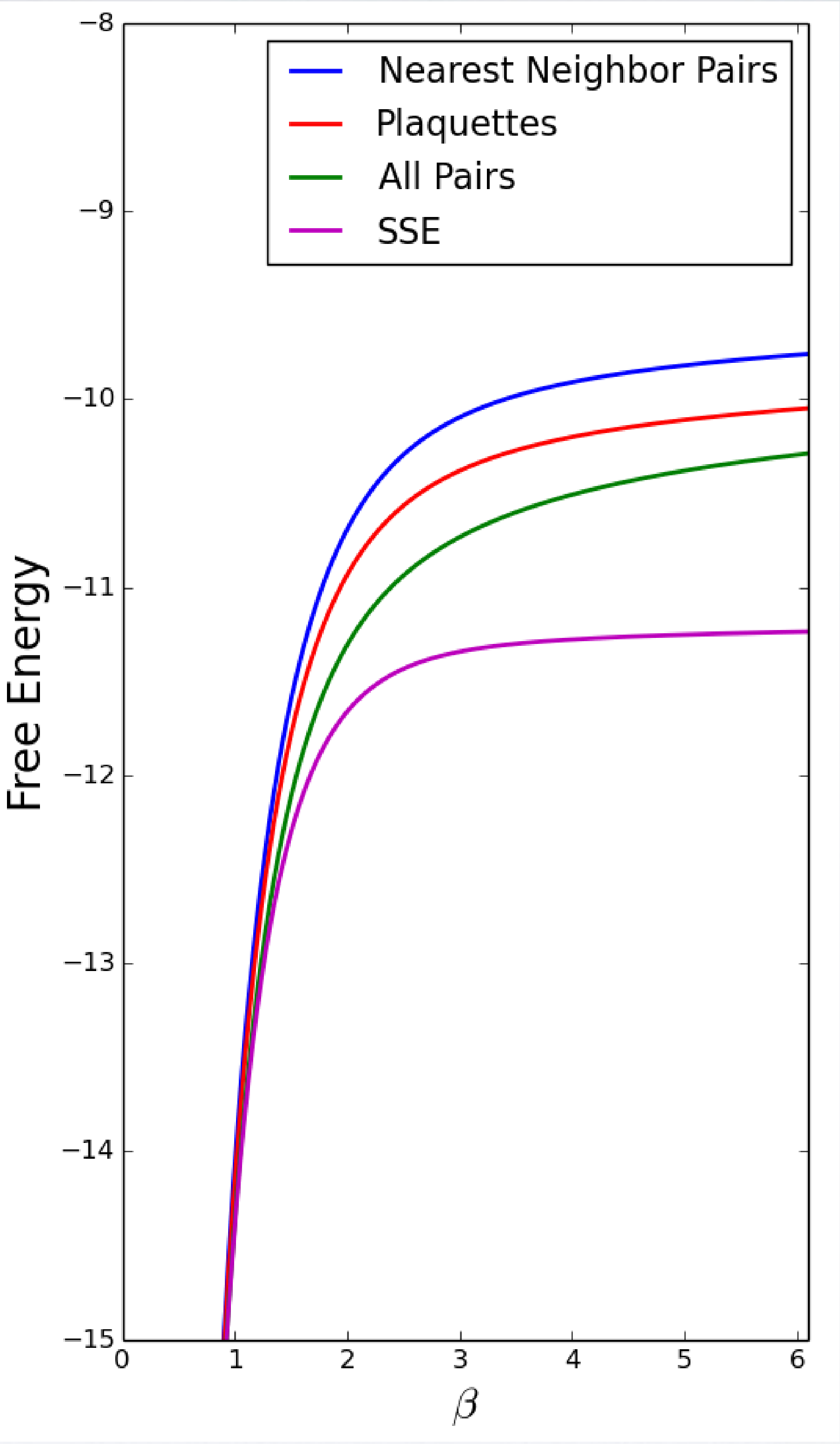


New product state



4 x 4 bipartite Heisenberg



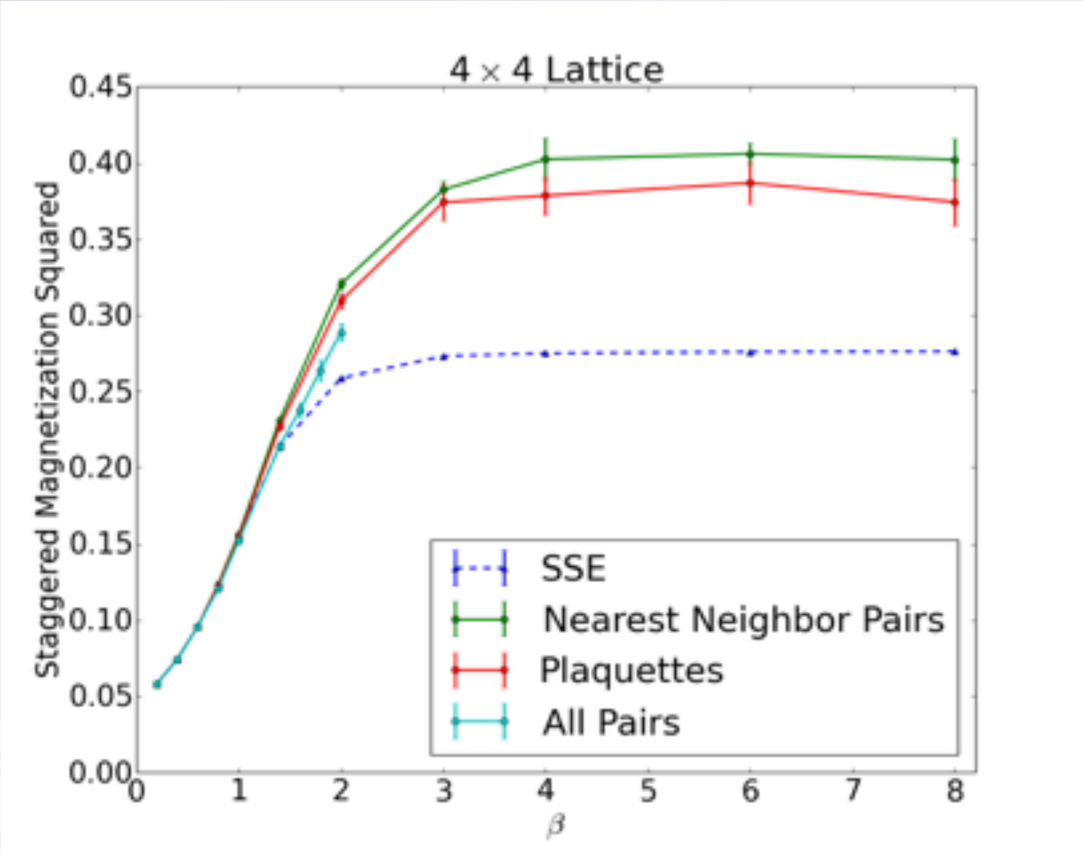


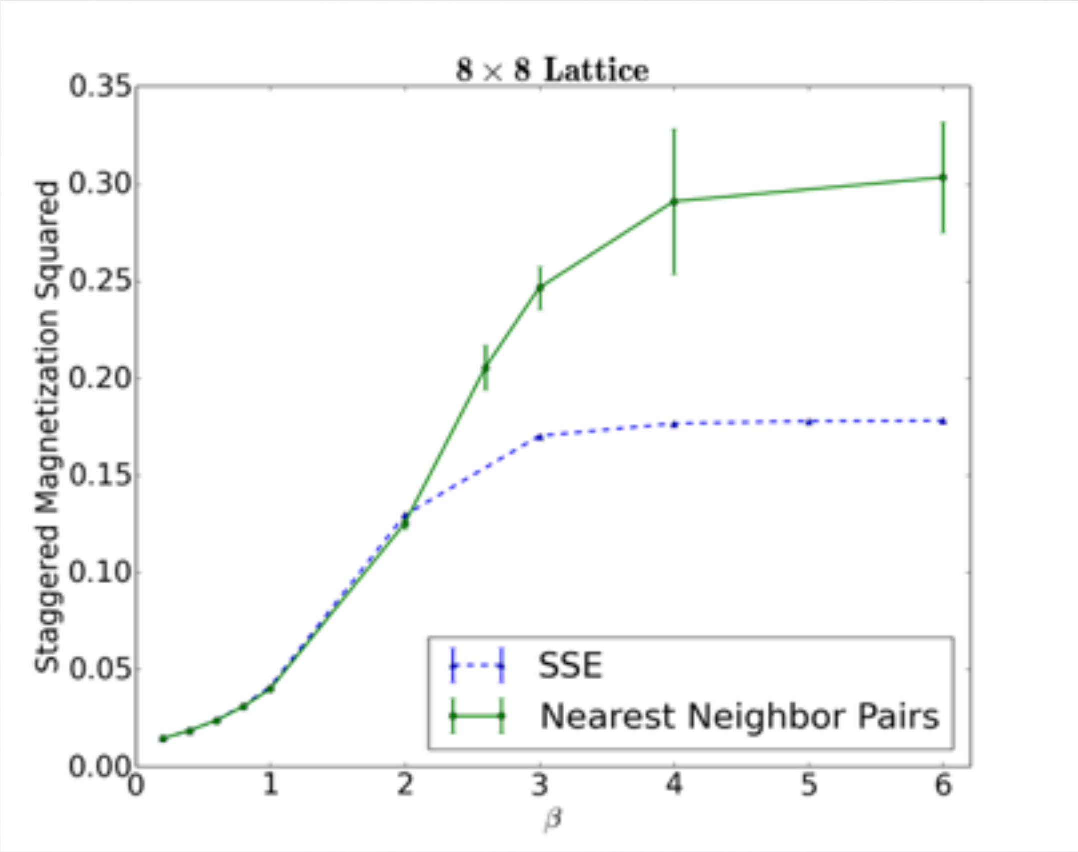
via thermodynamic integration

Free energy variational principle (tells you which variational manifolds are 'better')

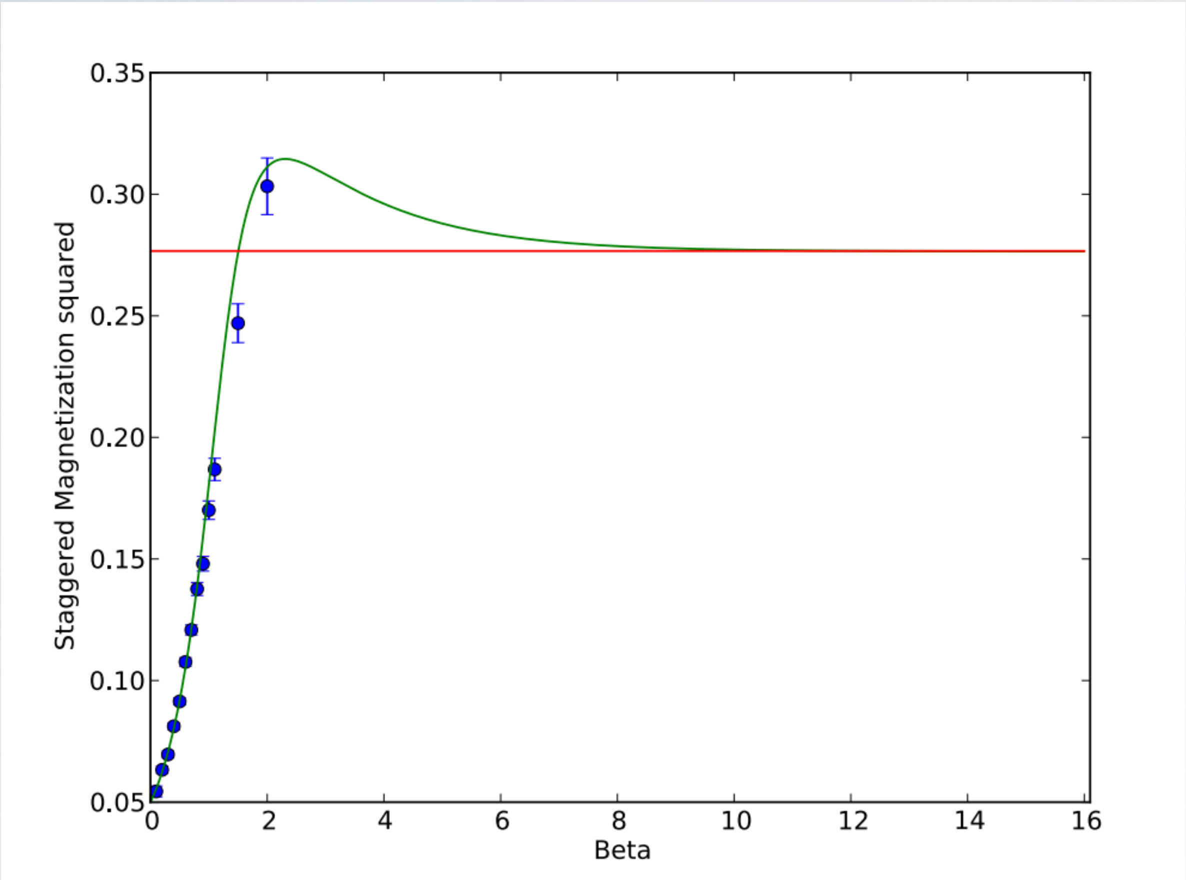
Can compute arbitrary properties of the "variational density matrix."

