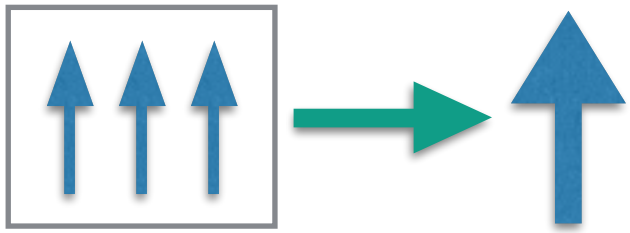
Introduction to DMRG

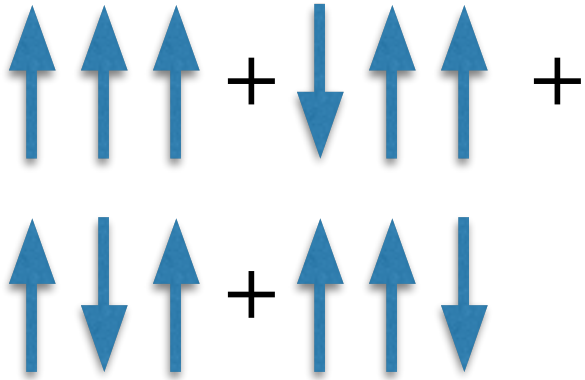
- A little history
  - DMRG in the context of real space RG methods
- The quantum information viewpoint:
  - Entanglement, the Area Law, Matrix Product states
- Some practical pointers for effective calculations
- Methods and results in 2D—mostly t-J model

What was understood before DMRG

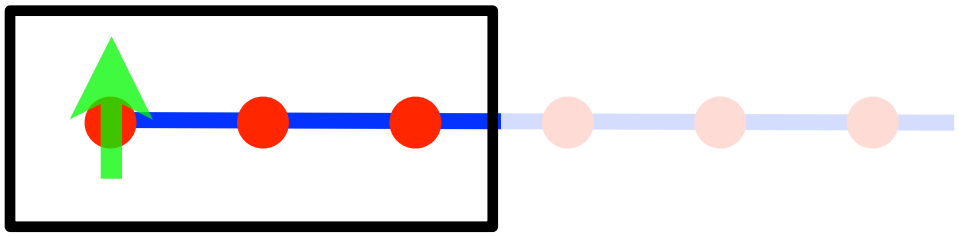
- The renormalization group was a Big Deal, and people wanted to apply it to quantum ground states. There were many possibilities… perturbation theory, path integrals, etc.
- Keeping an incomplete set of states was well known as an approximation: configuration interaction in quantum chemistry
  - CI keeps a thousands/millions of product states. This is a useful approximation for fermions if the single particle basis is chosen well (Hartree Fock)
  - Keeping sets of complicated non-product states was not thought about—and one didn't know how to think about it.
- Wilson's numerical RG treatment of the Kondo impurity problem solved a class of problems and also taught us how to keep track of complicated many particle bases.



How do you renormalize a block of sites?

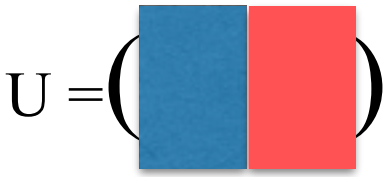


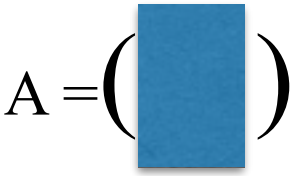
Wilson's numerical RG procedure



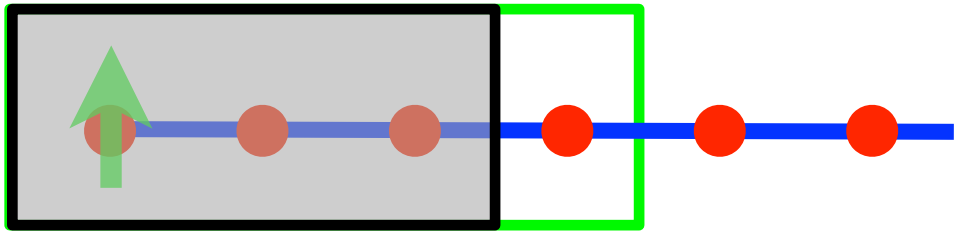
$$\tilde{H}_{\text{block}} = ADA^{\dagger}$$

Diagonalize H_{block}, keep m lowest energy states $H_{\text{block}} = UDU^{\dagger}$



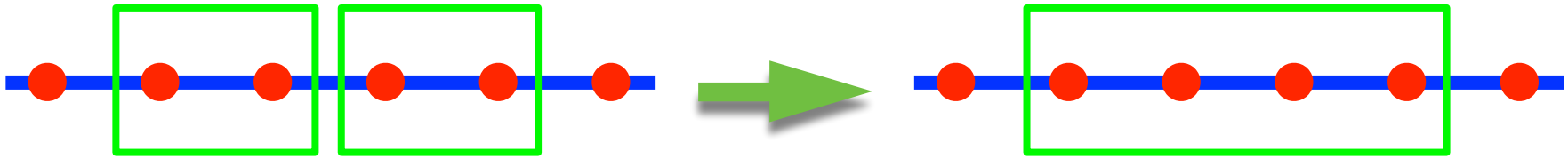


Columns = eigenvectors



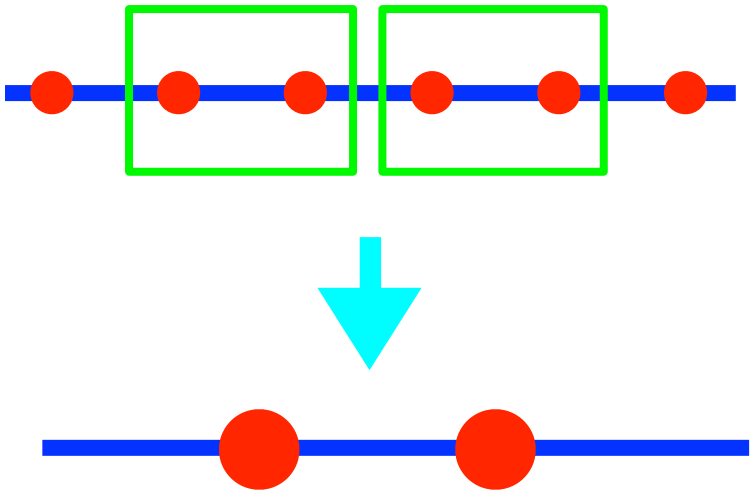
Repeatedly add sites, diagonalize H_{block}, keep lowest m states

- This procedure is justified (only) if the couplings as you move out along the chain decrease to zero (enough to solve Kondo impurity problem)



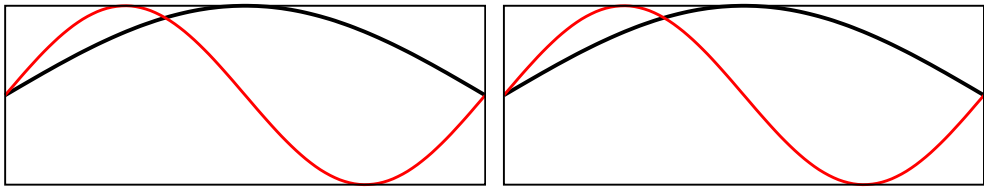
- Attempts to extend this to regular lattice problems failed

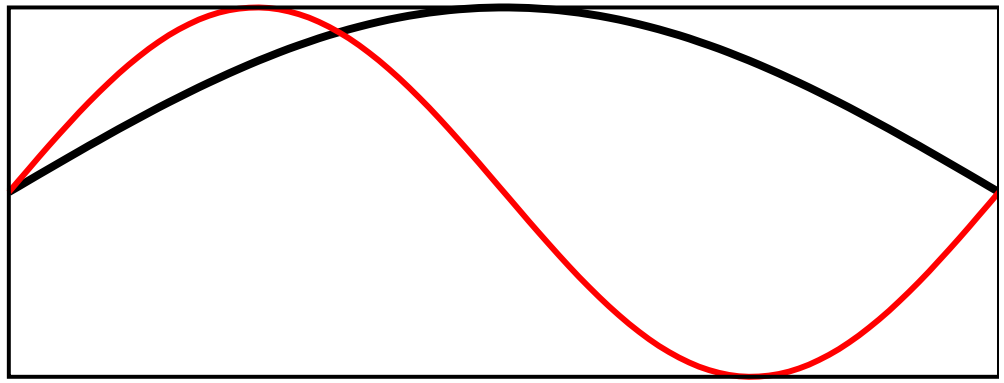
Wilson's approach applied in real space



Wilson's analysis: try it on a particle in a box!

$\Psi=0$

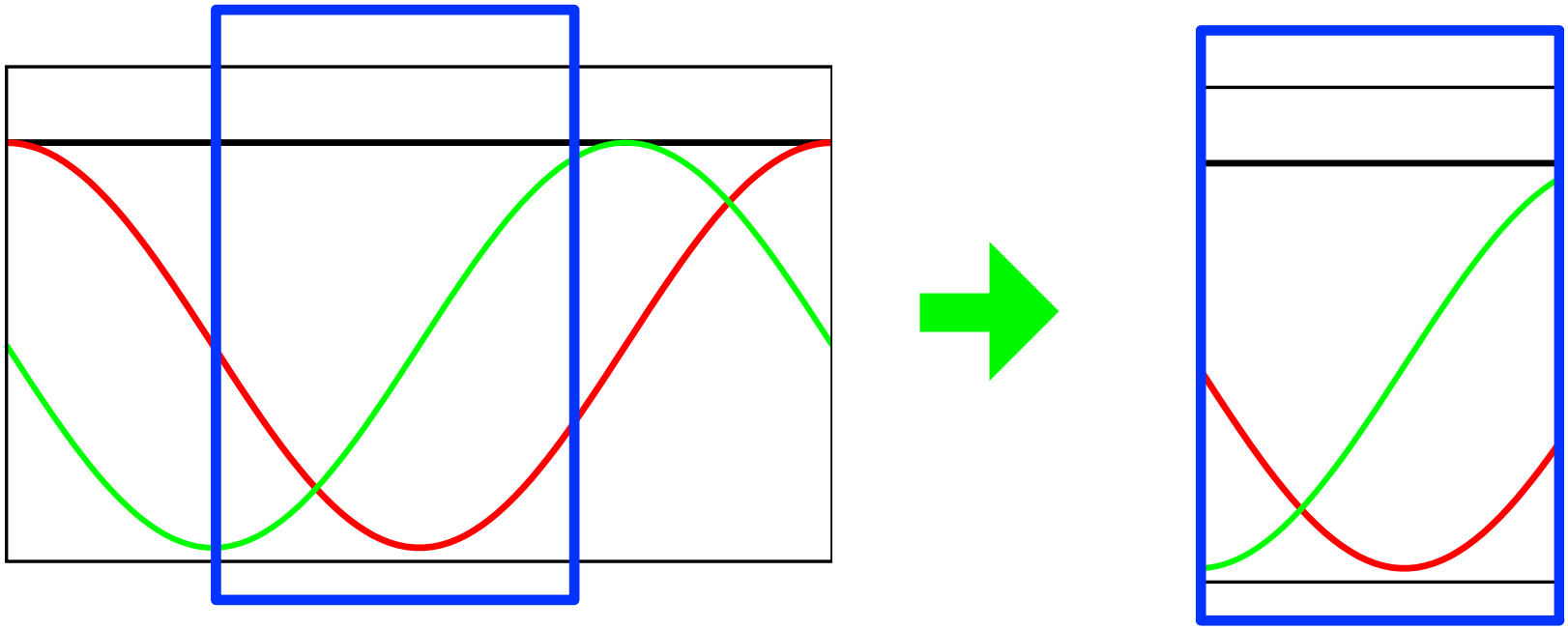




Any truncation yields "kinks" at larger scales.

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

- Combination of boundary conditions: fixed/free, etc
- Diagonalize a larger system, project out the parts of the wavefunctions in the block

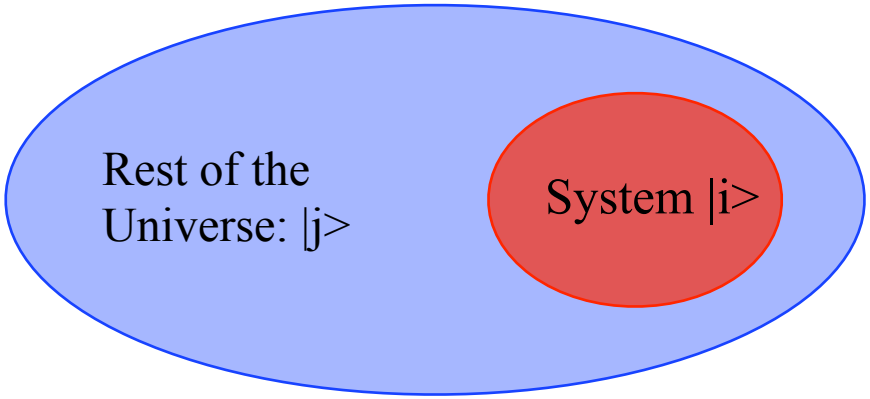


- These methods are building in the effects of the rest of the system—quantum fluctuations between the two parts, or entanglement between the two parts

Density matrix RG

What is the optimal way to truncate the states of a subsystem?

