# The density matrix renormalization group and tensor network methods

**Steve White**

## Outline

- Exploiting the low entanglement of ground states
- Matrix product states and DMRG
- 1D → 2D
- Tensor network states

Some of what I'm leaving out:

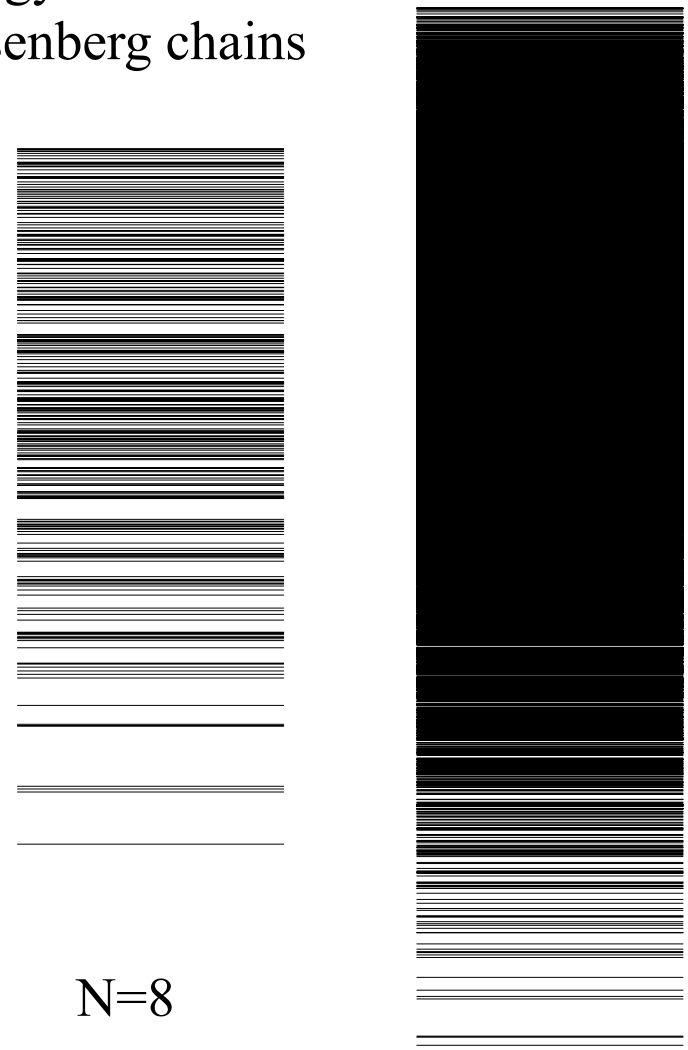
Historical connection to Wilson's NRG for the Kondo problem

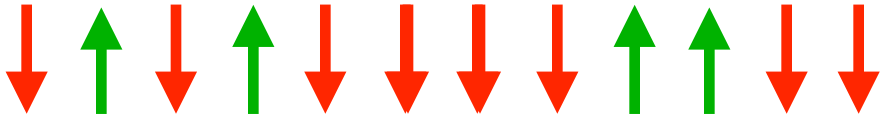
Applications to 1+1D field theories, including continuous MPS

DMRG for quantum chemistry

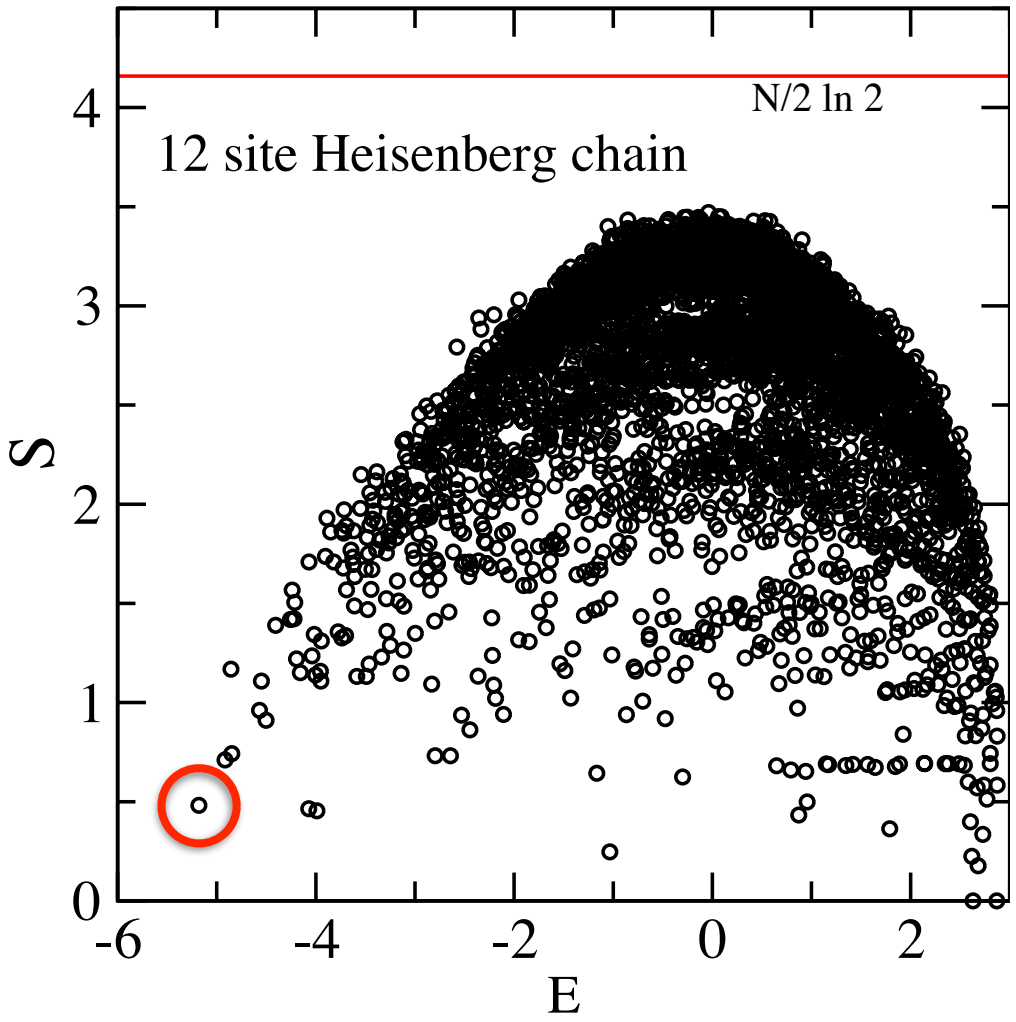
Real time solutions to time dependent Schrodinger eqn, including non equilibrium and spectral functions