Here is the staggered magnetization





We have versions of this with projector Monte Carlo
(sign problem but you can beat it down with FCIQMC)



Also developing fixed-phase AFQMC version

Some other extensions coming:

- Can use as the variational density matrix for PIMC
- (Should) solve ergodicity problem with PIMC
- Applications to Hubbard, etc.
- Finite Temperature quantum chemistry

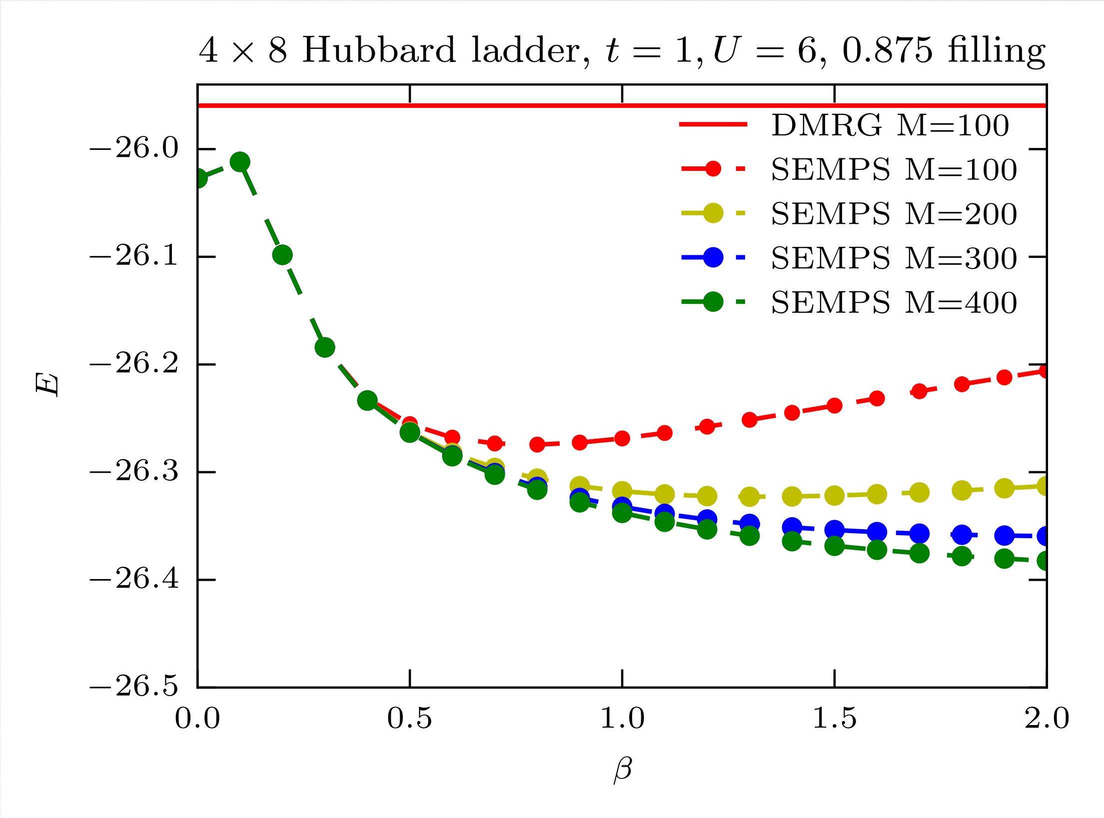
SEMPS: Stochastically evolved matrix-product states.   SEWF: Stochastically evolved wave-functions

To get the ground state, need to do $\exp[-\beta H]|\Psi_T\rangle \equiv \rho(\beta)|\Psi_T\rangle$

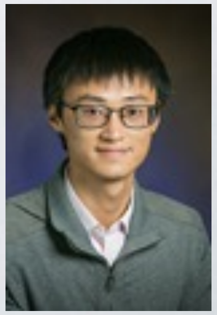
But we already know how to build $\rho(\beta \approx 1)$ which is essentially exact.

(Almost all the) steps:

1. Sample product states R from $|\langle\Psi_T|R\rangle|$ with weights $w = \text{sign}(\langle\Psi_T|R\rangle)$
2. Apply $\exp[-\beta H]|R\rangle$ **variationally**.
3. Sample R' from $\langle R'|\exp[-\beta H]|R\rangle$
4. Measure

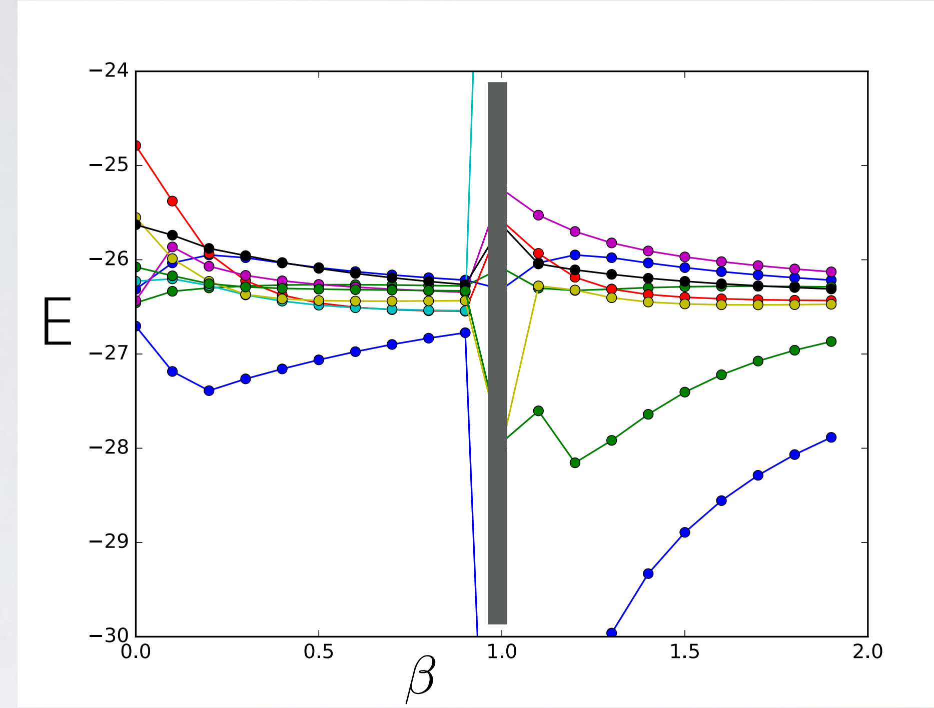


This will even work with a trial wave-function stochastically generated from fixed-node.



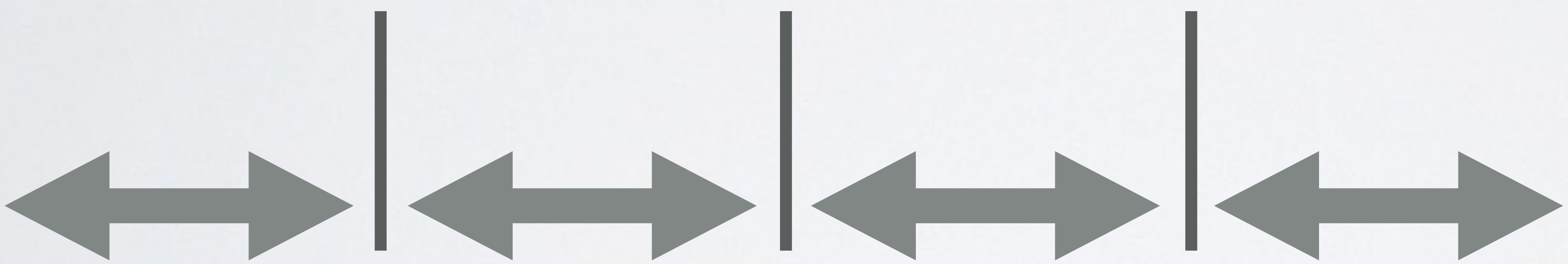
Also can replace variational with projector QMC (FCIQMC, AFQMC, PIMC, etc.)

(~~Almost~~ all the) steps:



1. Sample product states R from with weights $w = \text{sign}(\langle \Psi_T | R \rangle)$
2. Apply $\exp[-\beta H] | R \rangle$ **variationally**.
3. Sample R' from $\langle R' | \exp[-\beta H] | R \rangle$
4. R ⟵ R'; Go back to step 2.
5. Measure (occasionally)

This gives quantum Monte Carlo with large times steps. $\beta \sim 1$

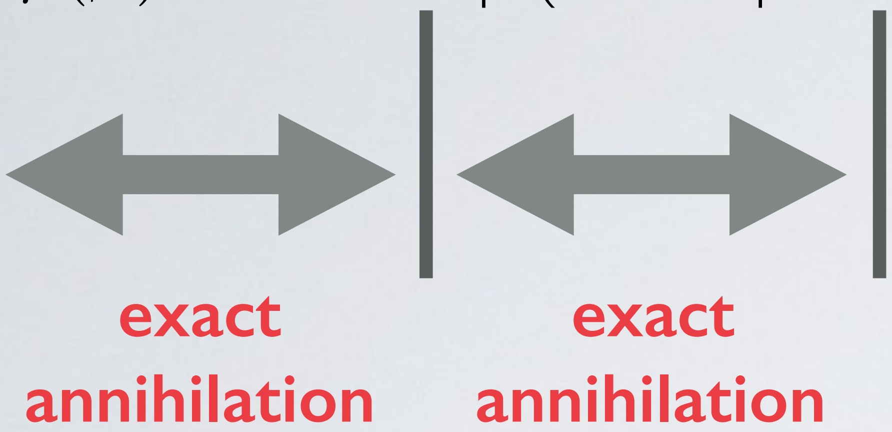


exact annihilation **exact annihilation** **exact annihilation** **exact annihilation**

Removes all sign-incoherent paths which start from R and go beta of 1.
Technical detail: Can Removes all sign-incoherent paths which start from many R's and go beta of 1
Attenuates the sign problem…

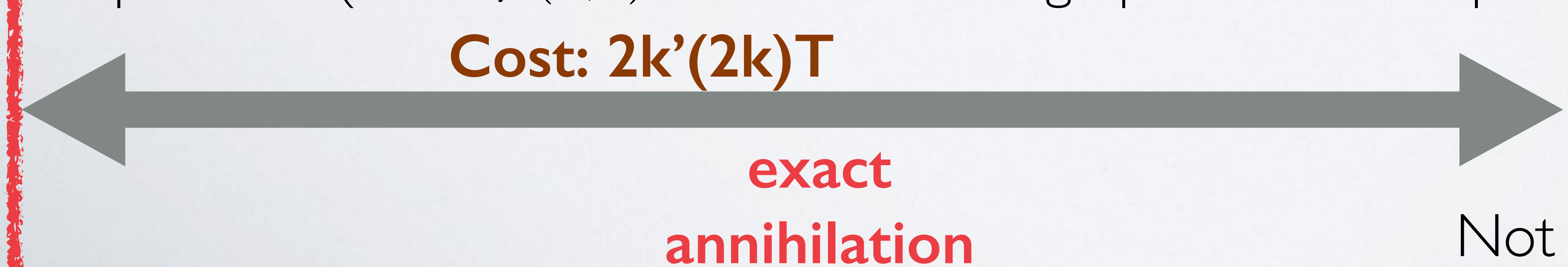
Technically this can be iterated (not variational though; pimc) (both for ground state and finite T)

$\rho(\beta)$ for one step (from a product state) is 'exact.' Takes time T



$\rho(2\beta)$ for two steps (from a product state) can be 'exact' by sampling all R' from $\rho(R,R';\beta)\rho(R',R'';\beta)$ by taking enough samples k to beat down the sign problem (recall $\rho(\beta)$ exact with no sign problem from product state.)

$\rho(2(2\beta))$ for two steps (from a product state) can be 'exact' by sampling all R' from $\rho(R,R';(2\beta))\rho(R',R'';(2\beta))$ by taking enough samples k' to beat down the sign problem (recall $\rho(2\beta)$ exact with no sign problem from product state.)



Not clear how much this saves you.

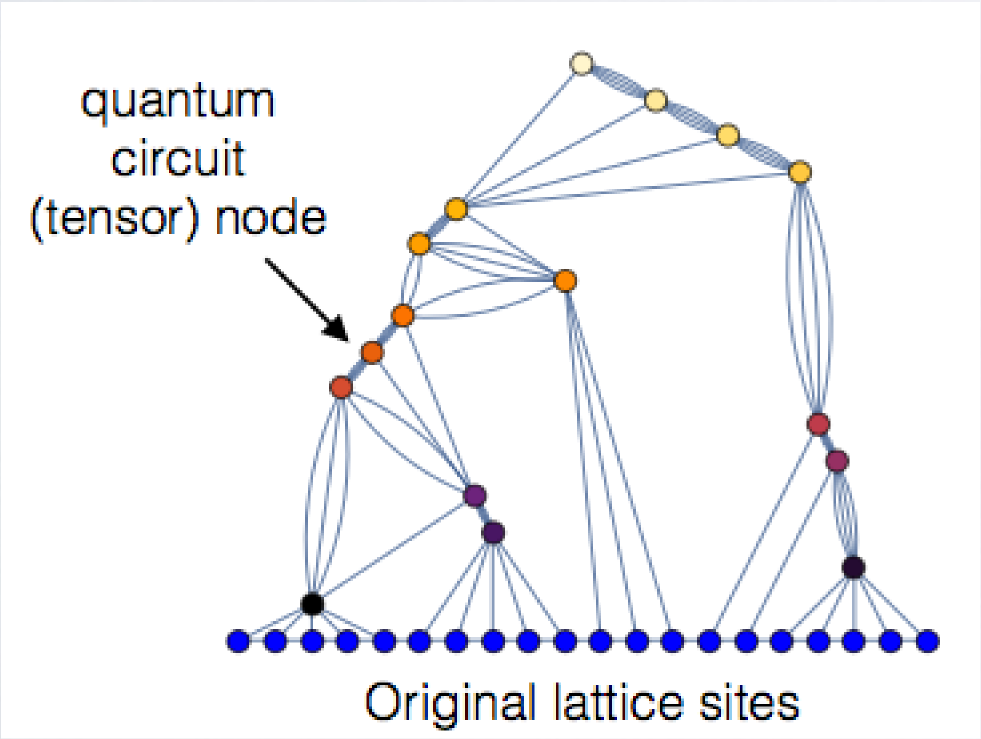
We'd really like to write down a wave-function for ground states (excited states). That's an important starting point for other propagating methods.