- Statistical Mechanics Viewpoint (Feynman SM lectures)



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

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

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

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

Starting around 2000, our view of DMRG changed dramatically

- Suddenly, it was realized that the ideas behind much of DMRG were already known in quantum information
- DMRG is now known as the natural 1D low entanglement approximation
- This has led to many major advances in what we can do with DMRG related methods…

Entanglement

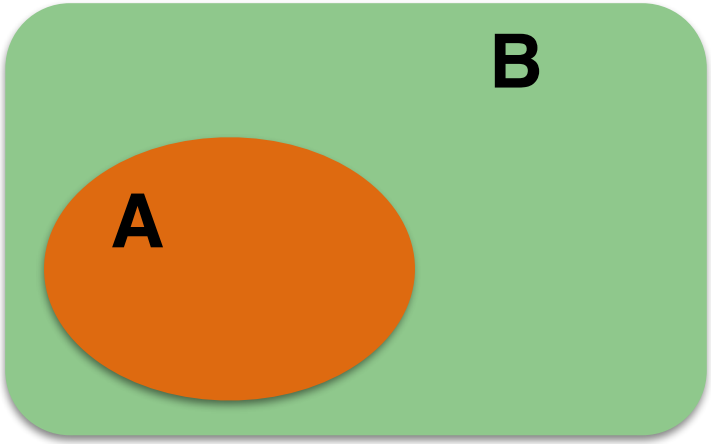
S = ln 2

$$\frac{1}{\sqrt{2}}(|\uparrow\rangle|\downarrow\rangle - |\downarrow\rangle|\uparrow\rangle)$$

Entanglement: Ψ is the sum of different terms with distinct states on the left and right

Measuring entanglement: the von Neumann entropy S ~ k ln(number of terms in Ψ) More precise defn later.

It turns out it is very interesting to look at S where there is no separation between the two parts—say, cutting a lattice spin model into two arbitrary parts



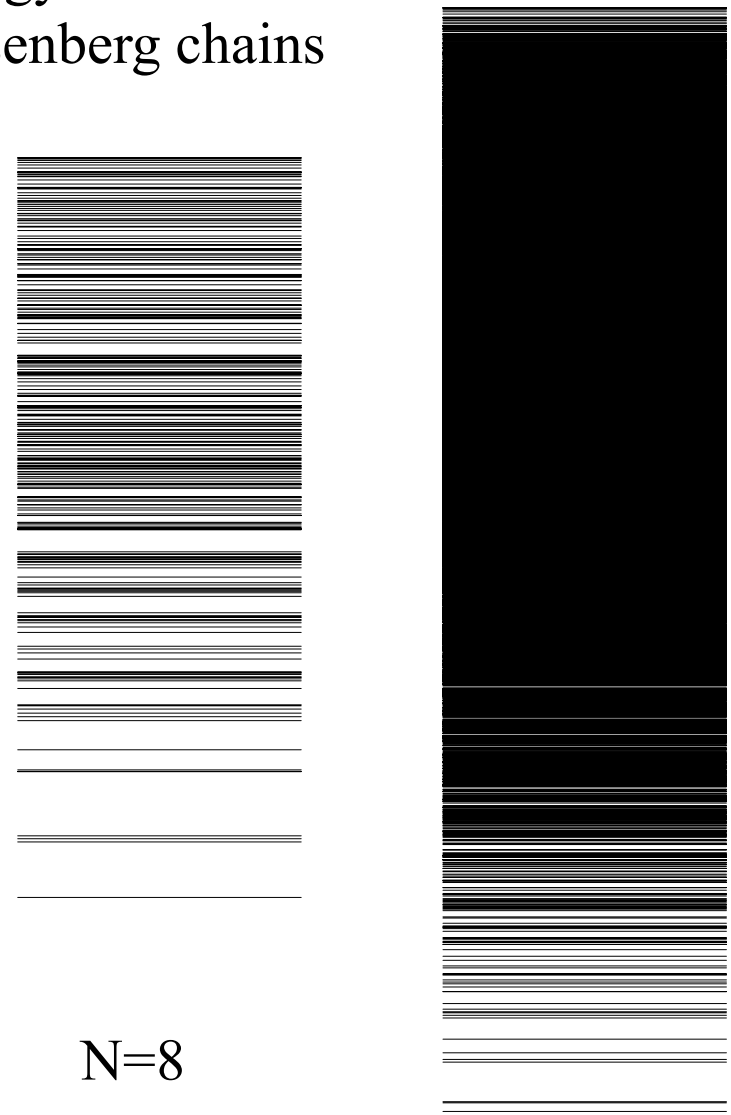
How should S depend on the size of A?

Thermodynamics: S is extensive, $S \sim N_A$

A random state: $S \sim N_A$

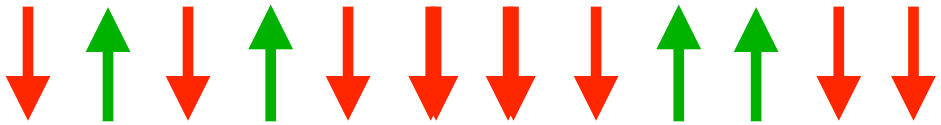
For ground states, these expectations are wrong: S ~ boundary (the "Area Law")

Energy levels of S=1/2
Heisenberg chains

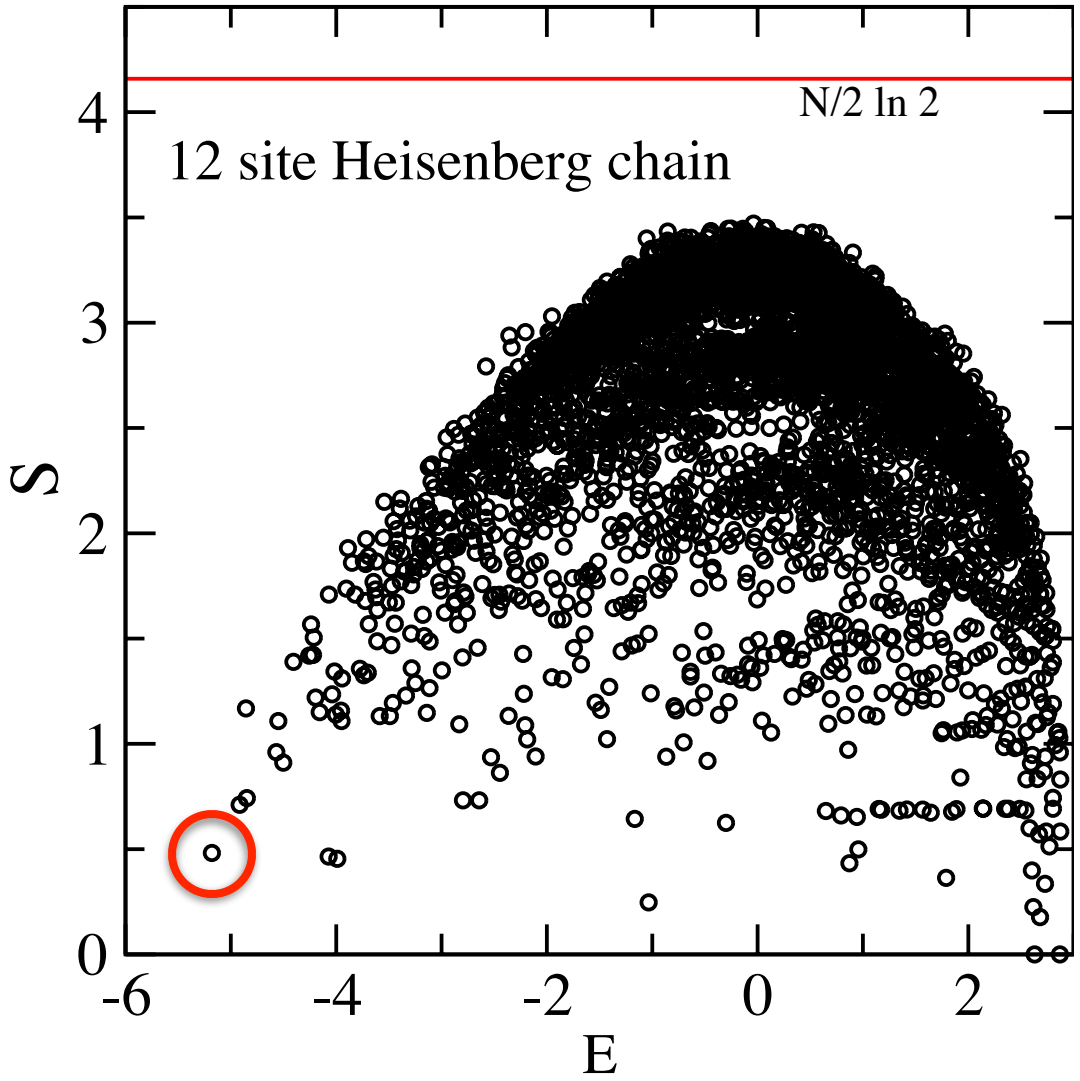


N=8

N=12



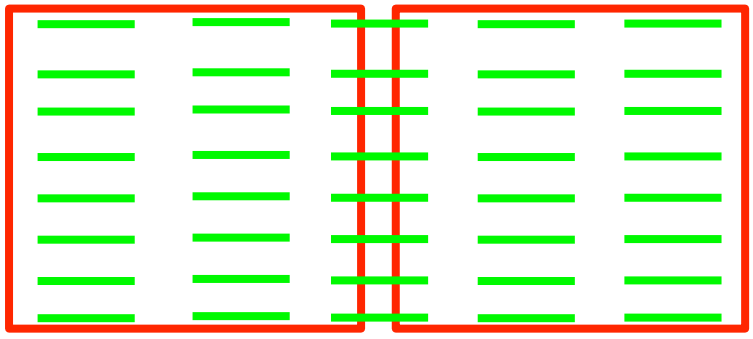
Ground states have low entanglement



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

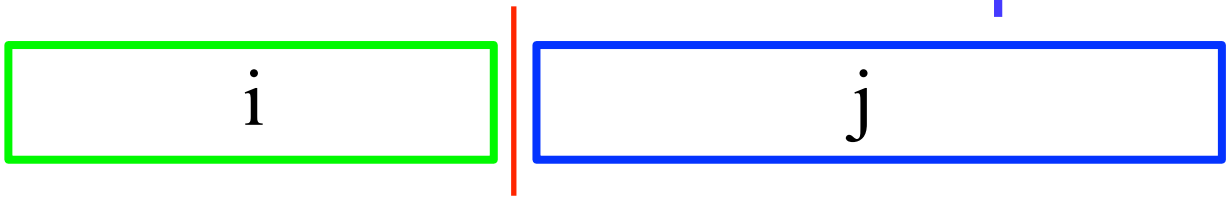
Why is the entanglement of ground states small?

- The short answer: High entanglement doesn't help reduce the energy for a physical Hamiltonian
  - Monogamy of entanglement: complicated, many-particle entanglement reduces the simple entanglement minimizing the energy
- **The Area Law**: *The entanglement entropy is proportional to the area of the cut separating the two subsystems*
  - Originally just a general expectation which seems to capture the leading behavior (and Fermi liquids have log corrections!)
  - Now proven in some cases (e.g. 1D and gapped, Hastings)
  - VB/RVB argument:



Singlet bond, ln 2 entanglement

The Schmidt decomposition

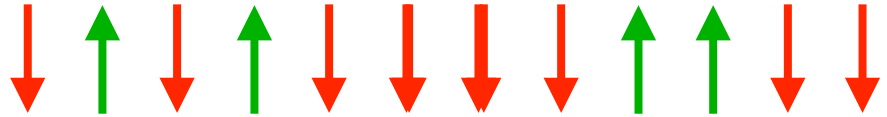


Bipartition of a quantum system

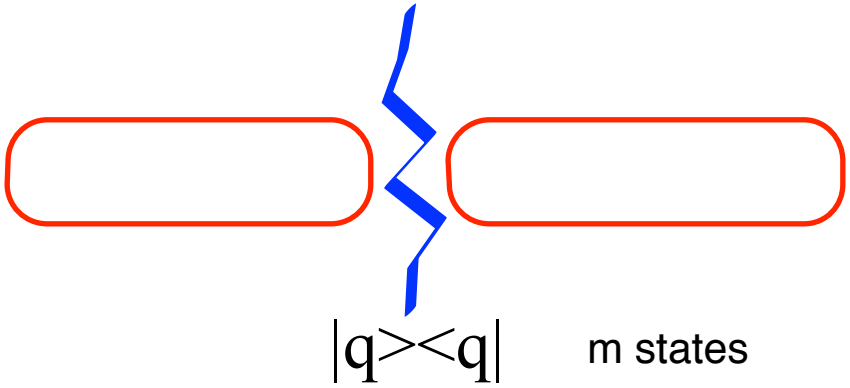
- Treat Ψ_{ij} as a matrix: perform the singular value decomposition" (SVD): $\Psi = U\,D\,V$, with U and V unitary, D diagonal, with elements λ_α
- Think of $(\lambda_\alpha)^2$ as the probability of the state $|\tilde{\alpha}\rangle\,|\alpha\rangle$; the von Neumann entanglement entropy is
  - $S = -\sum_\alpha (\lambda_\alpha)^2 \ln (\lambda_\alpha)^2$
- The Schmidt decomposition is equivalent to diagonalizing the reduced density matrix of one side (density matrix RG)

- How can we exploit this to simulate quantum systems?? Throw away the very low probability Schmidt states

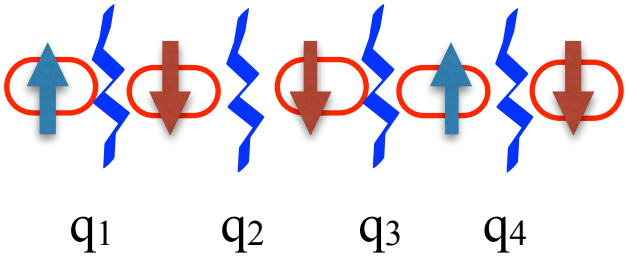
Exploiting low entanglement: 1D case



Low entanglement ⇒ Few quantum fluctuations across a cut ⇒ Represent state using a few (special) states



Repeat this "compression" on every link:



$A[s_1]_{q1\,q2}\ B[s_2]_{q2\,q3}\ C[s_3]_{q3\,q4}$

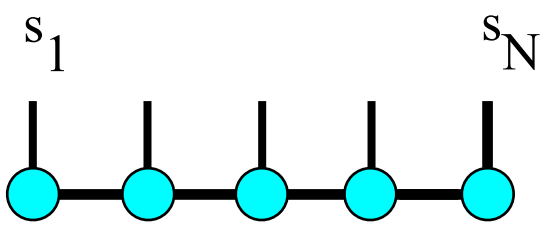
This is the "matrix product state" representation of the ground state

