The Density Matrix Renormalization Group

- Historical development: Numerical RGs, particle in a box analysis, density matrix idea and algorithm
- Quantum information, entanglement, matrix product states
- A few 2D examples and summary
- References:
  - S.R. White, PRL 69, 2863 (1992); PRB 48, 10345 (1993);
  - U. Schollwöck, RMP 77, 259 (2005).

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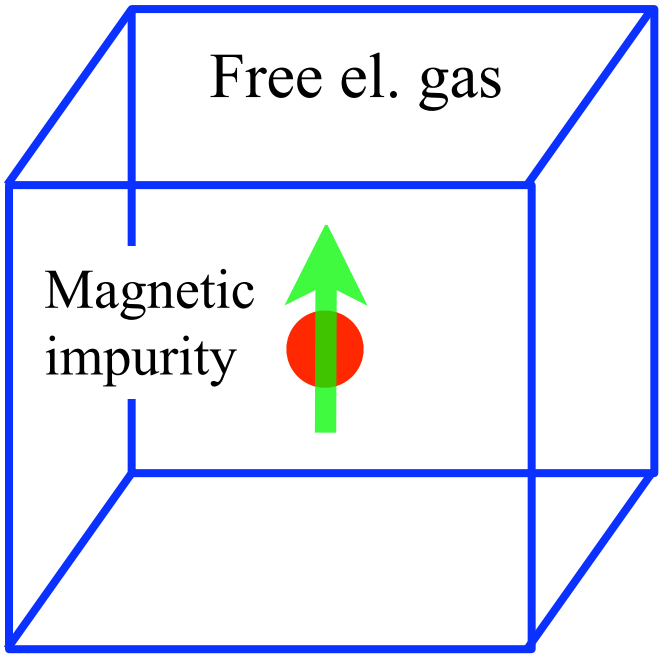
RG Approach

- Solve a high energy, short length part of the problem first
- Build solution into a new effective Hamiltonian which omits the highest energies
- Iterate, until you just have long-wavelength, low energies left
- [Fixed point analysis, scaling, critical behavior, etc]

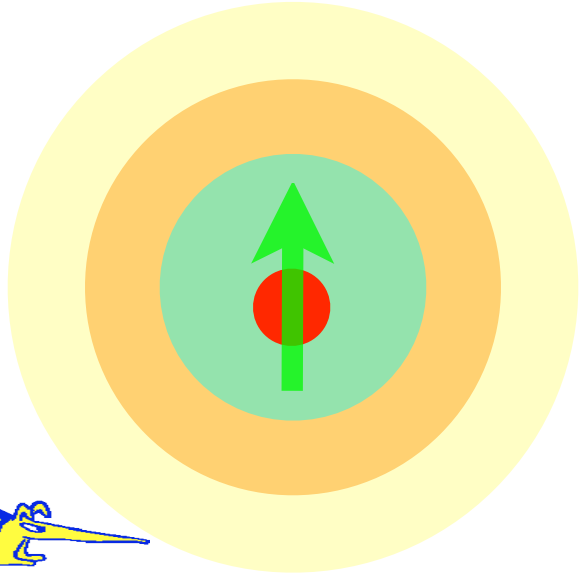
Wilson's numerical RG for a Kondo impurity



Standard Feynman diagrammatic perturbation approaches failed in the 60's.

Successes:

- "Poor man's scaling", Anderson et. al. 1970
- Wilson's NRG, 1975
- Exact Bethe ansatz solution, 1982



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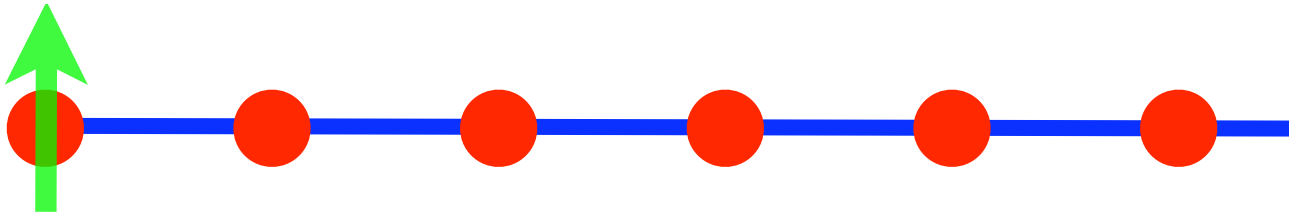
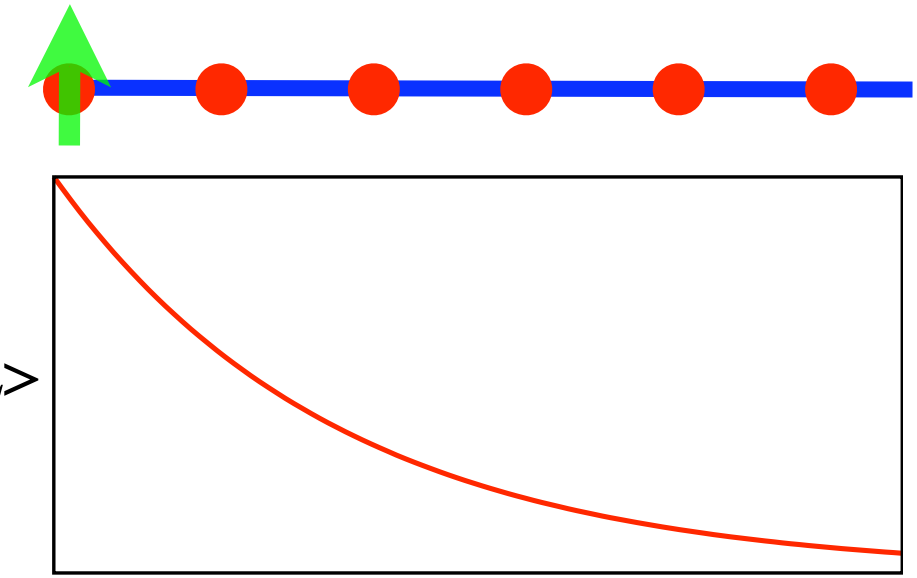
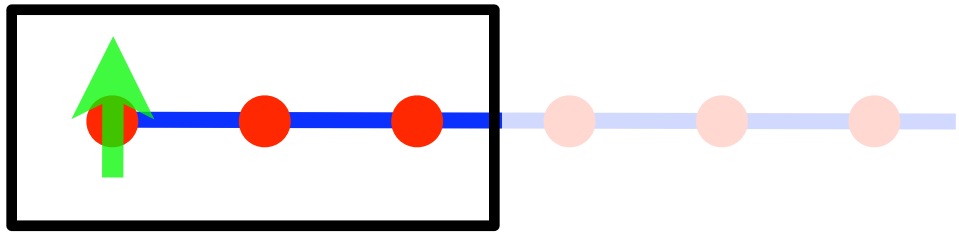