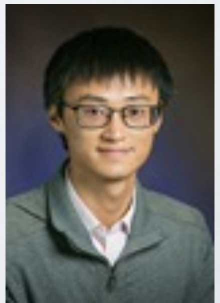
Tensor networks are amongst the most successful ways of pulling this off.

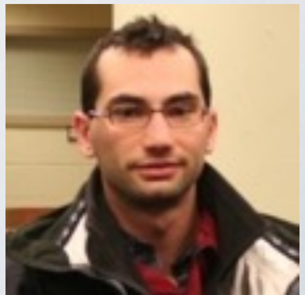
(All data here from many-body localization (i.e. Heisenberg model with disorder)

One of the problems with more complicated tensor networks (i.e. MERA) is the optimization is really difficult. This is particularly true for continuous space where there is a major difference in scale.

We have a new version of MERA which we build constructively (no optimization required)







Step 1: We will need local unitary matrices.

An important tangent about unitary matrices.

$$H_D = UHU^\dagger$$

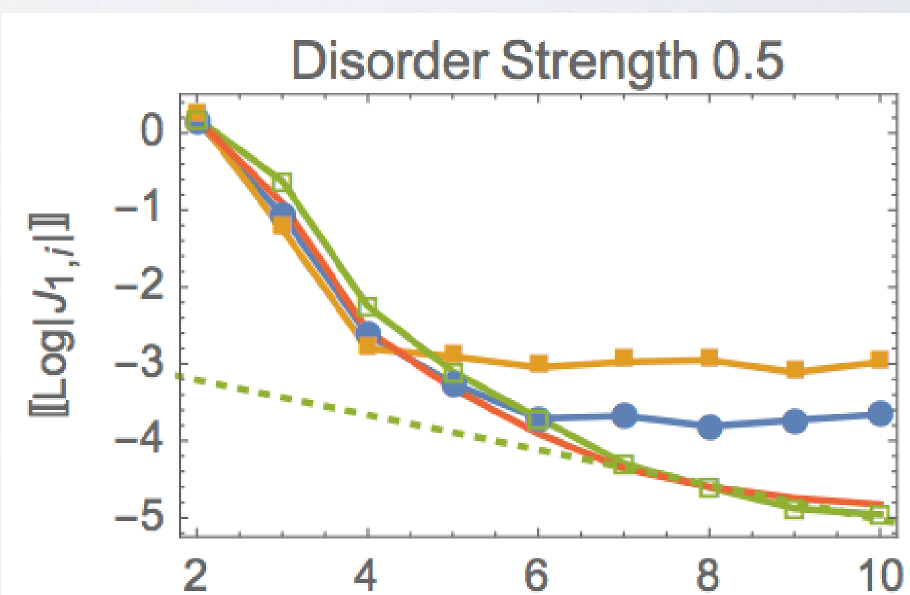
There are many such U

they differ from each other by permutations of columns/rows.

this difference matters in picking a ***local*** unitary transformation.

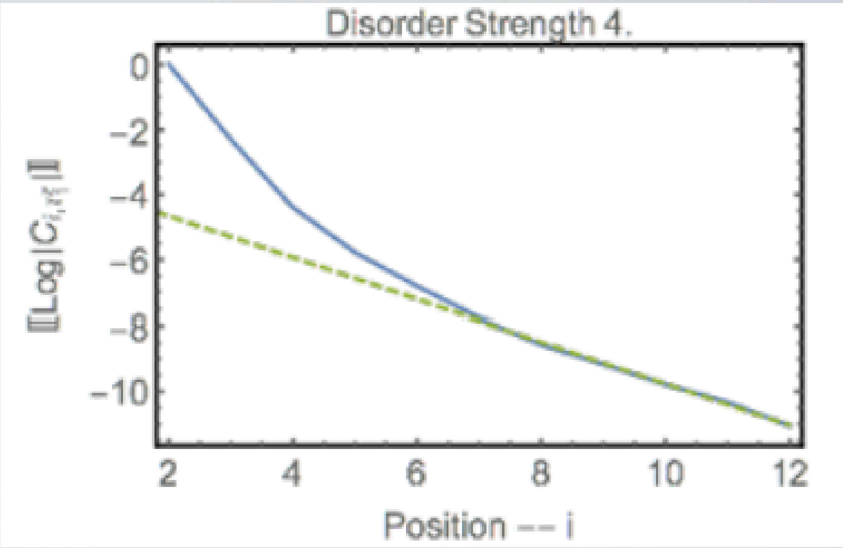
Wegner-Wilson Flow

$$\begin{aligned} H(\beta) &= H_0(\beta) + V(\beta), \\ \eta(\beta) &= [H_0(\beta), V(\beta)], \\ \frac{dU(\beta)}{d\beta} &= \eta(\beta), \\ \frac{dH(\beta)}{d\beta} &= [H(\beta), \eta(\beta)] \,. \end{aligned}$$



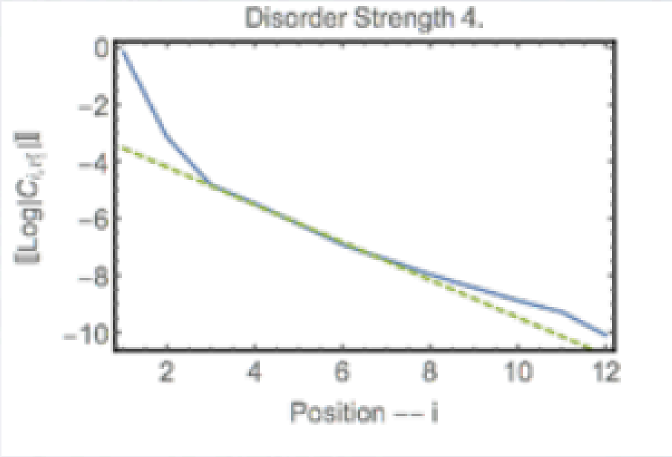
$$H = \sum_i \alpha_i \tau_i + \sum_{i,j} \alpha_{ij} \tau_i \tau_j + \ldots$$

decays exponential



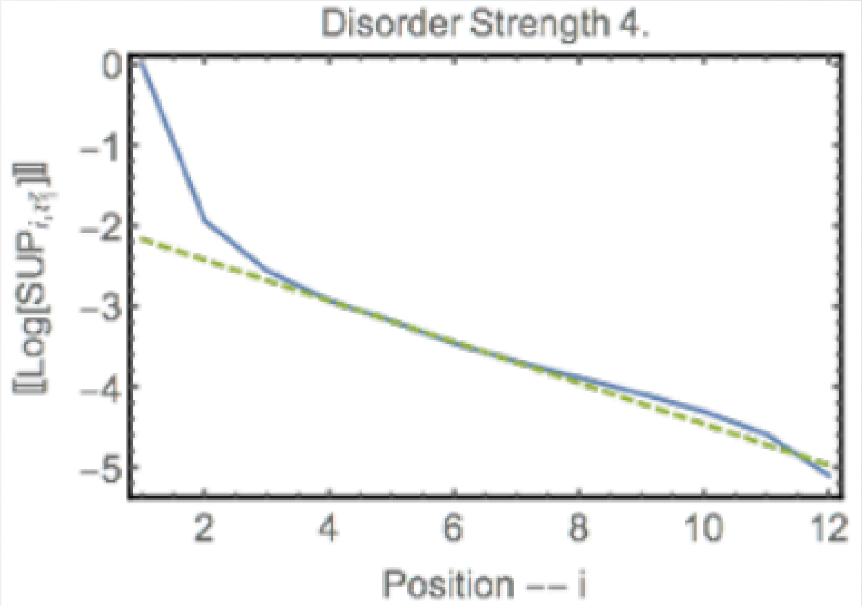
$$\tau_i = \sum_u a_i \sigma_z^i + \sum_{i,j} a_{ij} \sigma_i \sigma_j + \ldots$$

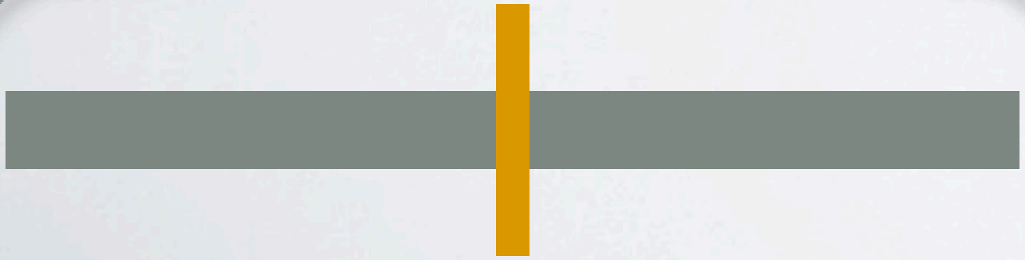
decays exponential



τ_i **is mainly supported on i (and it's nearby sites)**

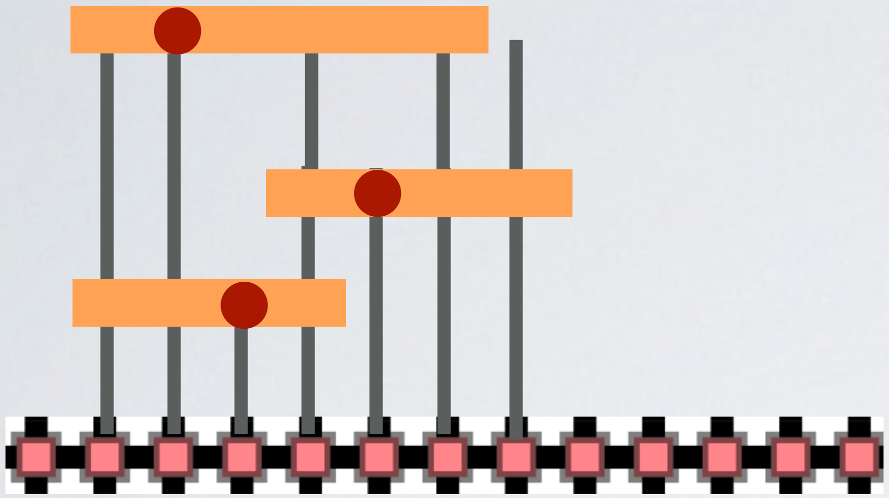
Consider how quickly it loses support: (1 - support)

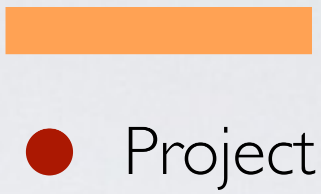




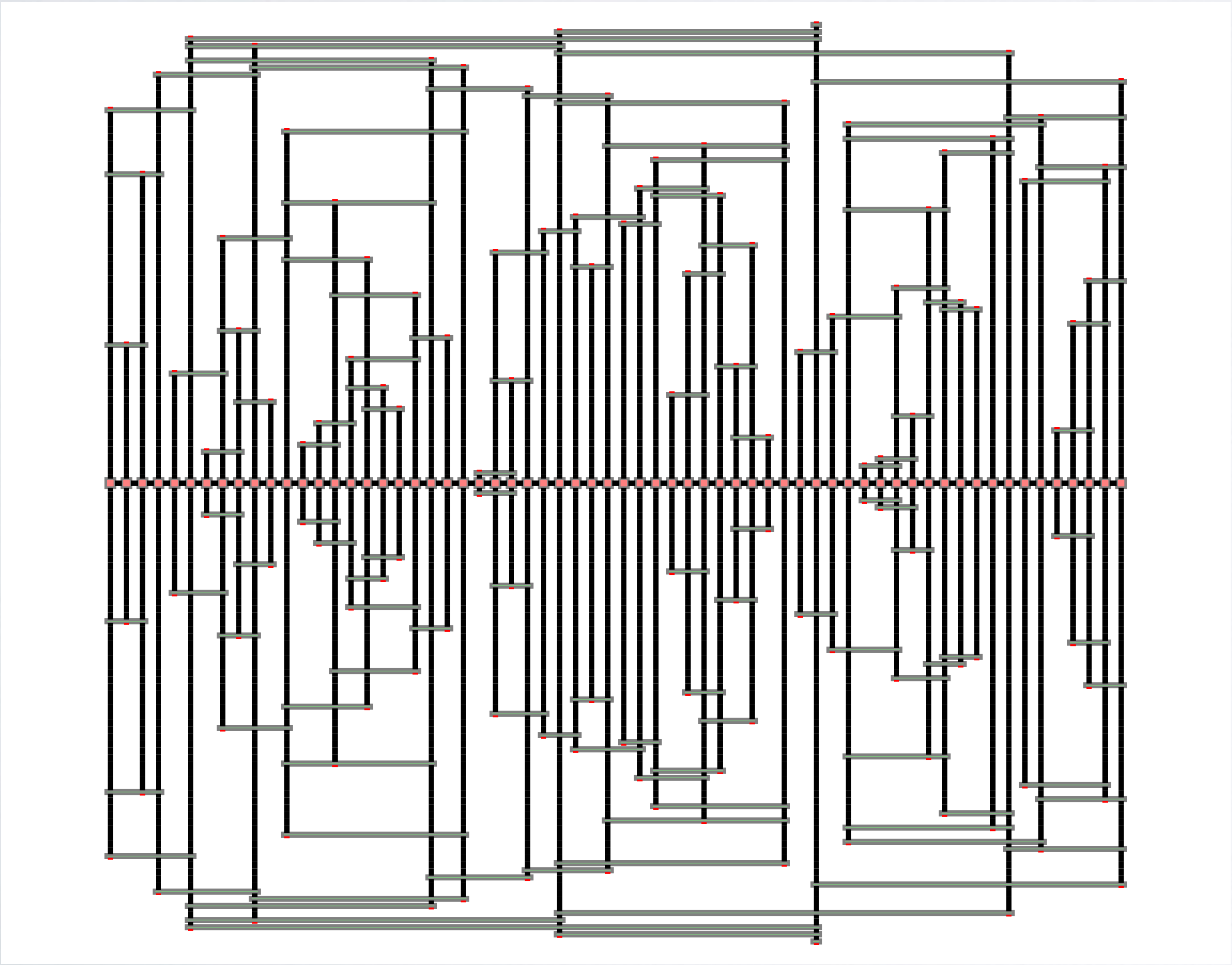
Entanglement (scaled)

