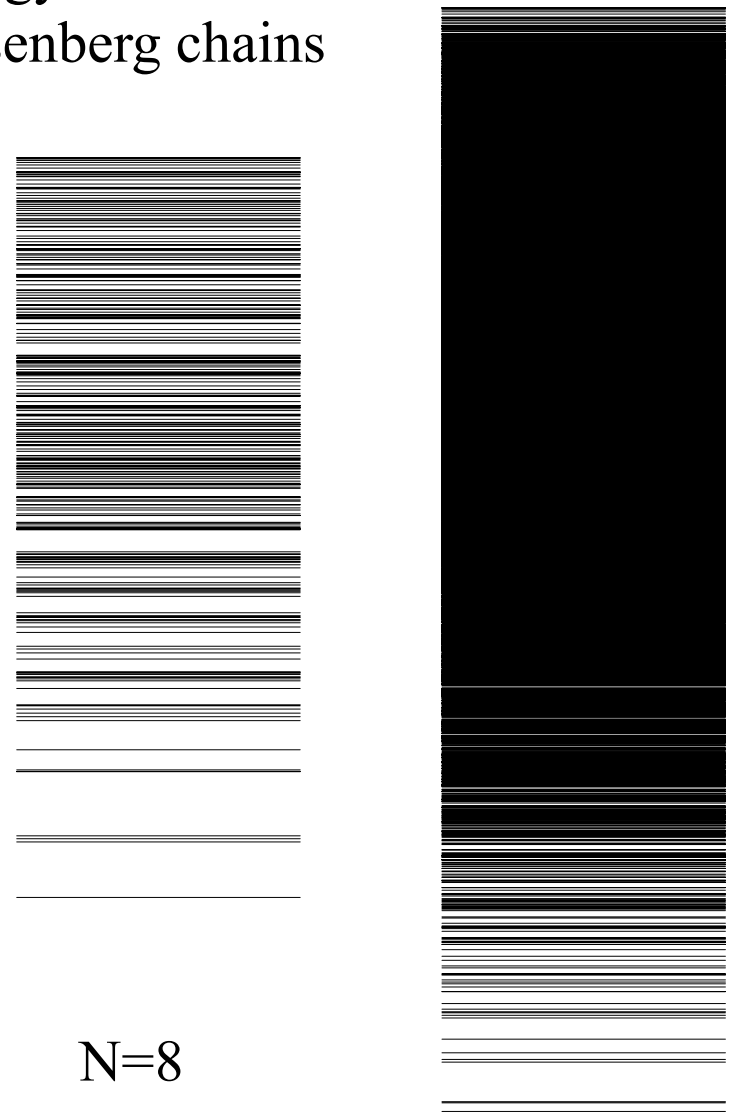
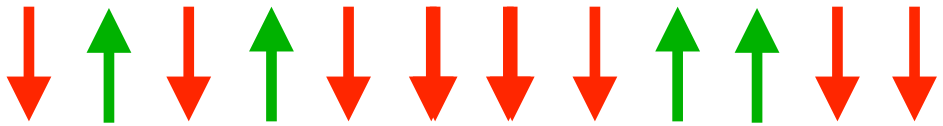
Energy levels of S=1/2
Heisenberg chains

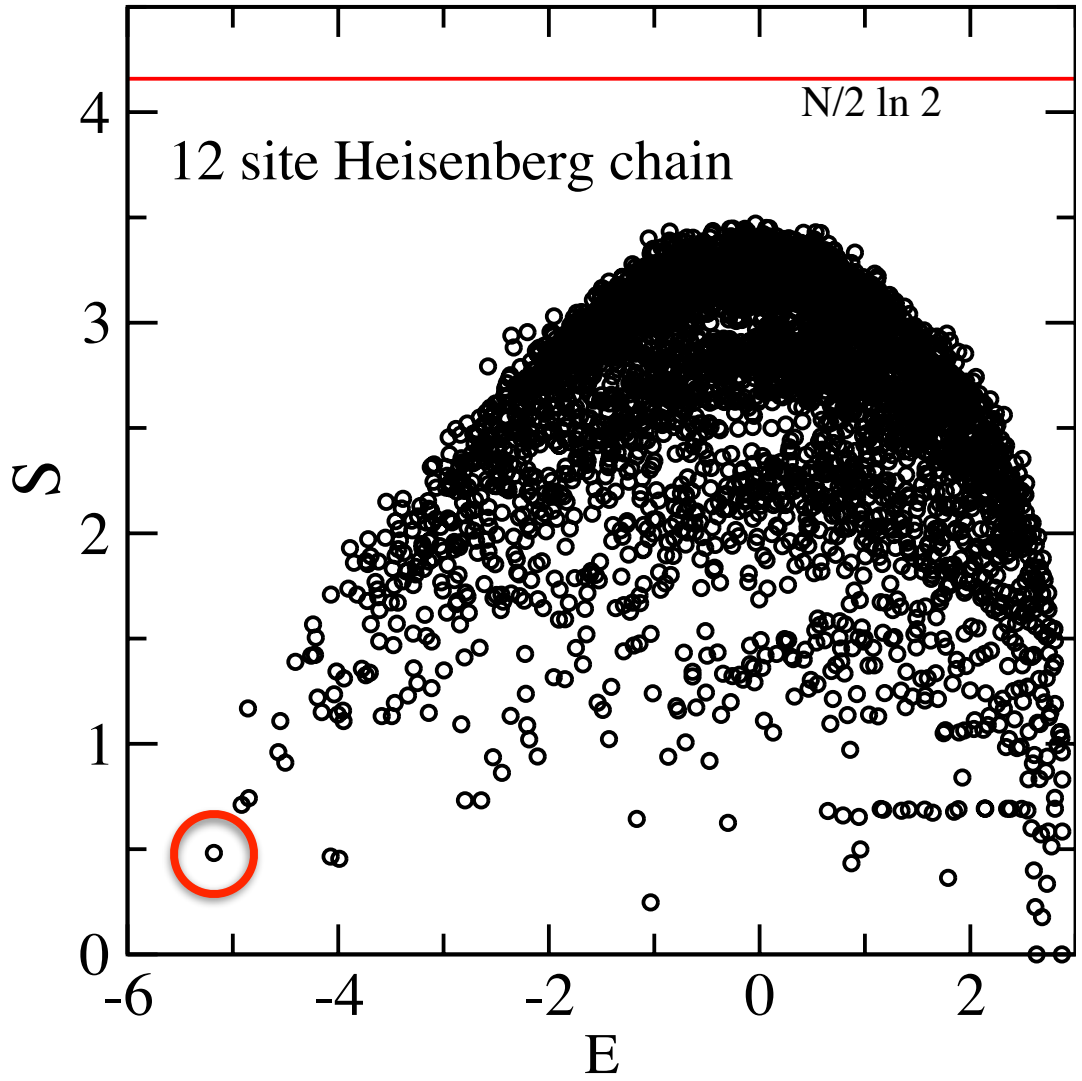


N=8

N=12



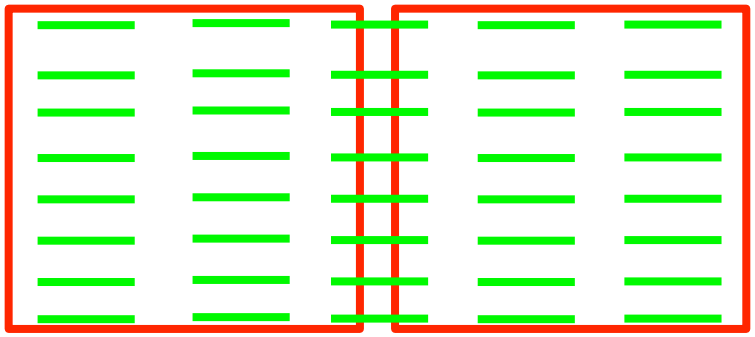
Ground states have low entanglement



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

Why is the entanglement of ground states small?

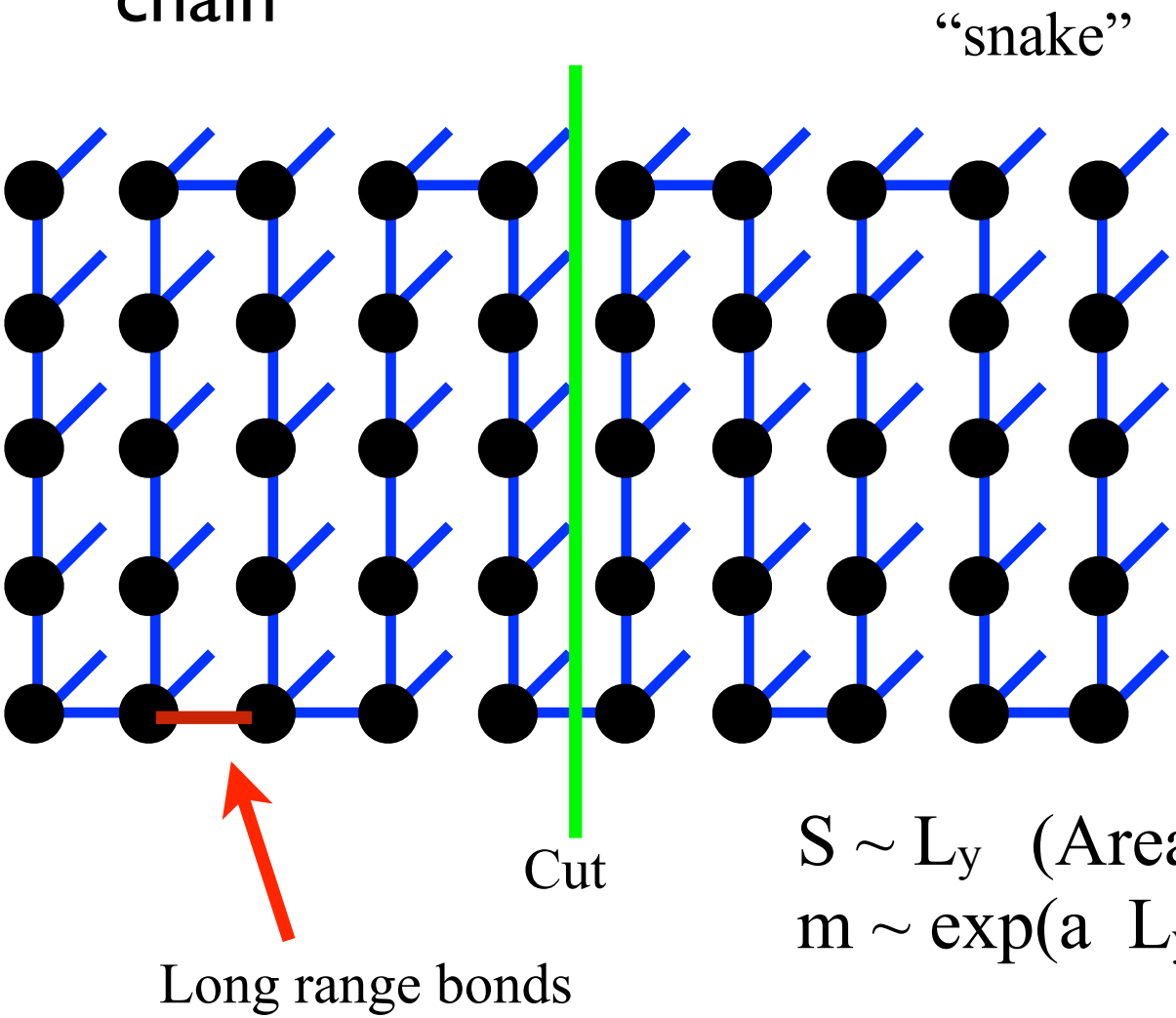
- The short answer: High entanglement doesn't help reduce the energy for a physical Hamiltonian
  - Monogamy of entanglement: complicated, many-particle entanglement reduces the simple entanglement minimizing the energy
- **The Area Law**: *The entanglement entropy is proportional to the area of the 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