Matrix Product States = DMRG

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

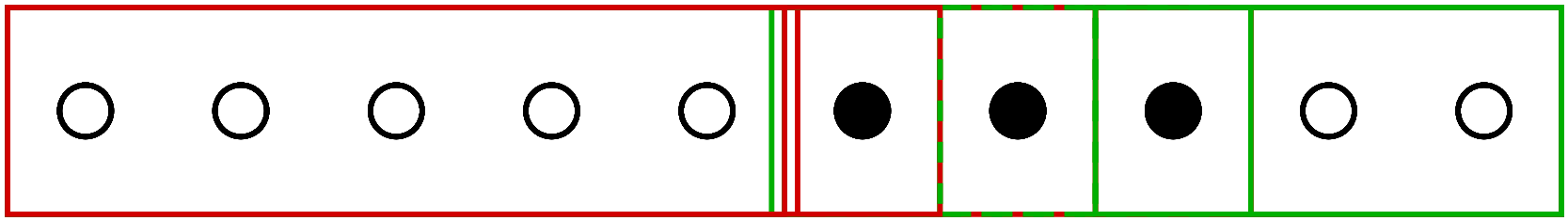
Exp'ly large

2^N



Highly compressed

N m^2

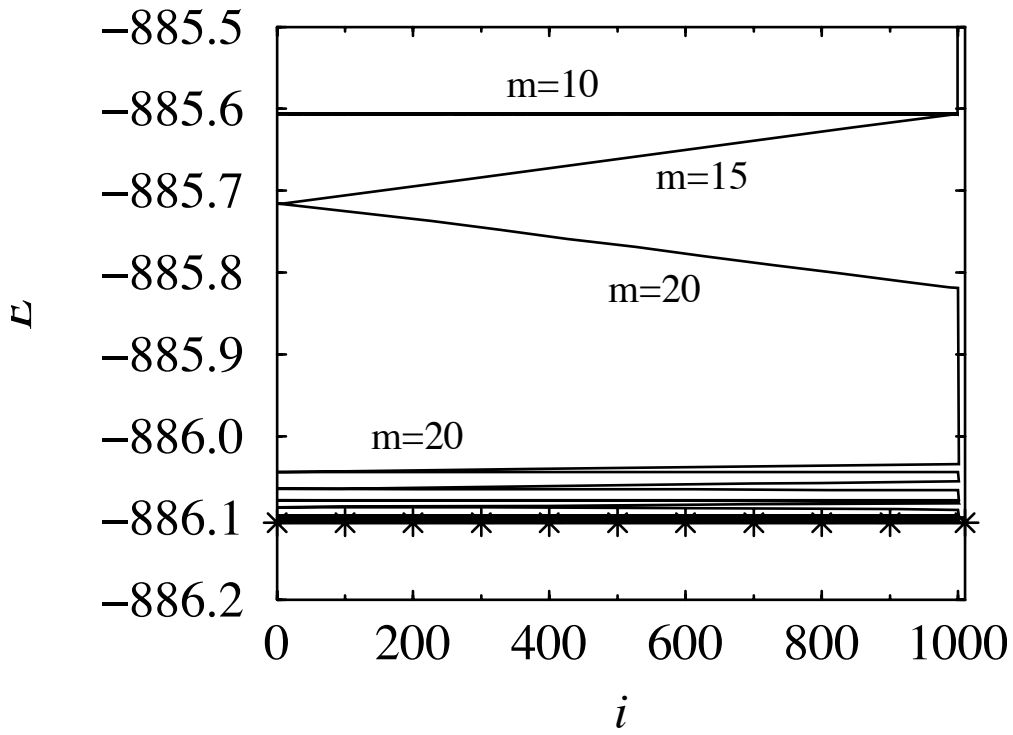


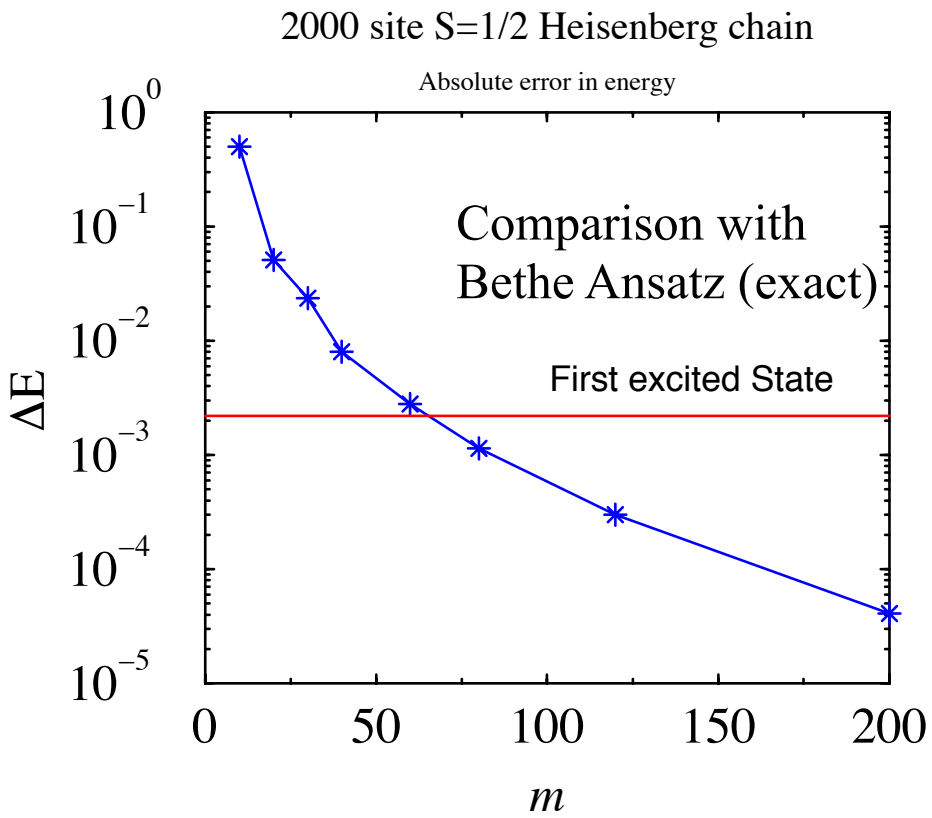
Sweeping

Matrix Product states and DMRG are the natural, optimal low-entanglement approach for studying (gapped) 1D systems.

Ground states can be obtained with double-precision accuracy on a laptop without plugging it in

DMRG Convergence in 1D





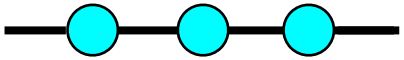
Note: the brute force way to solve this is to diagonalize a 2^{2000} x 2^{2000} matrix!

For 1D systems, we have learned how to get almost everything we want—finite temperature, **spectral functions**, out-of-equilibrium dynamics, disorder, … (but some things are hard)

Diagrams for Matrix Product States

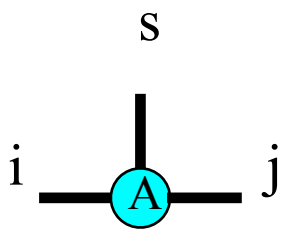
Vertices are matrices or tensors. All internal lines are summed over. External lines are external indices, usually associated with states

Ordinary Matrix Multiplication: ABC =

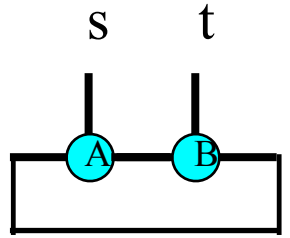


In an MPS, the basic unit has an extra index, like a Pauli spin matrix; or you can call it a tensor

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



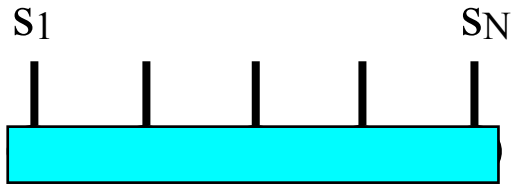
Simple diagram: gives f(s,t) $Tr[A^s B^t]$ =



Dimensions: i, j: m or D s: d

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

2^N



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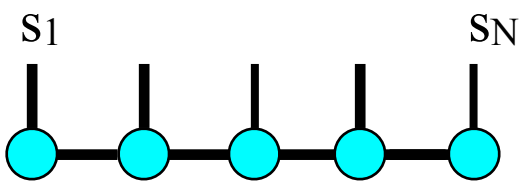
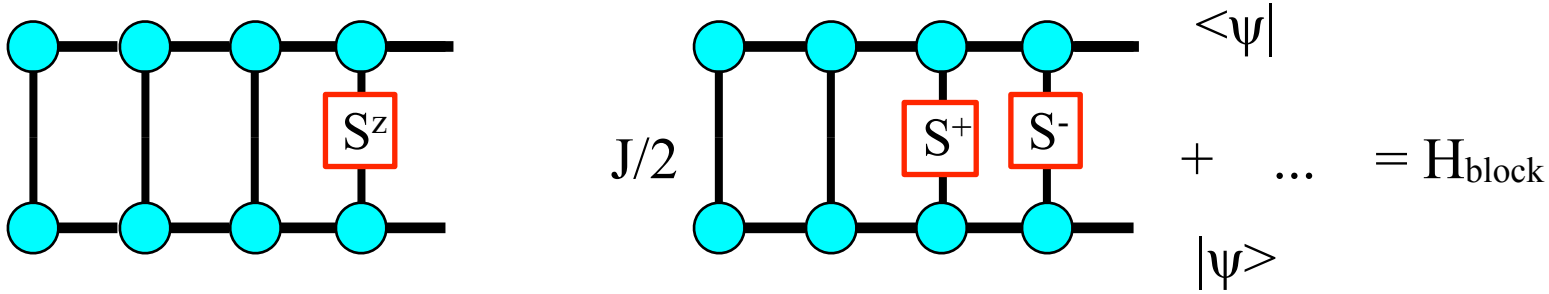


N m^2 for m x m matrices

MPS as Variational states

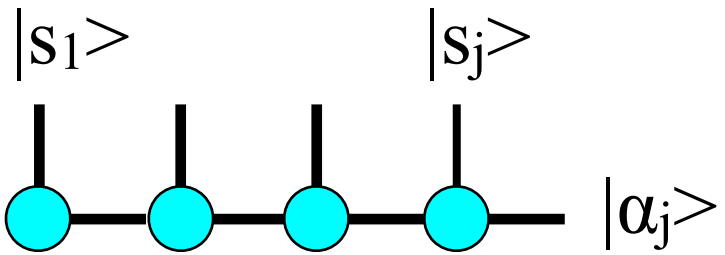
- Two things needed:
  - Evaluate energy and observables efficiently
  - Optimize parameters efficiently to minimize energy
- Observables:

Operators:



  - Working left to right, just matrix multiplies, N m^3
- Optimization:
  - General-purpose nonlinear optimization is hard
  - Lanczos solution to eigenvalue problem is one of the most efficient optimization methods (also Davidson method). Can we use that? Need an *orthonormal basis*.

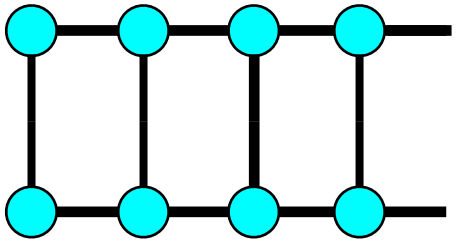
Matrix Product Bases



$$|\alpha_j\rangle = \sum_{s_1 \ldots s_j} [A[s_1] \ldots A[s_j]]_{\alpha_j} |s_1\rangle \ldots |s_j\rangle$$

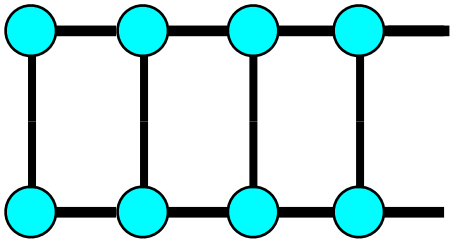
Left basis shown; also there are right bases

Orthonormality: $\langle \alpha_k | \alpha_j \rangle = \delta_{kj}$

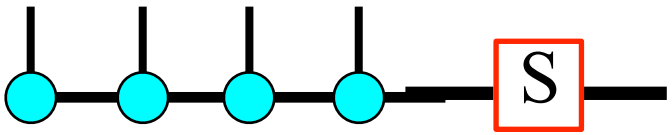


$= 1$

If its not orthonormal, you can make it so:



$= \mathrm{O}$ Let $S = O^{-1/2}$



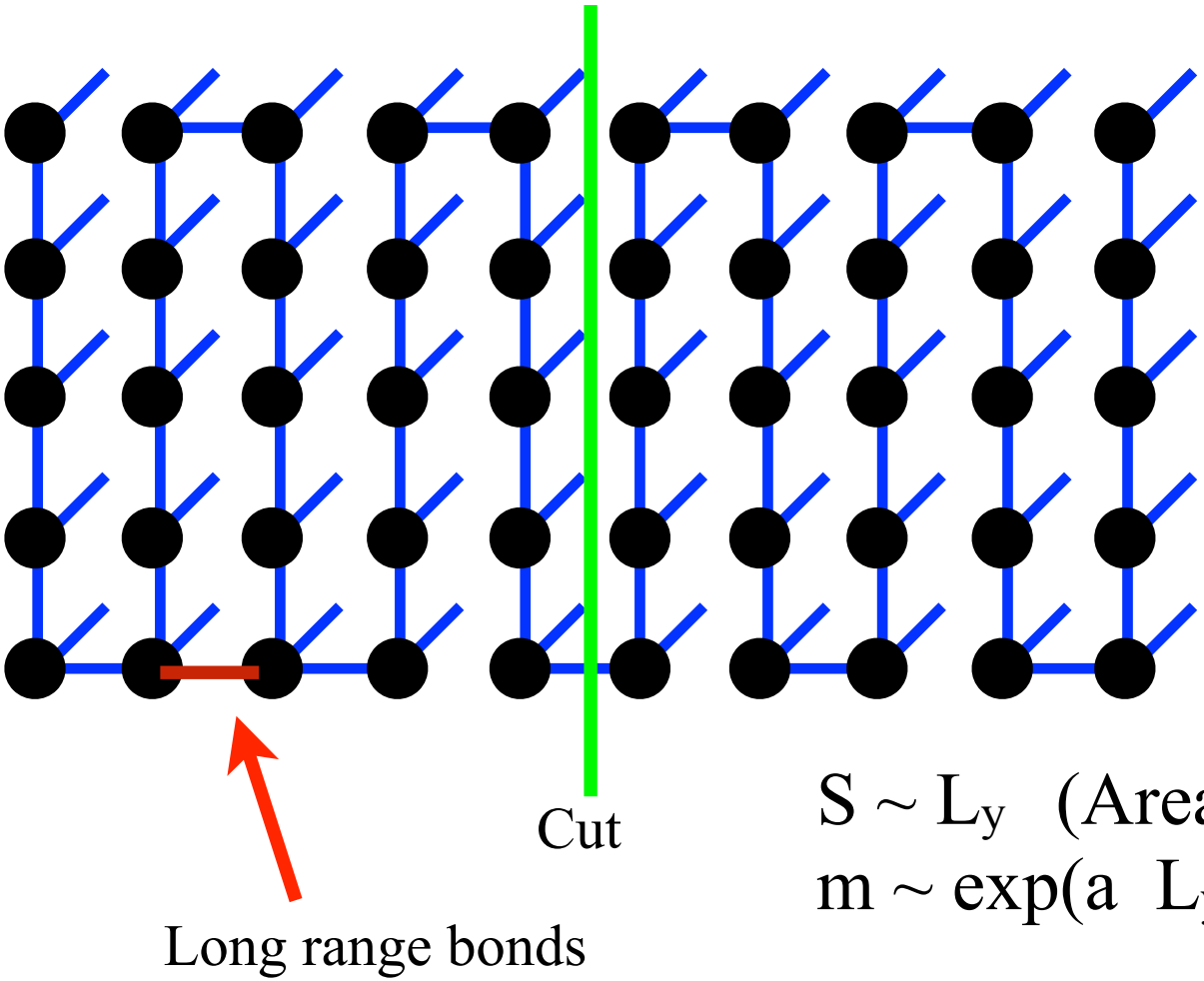
Can insert S S^{-1} anywhere w/o changing MPS
(but messes up right orthonormality...)