A conceptually simplified MERA (aka Quantum Circuit)

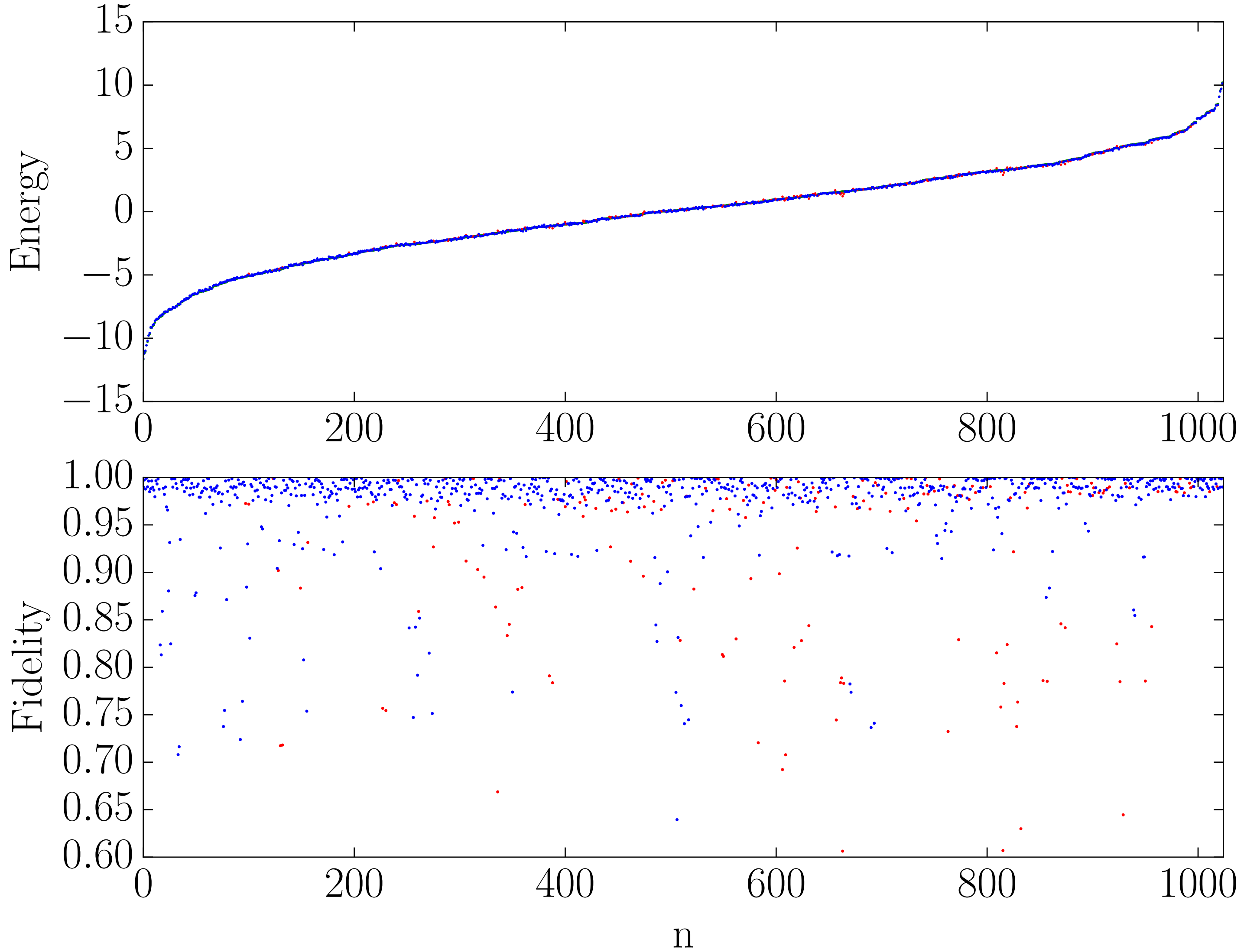




This can get any state in the spectrum.



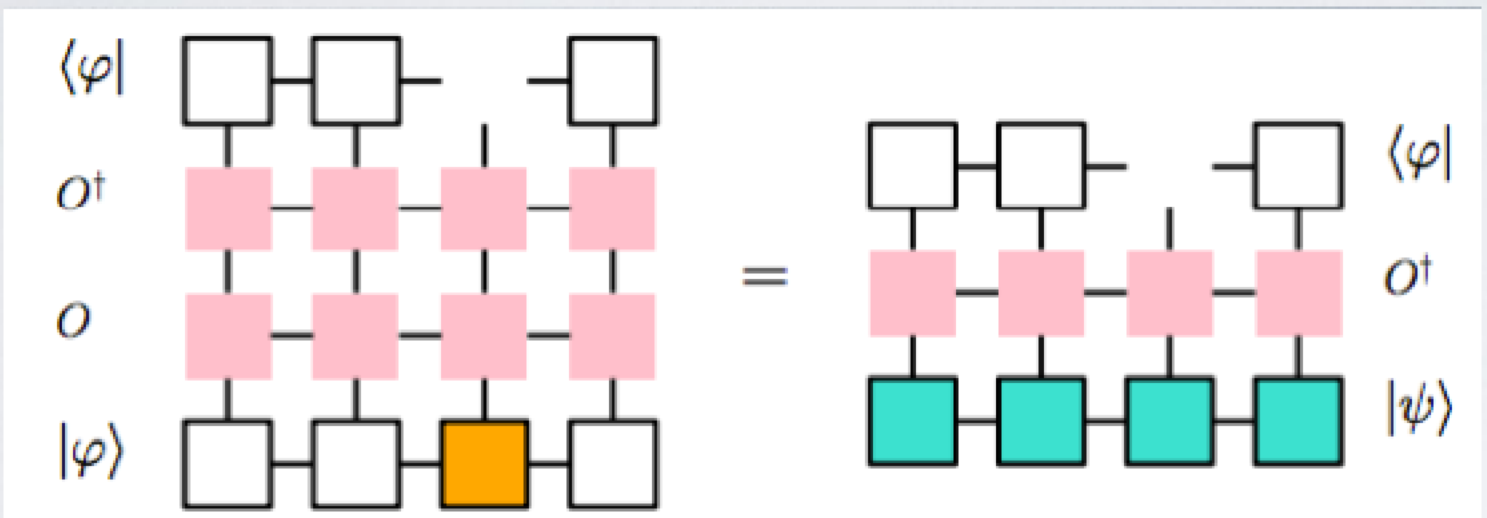
- Choose a set of sites
- Diagonalize with most local unitary
- Project "best" site
- Contract unitary gate into Hamiltonian
- Iterate

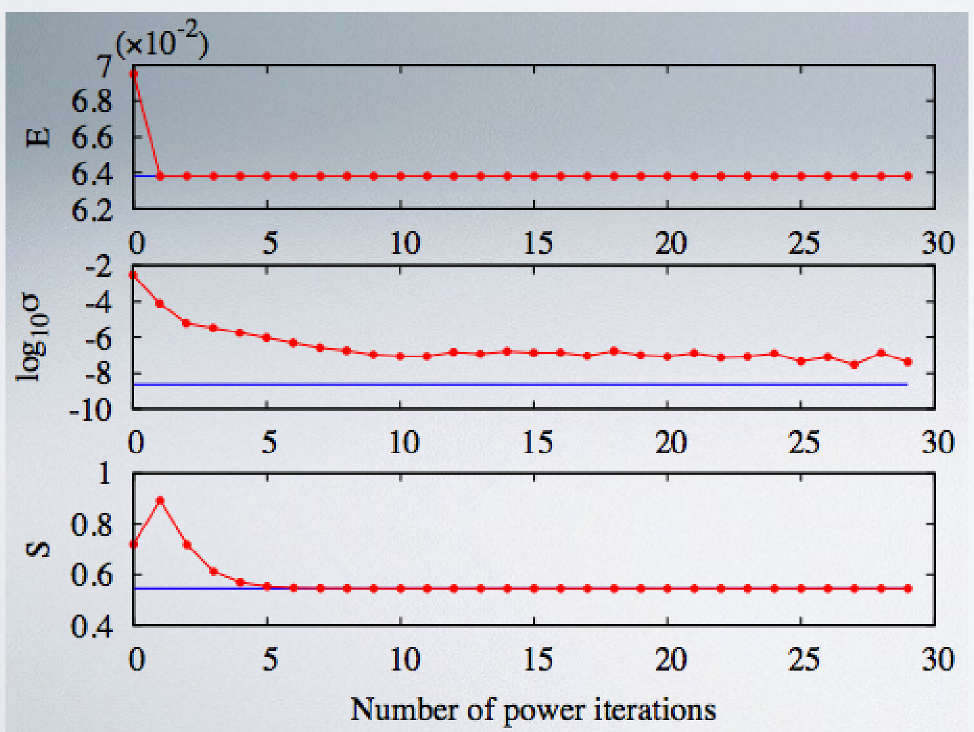

Energy
15
10
5
0
−5
−10
−15
0
200
400
600
800
1000
Fidelity
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
n