Wilson's logarithmic basis

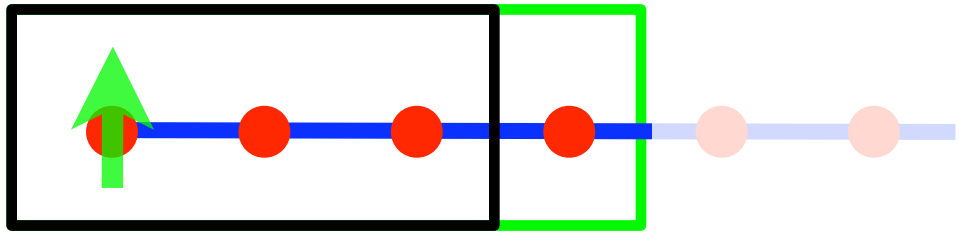
Wilson's numerical RG



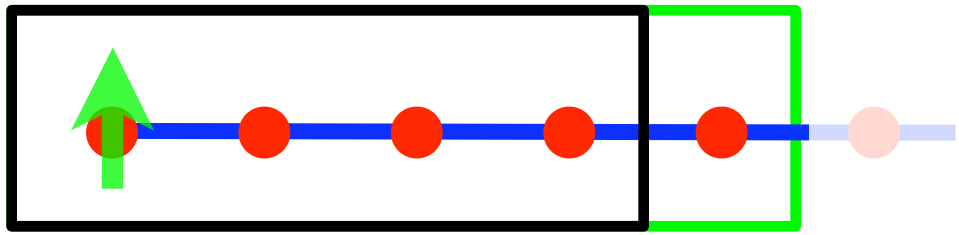
Treat short distance,
high energy scales first



Diagonalize block, keep m lowest energy states

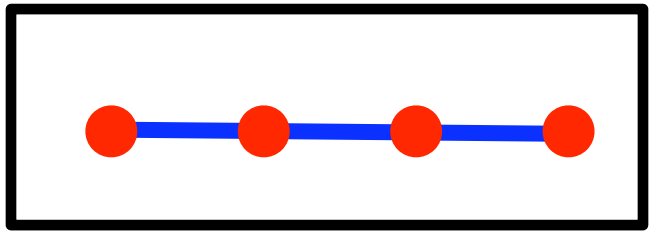


Add one site, diagonalize block Hamiltonian again, keeping m states

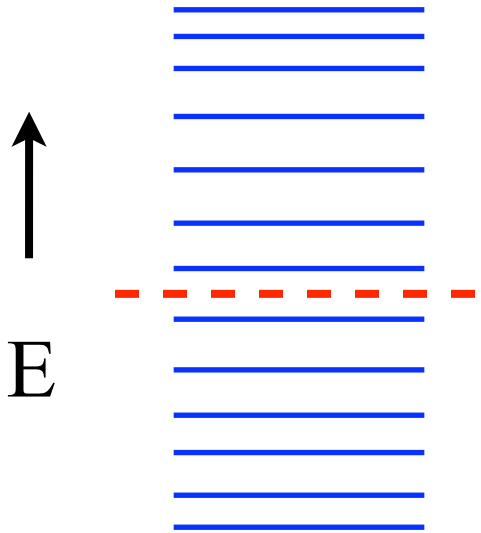


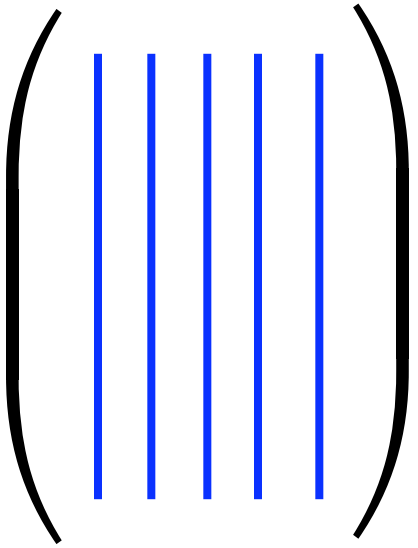
Key point:
Keep track of H through m x m operator and transformation matrices

Numerical RG in detail



Block Matrix H



$O =$ 

2^N or m^2 or $2m$

Eigenvectors

m

$$H' = O^T H O, \quad S'^{z}_{i} = O^T S^{z}_{i} O, \quad \text{etc}$$

4. Combine two adjacent B''s.

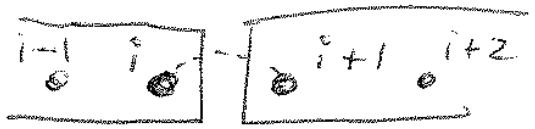
More Details-adding 2 blocks

$$B'' = B' \otimes B'; \qquad |i_1 i_2\rangle = |i_1\rangle |i_2\rangle$$

(B'': m^2; B': m; B': m)

$$H'' = H' \otimes \mathbf{1} + \mathbf{1} \otimes H' + \text{connecting terms}$$

Typical connecting term: $S_i^z S_{i+1}^z$ →

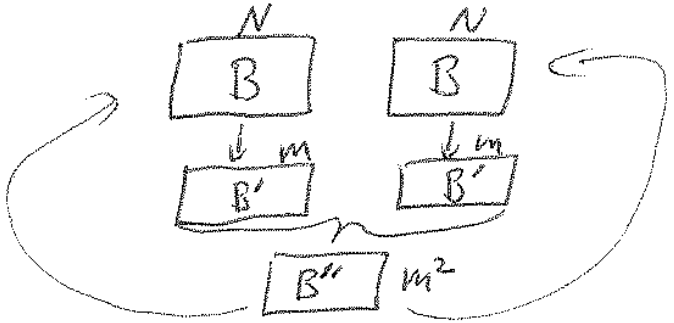


$$[S_i^z S_{i+1}^z]'' = S_i^{z\prime} \otimes S_{i+1}^{z\prime}$$

translation

$$[S_i^z S_{i+1}^z]''_{j_1 j_2, j_1' j_2'} = [S_i^{z\prime}]_{j_1 j_1'} [S_{i+1}^{z\prime}]_{j_2 j_2'}$$

5. Replace B by B'' and iterate.



After 1st iter, $N = m^2$

What justifies the truncation?

1. We want the ground state and we are throwing out high energy states (of small blocks).

2. In limit "connecting terms" are small, perturbation theory justifies it.

3. Detailed analysis of structure of H for impurity problems.

Wilson's Numerical RG: Successes and Failures

- Successes:
  - Impurity problems: falling energy scales
  - ?
- Failures:
  - Real space RG
    - Block + Block
    - Block + site
- Why does it fail?