DMRG: two ways of thinking about it

- I have explained two ways of think about DMRG:
  - The original view: Numerical RG; "Blocks" which have renormalized Hamiltonians (reduced bases) and operator-matrices in that basis
  - the MPS variational state point of view.
- The MPS point of view is now the most important—it connects with many new developments. The RG point of view is still also useful

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

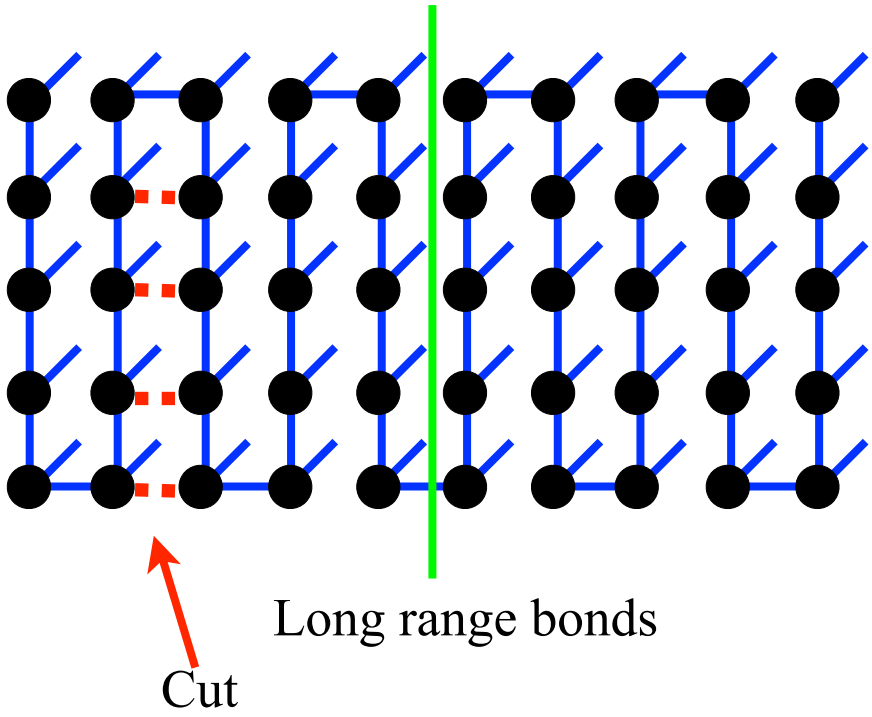
$S \sim L_y$ (Area Law)

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

Calc time: $L_x\ L_y^2\ m^3$; allows $m \sim 10000$, $L_y \sim 12$

Tensor network methods for 2D systems

Traditional DMRG method (MPS state)

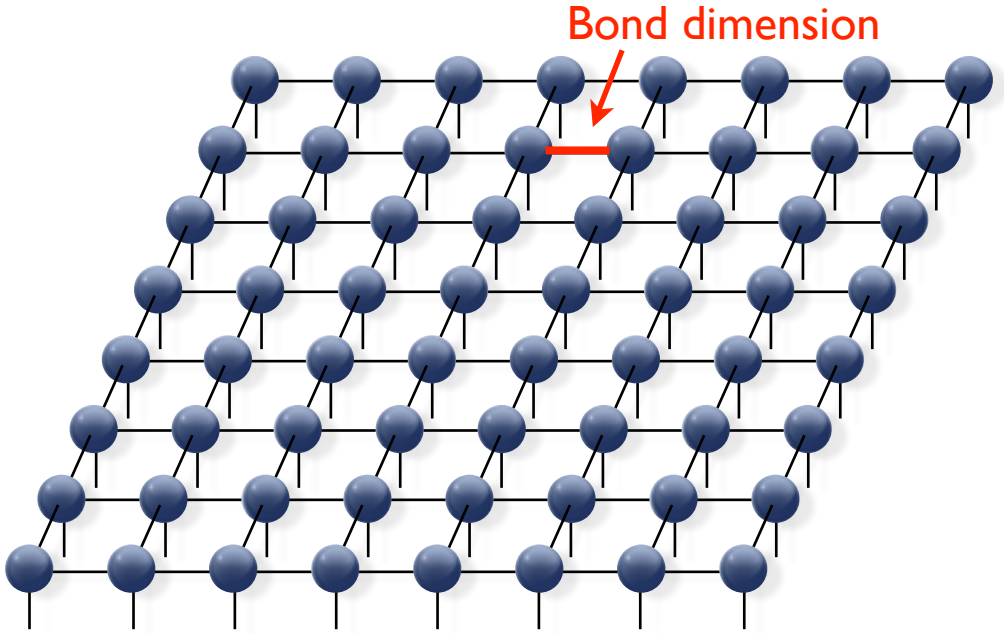


Entropy S ~ L_y ("area law")
Bond dimension m ~ exp(a L_y)

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

PEPS

projected entangled-pair state



Verstraete and Cirac, cond-mat/0407066

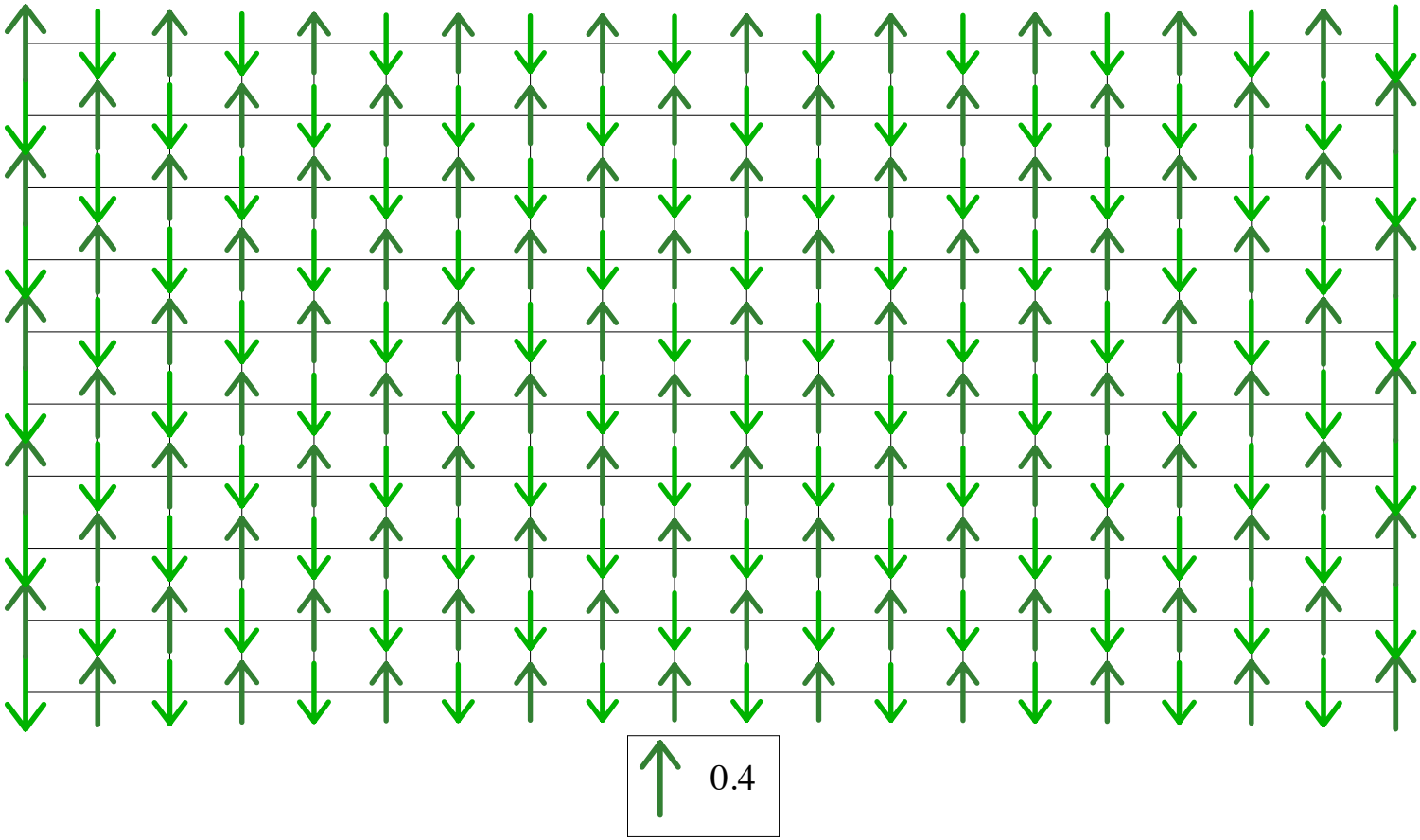
Naturally obeys Area Law
Can work directly with L_x ,$L_y \to \infty$
Calc time: ~m^{12};
Practical calculations: m ~ 15-20?,
(See Corboz' impressive work…)

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

Some Practical aspects of DMRG for hard systems and Applications to 2D

- Extrapolation in truncation error for energy and observables
- Tips for very efficient calculations
- Example systems:
  - Square lattice
  - Triangular lattice
  - Kagome lattice