Accessing Excitations

SIMPS and ES-DMRG and ES-VMC

SIMPS $(H - E)^{-1}$

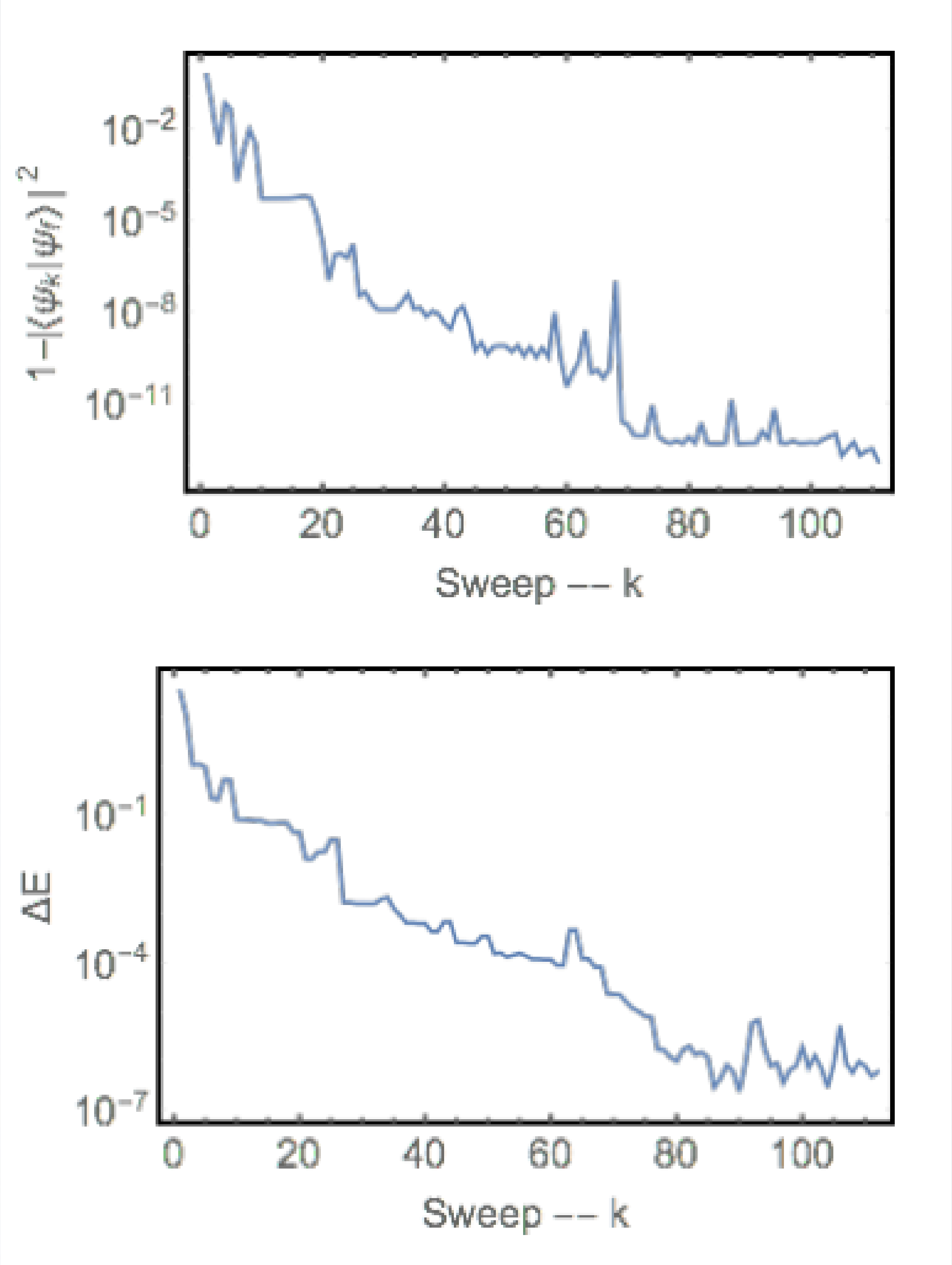




ES-DMRG

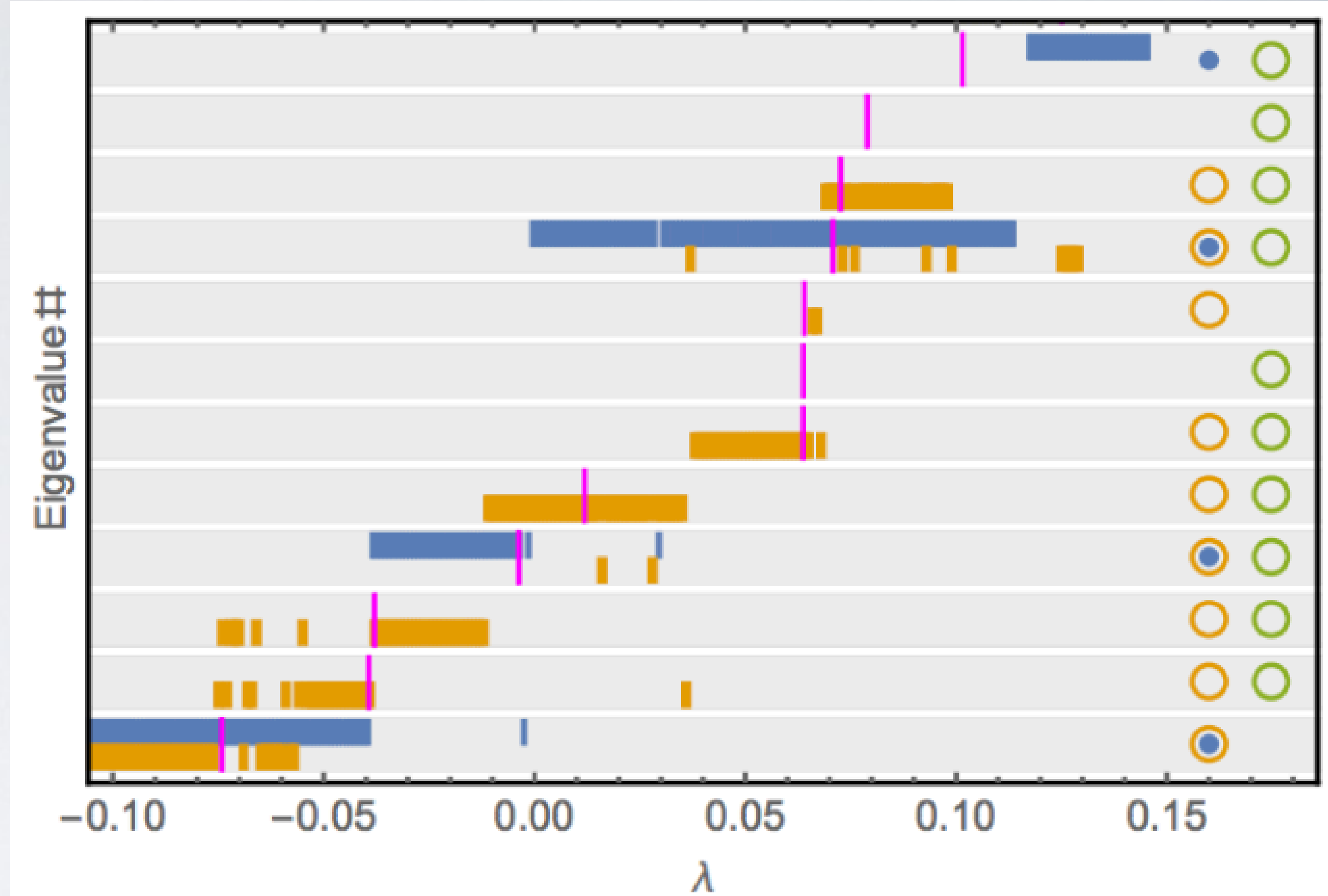
Typical DMRG: For a site produce an effective Hamiltonian H' and solve for the ground state of H'

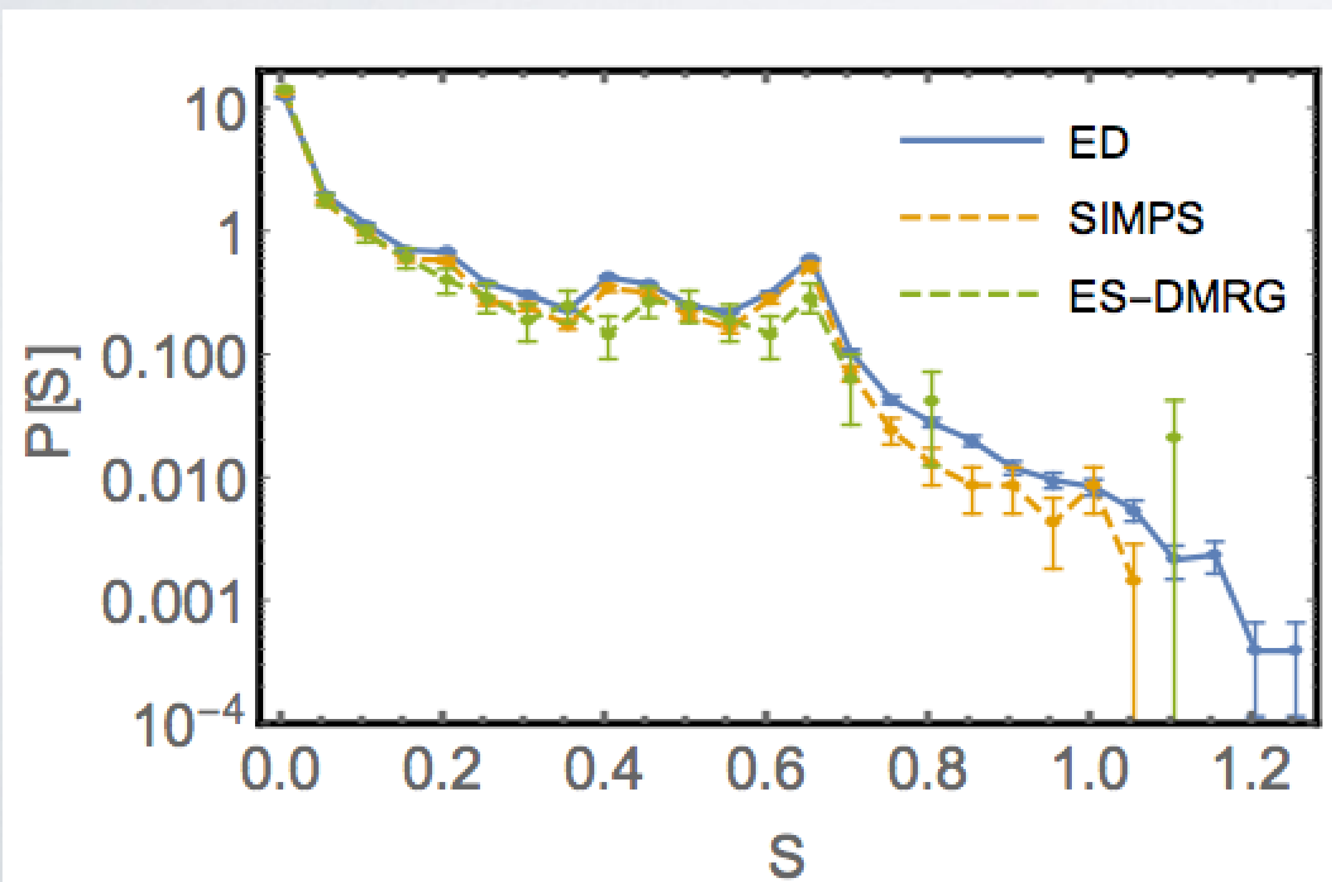
Modified DMRG: For a site produce an effective Hamiltonian H' and choose the eigenstate of H' closest to the current energy of your state.

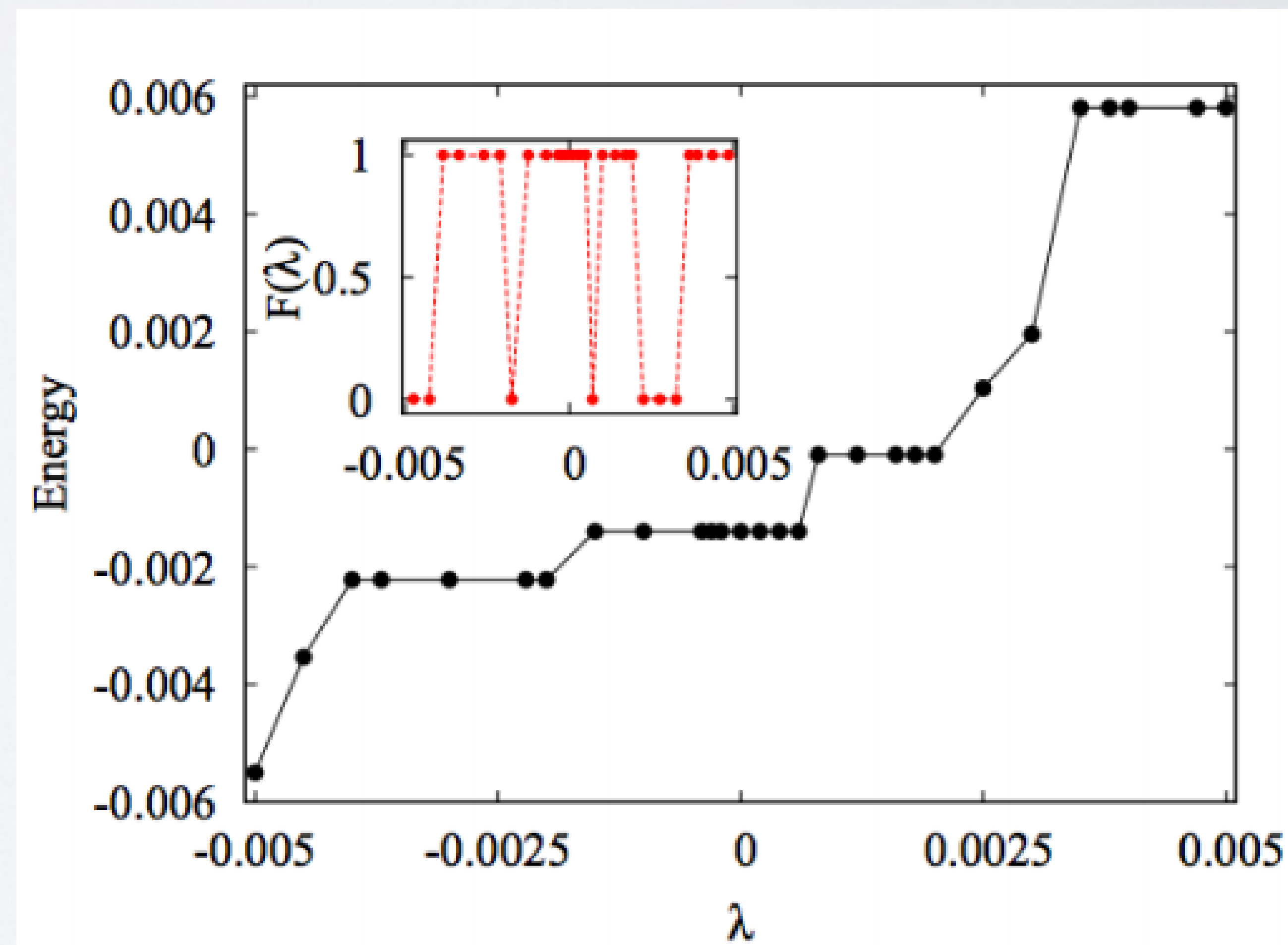


Does it work?

The question: Do you get an eigenstate?