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

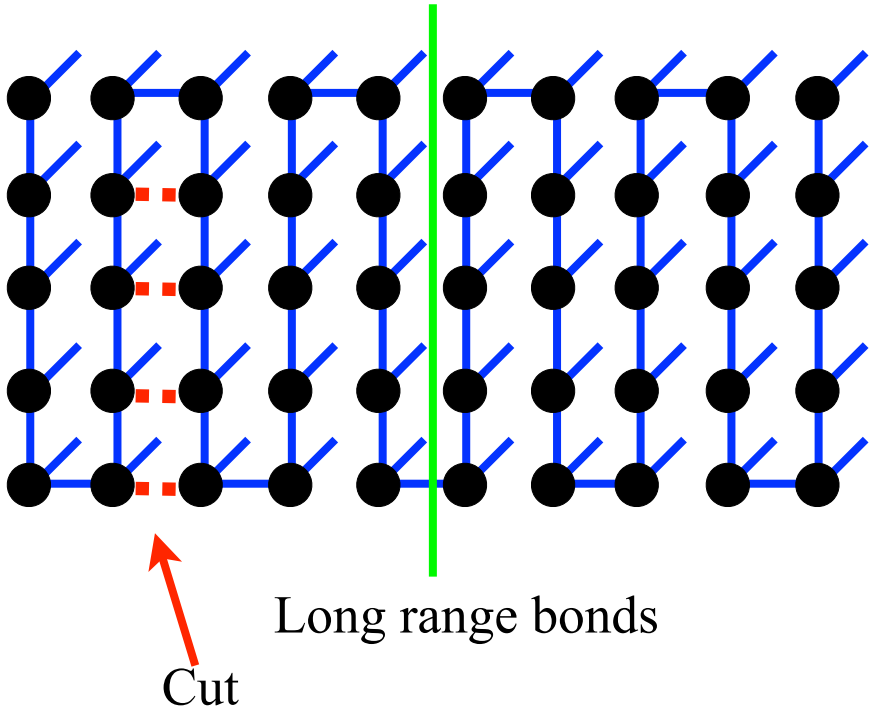
$S \sim L_y$ (Area Law)

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

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)



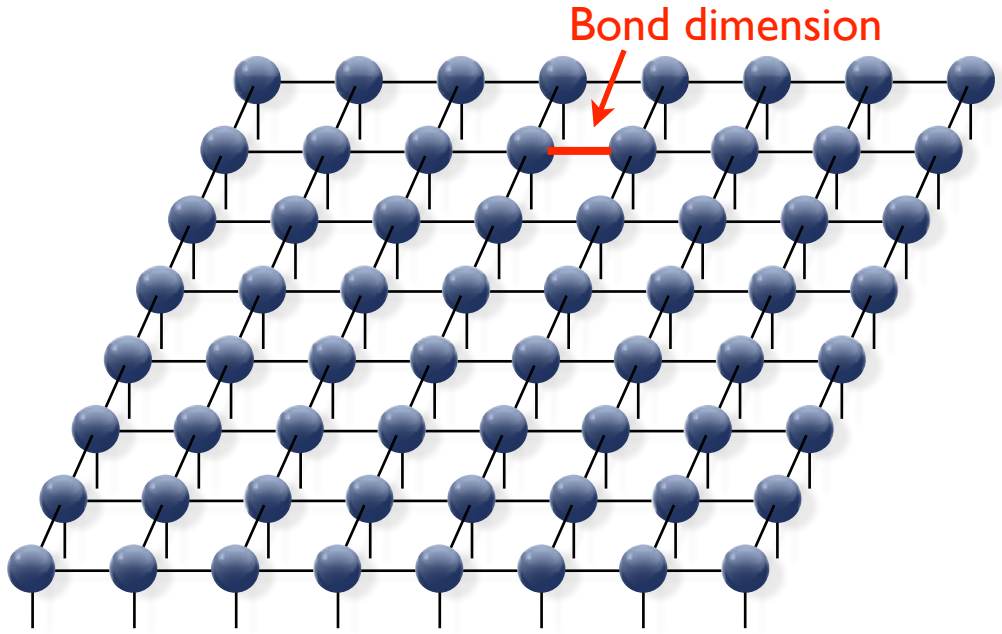
Entropy S ~ L_y ("area law")
Bond dimension m ~ exp(a L_y)

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

PEPS

tensor network states

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…)

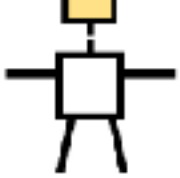
Crossover in accuracy as a function of width for DMRG, L_y ~ 10

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

- DMRG codes: ITensor, AutoMPO
- Extrapolation in truncation error for energy and observables
- Tips for very efficient calculations
- Example systems:
  - Square lattice
  - Triangular lattice
  - Kagome lattice
  - tJ model

The ITensor library (itensor.org; Miles Stoudenmire, Now at Simons)

- ITensor started out based on the simple idea of autocontraction of tensor: You should be able to contract tensors, including vectors and matrices, with code that looks like: A = B * C * D * E;
- How can you do that? Each tensor knows its indices, and indices have names, like "i", or "j", or "Joe"
- Then used the Einstein summation convention and automatically contract over repeated indices:
- Cik = Aij Bjk can automatically become C = A * B; (or C = A * B;)
- It also has DMRG, standard MPS and MPO algorithms, Abelian symmetries, fermions, long range interactions/MPO-compression, sums of MPOs, time evolution, and AutoMPO



ITensor

Learn to Use ITensor

How to use AutoMPO

Thomas E. Baker—August 18, 2015

Instead of programming an MPO by hand, ITensor has AutoMPO which allows for the automatic generation of an MPO. This feature allows for the typing of a chain of input which AutoMPO converts into an MPO for the full system.

Here is a code snippet for making an MPO for the Heisenberg model on a spin-half chain.

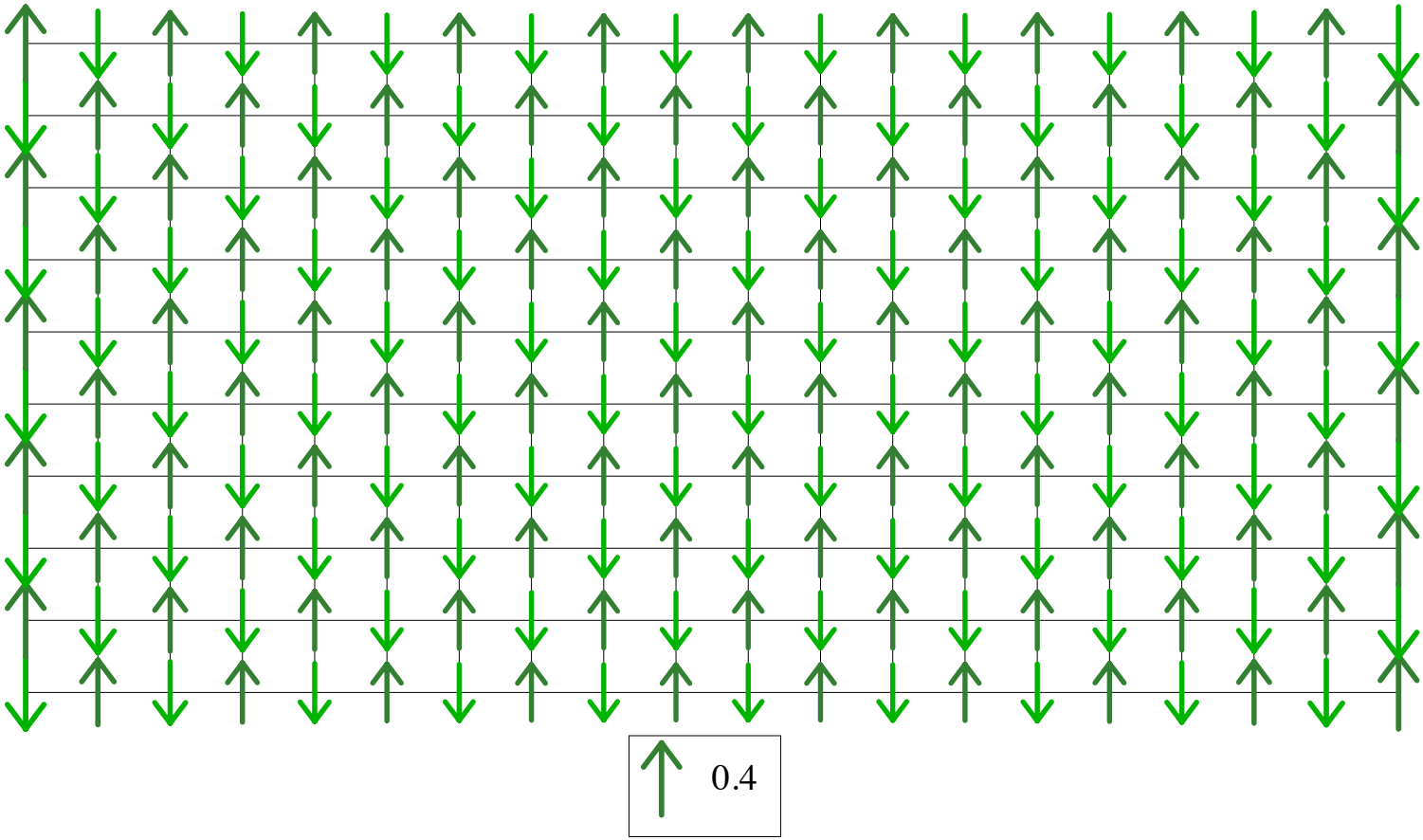
```
SpinHalf sites(N);
AutoMPO ampo(sites);
for(int j = 1; j < N;++j)
  {
  ampo += 0.5,"S+",j,"S-",j+1;
  ampo += 0.5,"S-",j,"S+",j+1;
  ampo +=     "Sz",j,"Sz",j+1;
  }
auto H = MPO(ampo);
```