Test case–1D particle in a box

Continuum version: $H = -\frac{\partial^2}{\partial x^2}$; $\psi(0) = \psi(L) = 0$.

Lattice version:

Ground state:

excited state:

$$H = \begin{pmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ 0 & & & & \ddots \end{pmatrix}$$

Exercise: find exact E-vals.

This problem was studied as a test case for why RG fails by Wilson in 1986 (unpublished).

In this 1 particle problem, instead of adding blocks using direct products $\otimes$, we use direct sums $\oplus$. Number of states $= L$, not 2^L or 4^L.

Before $\psi_{ij} = u_i v_j$

now $\psi = \begin{pmatrix} u \\ \hline v \end{pmatrix}$

Procedure

$$H_{\text{system}} = \begin{pmatrix} H & T & & & 0 \\ T^\dagger & H & T & & \\ & T^\dagger & H & T & \\ & & T^\dagger & H & T \\ 0 & & & & \ddots \end{pmatrix}$$

Initially $H = (2)$ and $T = (-1)$.

1. Combine two blocks:

$$H' = \begin{pmatrix} H & T \\ T^\dagger & H \end{pmatrix} \qquad T' = \begin{pmatrix} 0 & 0 \\ T & 0 \end{pmatrix}$$

2. Diagonalize H', getting eigenvectors V_ℓ
3. Form matrix O

$$O = \begin{pmatrix} \vdots & \vdots & & \vdots \\ V_1 & V_2 & \dots & V_m \\ \vdots & \vdots & & \vdots \end{pmatrix}$$

discard V_{m+1} to V_N

(After 1st couple of iters, $N = 2m$.)

4. Change basis and truncate:

O assumed real

$$H'' = O^T H O \qquad T'' = O^T T O$$

$m \times m \quad m \times N \quad N \times N \quad N \times m$

5. Replace H and T by H'' and T'' and iterate.

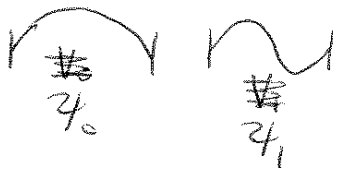
How does it do?

Test calculation: 10 blockings, keeping $m = 8$ states:

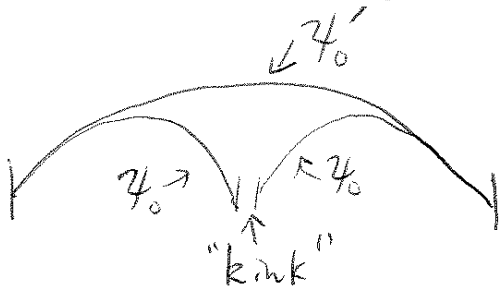
	Exact	RG
E_0	2.351×10^{-6}	1.9207×10^{-2}
E_1	9.403×10^{-6}	1.9209×10^{-2}
E_2	2.116×10^{-5}	1.9214×10^{-2}
E_3	3.761×10^{-5}	1.9217×10^{-2}

It performs terribly. Why? Look at continuum states.

Isolating a block sets ψ to 0 at the edges (fixed BCs).



→ Particle-in-a-box eigenstates.



Any state formed by low-lying states has a "kink" in the middle. To remove kink, need to keep almost all states.

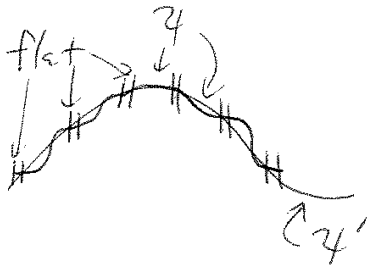
How to fix it (White and Noack, PRL **68**, 3487 (1992).)

One approach involves different boundary conditions.

Periodic BCs? Only slightly better. Get "staircases" in excited states.

Free BCs? (Slope vanishes at edges.) Again, only slightly better (flat spots).

$$\begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & \\ & & & \ddots \end{pmatrix} \longrightarrow \begin{pmatrix} 1 & -1 & & \\ -1 & 2 & -1 & \\ & -1 & 2 & \\ & & & \ddots \end{pmatrix}$$



One solution: Combine states from different BCs.

- States must be orthogonalized.

Example: Fixed-Free combination.

Use $m/4$ states from each of Free-Free, Fixed-Free, Free-Fixed, Fixed-Fixed BC's. (4 diagonalizations each iteration)

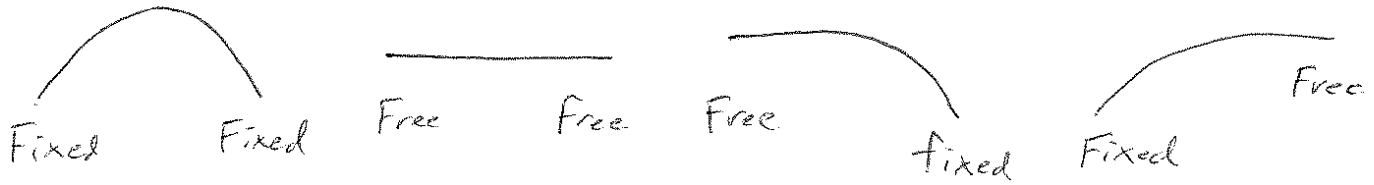
$$\tilde{O} = \begin{pmatrix} \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\ V_1^{ff} & \cdots & V_{m/4}^{ff} & V_1^{fo} & \cdots & V_{m/4}^{fo} & V_1^{of} & \cdots & V_{m/4}^{of} & V_1^{oo} & \cdots & V_{m/4}^{oo} \\ \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \end{pmatrix}$$

$O = \text{Gram-Schmidt}(\tilde{O})$ (Otherwise procedure is identical)

Test case: $m = 8$ states, 10 blockings:

	Exact	Standard RG	Fixed-Free
E_0	2.3508×10^{-6}	1.9207×10^{-2}	2.3508×10^{-6}
E_1	9.4032×10^{-6}	1.9209×10^{-2}	9.4032×10^{-6}
E_2	2.1157×10^{-5}	1.9214×10^{-2}	2.1157×10^{-5}
E_3	3.7613×10^{-5}	1.9217×10^{-2}	3.7613×10^{-5}

Results correct to 10 or 12 places.

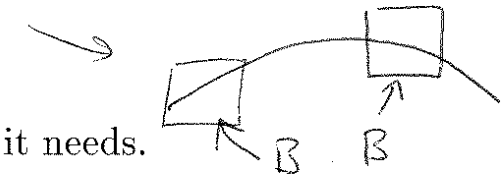


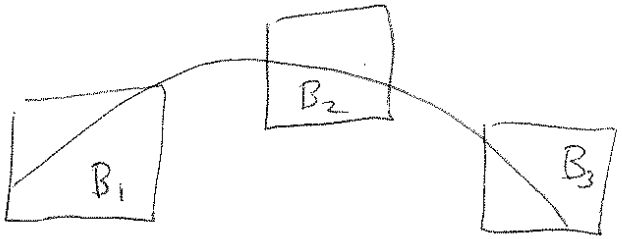
→ Other variations: periodic-antiperiodic works almost as well.