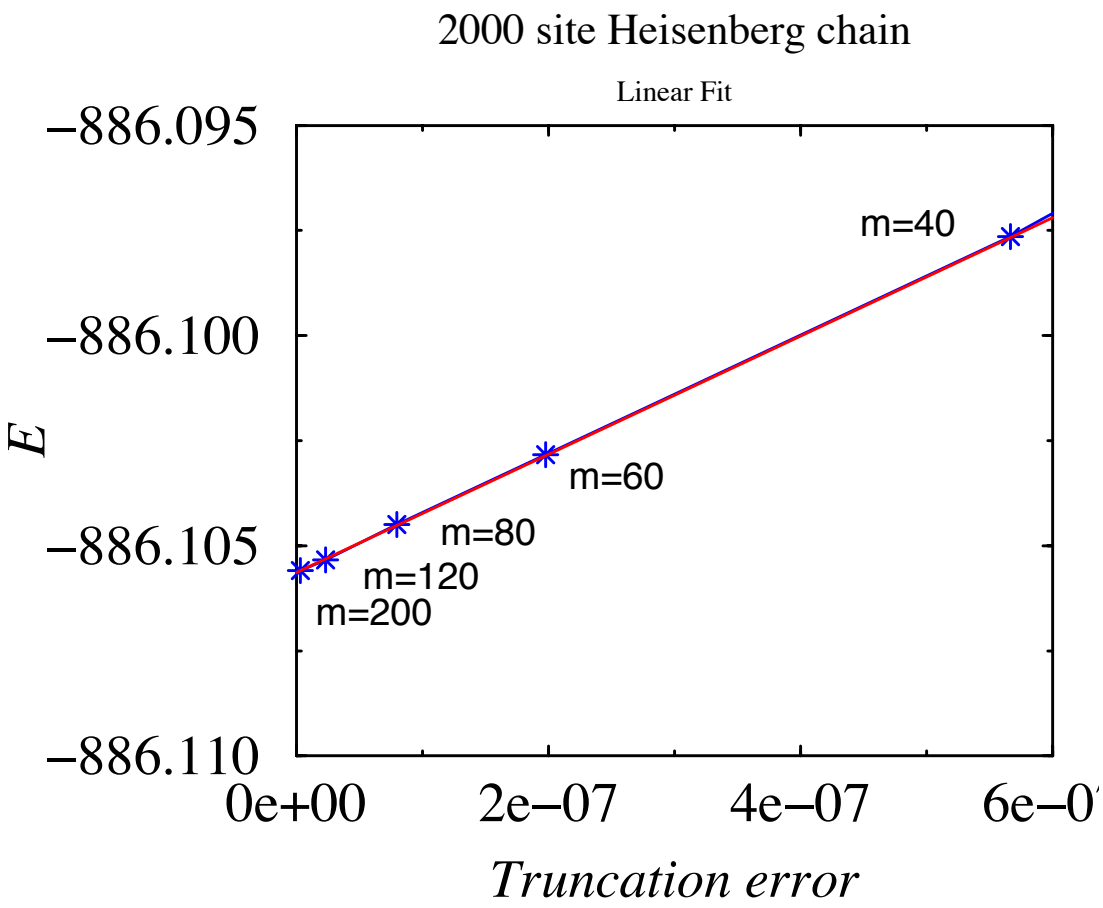
Square lattice: benchmark against



20 x 10

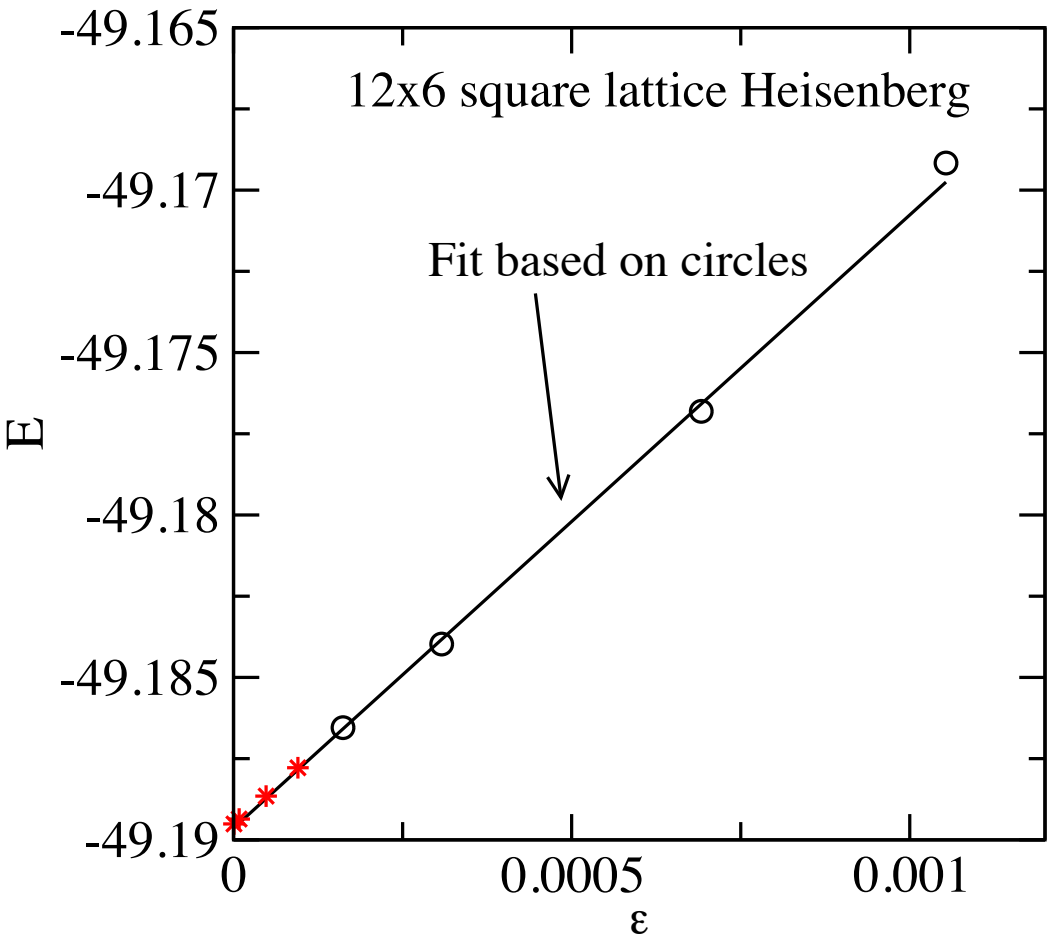
- Cylindrical BCs: periodic in y, open in x
- Strong AF pinning fields on left and right edges
- 21 sweeps, up to m=3200 states, 80 hours

Extrapolation of the energy



Extrapolation improves the energy by a factor of 5-10 and provides an error estimate.

Energy extrapolation



Probability of states thrown away
= truncation error (function of m)

Assign error bars to result: if the fit is this good, assign (extrapolation from last point)/5

(no derivation, just experience that this works on lots of systems)

If the fit looks worse, increase the error bar (substantially) or don't use that run/keep more states or smaller size system.

Extrapolation of local observables(ref: White and Chernyshev, PRL 99, 127004 (2007))

- Standard result for a variational state

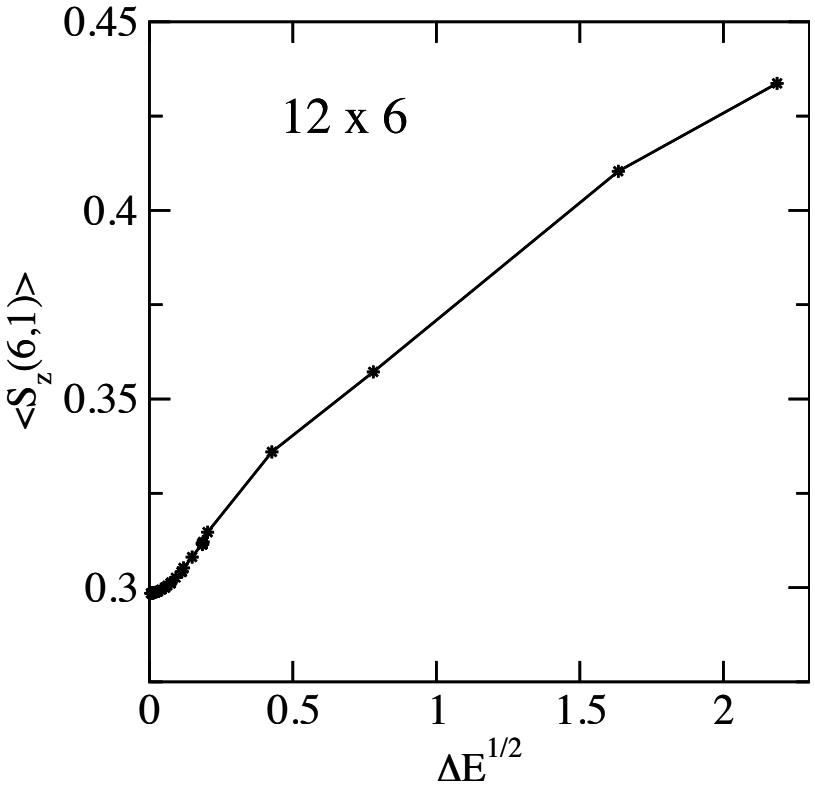
$$|\psi\rangle = |G\rangle + |\delta\rangle, \quad \langle G|\delta\rangle = 0,$$

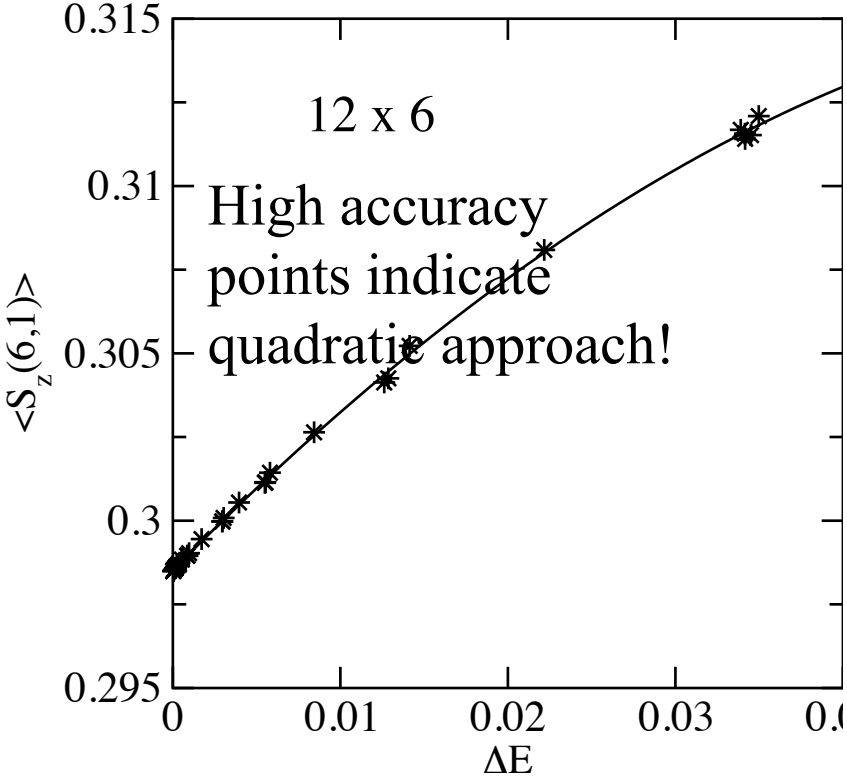
$$A = (1 + \langle\delta|\delta\rangle)^{-1}(A_G + 2\langle G|\hat{A}|\delta\rangle + \langle\delta|\hat{A}|\delta\rangle)$$

$$E = (1 + \langle\delta|\delta\rangle)^{-1}(E_G + \langle\delta|\hat{H}|\delta\rangle)$$

- Consequences:
  - Variational calculations can have excellent energies but poor properties
  - Since DMRG truncation error $\varepsilon \sim \langle\delta|\delta\rangle$ $E \sim \varepsilon$, but otherwise extrapolations vary as $A \sim \varepsilon^{1/2}$
- These $\varepsilon^{1/2}$ extrapolations have never worked well.

Typical extrapolation of magnetization

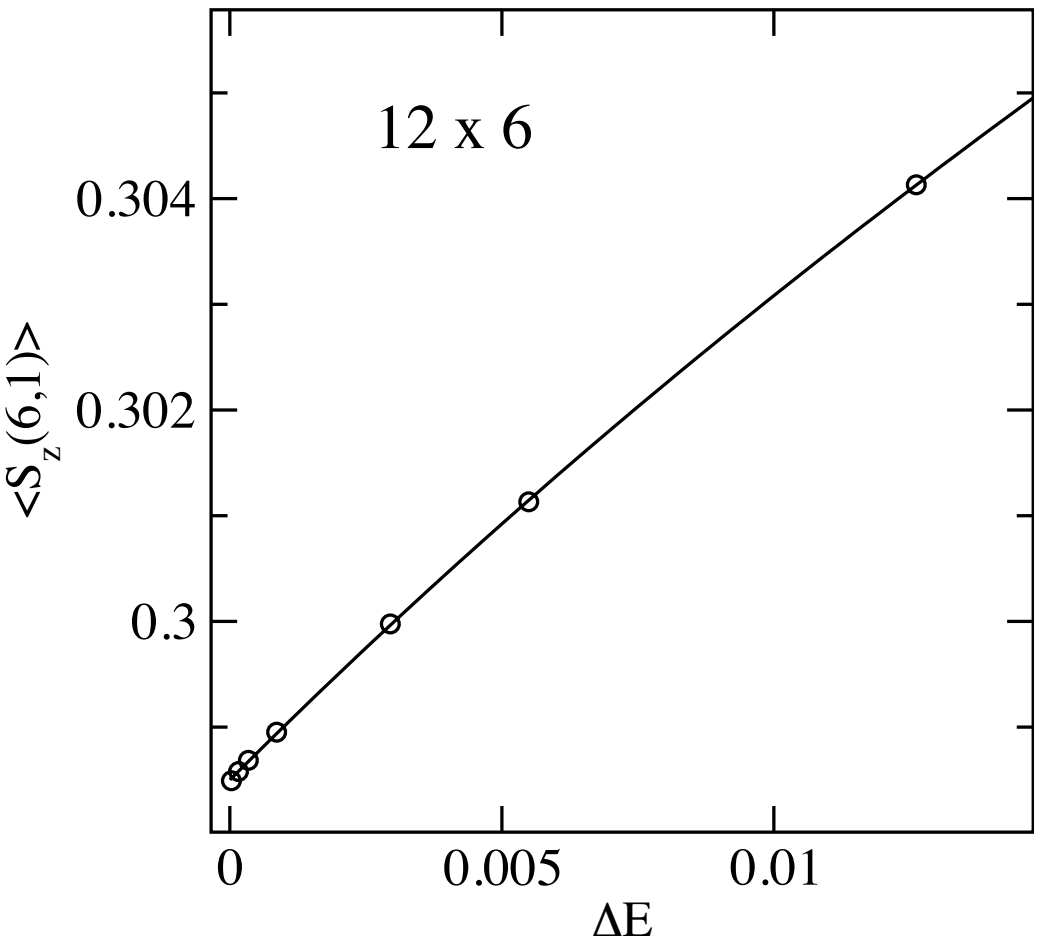




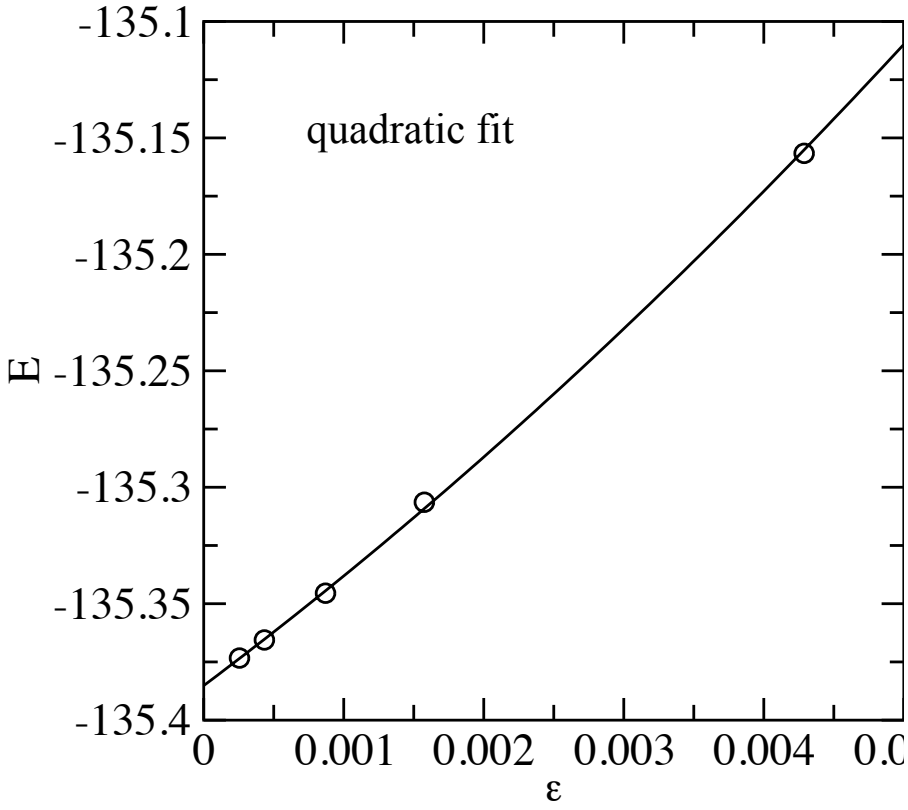
Pinning AF fields applied to edges, cylindrical BCs