This works just as well for a 2D cluster as for a chain

You need to translate your 2D lattice to 1D for it.

Let's go line by line through it and see what AutoMPO is doing. Here, we are just showing the part that makes the MPO. Higher up in the code (maybe the previous line), we must initialize a number N

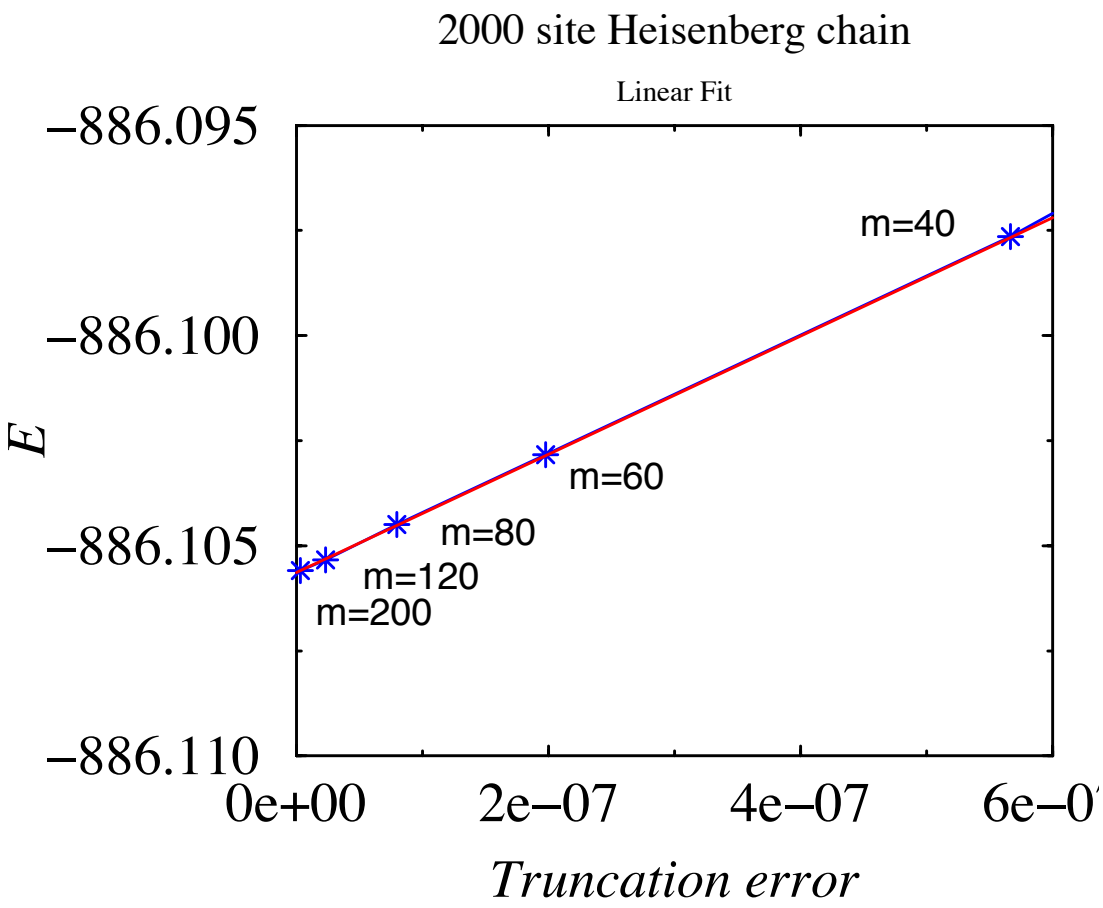
Square lattice: benchmark against QMC



20 x 10

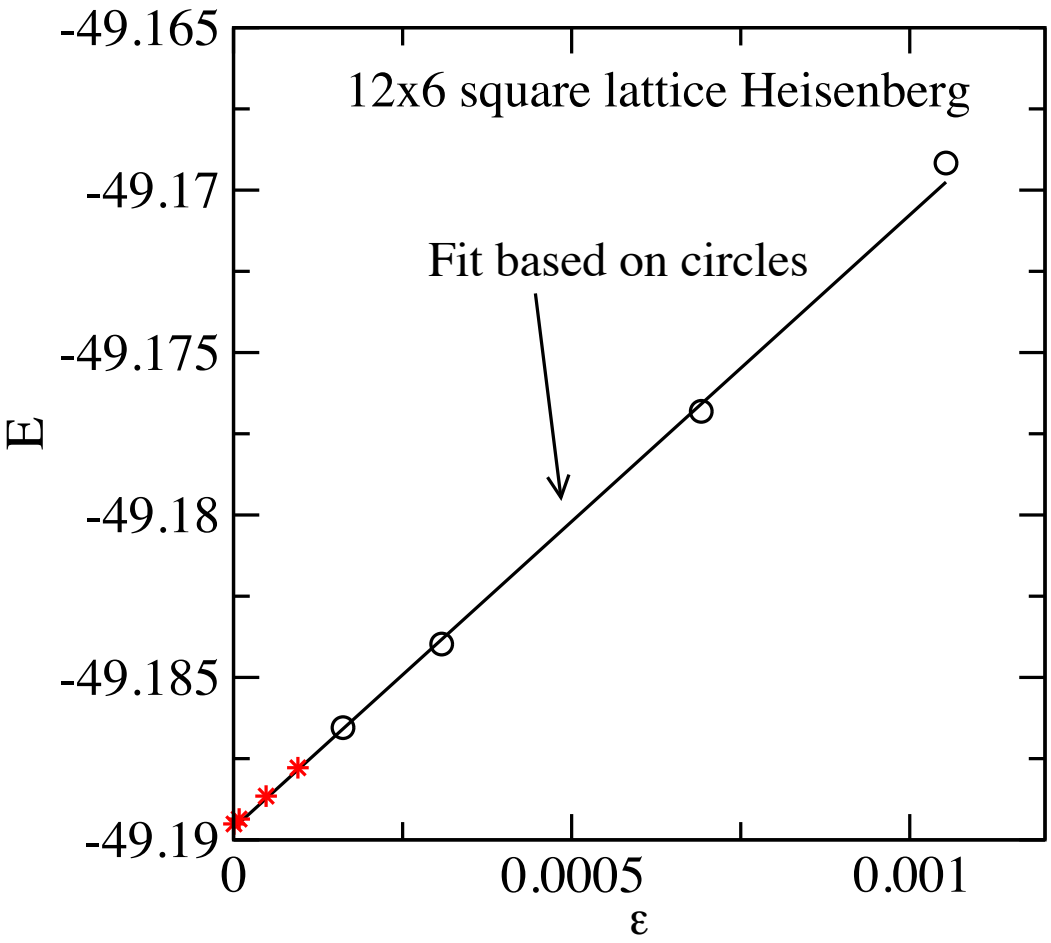
- Cylindrical BCs: periodic in y, open in x
- Strong AF pinning fields on left and right edges
- 21 sweeps, up to m=3200 states, 80 hours

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

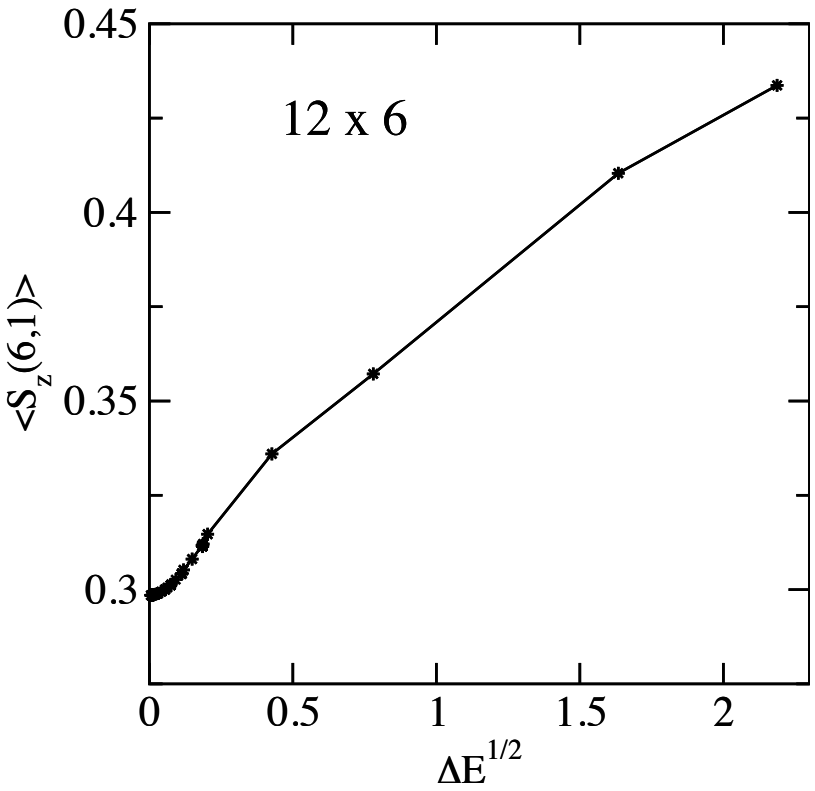
$$|\psi\rangle = |G\rangle + |\delta\rangle, \quad \langle G|\delta\rangle = 0,$$