Why does varying the boundary conditions work?

When you isolate a block, that applies a particular BC to the block. The rest of the lattice, if it were there, would apply different BCs, so the states you keep aren't appropriate. You have two ways to rectify this.

1. Make each block able to represent a variety of BCs. This is what we just did with the fixed-free method.
   "Complete set" of BC's
2. Design each block to represent the exact BC it needs.





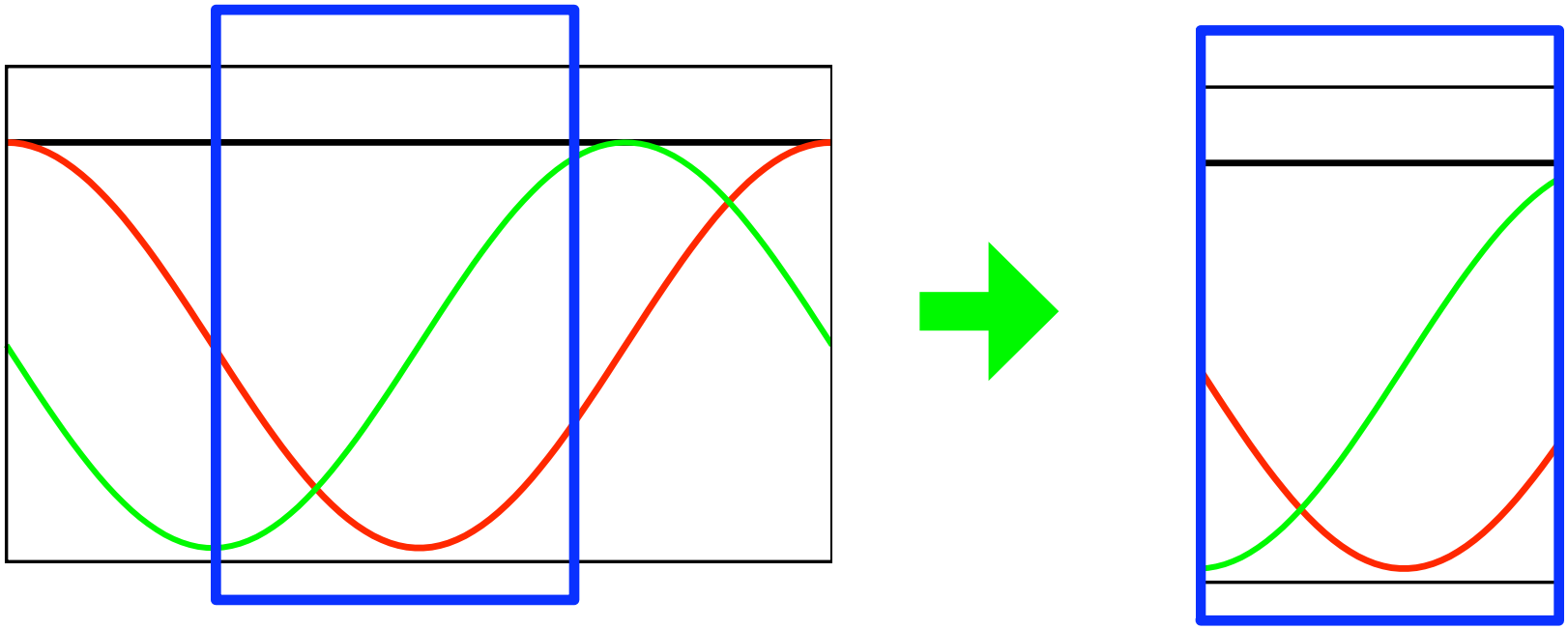
For noninteracting system to get one state, need only one style per block!

In method 2, block must know where it goes. Clearly method 2 must be iterative.

Method 1 doesn't work well for interacting systems–need too many states to represent response to lots of possible BCs. Also, it's not clear how to choose to vary the BC's in interacting systems. I tried several methods for Heisenberg chains—none worked.

Solutions to particle in a box RG (White & Noack, 1991)

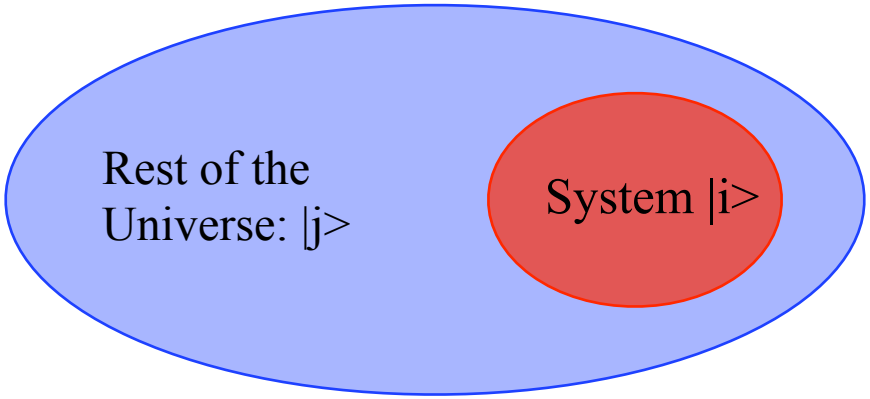
- Combination of boundary conditions
- Diagonalize a larger superblock, project out the parts of the wavefunctions in the block



- Interacting systems: multivalued projection?

Density matrix RG

- Statistical Mechanics Viewpoint (Feynman SM lectures)



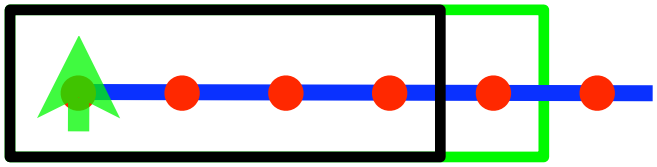
$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

$$\rho_{ii'} = \sum_{j}^{m} \psi^*_{ij} \psi_{i'j}$$

$$\langle A \rangle = \sum_{\alpha=1} w_\alpha \langle \alpha | A | \alpha \rangle$$