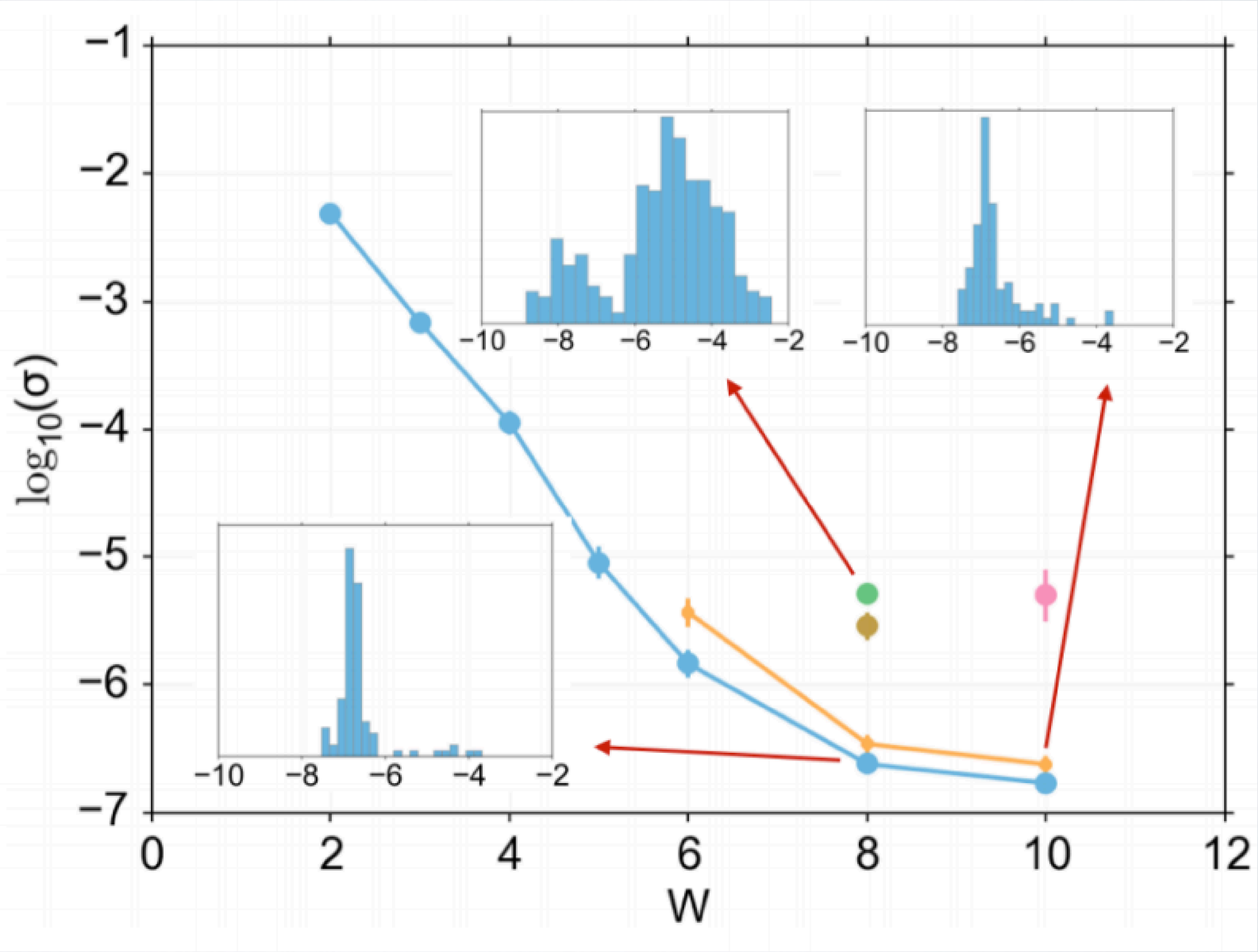
N=100 ES-DMRG

N=30 - SIMPS M=20

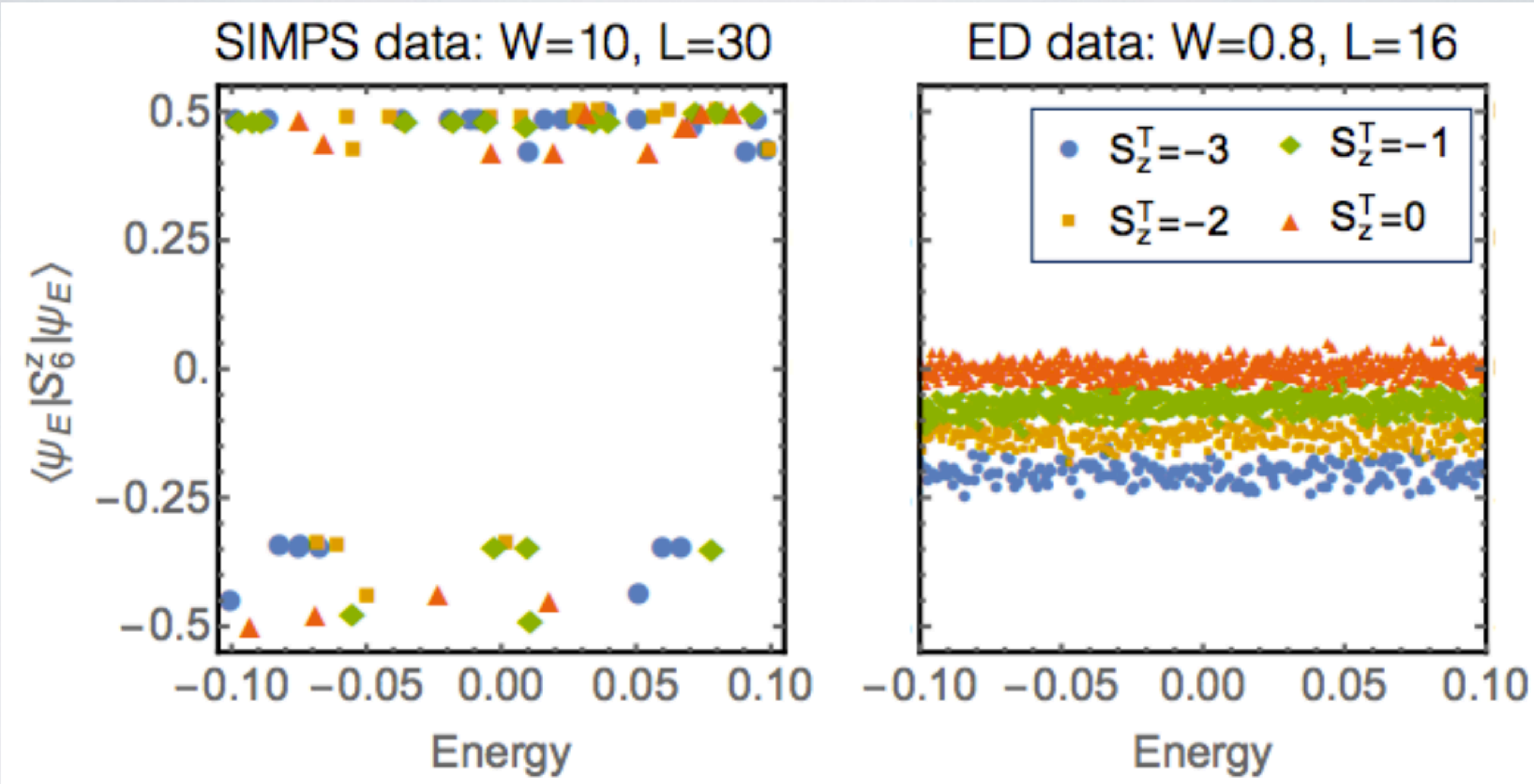
N=30 - ES-DMRG M=20

N=30 - SIMPS
M=60

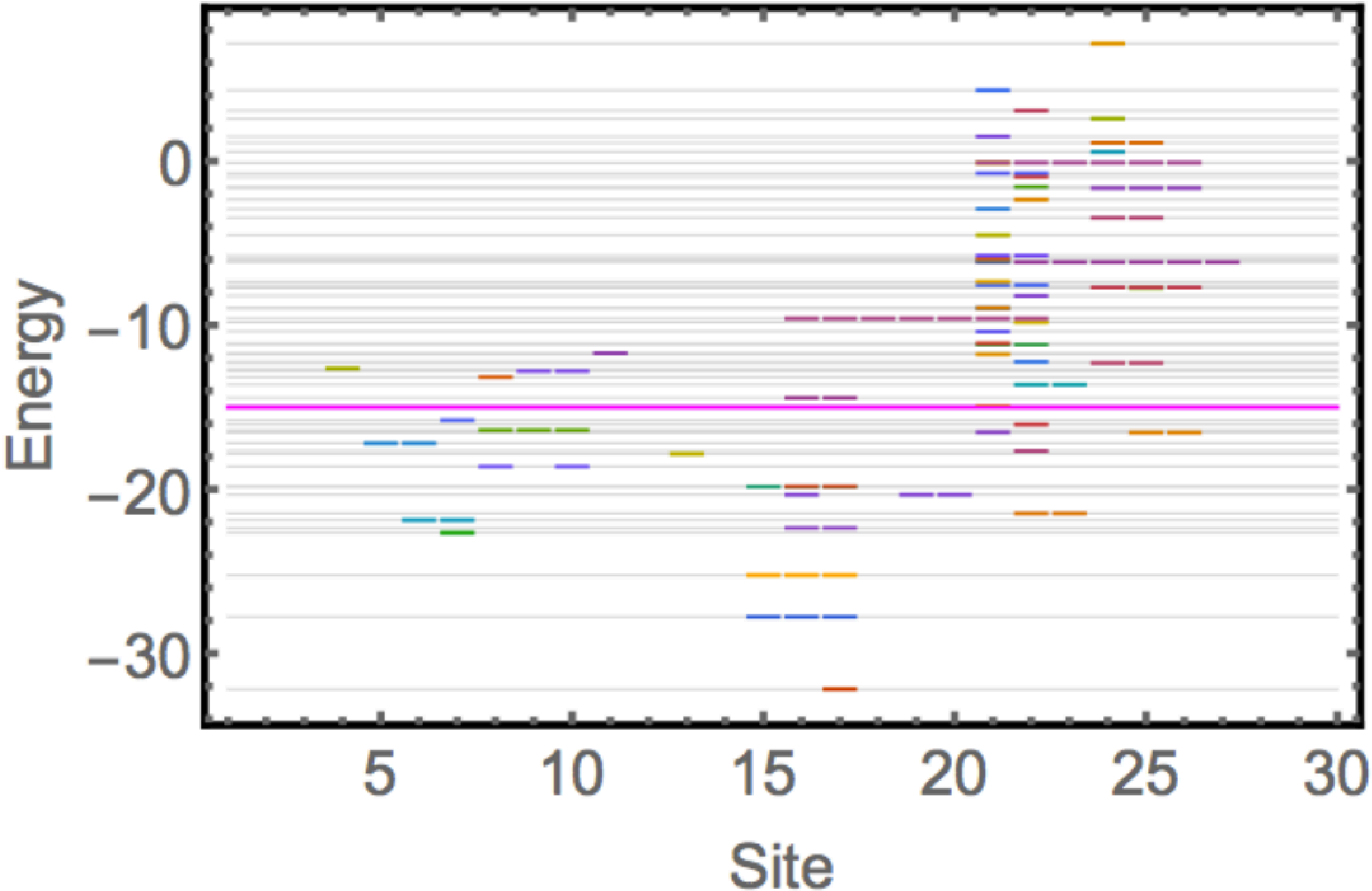
N=40 - SIMPS
M=60



ETH



SIMPS data: W=10, L=30
ED data: W=0.8, L=16
$\langle\psi_E|S_6^z|\psi_E\rangle$
0.5
0.25
0.
−0.25
−0.5
−0.10
−0.05
0.00
0.05
0.10
Energy
S_z^T=−3
S_z^T=−1
S_z^T=−2
S_z^T=0

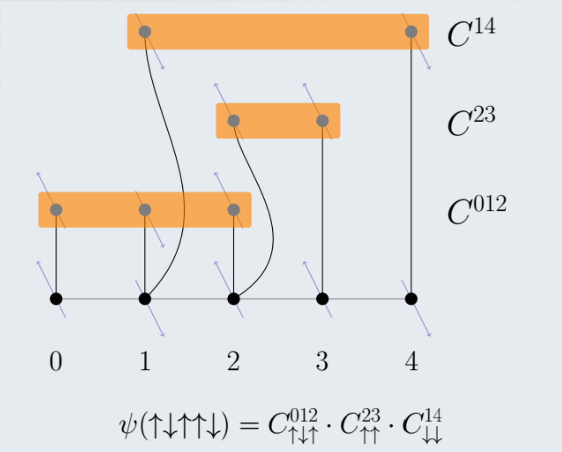


Energy
0
−10
−20
−30
5
10
15
20
25
30
Site

ES-VMC

Want an excitation method that works in many dimensions…

Let's use a tensor network that works in two dimensions:



Huse-Elser states again.

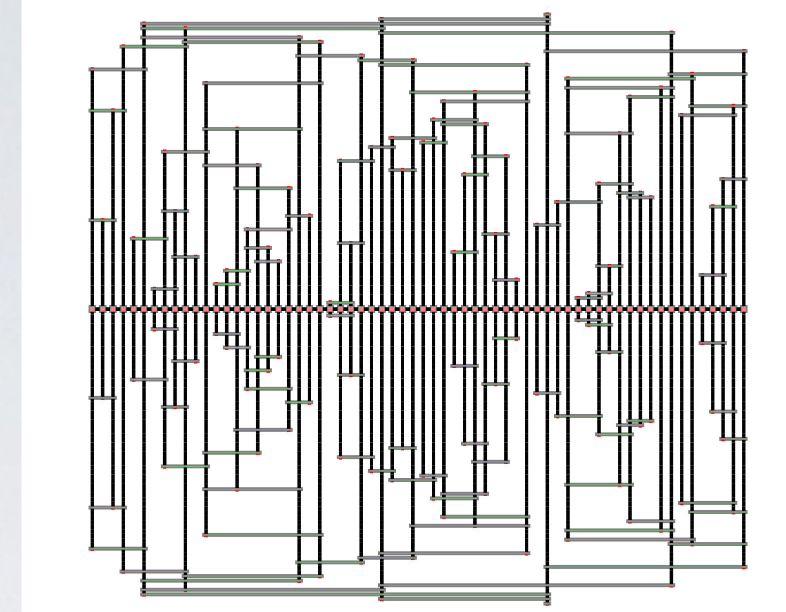
Use variational Monte Carlo to compute H and S for a set of correlators.

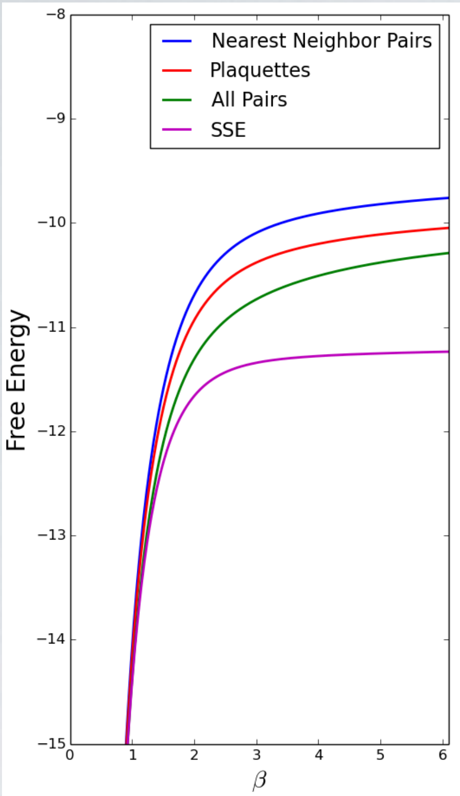
Solve the generalized eigenvalue problem to pick new parameters that are close to the current state.