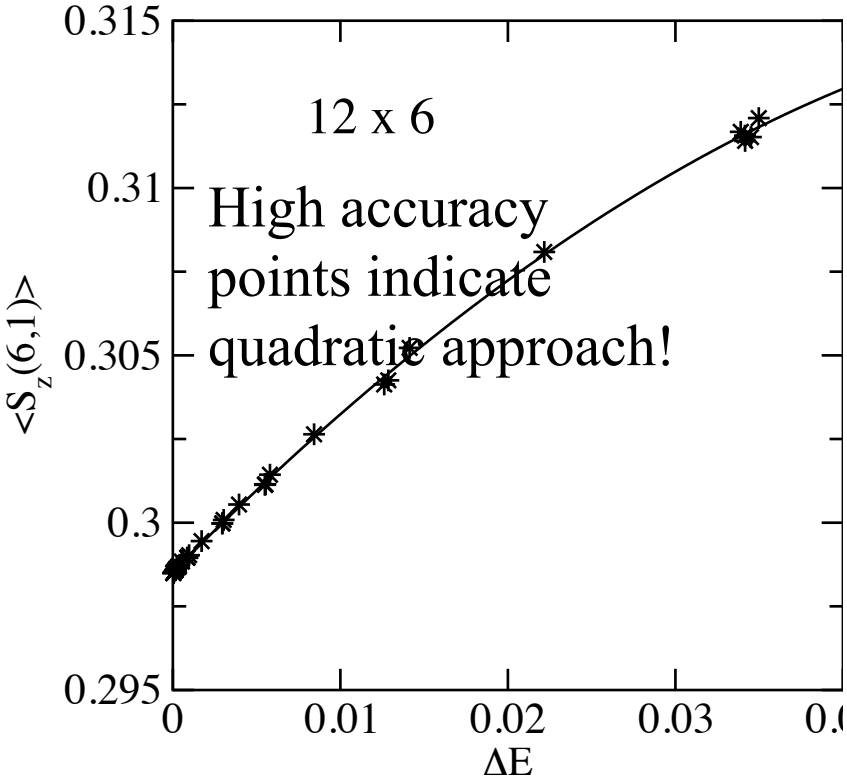
$$A = (1 + \langle\delta|\delta\rangle)^{-1}(A_G + 2\langle G|\hat{A}|\delta\rangle + \langle\delta|\hat{A}|\delta\rangle)$$

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

- 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

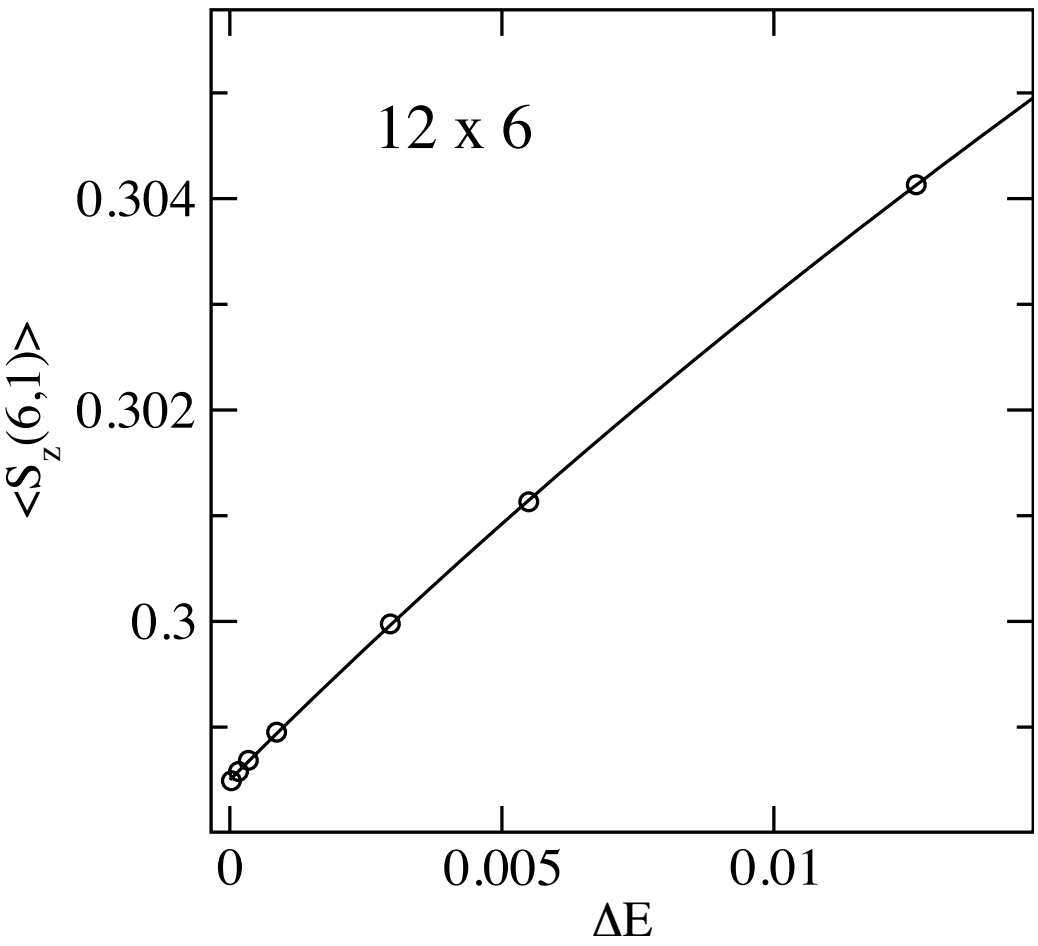




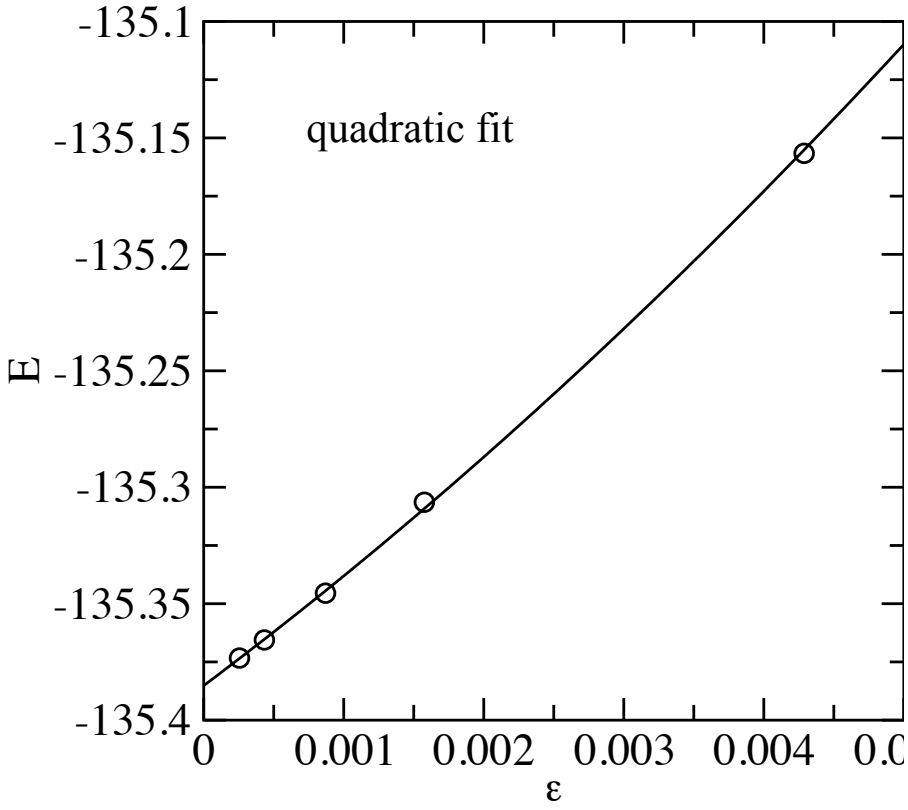
Pinning AF fields applied to edges, cylindrical BCs

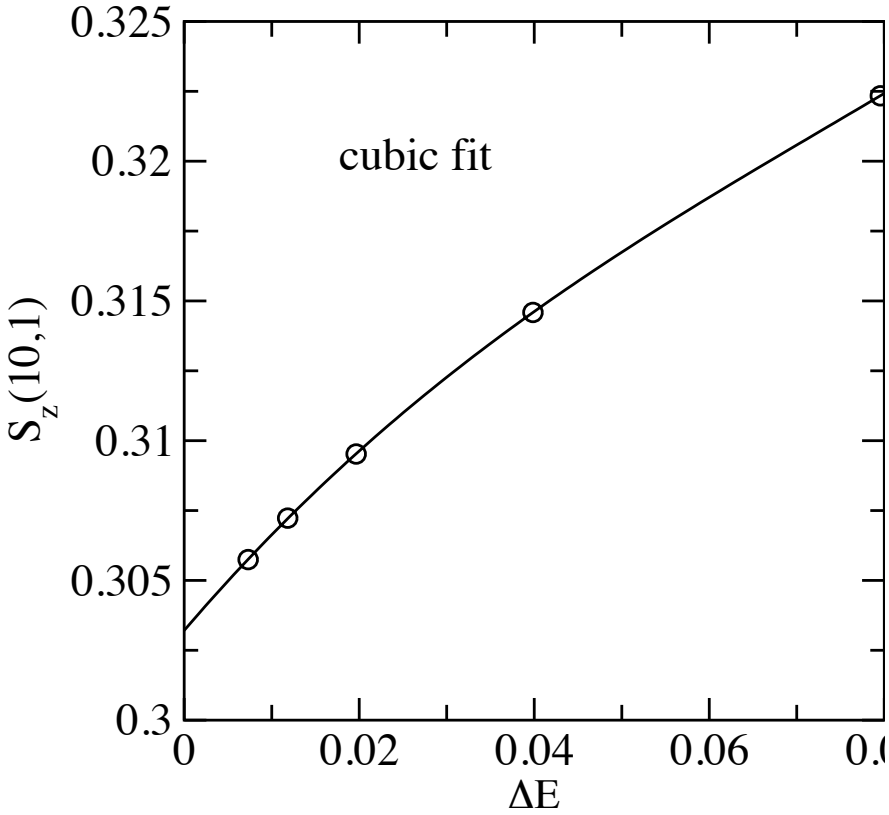
Now we understand why the local measurements converge fast; see White & Chernyshev