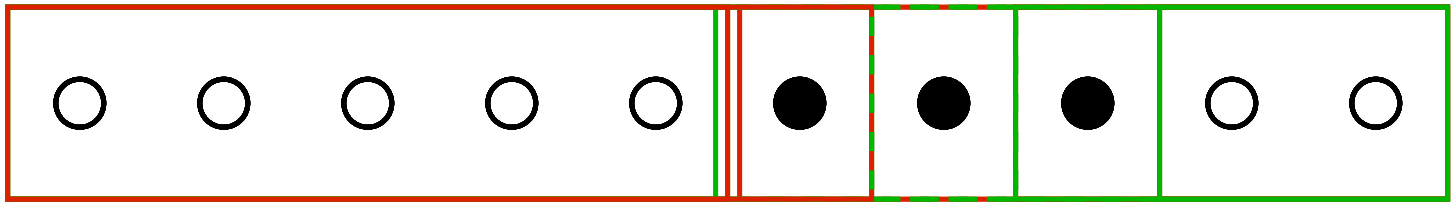
- Key idea: throw away eigenstates with small probability
- Algorithm based on this: density matrix renormalization group (DMRG, srw(1992))

DMRG Algorithm



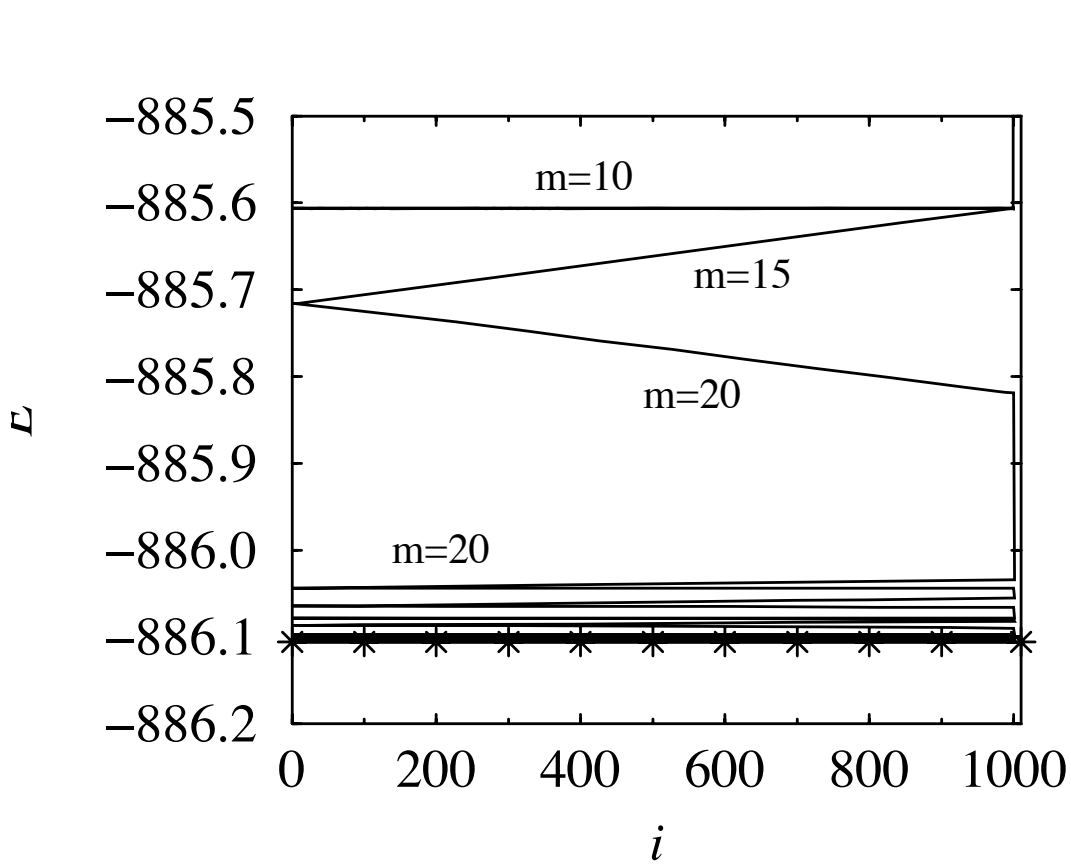
Wilson's algorithm

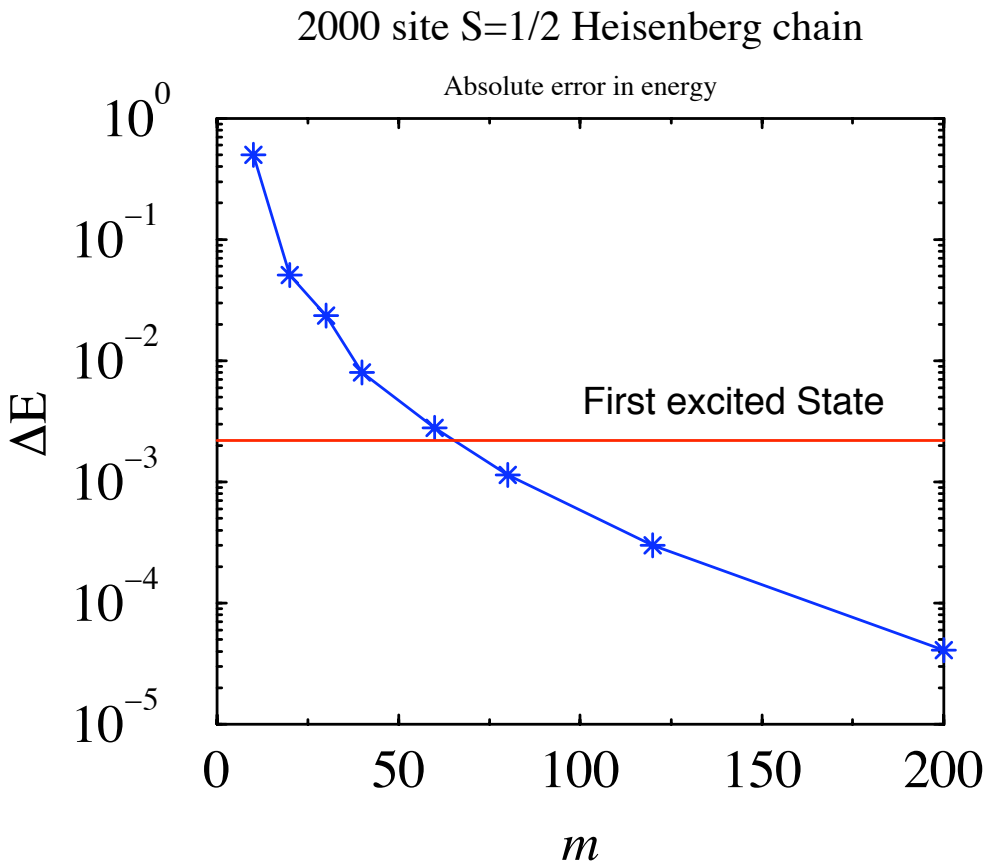
DMRG sweeps



- Diagonalization of entire system
- Construction of density matrix for block
- Transformation to new density matrix states
- Sweeps back and forth

Convergence in 1D





Comparison with Bethe Ansatz

Matrix Product States

Wilson, 1975 (NRG), Accardi (1981), Affleck et al (1988), Fannes et al(1989), Ostlund and Rommer (1995), ...