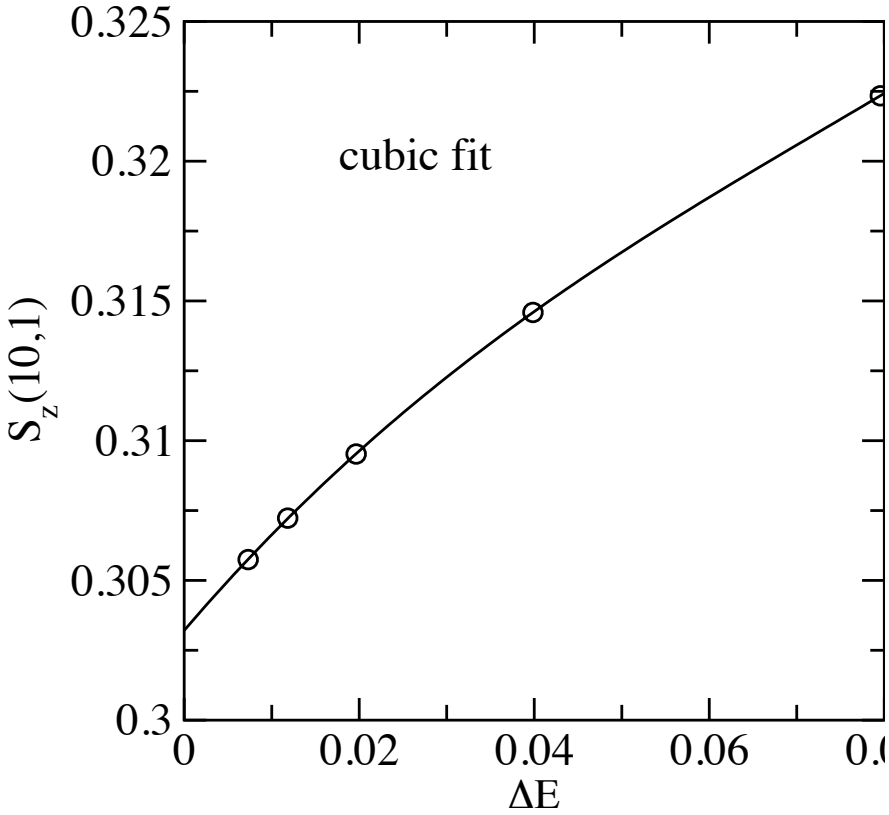
Now we understand why the local measurements converge fast; see White & Chernyshev

Cubic fit to well-converged measurements



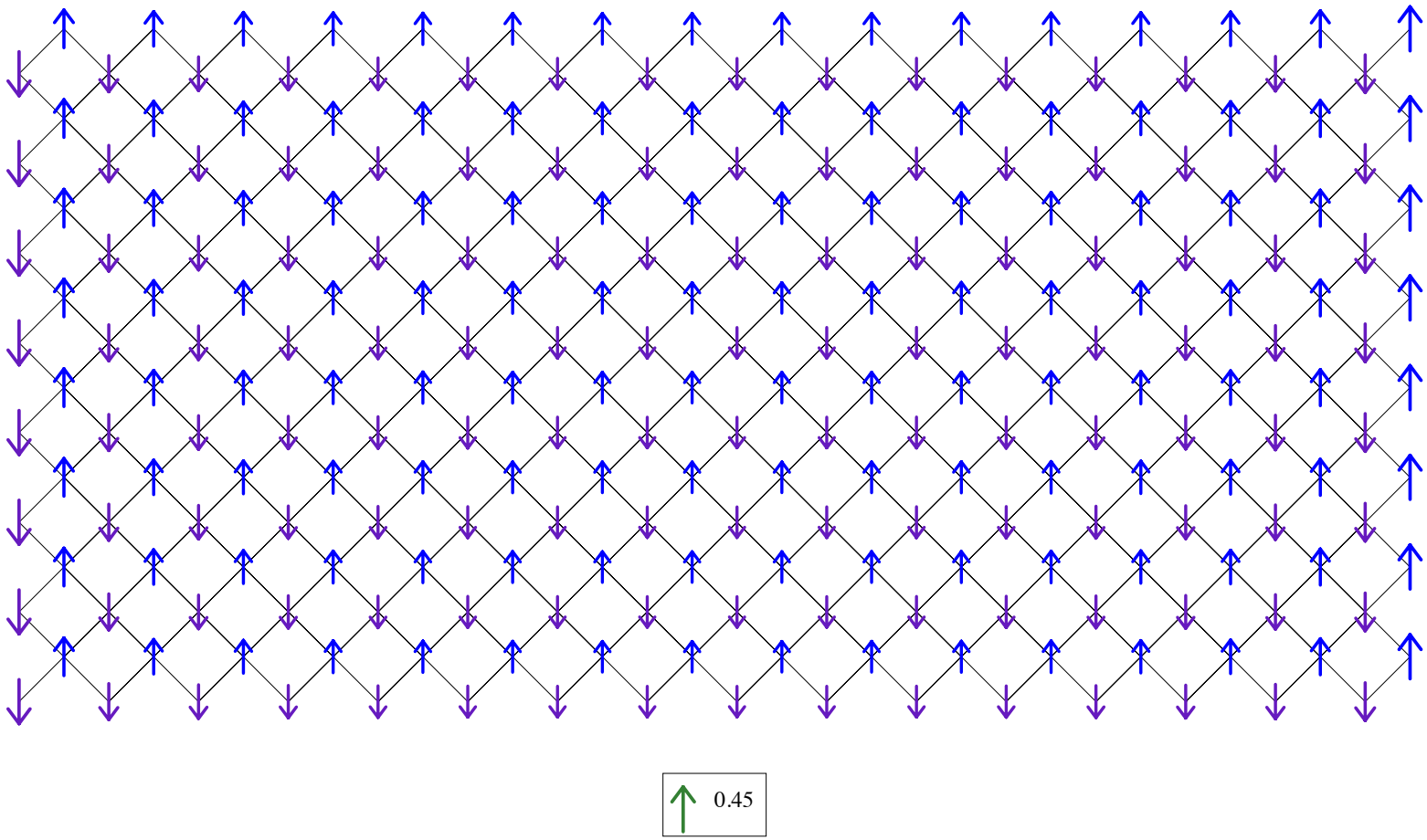
20x10 square lattice Heisenberg





Result: central M = 0.3032(9)

Tilted square lattice

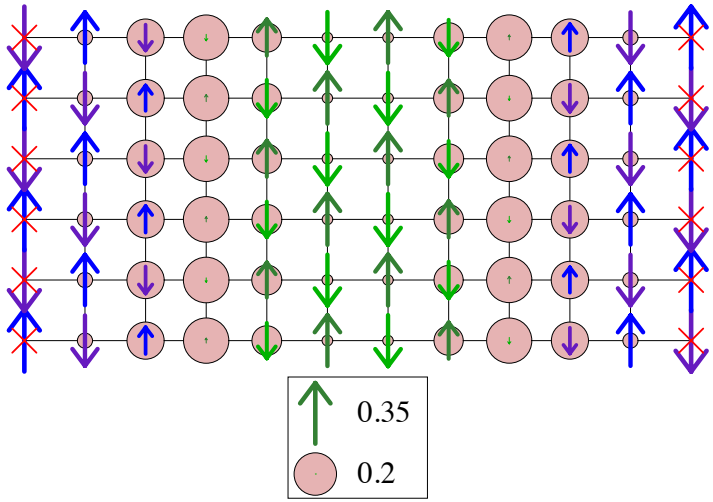


- Tilted lattice has smaller DMRG errors for its width
- For this "16 $\sqrt{2}$ x 8 $\sqrt{2}$" obtain M = 0.3052(4)

Applications of DMRG in 2D

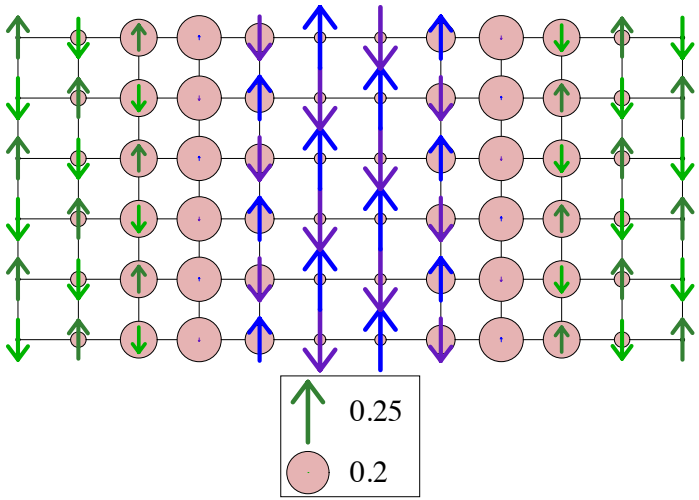
- t-J model—stripe formation
- Thursday—spin liquids

t-J model: stripes on width 6 cylinders



12 x 6 system, Vertical PBC's
J/t = 0.35, 8 holes

Pinning AF fields

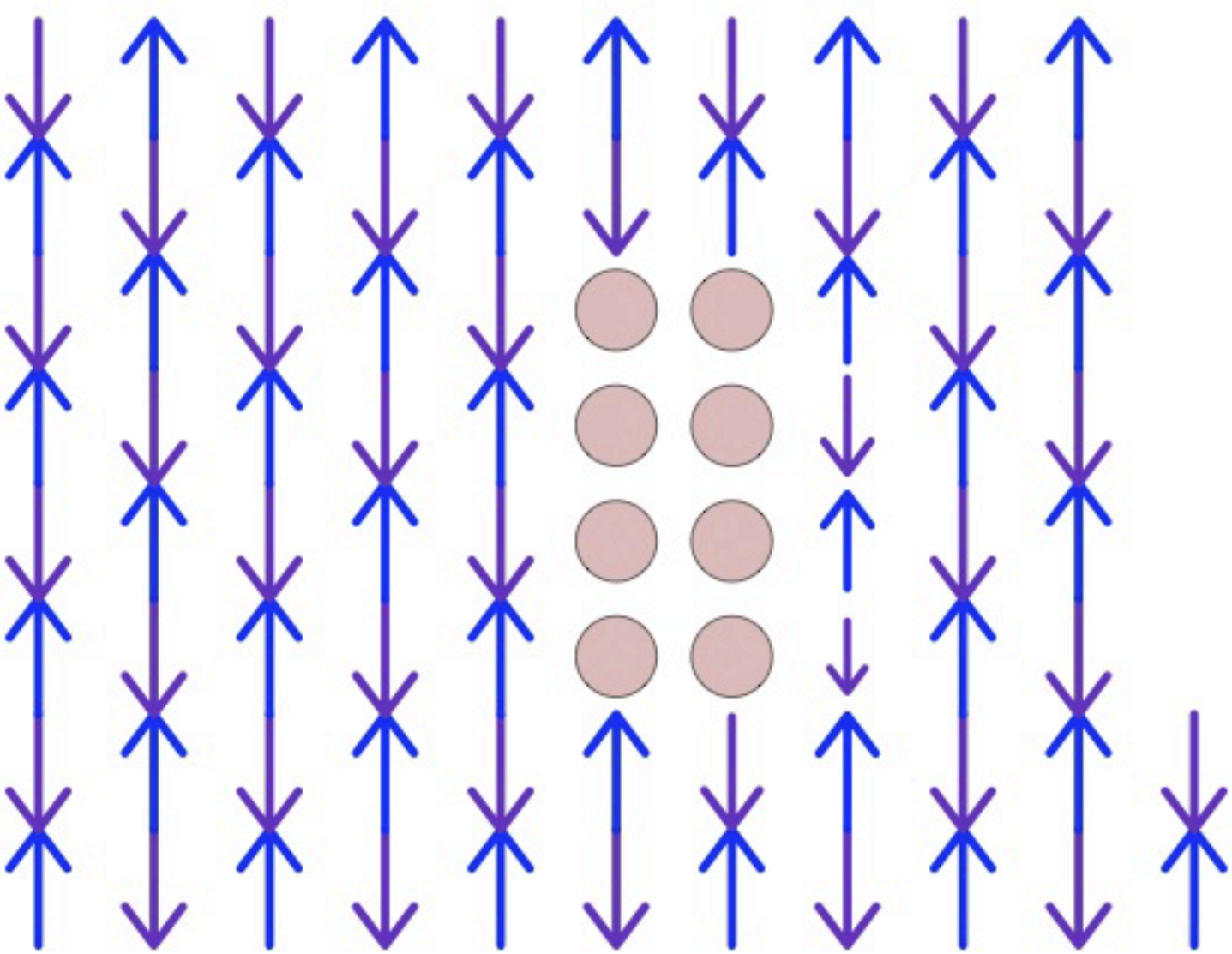


12 x 6 system, Vertical PBC's
J/t = 0.35, 8 holes

No Pinning AF fields
m=1600

- Issues: How well converged are the results with m?
- Are these just finite size artifacts? (i.e. are they just Friedel oscillations?)
- Do the stripes destroy pairing?