Cubic fit to well-converged measurements



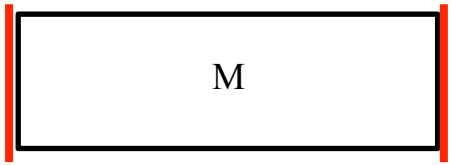
20x10 square lattice Heisenberg



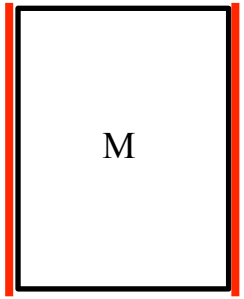


Result: central M = 0.3032(9)

Improved finite size scaling: choosing aspect ratios to reduce finite size effects



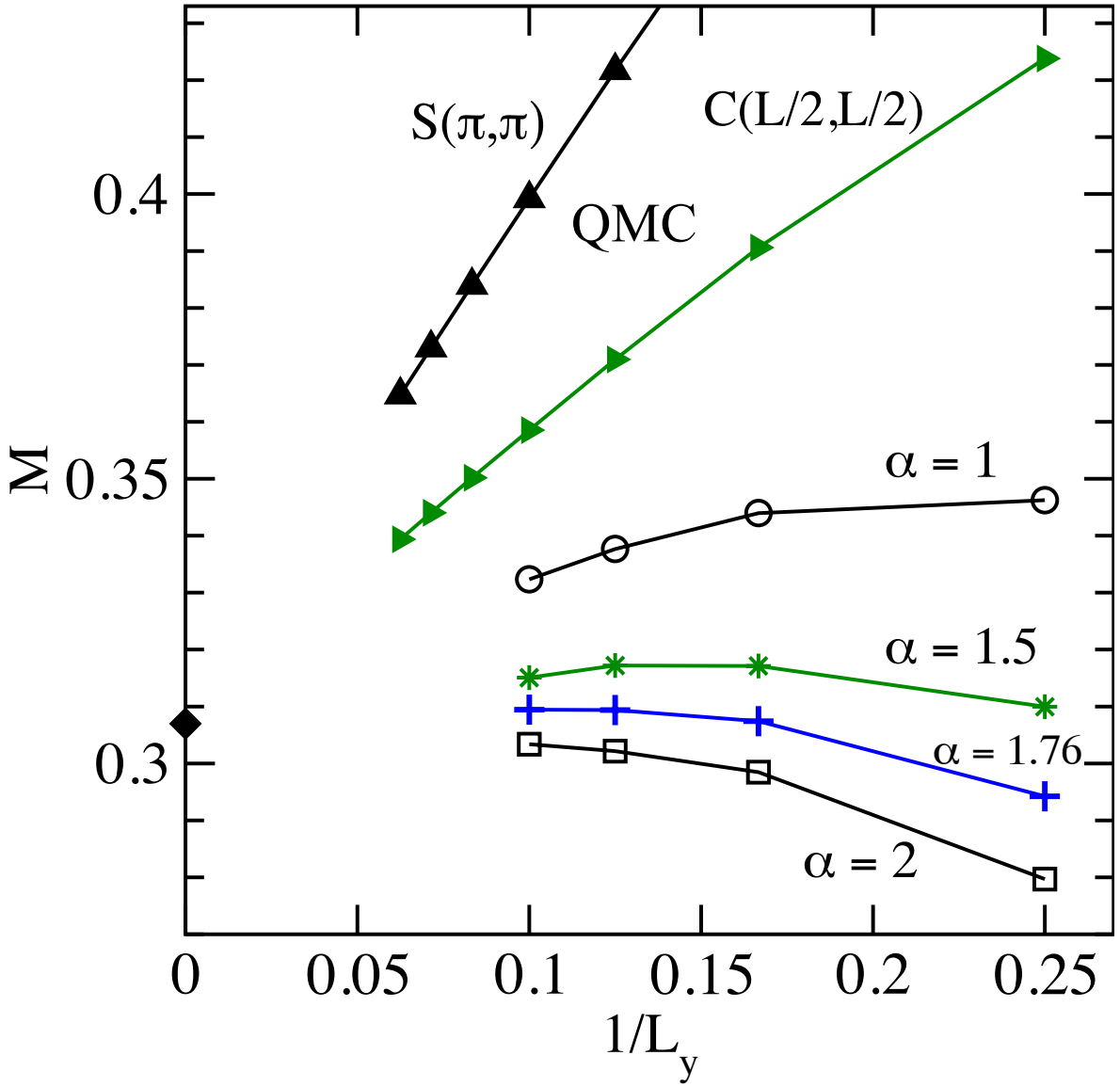
Long: 1D makes M small



Short: proximity to strong pinning makes M large

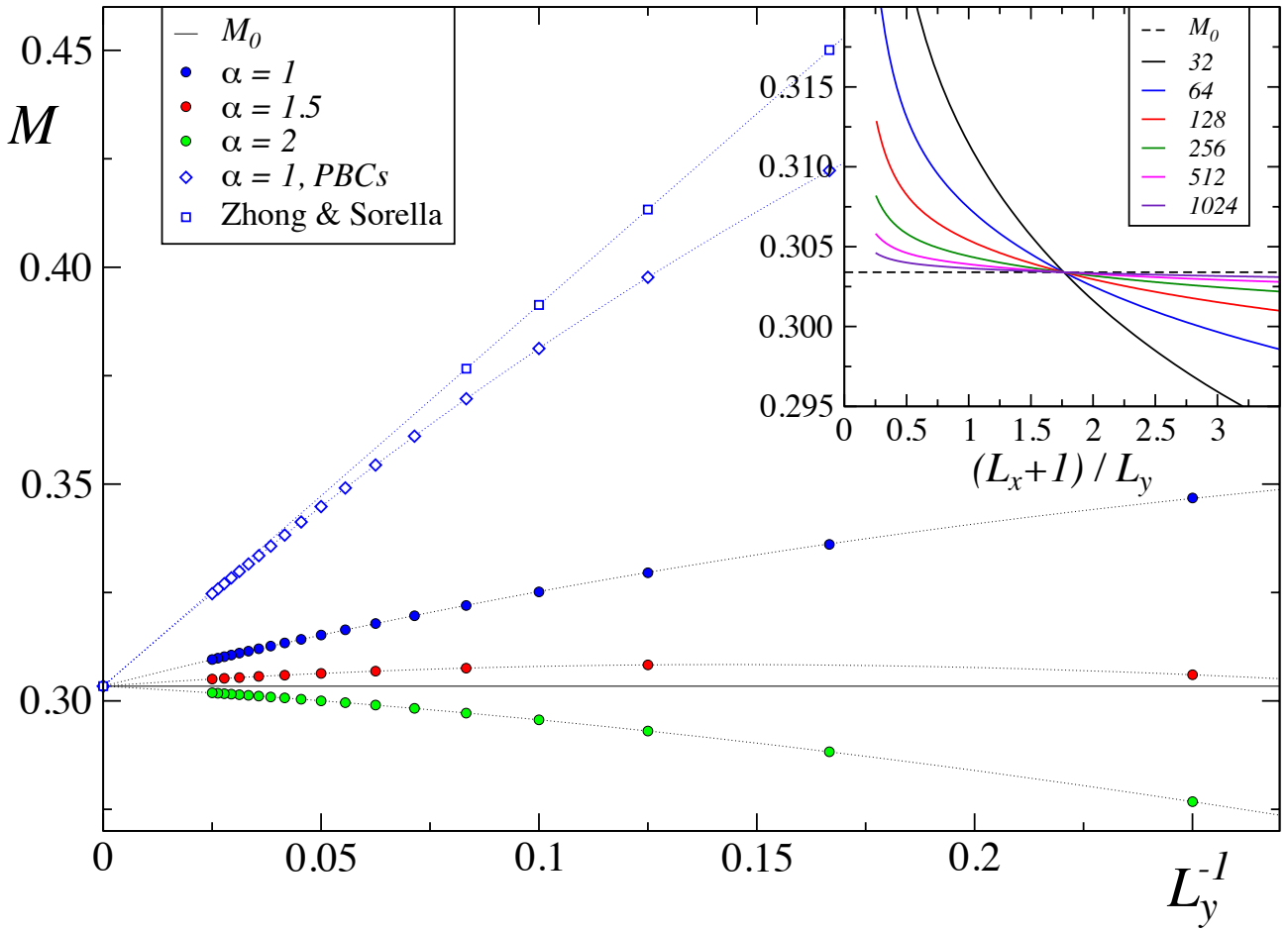
- "Standard" measurements in QMC estimate M^2 using correlation functions and have large finite size effects $O(1/L_y)$
- Can one choose a special aspect ratio to eliminate $O(1/L_y)$ term?
- What is behavior at large length scales? Use finite system spin wave theory as a guide.