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

Vector Matrix Vector

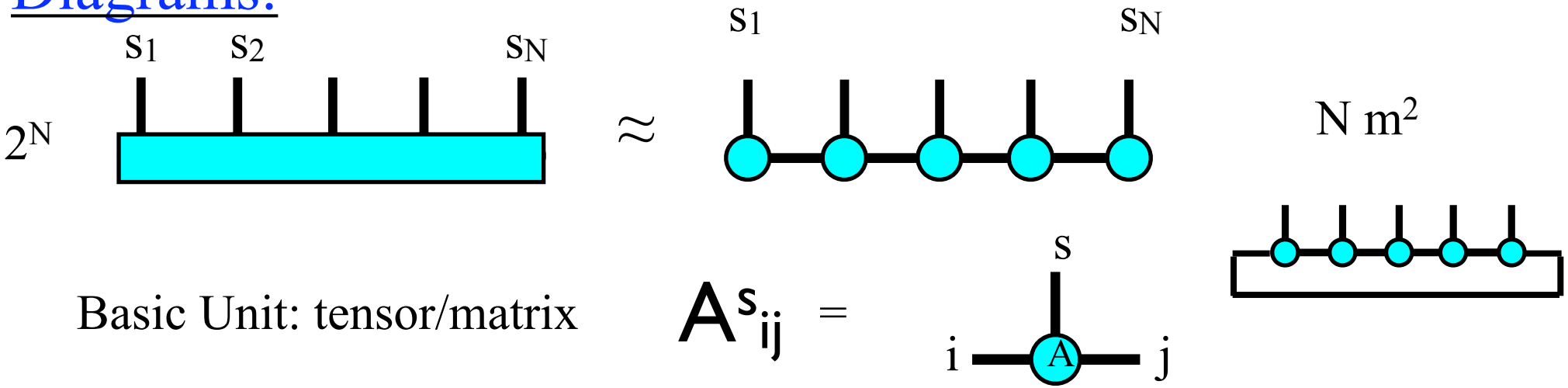
or:

$$\Psi(s_1,s_2,..s_N) = \mathrm{Tr}\{A^1[s_1]\, A^2[s_2] \ldots A^N[s_N]\}$$

All Matrices

Matrix dimension: m x m

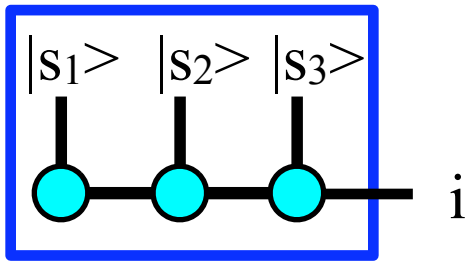
Diagrams:



What do Matrix Product states have to do with DMRG?

Both Wilson's NRG and DMRG implicitly use an MPS

Matrix A[s] represents change of basis matrix when adding one site



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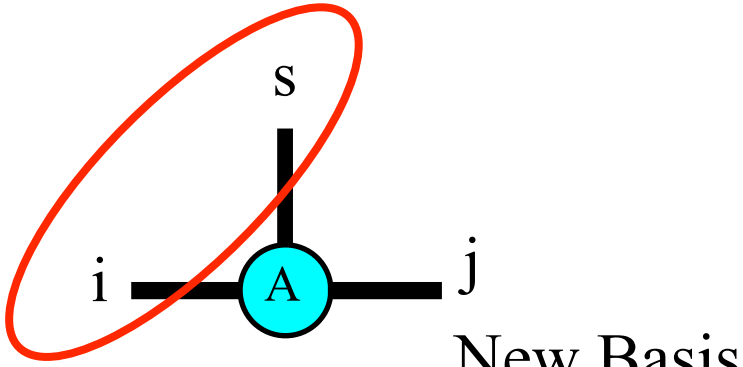
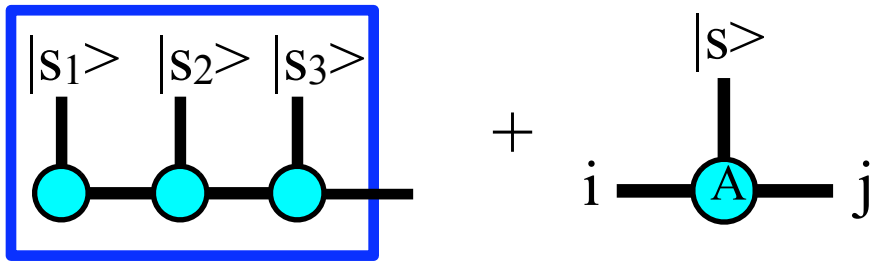




$=$ New Block

DMRG as a low entanglement approximation

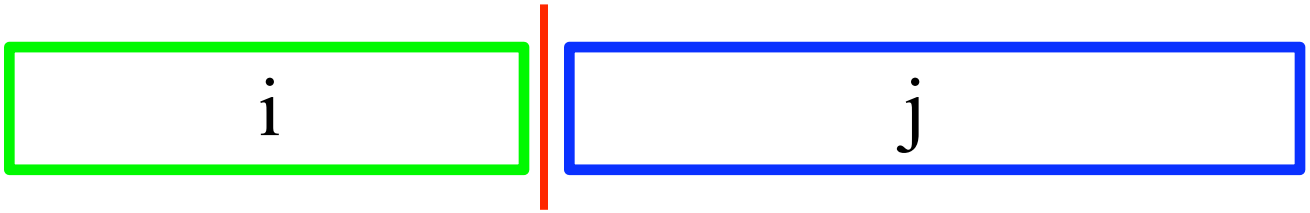
- Vidal, Verstraete, Cirac: DMRG and QI entangled.
- Entanglement: Which is more entangled?
  - 1) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle$ or
  - 2) $|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$??