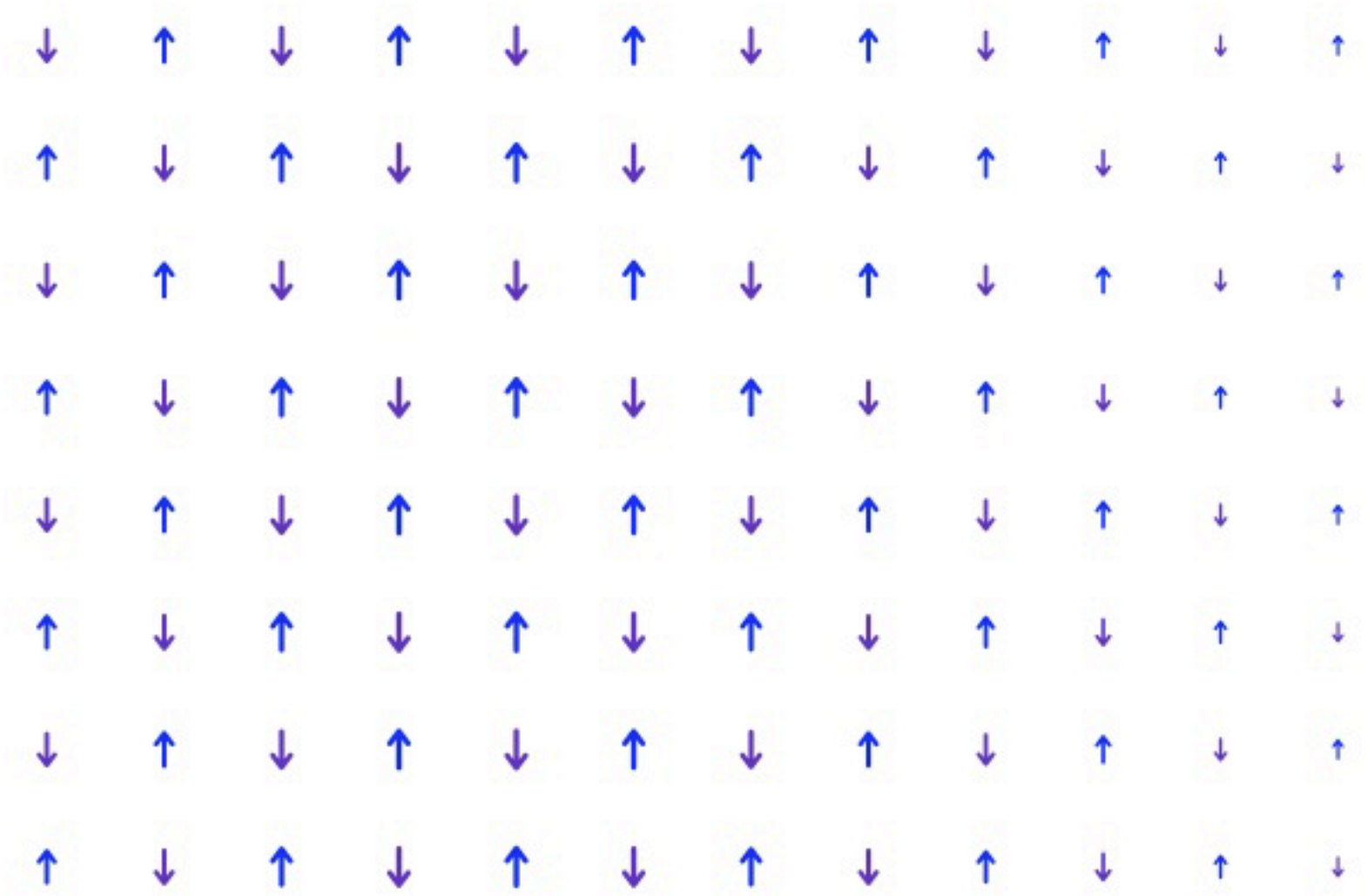
Stripes forming from a blob of 8 holes



E = -30.7350 m = 40

12x8
Cylindrical BCs
t=1, J=0.35
t'=t''=0
8 holes
AF edge pinning fields applied for two sweeps to favor one stripe

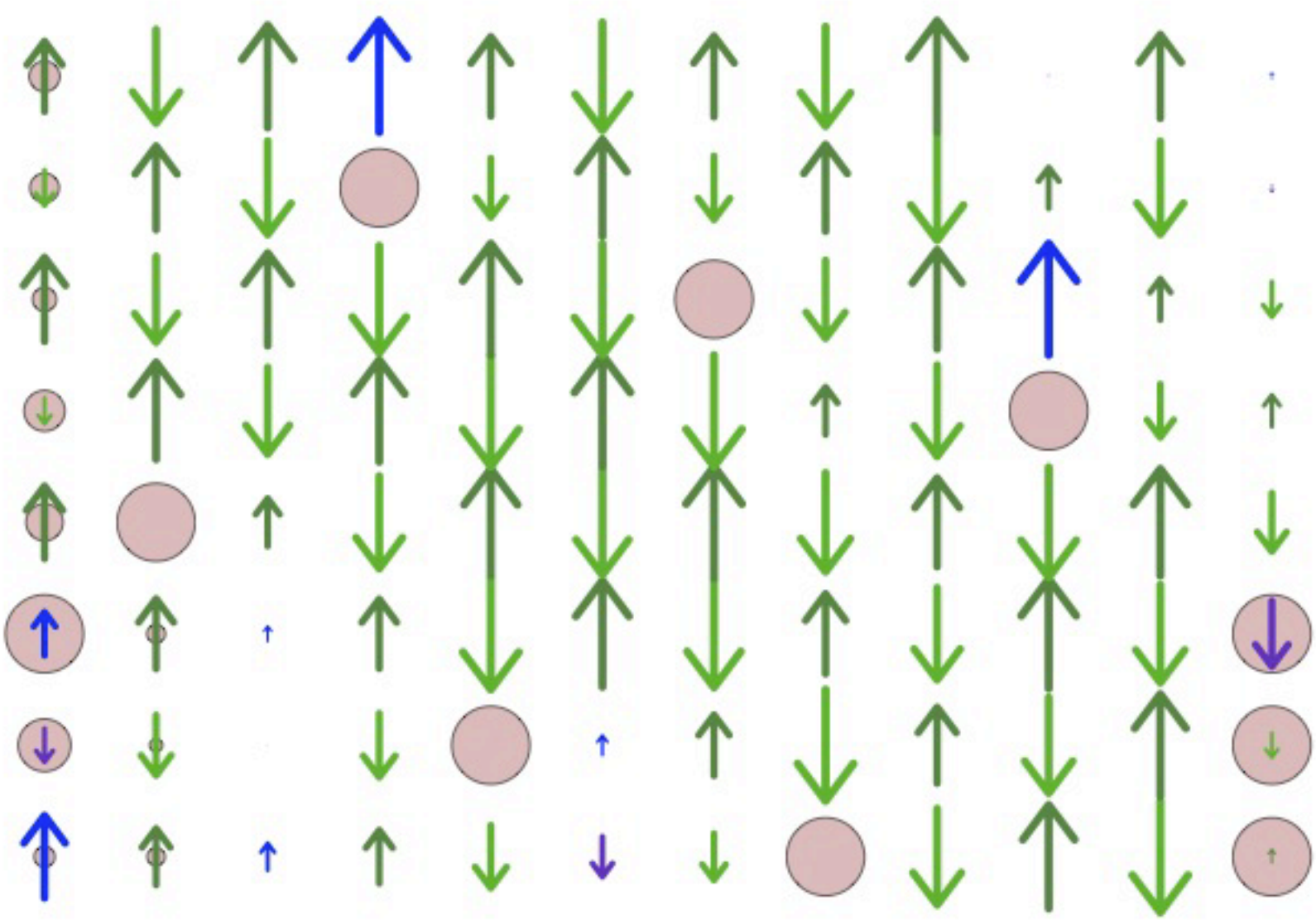
Undoped system: Restoration of SU(2) symmetry



12x8
Cylindrical BCs
J=0.35
0 holes
No pinning fields

E = -38.0681 m = 600

Stripes not forming from a bad initial state

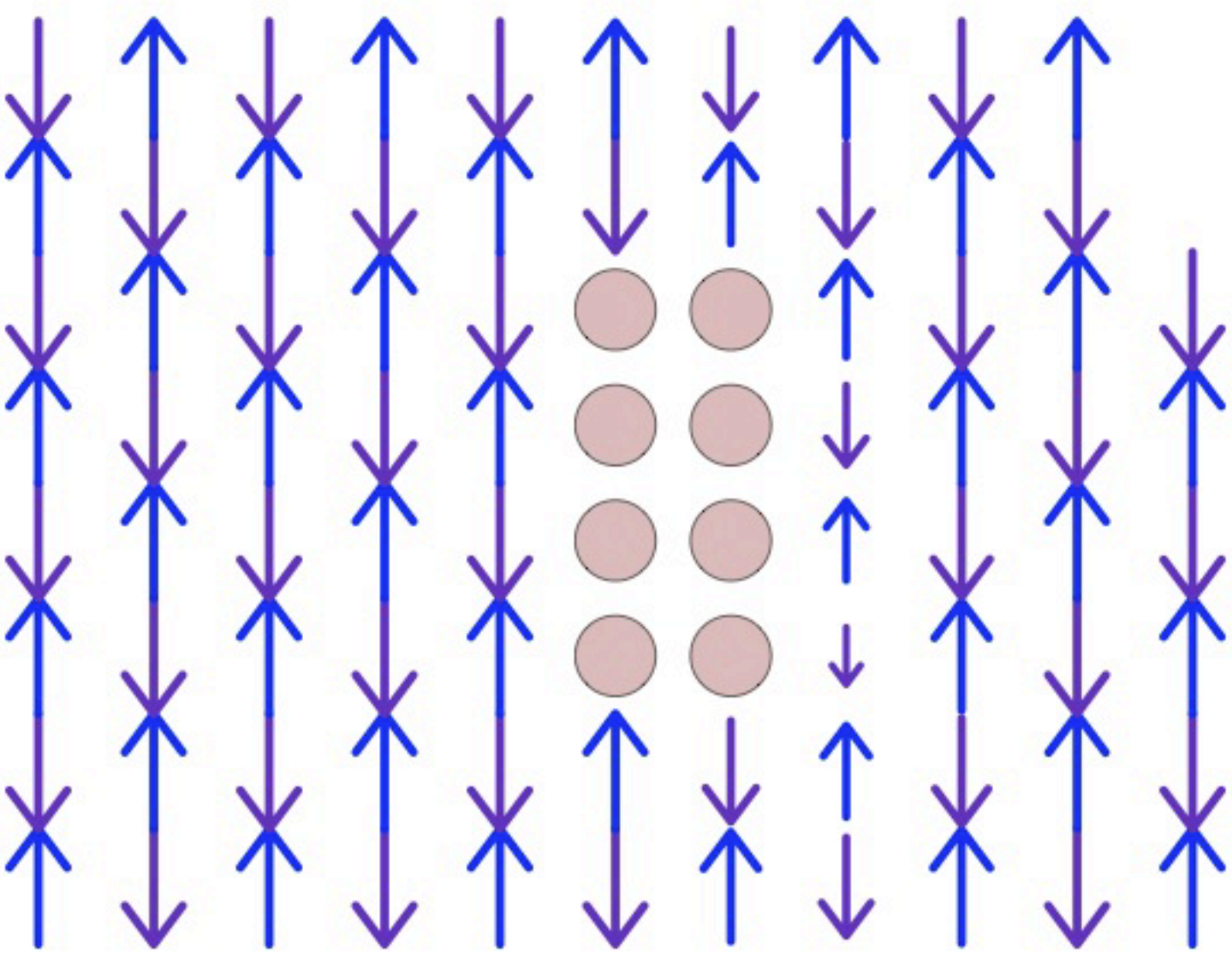


E = -30.6370

m = 70

12x8
Cylindrical BCs
t=1, J=0.35
t'=t''=0
8 holes
No pinning fields.
Initial state has holes spread out so favored striped state is hard to find.
Energy higher by ~0.3 t.