Square lattice



$\alpha = L_x / L_y$

Finite size spin wave theory

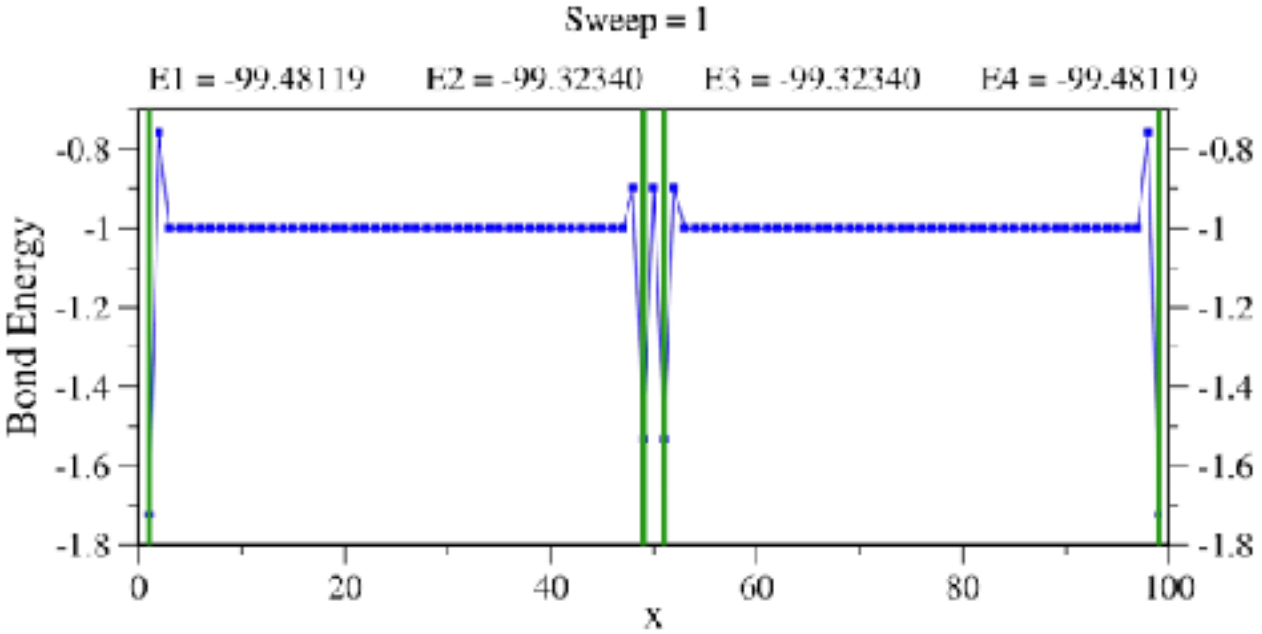


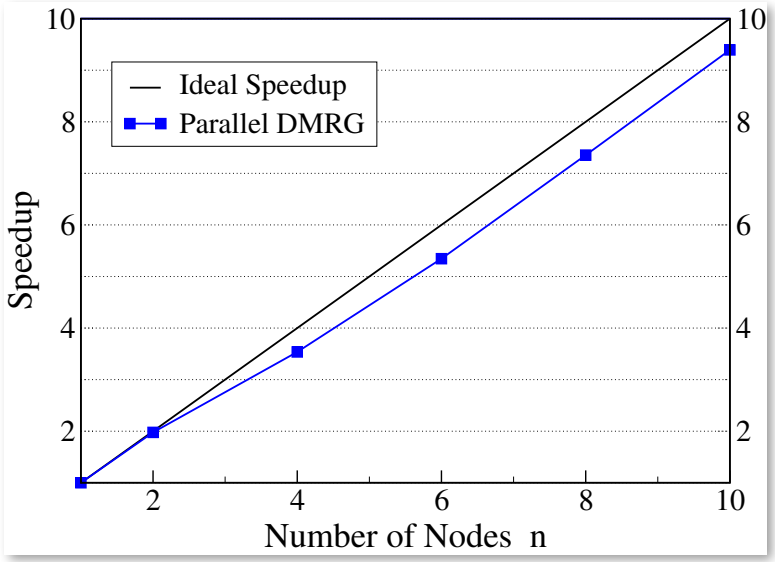
- Optimal choice $\alpha = 1.764$ eliminates linear term
- Even $\alpha = 1$ has much smaller finite size effects

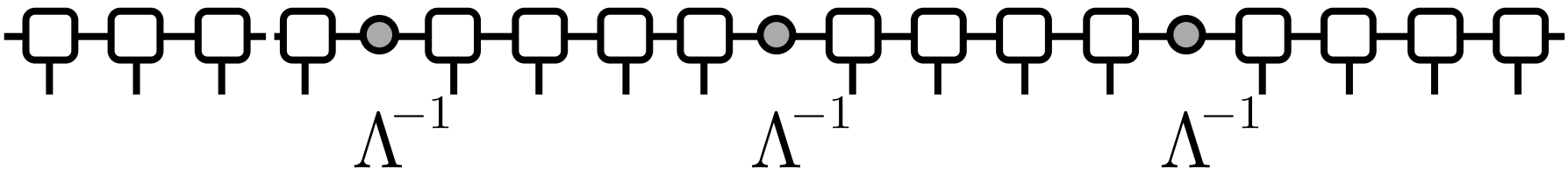
Parallel DMRG

Stoudenmire & White, PRB **87**, 155137 (2013)

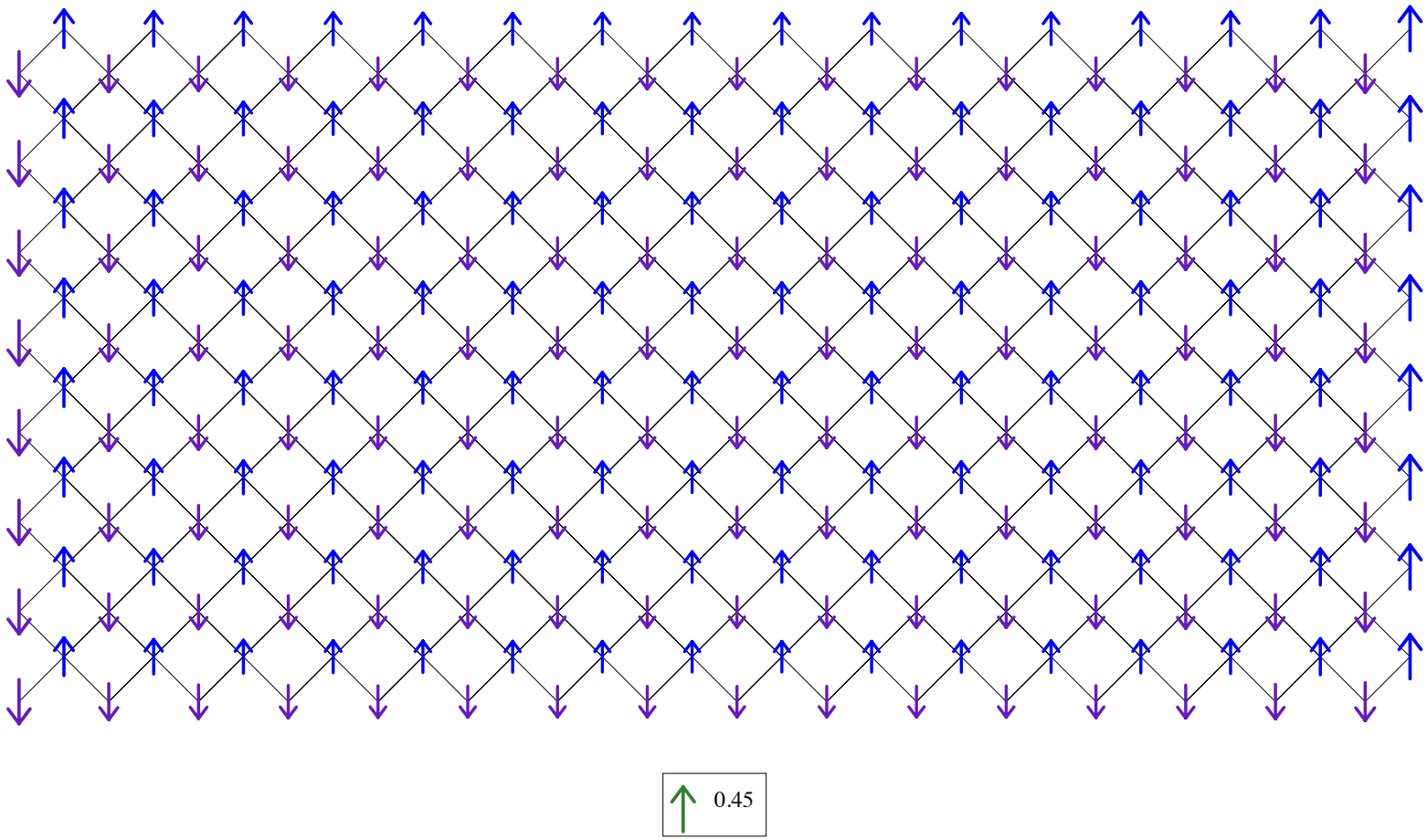
- Parallelize single DMRG calculation across **real space** blocks
- Nearly ideal speedup
- Key step: MPS gauge transformation at block boundaries, each block has orthogonal environment