Energy levels of S=1/2
Heisenberg chains



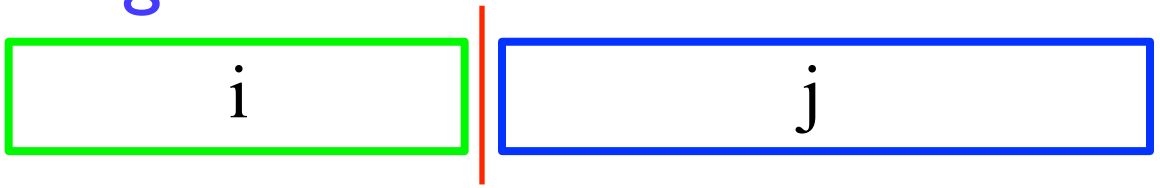



## Ground states have low entanglement




Von Neumann Entanglement entropy S for every eigenstate (system divided in center)

# Entanglement and the Schmidt decomposition



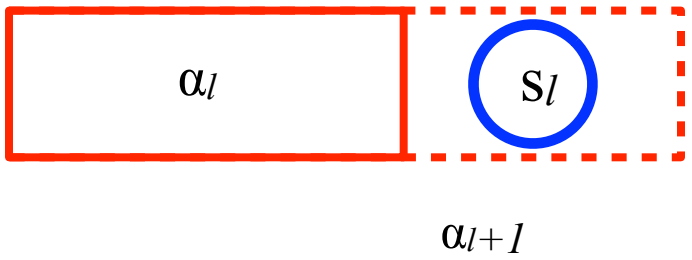

Bipartition of a quantum system

- Treat $\Psi_{ij}$ as a matrix: perform the singular value decomposition" (SVD): $\Psi = U D V$, with U and V unitary, D diagonal, with elements $\lambda_\alpha$
- Think of $(\lambda_\alpha)^2$ as the probability of the state $|\tilde{\alpha}\rangle |\alpha\rangle$; the von Neumann entropy
  - $S = -\sum_\alpha (\lambda_\alpha)^2 \ln (\lambda_\alpha)^2$
- Thus we have a natural *low entanglement approximation:* approximate the wavefunction by keeping a small number of $|\alpha\rangle$ (with largest $\lambda_\alpha$).
- In DMRG we do an approximate version of this Schmidt decomposition for all positions of the dividing line between left and right.

# Matrix Product States

- For a 1D system, at every link, truncate the states to be the m largest Schmidt states
- The Schmidt basis states for position $l+1$ must be linear combinations of those at $l$

$$|\alpha_{l+1}\rangle = \sum_{\alpha_l, s_l} A[s_l]_{\alpha_{l+1}\alpha_l} |s_l\rangle |\alpha_l\rangle$$




- This produces a Matrix Product State (MPS) formula for the wavefunction:

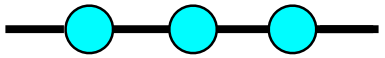
$$\Psi(s_1,s_2,..s_N) \approx A^1[s_1]\, A^2[s_2] \ldots A^N[s_N]$$

- A function is just a rule for giving a number from the inputs--here the {s} tell which matrices to multiply (first and last A's are vectors).

# Diagrams for Matrix Product States

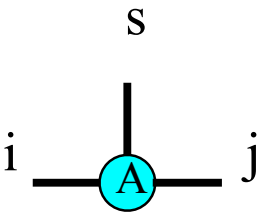
Vertices are matrices or tensors. All internal lines are summed over. External lines are external indices, associated with physical states

Ordinary Matrix Multiplication: ABC =

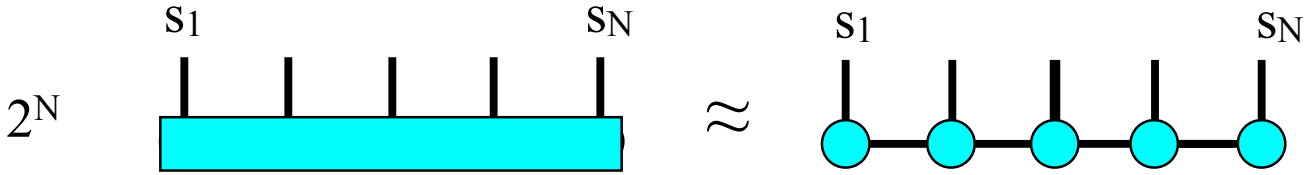


In an MPS, the basic unit is a matrix with an extra index, representing the state of a site

$A^{[s]}_{ij} =$

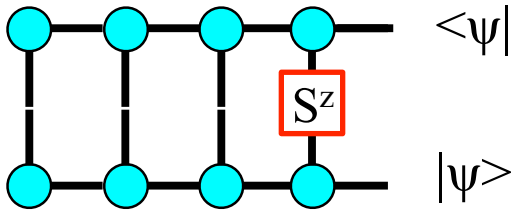



Matrix Product State: $\Psi(s_1,s_2,..s_N) \approx A^1[s_1]\, A^2[s_2] \ldots A^N[s_N]$