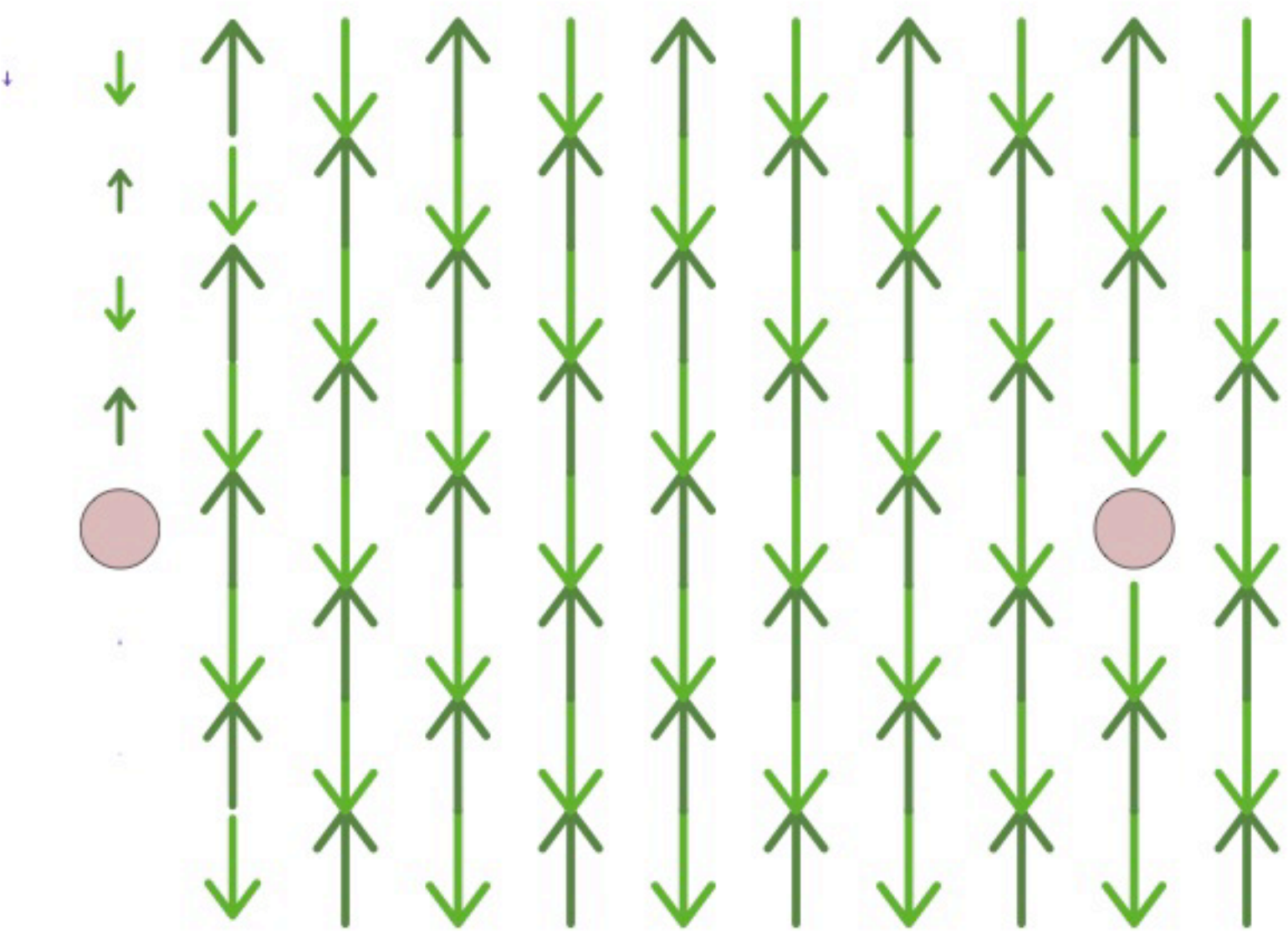
Curved Stripe forms due to open BCs



E = -30.8532 m = 40

12x8
Open BCs
t=1, J=0.35
t'=t''=0
8 holes
No pinning fields

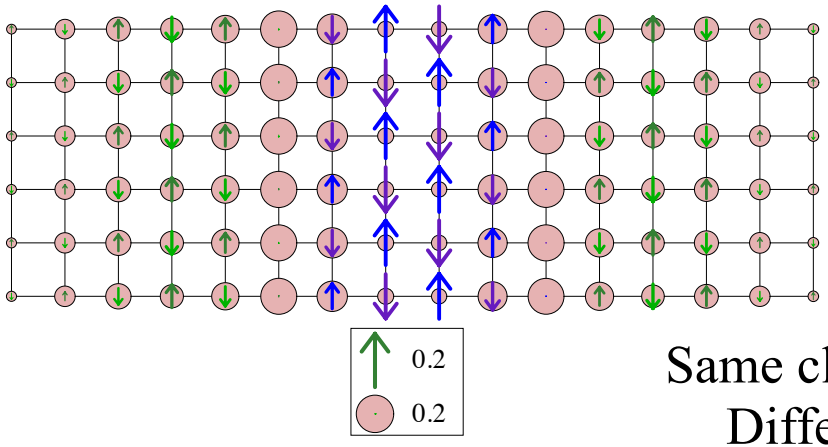
t'=0.3: two holes attract

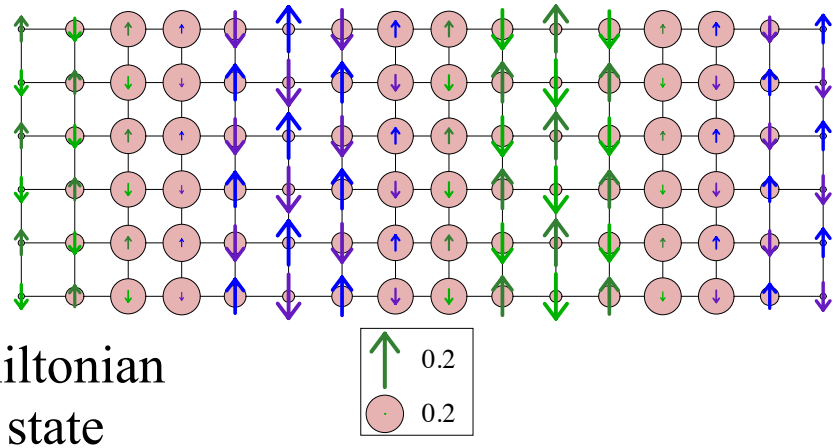


E = -31.0529 m = 40

12x8
Open BCs
t=1, J=0.35
t'=0.3
2 holes
No pinning
fields

t-J model: stripes on width 6 cylinders

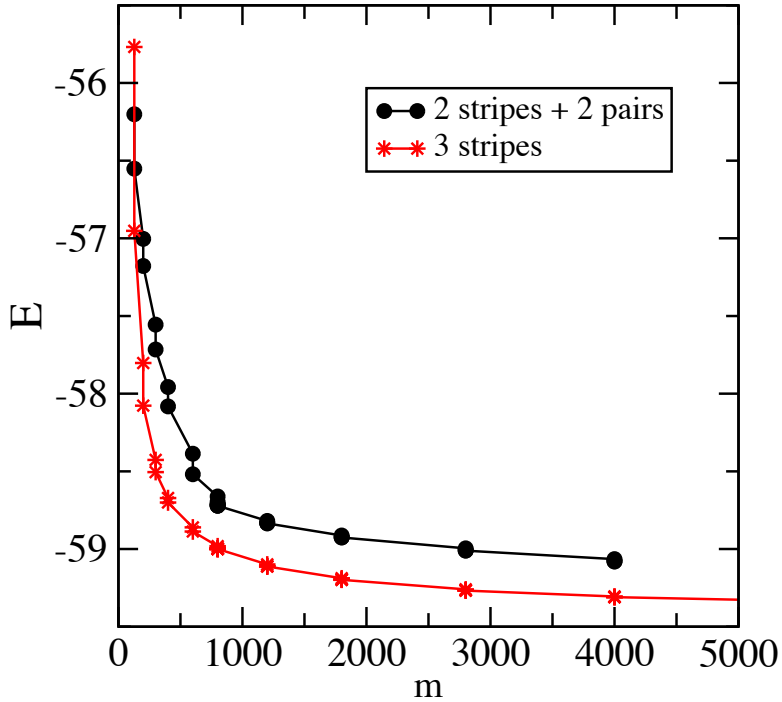




Same cluster, Hamiltonian
Different initial state

16 x 6 system, Vertical PBC's
J/t = 0.35, 12 holes

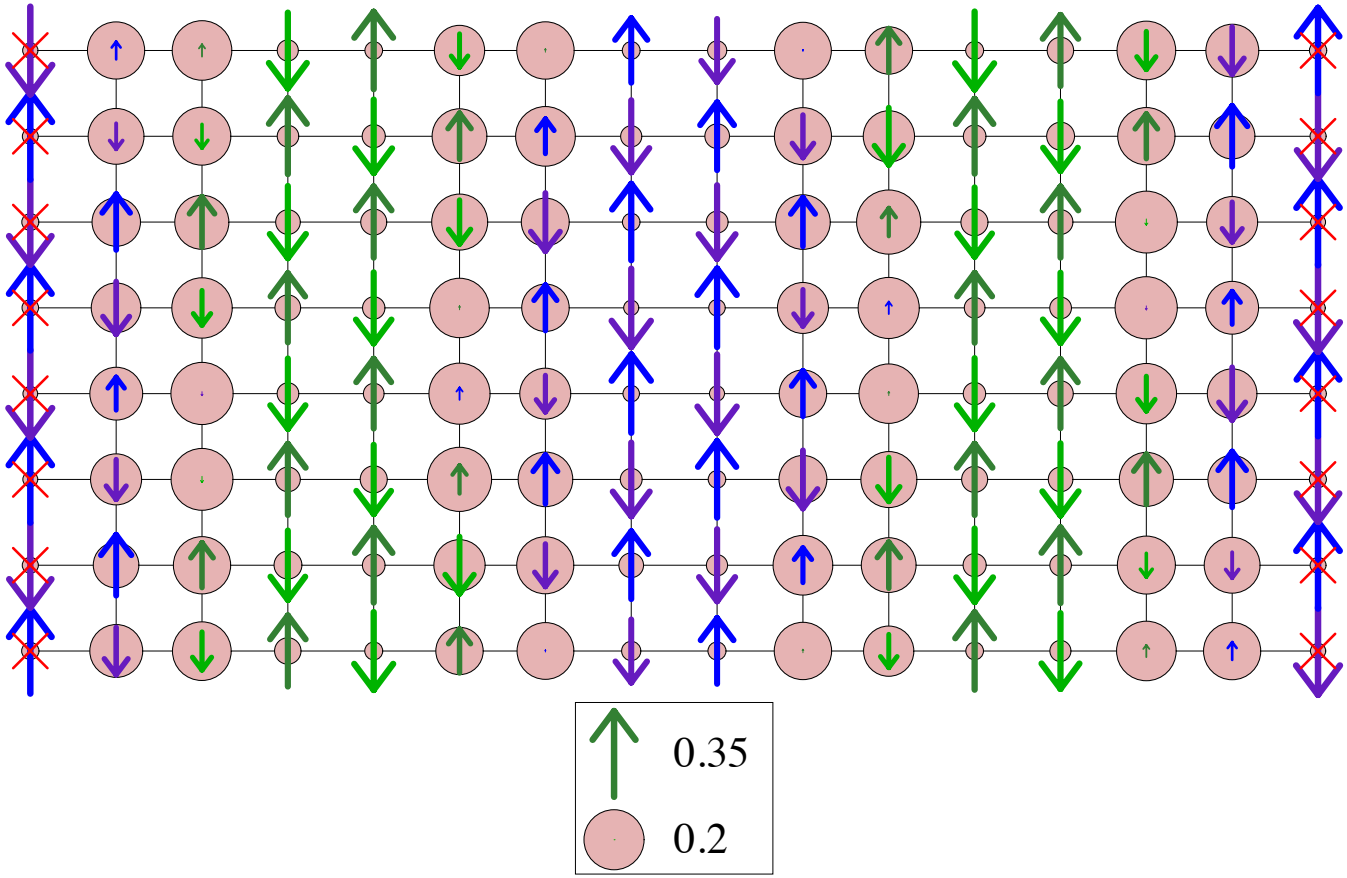
16 x 6 system, Vertical PBC's
J/t = 0.35, 12 holes



Convergence to metastable state: excellent

Tunneling between metastable states: can be very hard—need to try many initial states

Stripes on 8 leg ladders



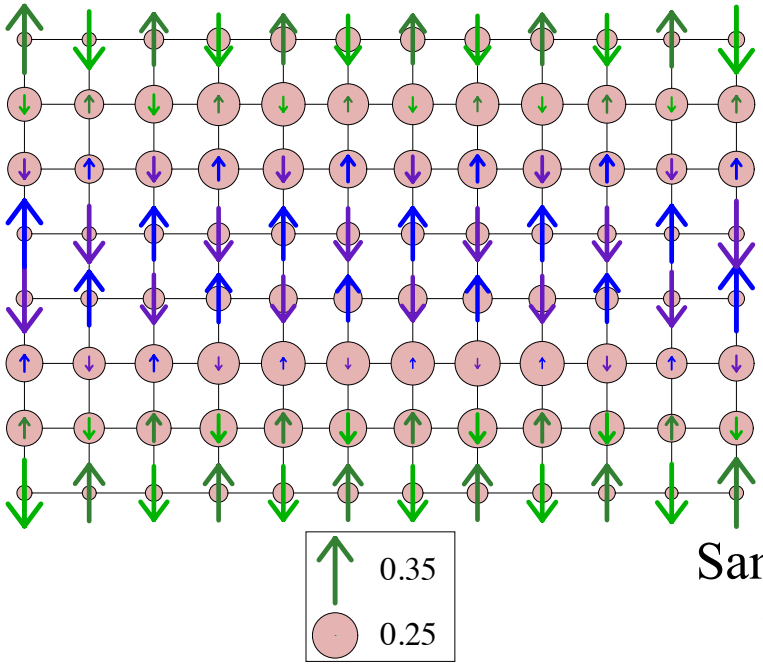
16 x 8 system, Vertical PBC's

J/t = 0.35, 16 holes

White and Scalapino,PRL '98

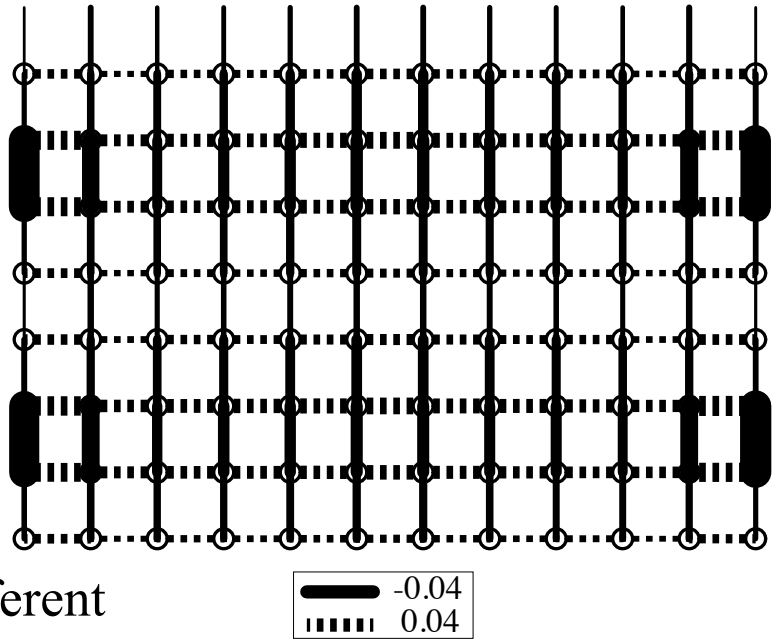
m ~ 2000 → m ~ 10000-15000 still striped

Pairing and stripes, 2 stripes, cylindrical BCs
Particle numbers not conserved



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

Same state, different measurements



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

Bond thickness shows pairing strength (dashed = negative)

- To orient the stripes longitudinally, we use Jx>Jy.
- Larger J gives stronger pairing.
- Local measurements of response converge much more quickly than correlations, especially for pairing.

Conclusions

- DMRG developed out of real space RG—finding a better set of states to keep, and building up the state iteratively
- Now we understand it as a variational ansatz which is ideal for 1D systems with low entanglement
- DMRG is now the simplest/original tensor network algorithm
- We have discussed many practical aspects of pushing DMRG to its limits in 2D