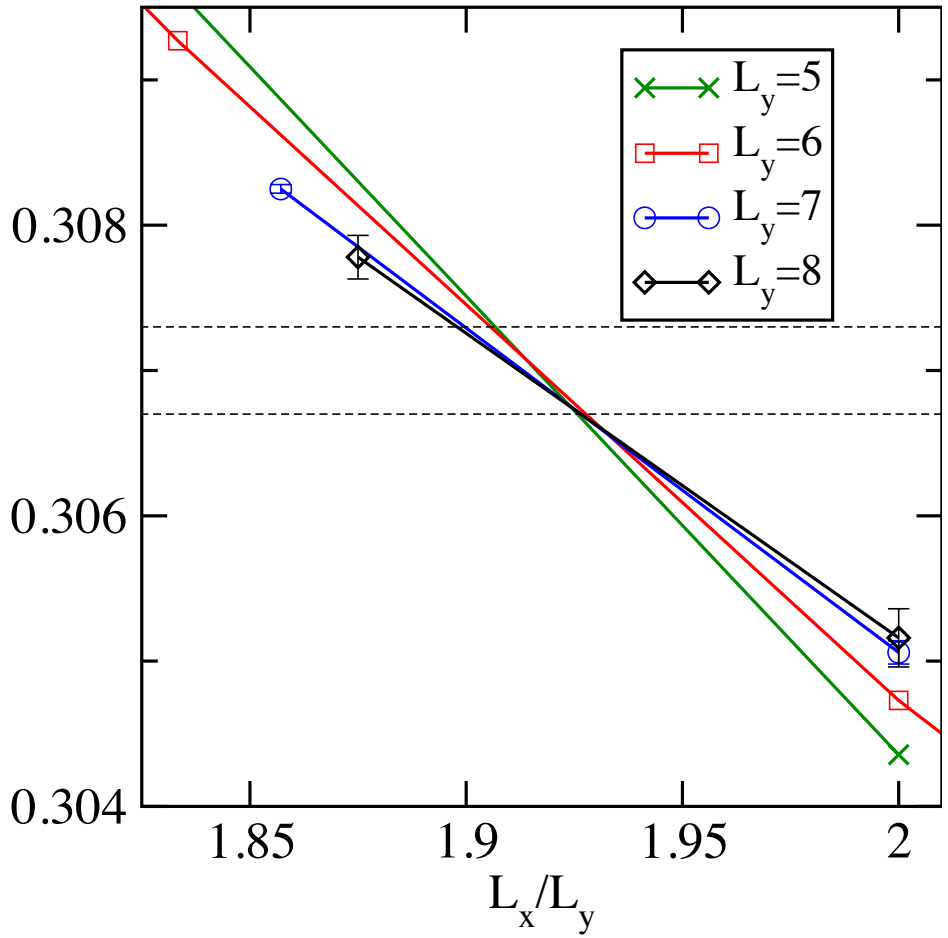


Tilted square lattice



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

Tilted square lattice



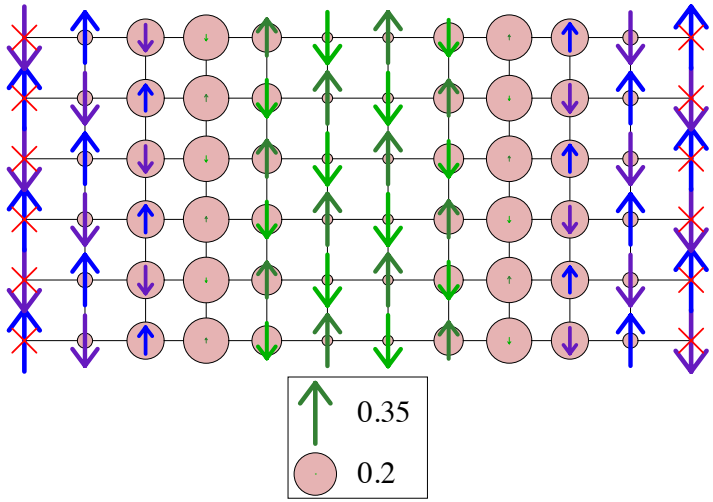
Sandvik, QMC

Energy, extrapolated to thermo limit: -0.669444(5)

Sandvik (1997): -0.669437(5)

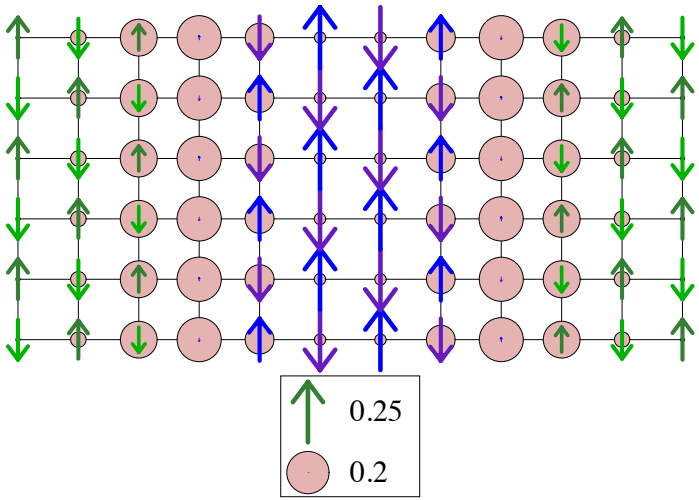
- Results are consistent with and with comparable accuracy to QMC! (of 1997, at least)
- Latest QMC (Sandvik&Evertz) -0.30743(1) (No new E)

t-J model: stripes on width 6 cylinders



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

Pinning AF fields

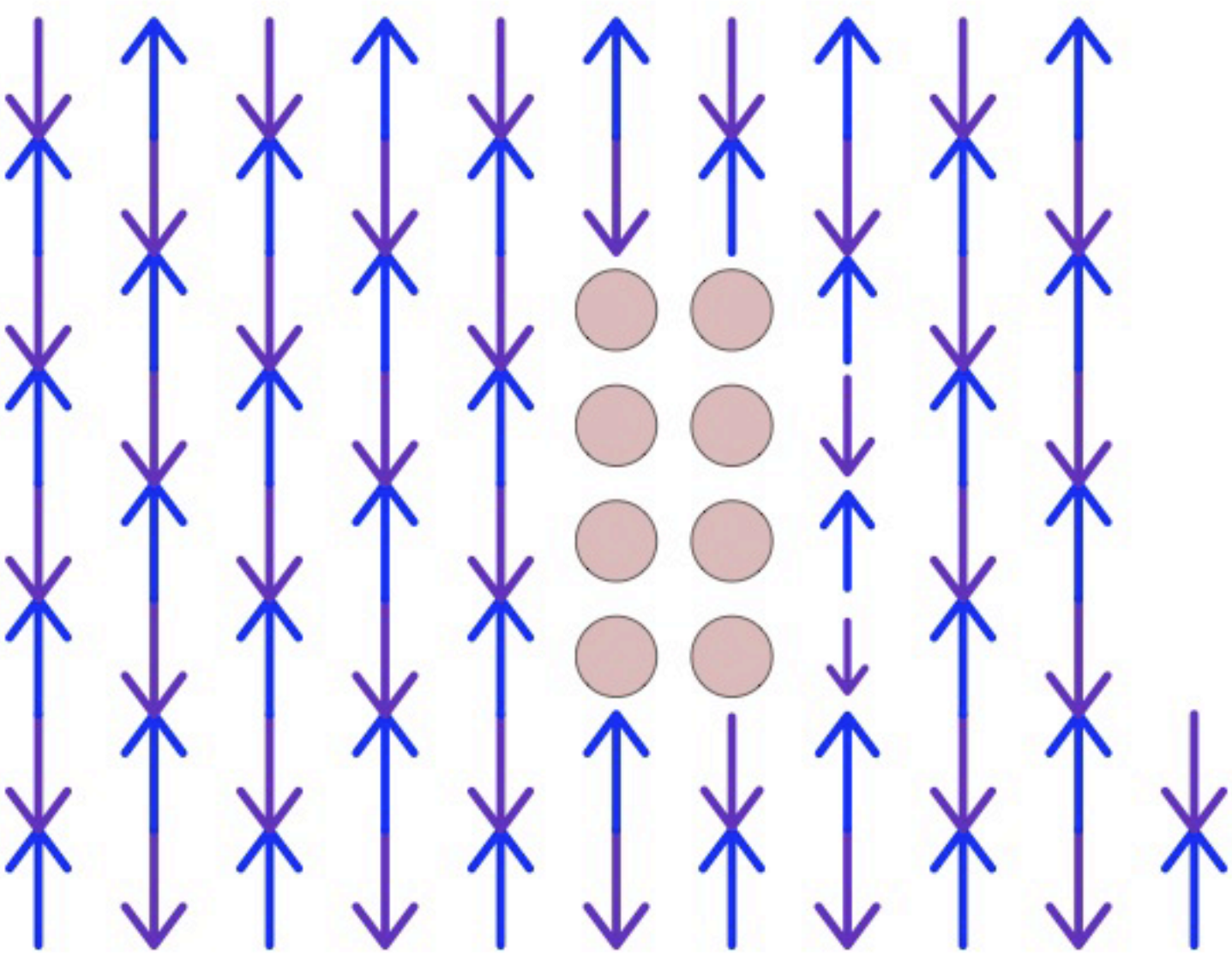


12 x 6 system, Vertical PBC's
J/t = 0.35, 8 holes

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?