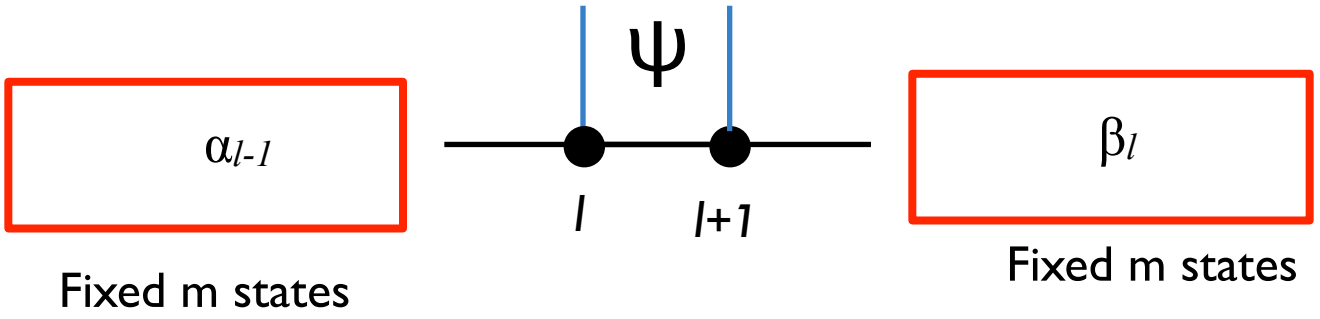

N $m^2$ for m x m matrices

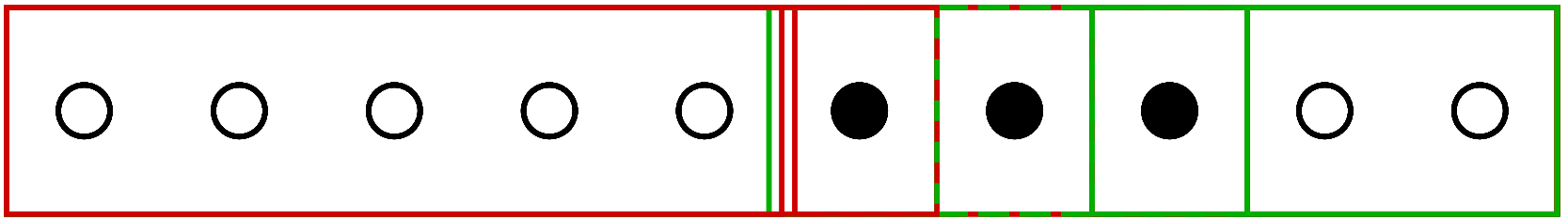
Contractions:




– Working left to right, just matrix multiplies, N $m^3$

# Matrix Product States + sweeping optimization algorithm = DMRG

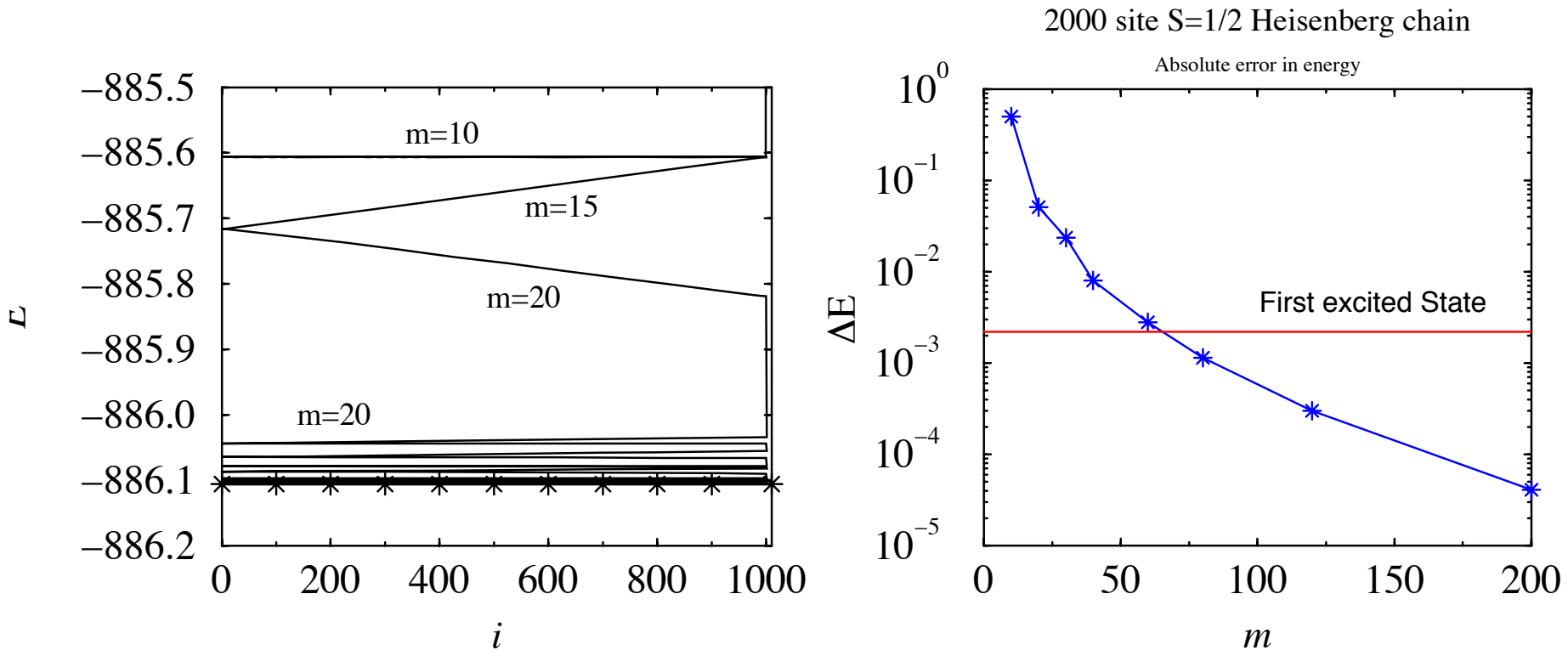


Sweeping

Each step: Lanczos to get ground state in reduced basis; SVD splits Ψ in two; left half gets absorbed into left block