Iterate

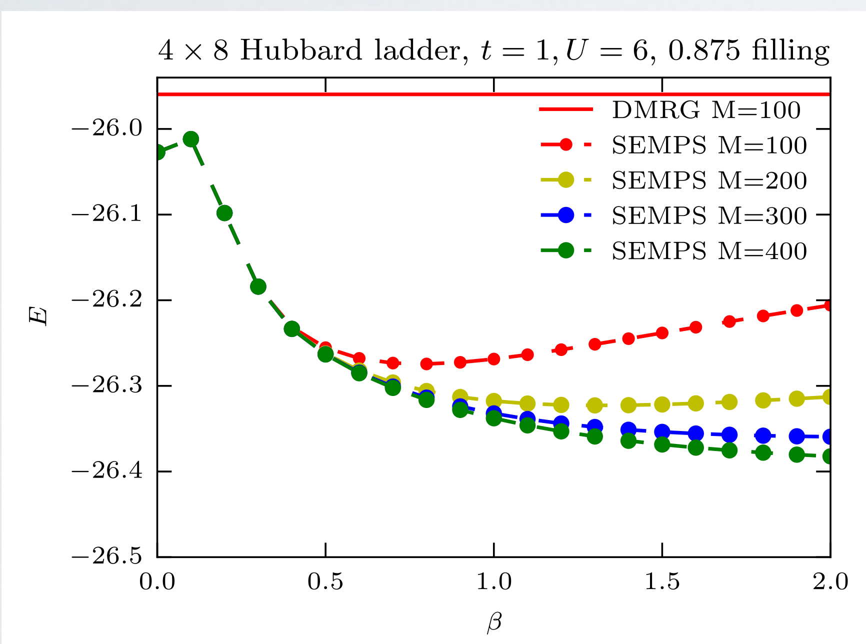
Conclusions….

Constructive MERA





WAFT



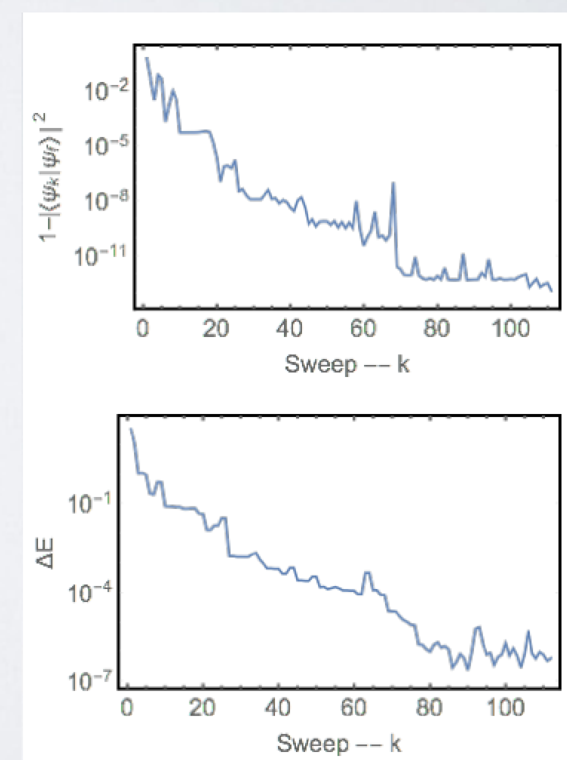
SEMPS

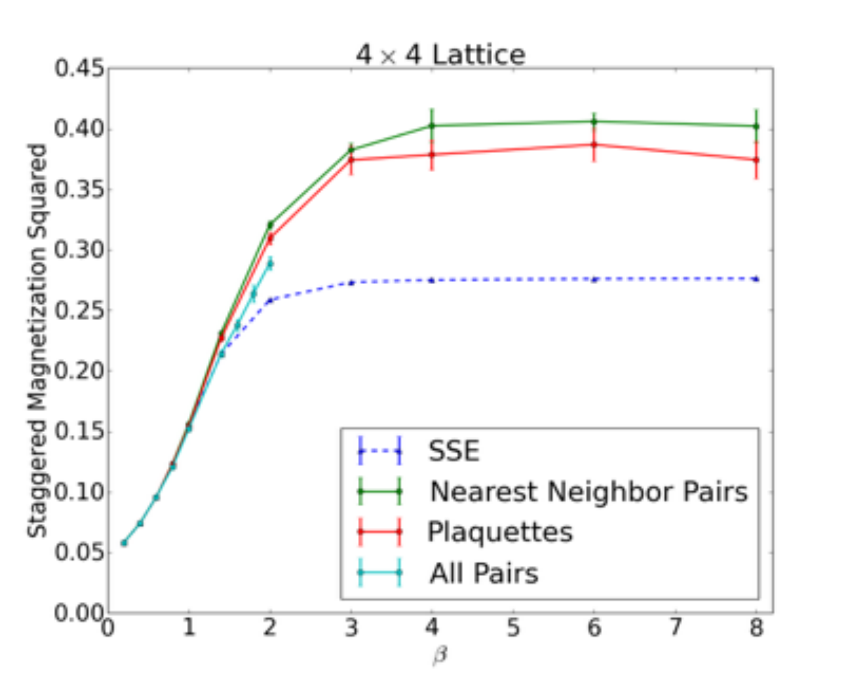
SEWF

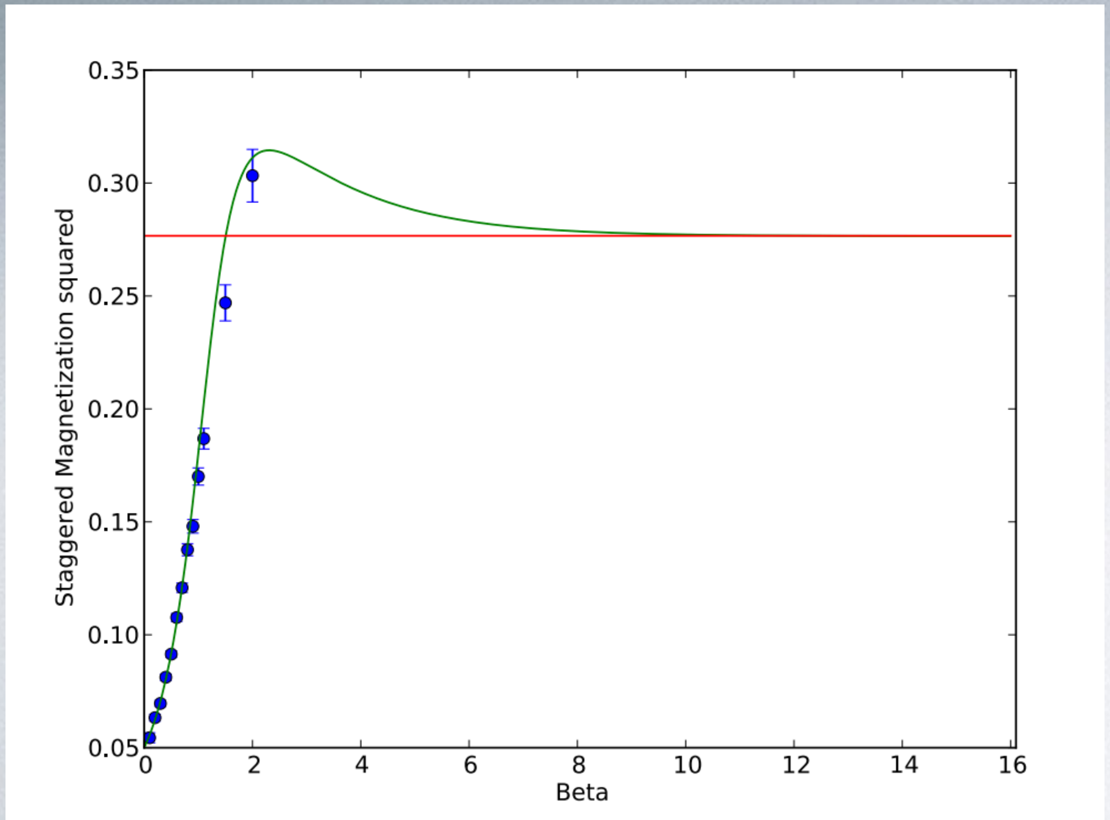
ES-DMRG

ES-VMC

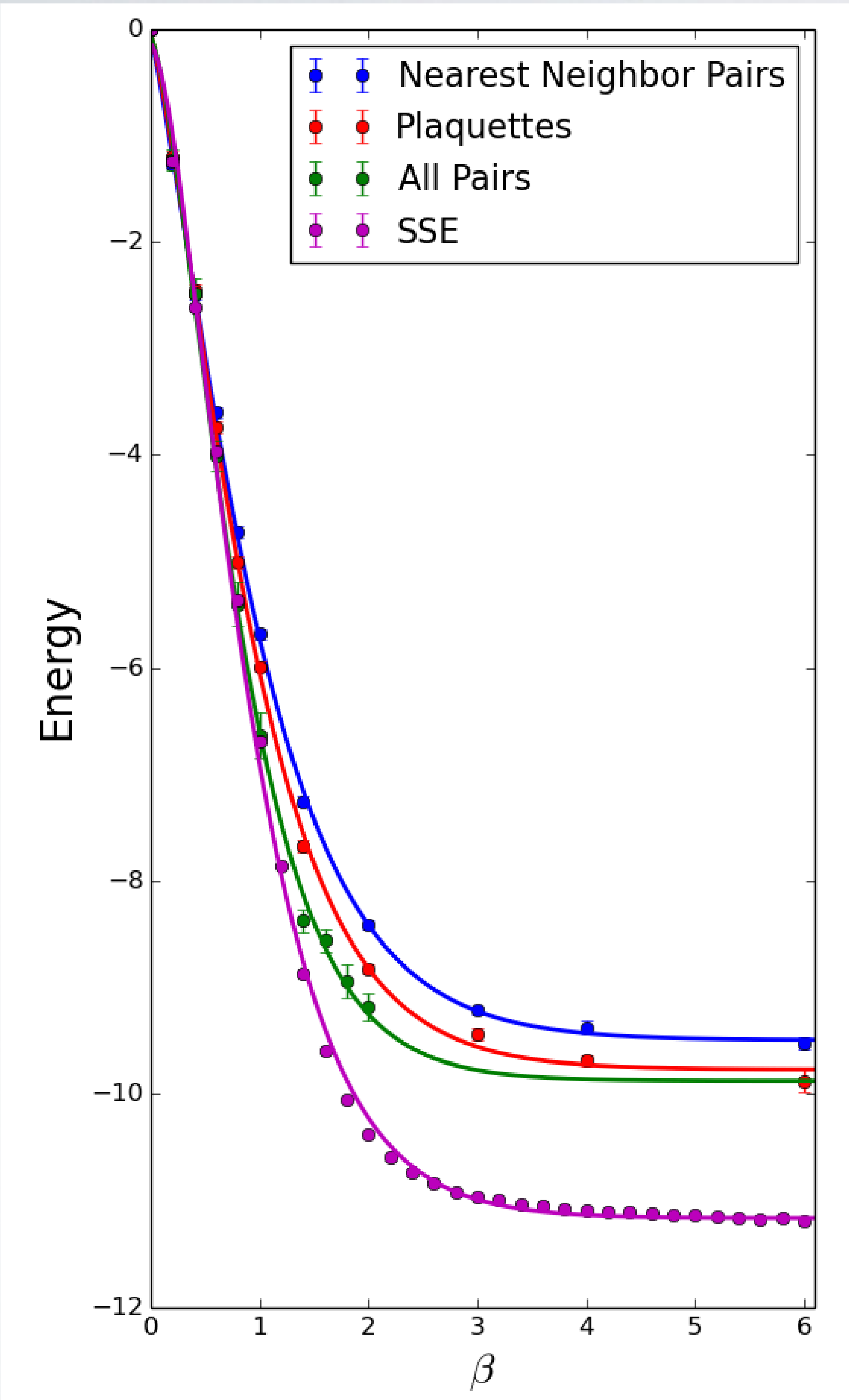
SIMPS



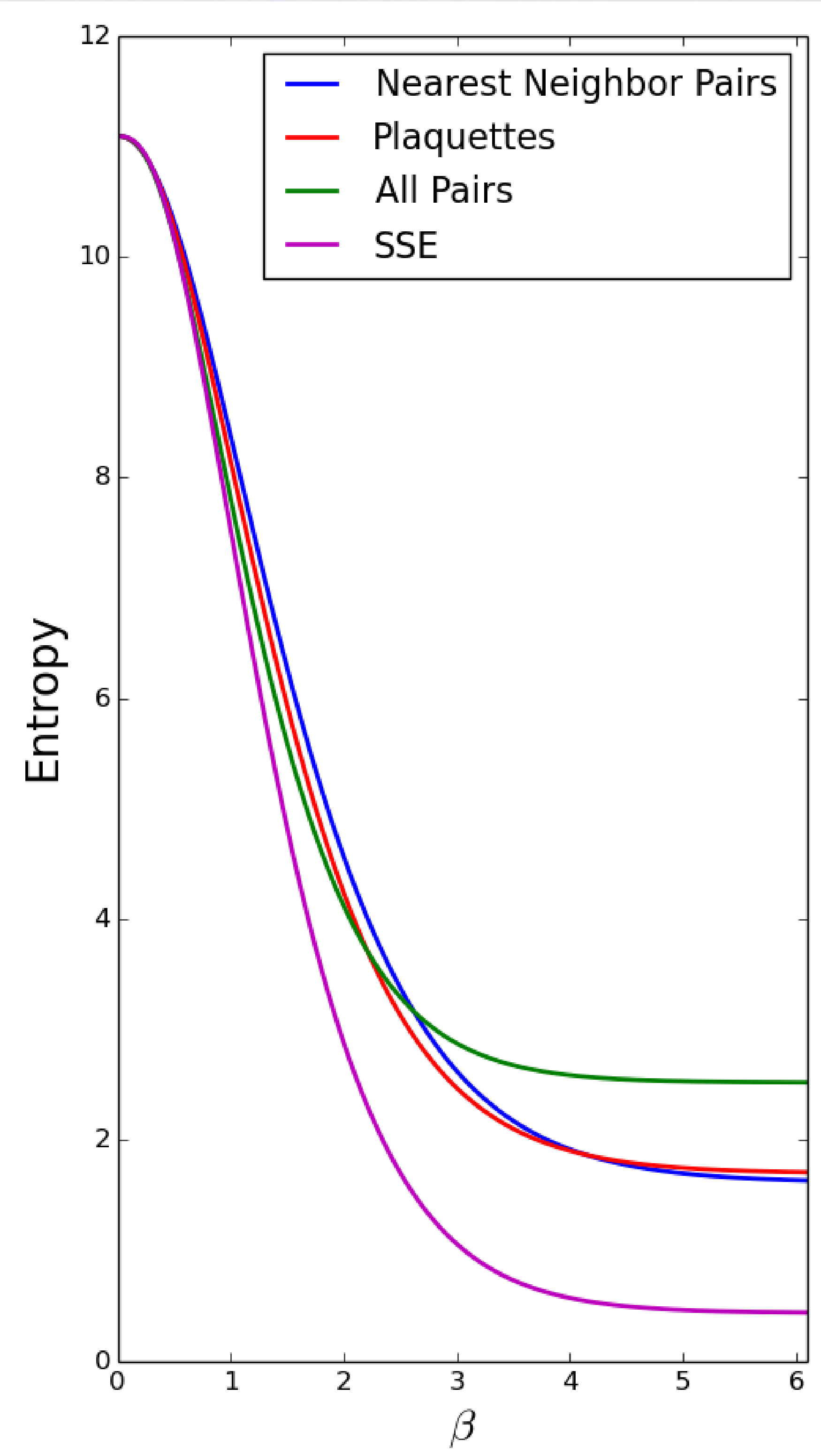

4 × 4 Lattice
Staggered Magnetization Squared
β
SSE
Nearest Neighbor Pairs
Plaquettes
All Pairs