Entanglement

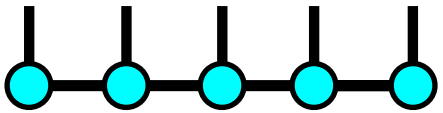
- To measure entanglement, must change to the Schmidt basis where the Ψ is diagonal:
- $\Psi=\Psi(i,j)$ i, j states of left, right subsystem
- Singular value decomposition: $\Psi = U D V$
- Singular values characterize entanglement (entropy) U,V transform to Schmidt bases
- Density matrix eigenvalues are square of singular values!
  - $\rho=U D^2 U^\dagger$
- From QI viewpoint: DMRG is a natural low entanglement approximation

A Low entanglement approximation

Measuring entanglement (QI): Schmidt decomposition

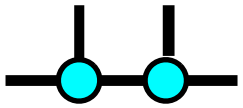


- Entropy S depends on partition and state: defined by Schmidt Decomp: $\Psi_{ij} = \sum_\alpha U_{i\alpha}\, w_\alpha\, V_{\alpha j}$ (SVD)
- $w_\alpha \geq 0$; $\sum_\alpha w_\alpha^2 = 1$; $S = -\sum_\alpha w_\alpha^2 \ln w_\alpha^2$
- <u>If entanglement is small</u>, the w_α decay fast, so truncate
- Repeat at every link: MPS !
- m ~ exp(S)
- 1D non critical: S ~ const
- 1D critical: S(N) ~ ln(N)



MPS as a class of optimal variational states

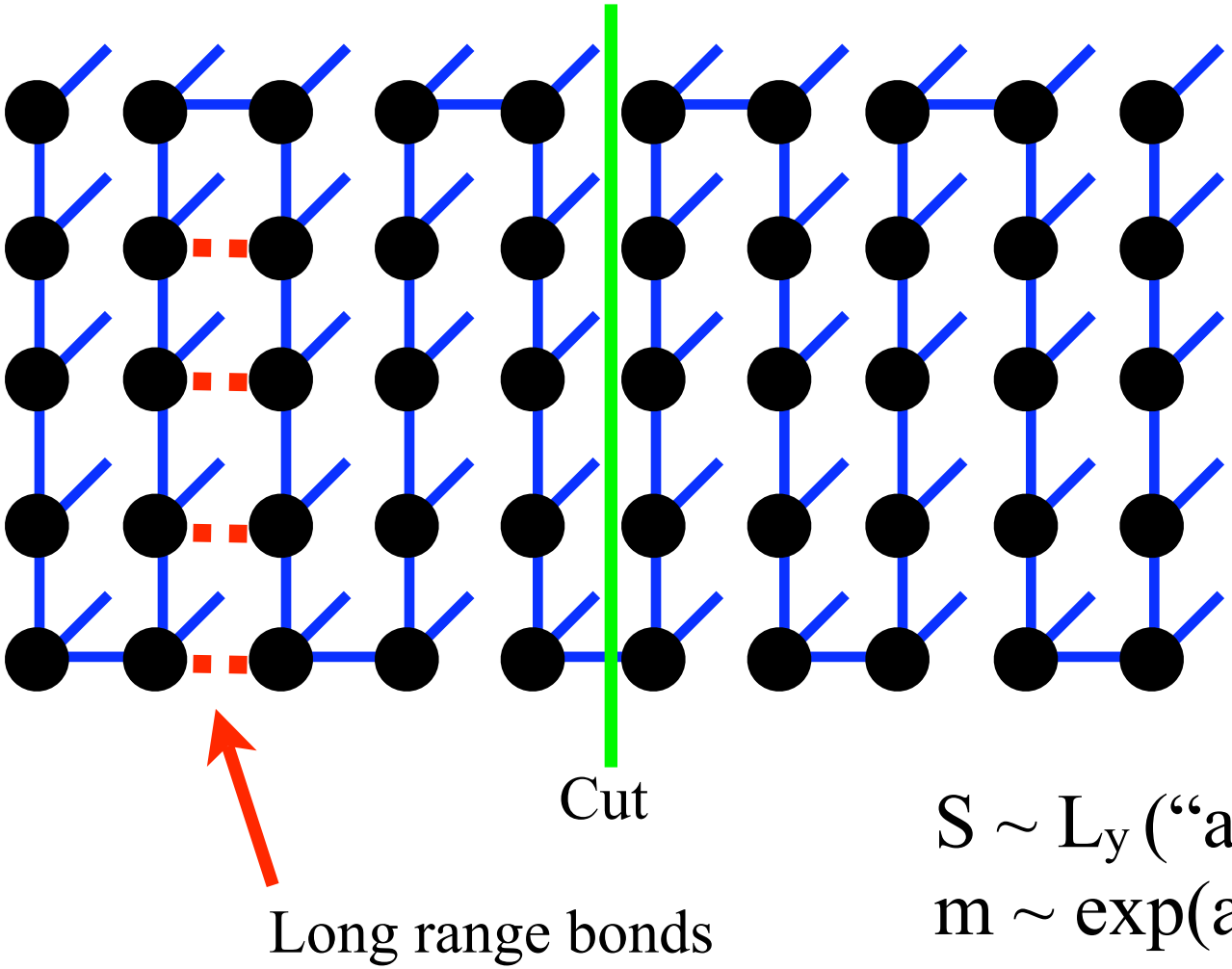
- Desirable properties of variational states
  - Completeness: exact when number of d.of f. increased ✔
  - Rapid convergence
    - 1D m ~ const, 1D non critical, m(N) ~ N^k, critical ✔
    - 2D S ~ width (area law), m ~ exp(width) ✕
  - Physical motivation ✔



    - summation over index ~ summation over fluctuations
    - near neighbor links support correlations for local Hamiltonians
    - Larger m: extra states act as conduit for longer range correlations
  - Compactness (compression, zipping) ✔
  - Computational convenience ✔
    - DMRG CPU time ~ N m^3, up to m ~ 10^4 feasible
    - Optimize one A at a time, sweep

2D algorithms

- Traditional DMRG method (MPS state)