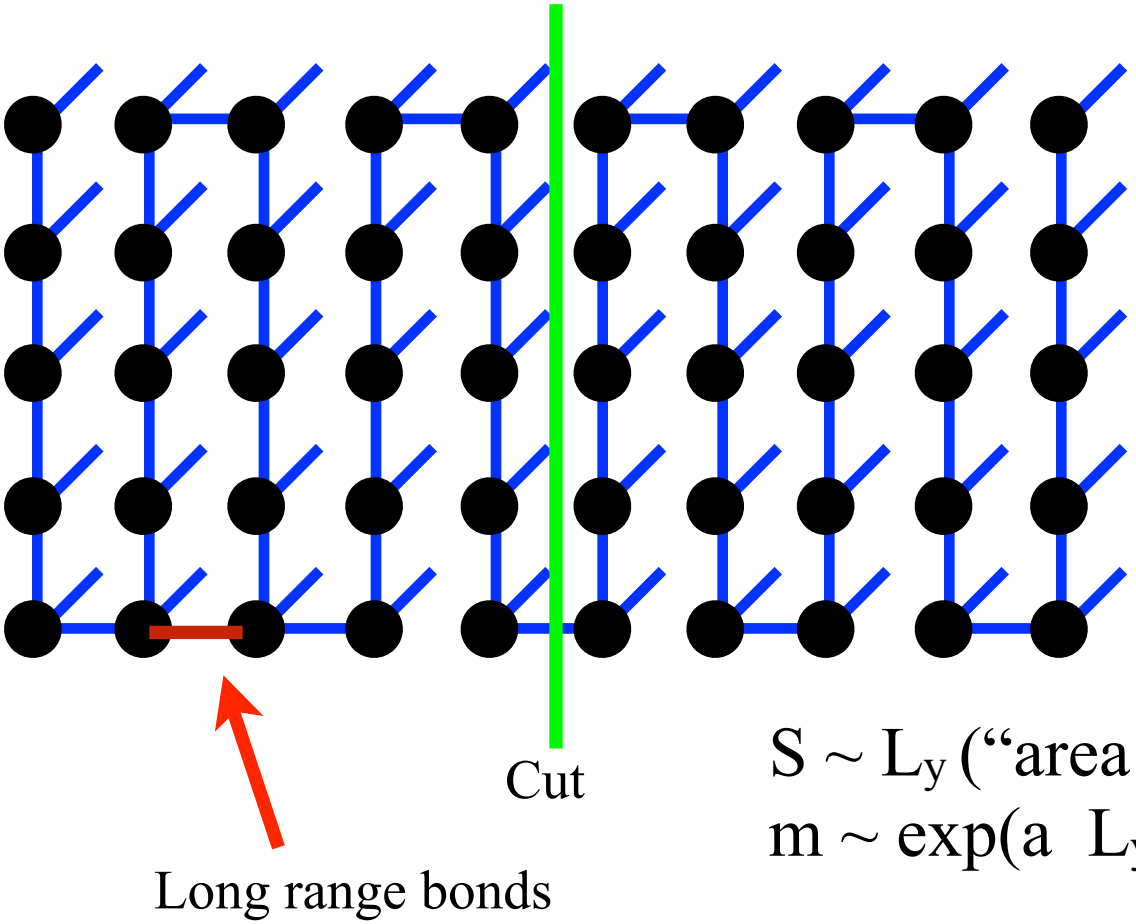
# DMRG Convergence in 1D




Comparison with Bethe Ansatz

# DMRG for 2D systems

- Map a finite width cylinder (vertical pbc's only) onto a chain



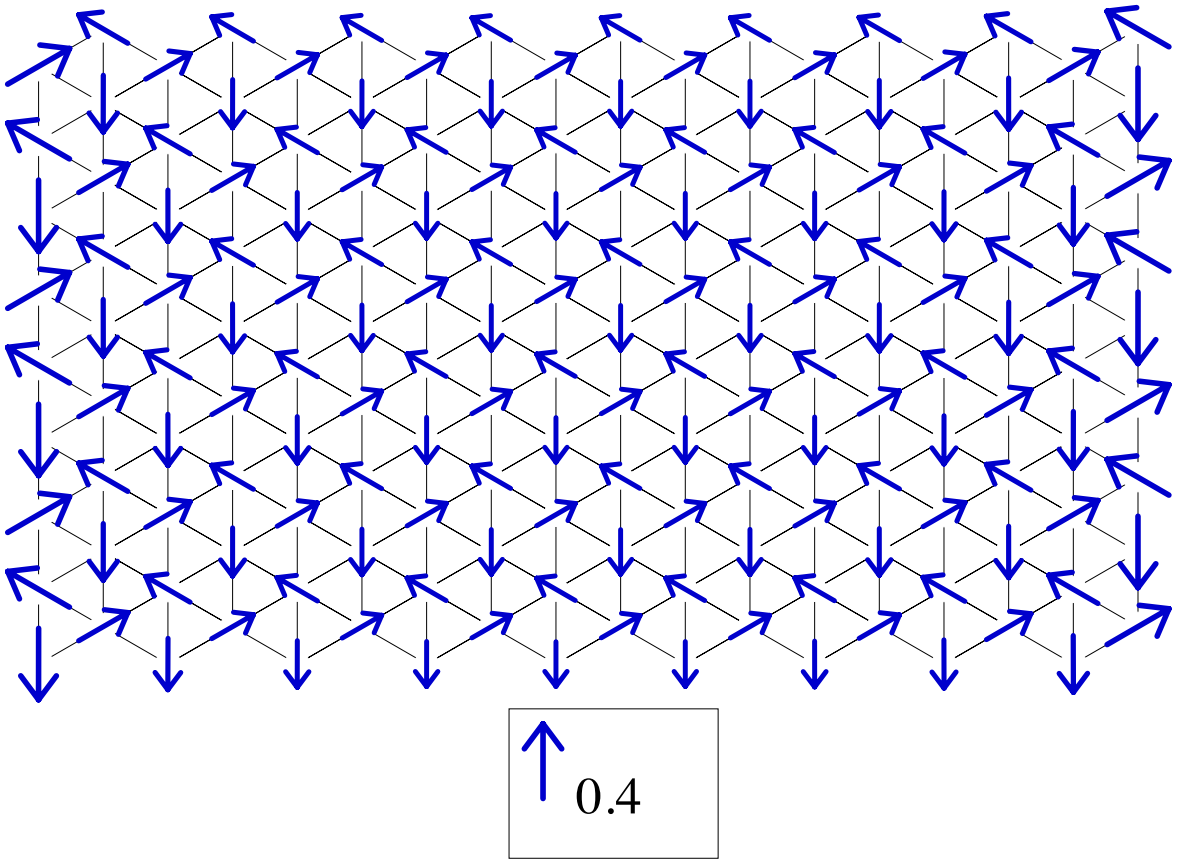

Key problems: 2D system with a sign problem: frustrated magnetic systems; doped fermion systems

$S \sim L_y$ ("area law")

$m \sim \exp(a\ L_y)$

Calc time: $L_x\ L_y^2\ m^3$; allows $m \sim 10000$, $L_y \sim 10\text{-}12$

# Traditional DMRG for triangular lattice Heisenberg model




See White & Chernyshev, PRL 99, 127004 (2007)