Staggered Magnetization squared
Beta

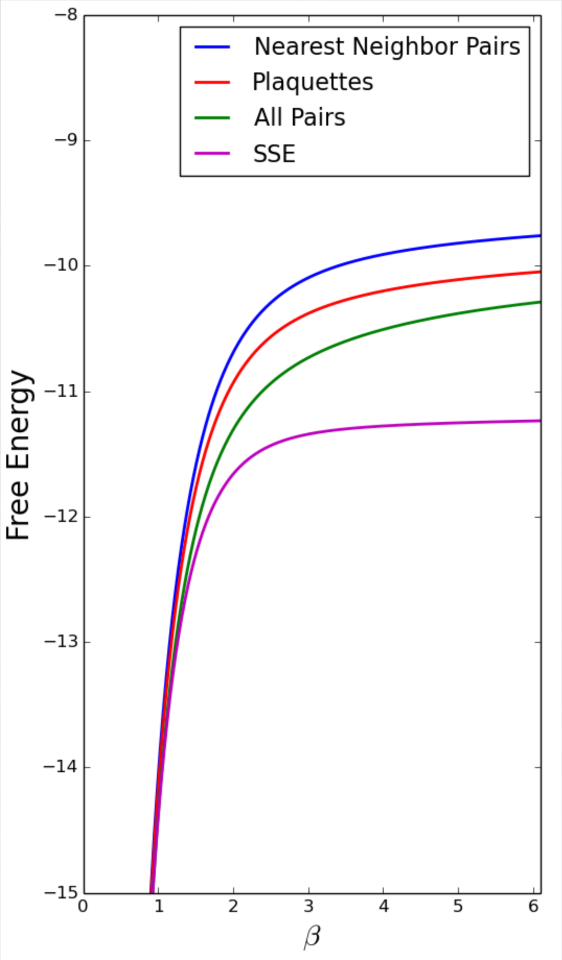
Finite T VMC



Energy
β
Nearest Neighbor Pairs
Plaquettes
All Pairs
SSE
0
−2
−4
−6
−8
−10
−12
0 1 2 3 4 5 6

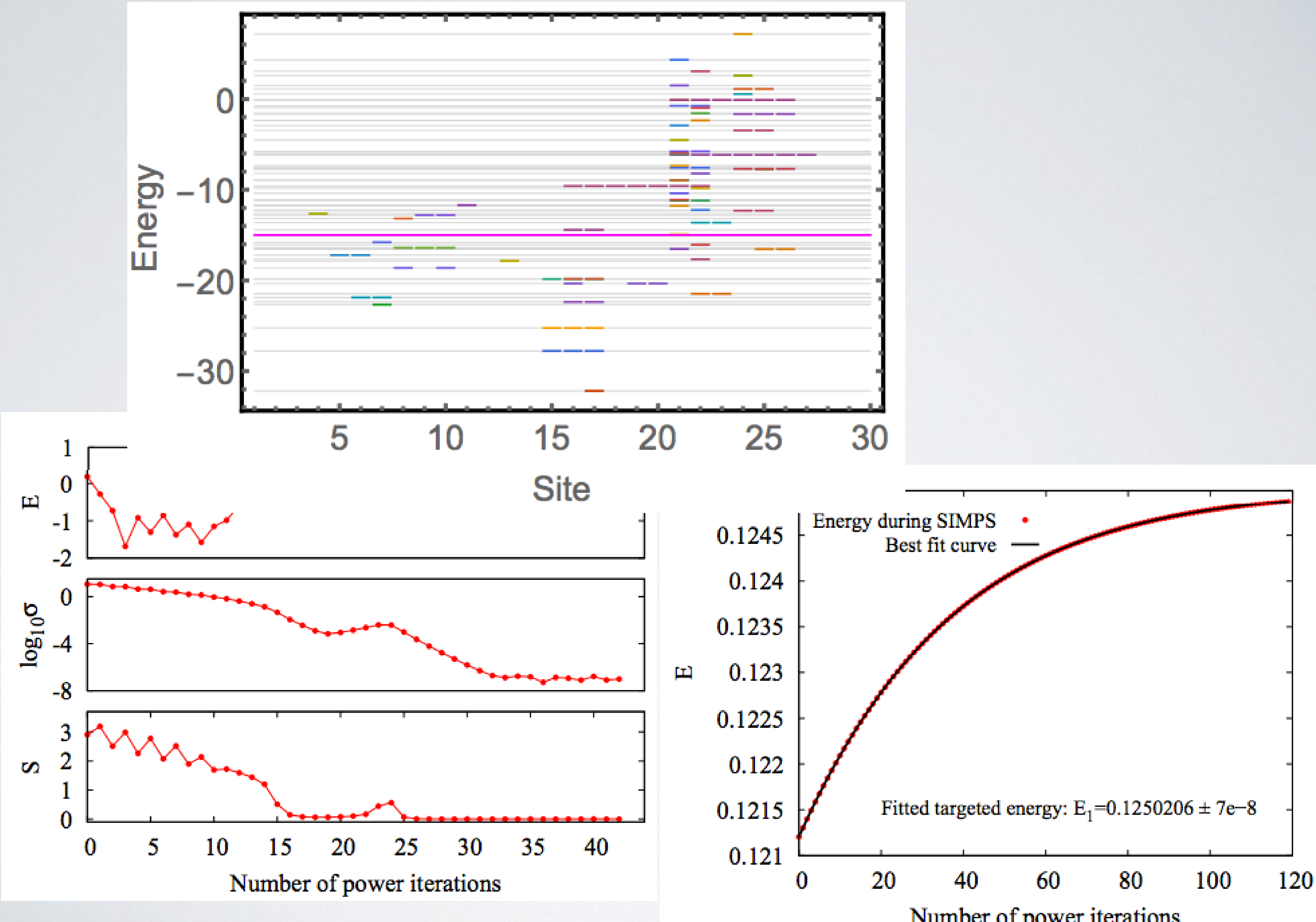


Entropy
β
Nearest Neighbor Pairs
Plaquettes
All Pairs
SSE
0 2 4 6 8 10 12
0 1 2 3 4 5 6



Free Energy
β
Nearest Neighbor Pairs
Plaquettes
All Pairs
SSE
−8 −9 −10 −11 −12 −13 −14 −15
0 1 2 3 4 5 6

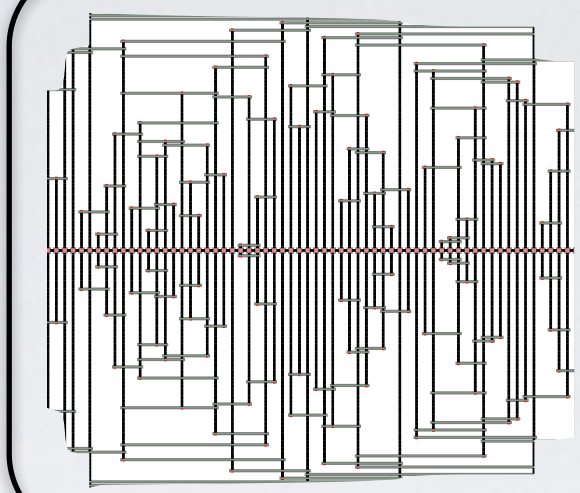
SIMPS



Energy
0
−10
−20
−30
5
10
15
20
25
30
Site
E
log$_{10}$σ
S
Number of power iterations
Energy during SIMPS
Best fit curve
Fitted targeted energy: E$_1$=0.1250206 ± 7e−8
Number of power iterations

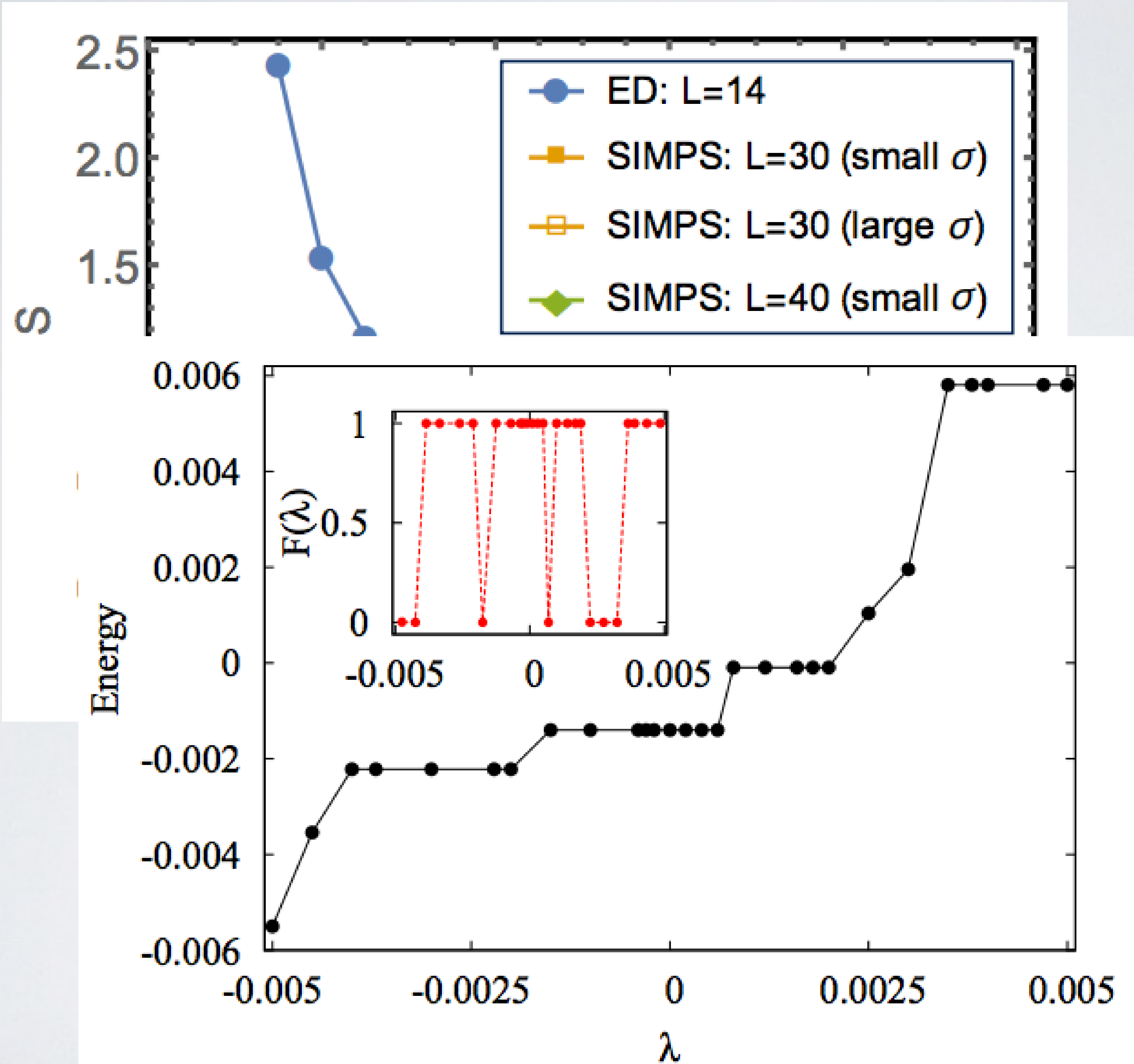
Propagators…

$$\rho \equiv \exp[-\beta H]$$



quantum circuit

$$(H - E)^{-1}$$



S
2.5
2.0
1.5
ED: L=14
SIMPS: L=30 (small σ)
SIMPS: L=30 (large σ)
SIMPS: L=40 (small σ)
Energy
0.006
0.004
0.002
0
-0.002
-0.004
-0.006
-0.005
-0.0025
0
0.0025
0.005
λ
F(λ)
1
0.5
0
-0.005
0
0.005

ES-VMC

Quantum Blocks

Constructive MERA

Variational Density Matrix

SEMPS

$$\rho(R,R) = \rho(R,R_1)\rho(R_1,R_2)\rho(R_2,R_3)...\rho(R_{n-1},R)$$

Lanczos

SIMPS

ES-DMRG

ES-VMC