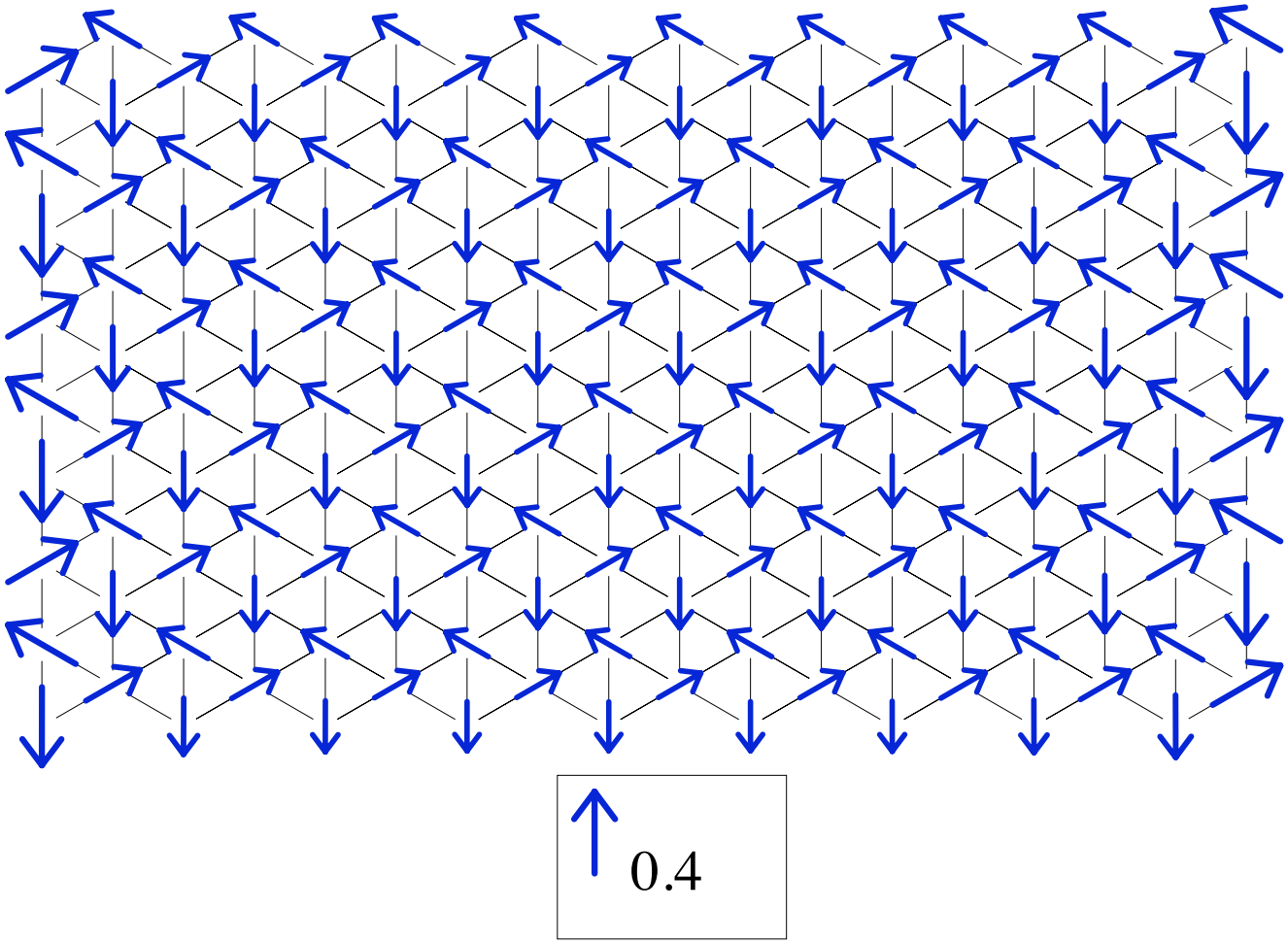


$S \sim L_y$ ("area law")

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

Calc time: $L_x\ L_y^2\ m^3$; allows $m \sim 5000$, $L_y \sim 8$-10

Traditional DMRG for triangular lattice Heisenberg model

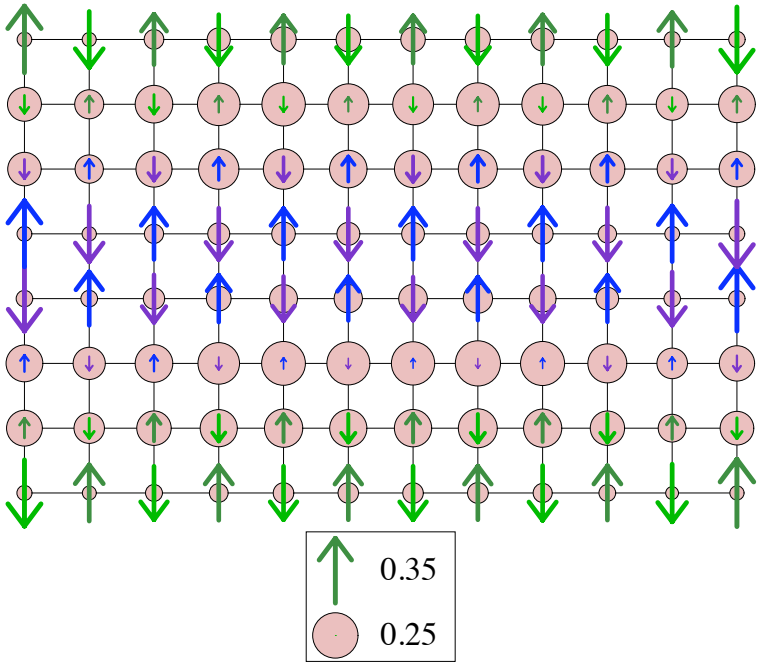


See White & Chernyshev, PRL 99, 127004 (2007)

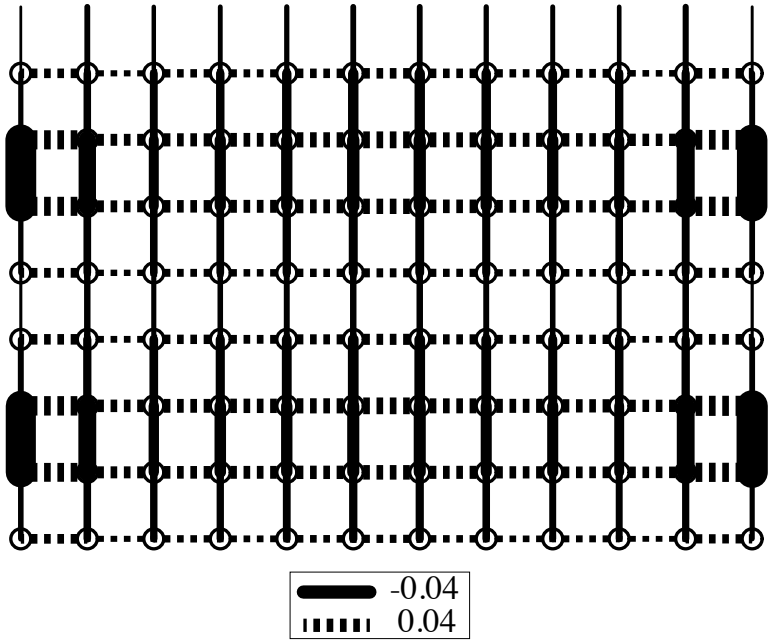
$\Delta E \sim 0.3\%, \quad \Delta \langle S_z \rangle \sim 0.01$

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

Traditional DMRG: t-J model



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

Stripes with pairing! (White and Scalapino, arxiv 810.0523)

Questions and extensions

- Extension to 2D: projected entangled pair states
  - More natural, more compact
  - High power-law computational effort
  - Which currently works better for 2D, 1D-DMRG or PEPS?
    - Latest answers: Vidal, Verstraete, Orus
- Time evolution (Schollwöck)
  - Out-of-equilibrium
  - Spectral functions
  - Finite temperature
- Matrix Product Operators (McCulloch)
- Infinite systems, scaling, disorder, QMC+DMRG...

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