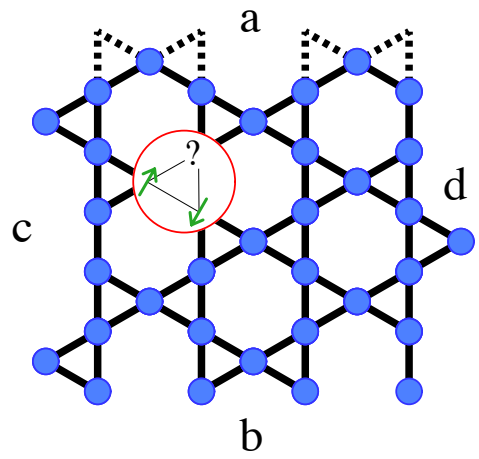
$\Delta E \sim 0.3\%$, $\Delta \langle S_z \rangle \sim 0.01$

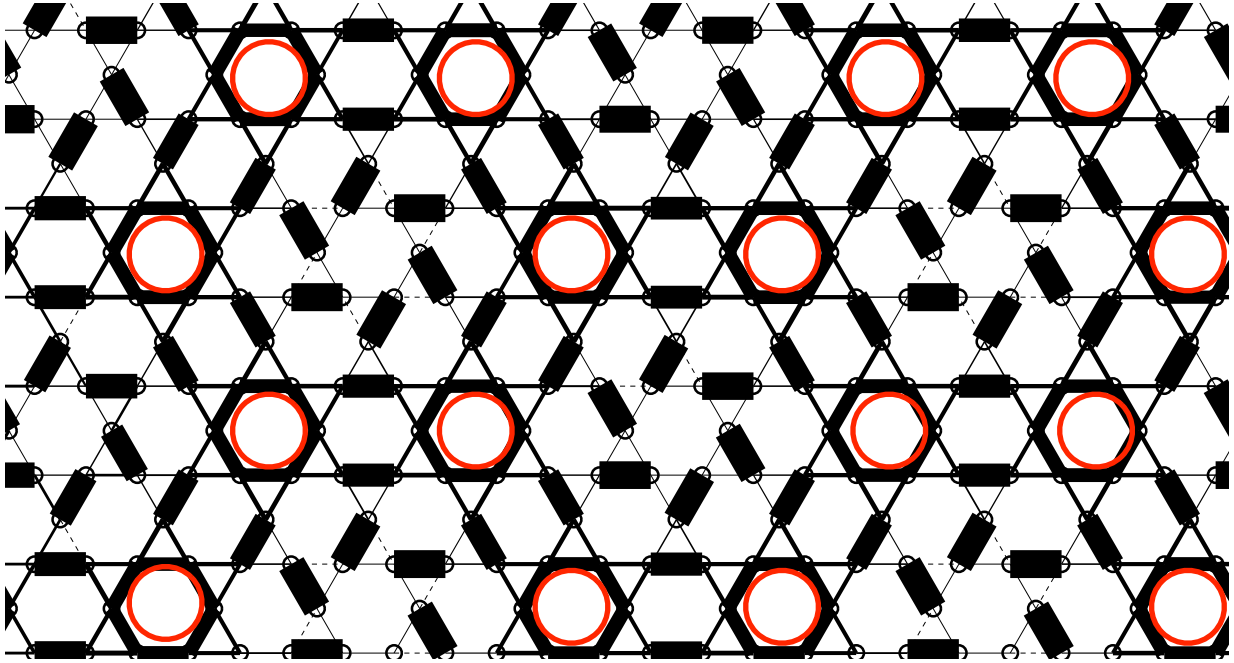
Extrap order param to thermodynamic limit: $M = 0.205(15)$

# Heisenberg model on the kagome lattice

- The Heisenberg model on the kagome lattice is one of the most frustrated systems
  - Proposed as a possible spin liquid in late 80's, support from field theory ($Z_2$...)(Sachdev, Read)

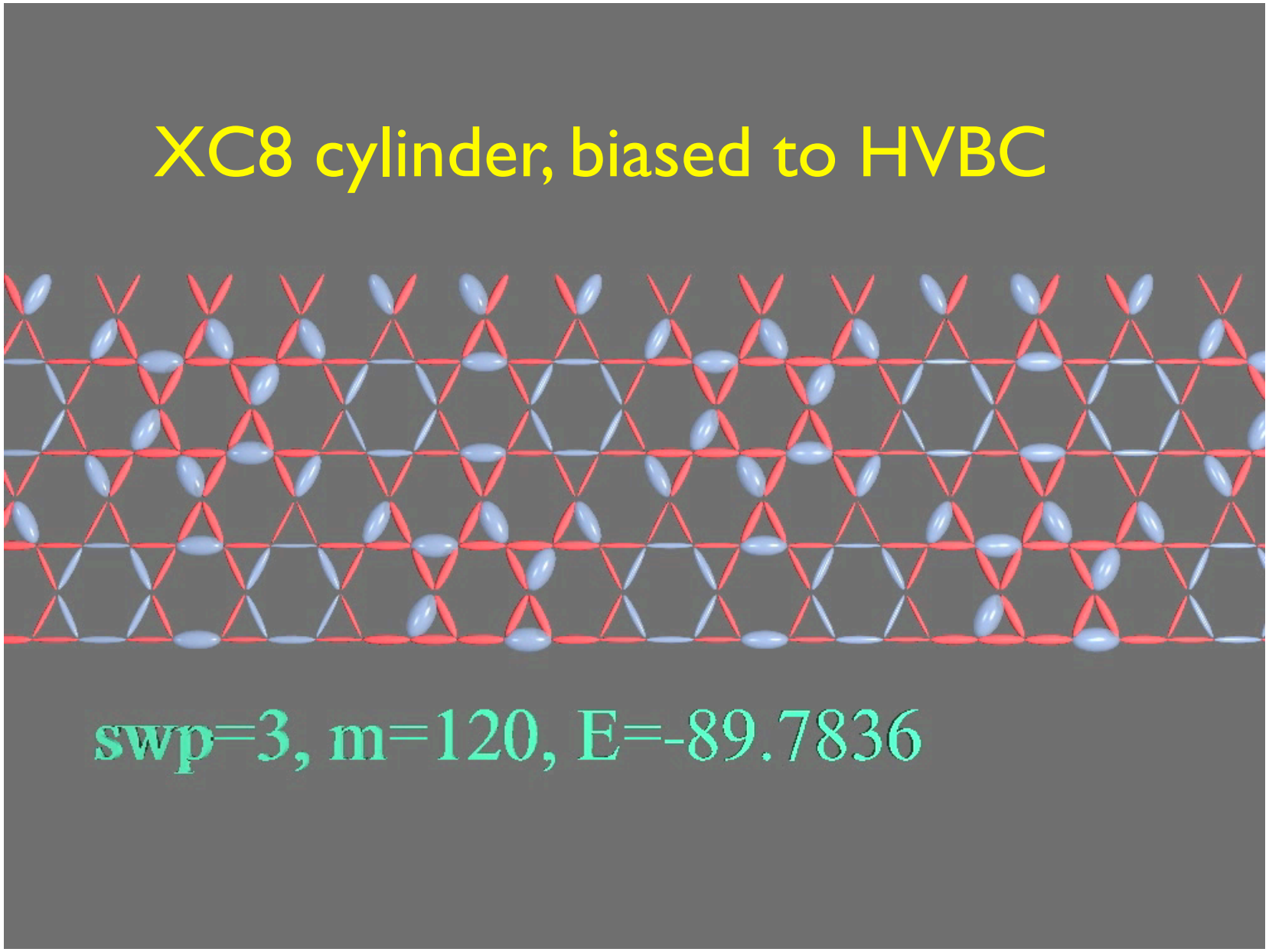
But is it instead a valence bond crystal??

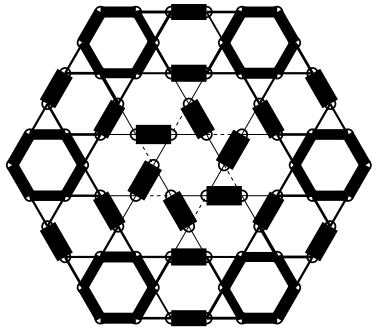


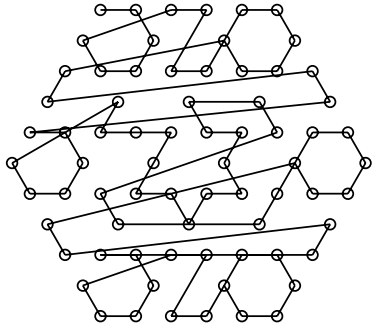



Honeycomb VB crystal: maximizes 6 site (hexagon) resonance configurations

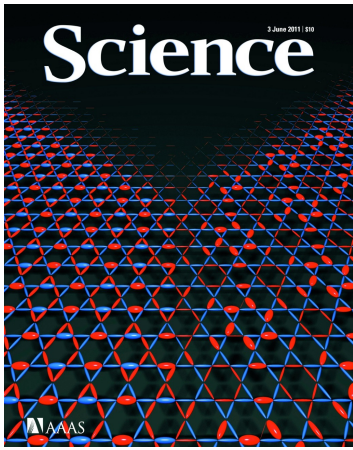
# Sample DMRG simulation on Kagome





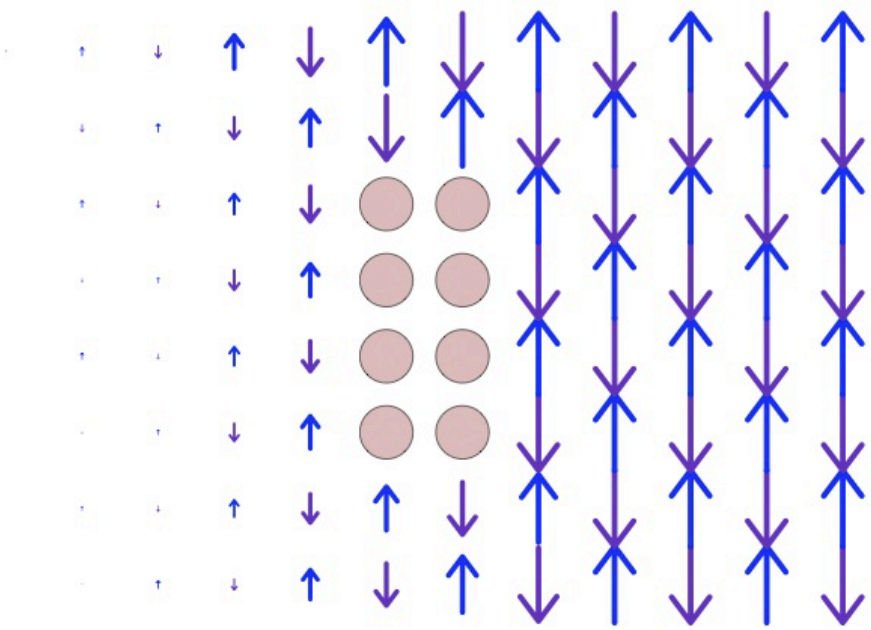
Highly biased path



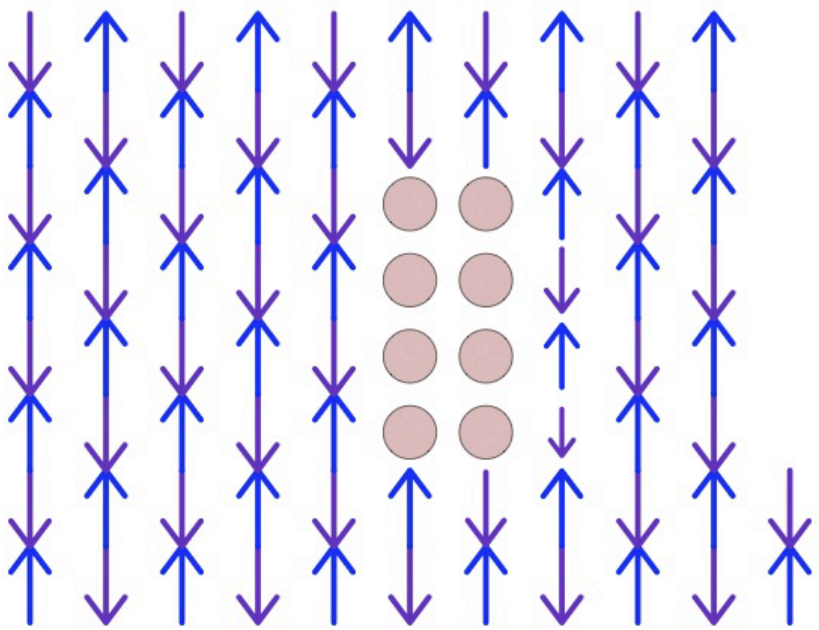

Lots more numerical experiments were performed to build a very strong case that the ground state is a spin liquid

Yan, Huse, White, Science June 5, 2011

# Doped Fermion systems: Hubbard models, etc: Stripes forming in a t-J cylinder with 8 holes



E = -31.7287 m = 70



E = -30.7350 m = 40

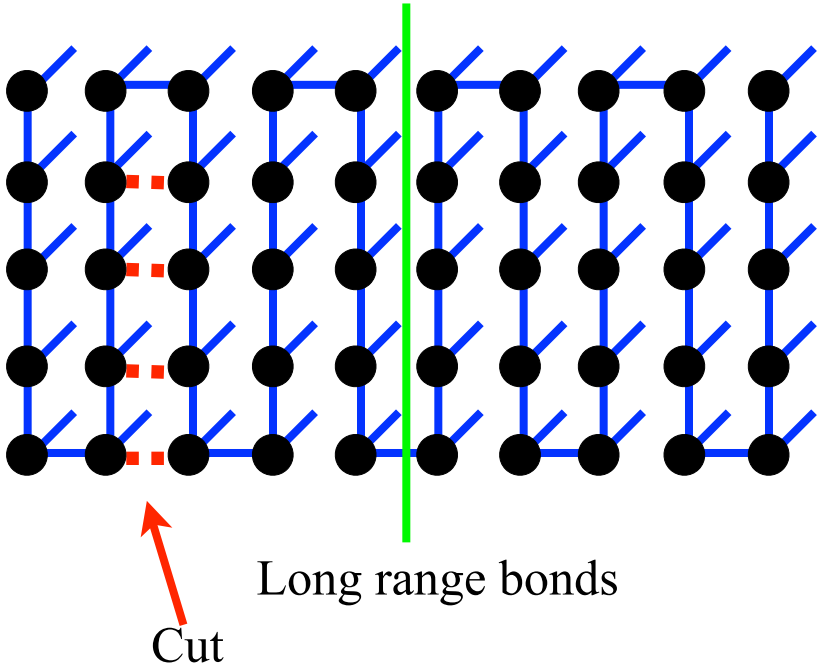
t=1, J=0.35
t'=t''=0
8 holes
No pinning fields

Same system, but initial magnetic pinning favors a single anti phase stripe

White and Scalapino

# Tensor networ methods for 2D systems

Traditional DMRG method (MPS state)

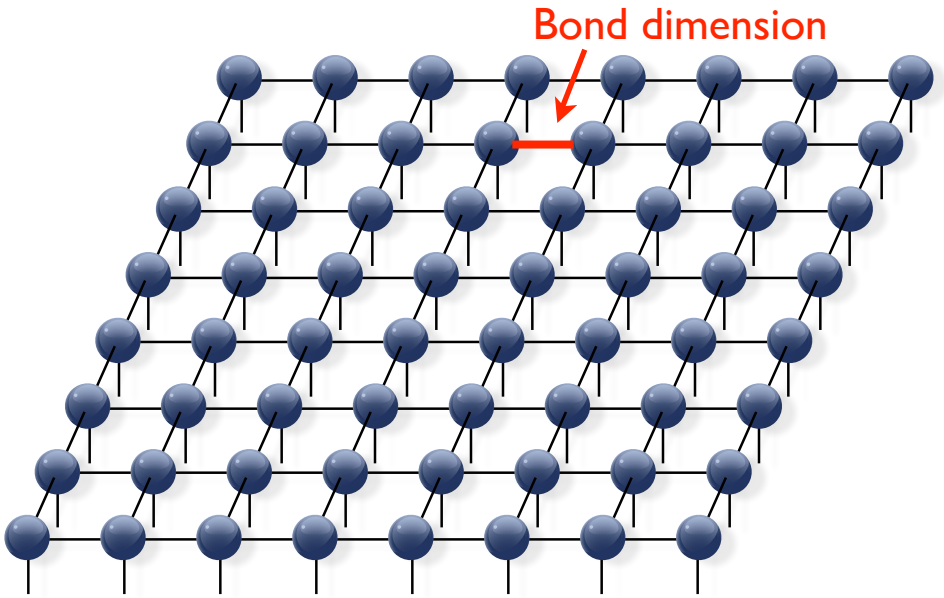



Entropy S ~ $L_y$ ("area law")
Bond dimension m ~ exp(a $L_y$)

Calc time: $L_x L_y^2 m^3$;
Practical calculations: m ~ 10000,
$L_y$ ~ 12-14 for S=1/2 Heisenberg

## PEPS

projected entangled-pair state

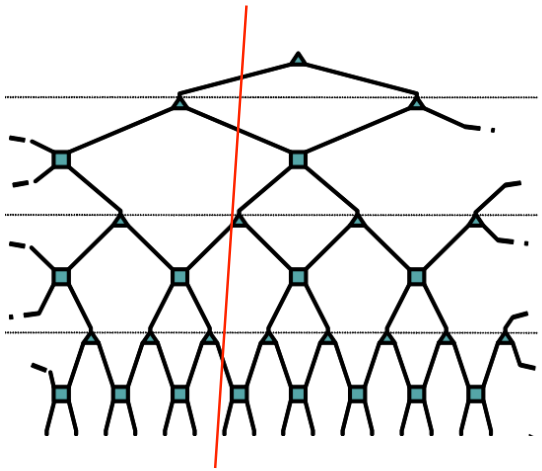



Verstraete and Cirac, cond-mat/0407066

Naturally obeys Area Law
Can work directly with $L_x$ ,$L_y \to \infty$
Calc time: ~$m^{12}$;
Practical calculations: m ~ 15,
S=1/2 Heisenberg

Crossover in accuracy as a function of width for DMRG, $L_y$ ~ 10

# MERA: multiscale entanglement renormalization ansatz

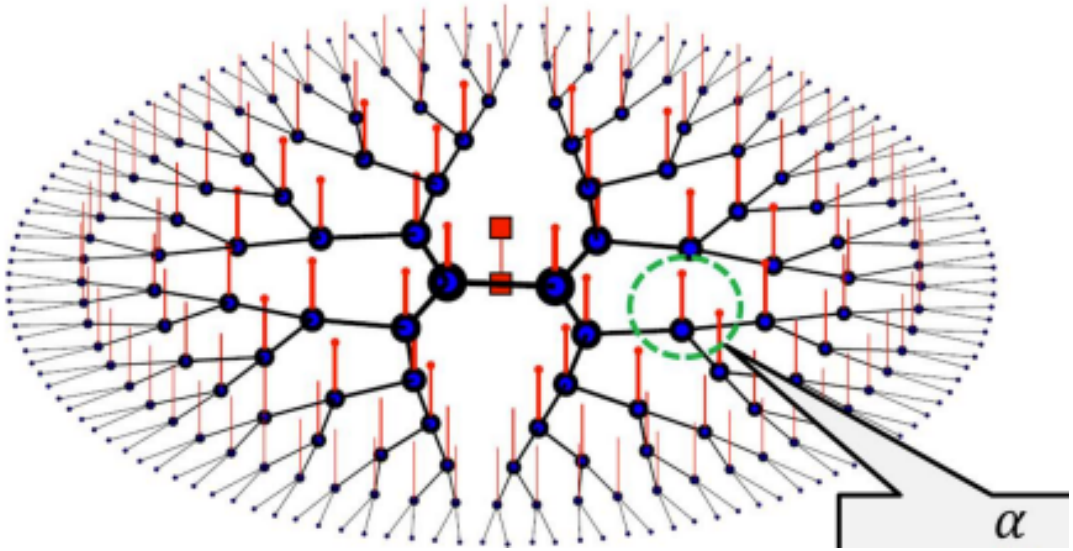


Each link cut by the red line carries entanglement across the system

Vidal, PRL 99, 220405 (2007)

Optimally encodes quantum critical systems with ln(L) corrections to the area law

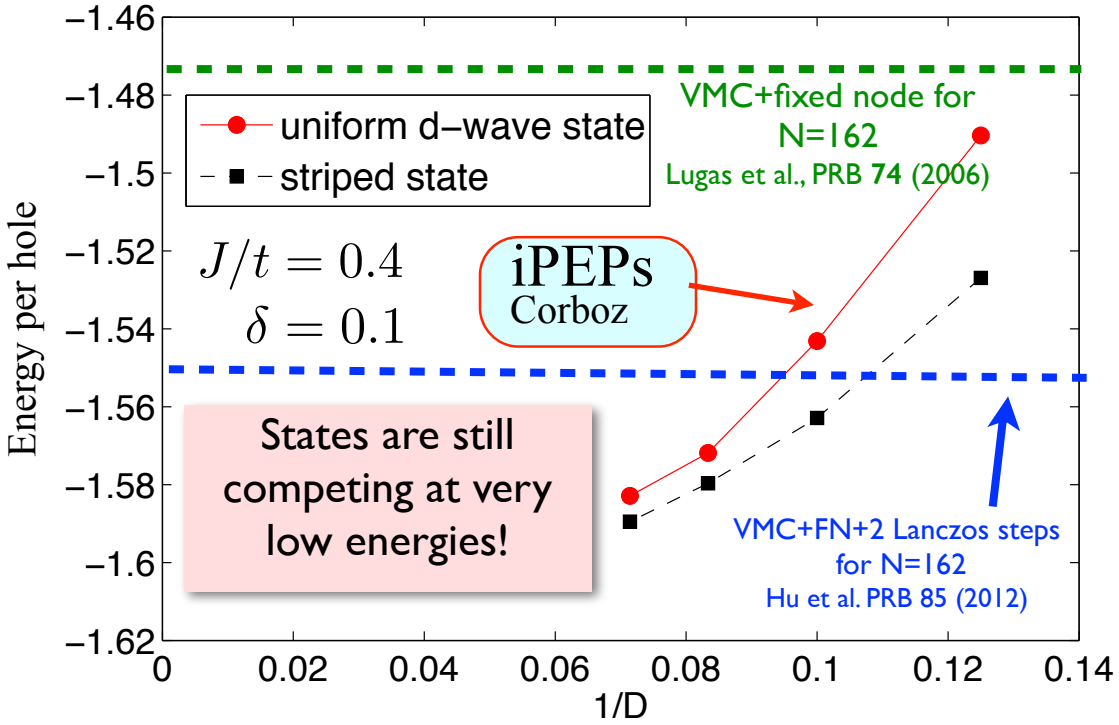
MERA encodes CFT's beautifully. It also may tell us how the AdS/CFT correspondence works (Swingle)

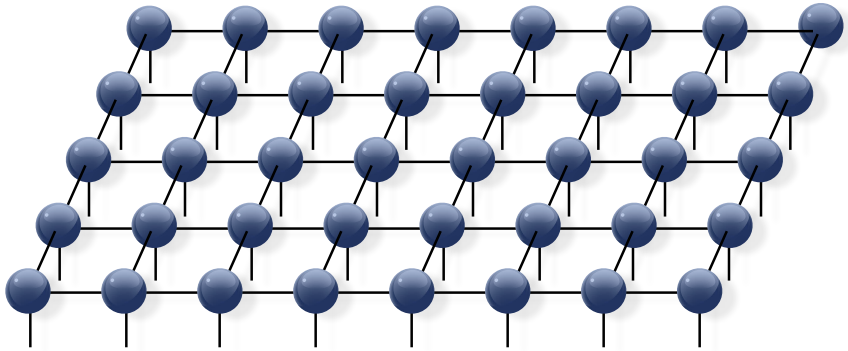



Exact holographic map
Qi, arxiv 1309.6282

Note: close relationship to wavelet transforms; see my Perimeter talk, August '13

# PEPS applied to the t-J model (Corboz, et al)



**Simple t-J model: energy differences are too close to resolve competing states, despite excellent accuracy!**

**PEPS is clearly competitive with the best alternative approaches for the t-J model. If the competition between phases wasn't so close, we would know the answer!**

# Summary

- Tensor networks methods (including DMRG) are natural low entanglement methods which are having a very big impact on computational condensed matter and are now becoming crucial conceptual tools to understand quantum phases.