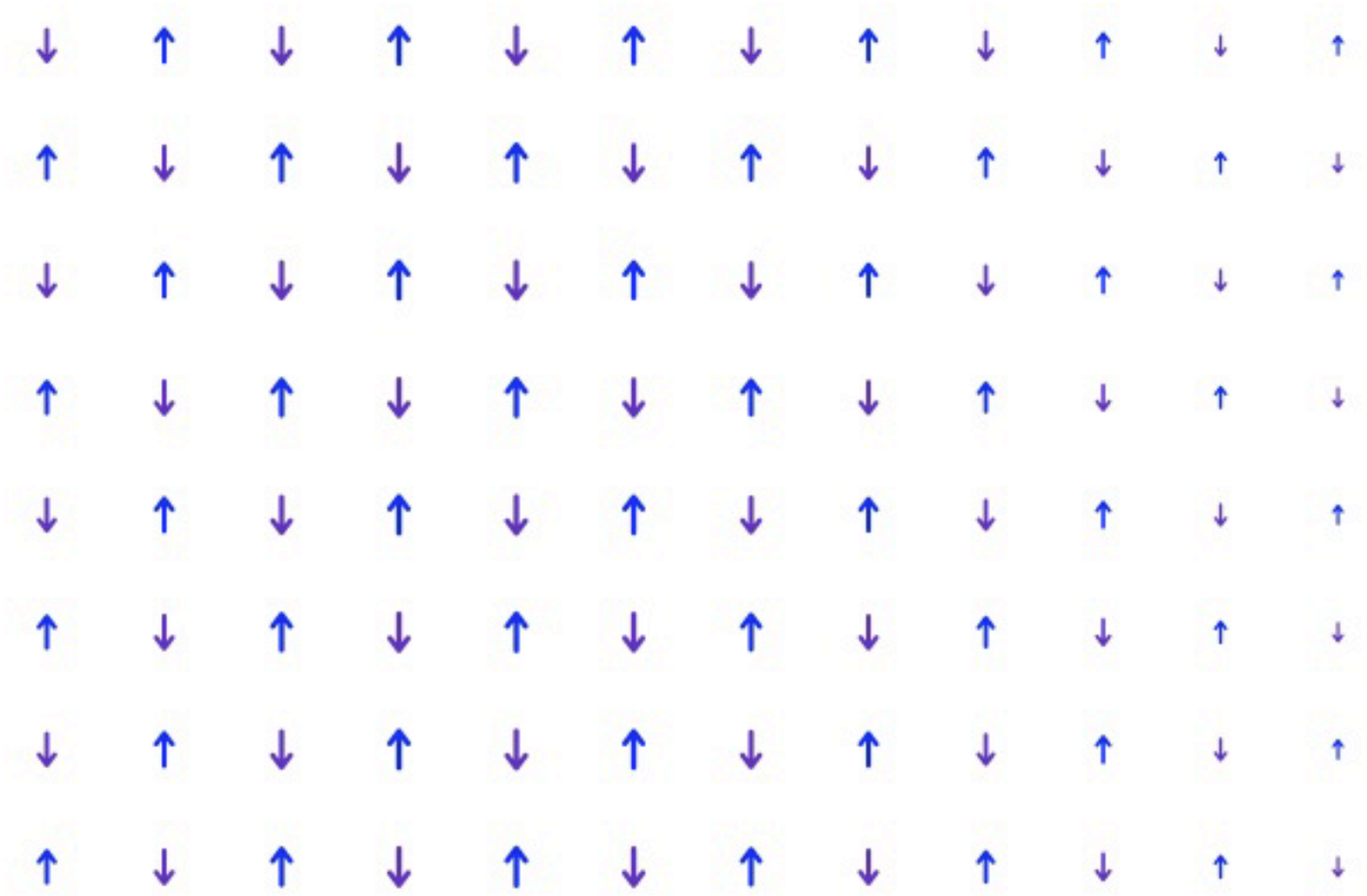
Stripes forming from a blob of 8 holes



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

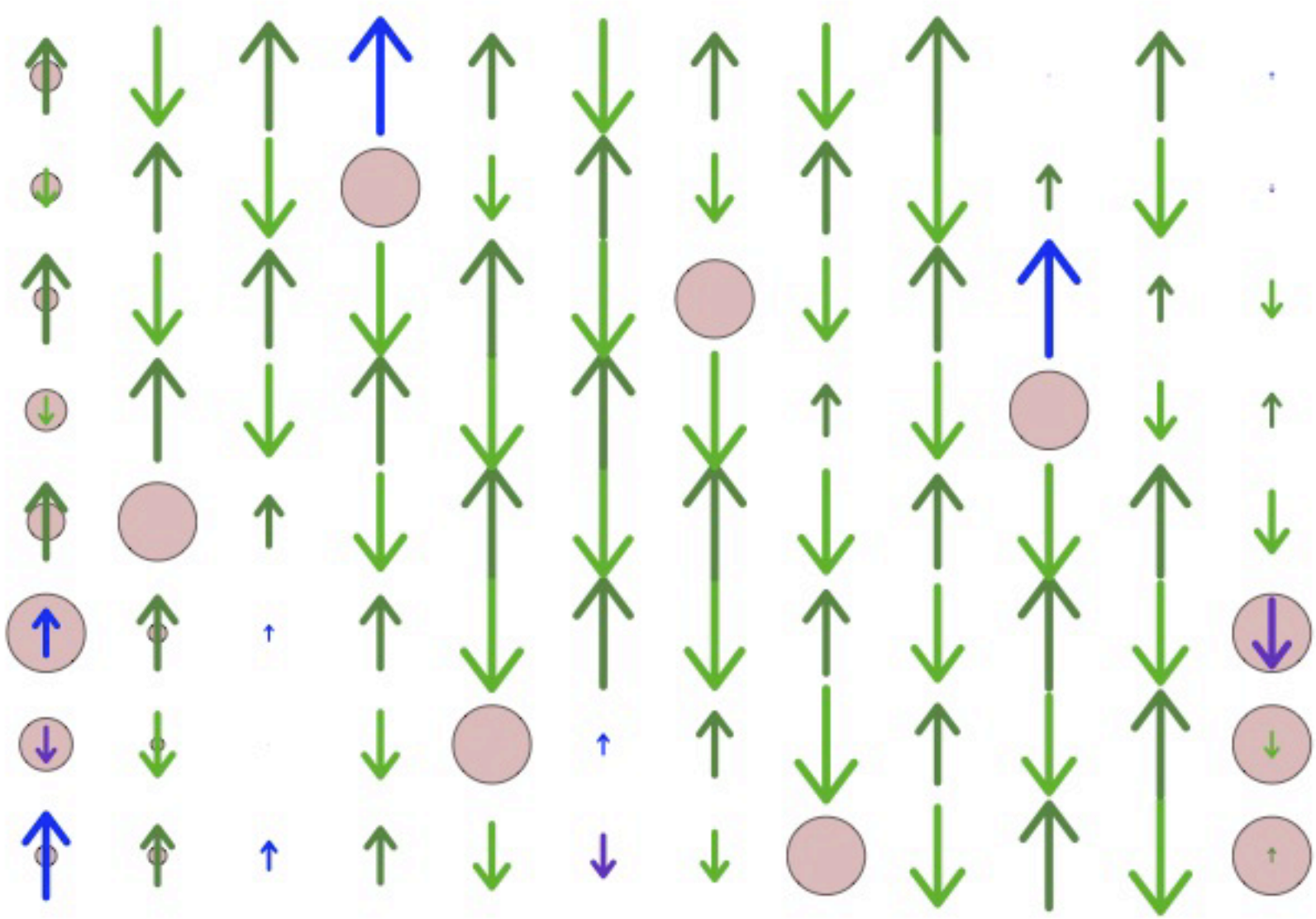
Undoped system: Restoration of SU(2) symmetry



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

E = -38.0681 m = 600

Stripes not forming from a bad initial state

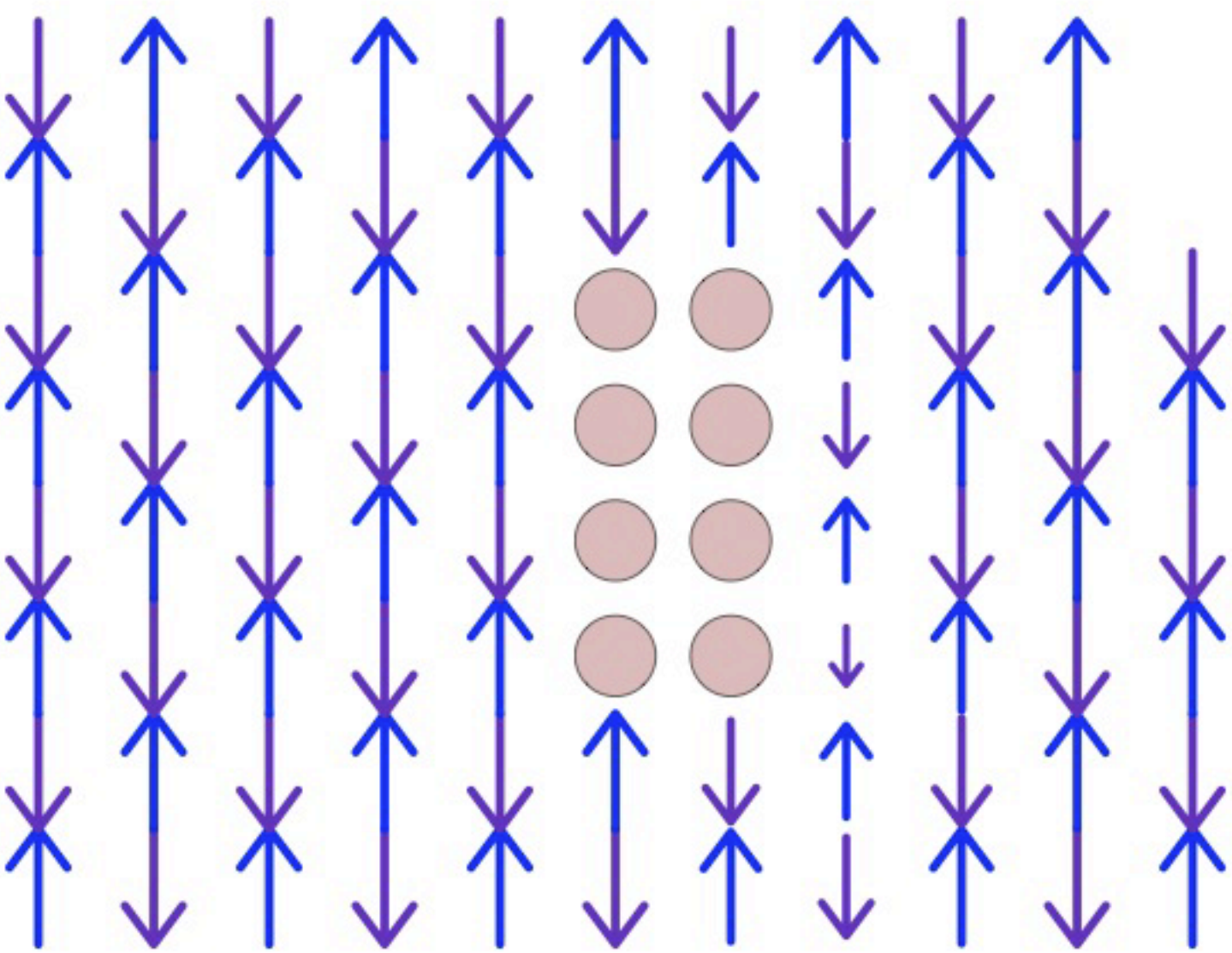


E = -30.6370

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.

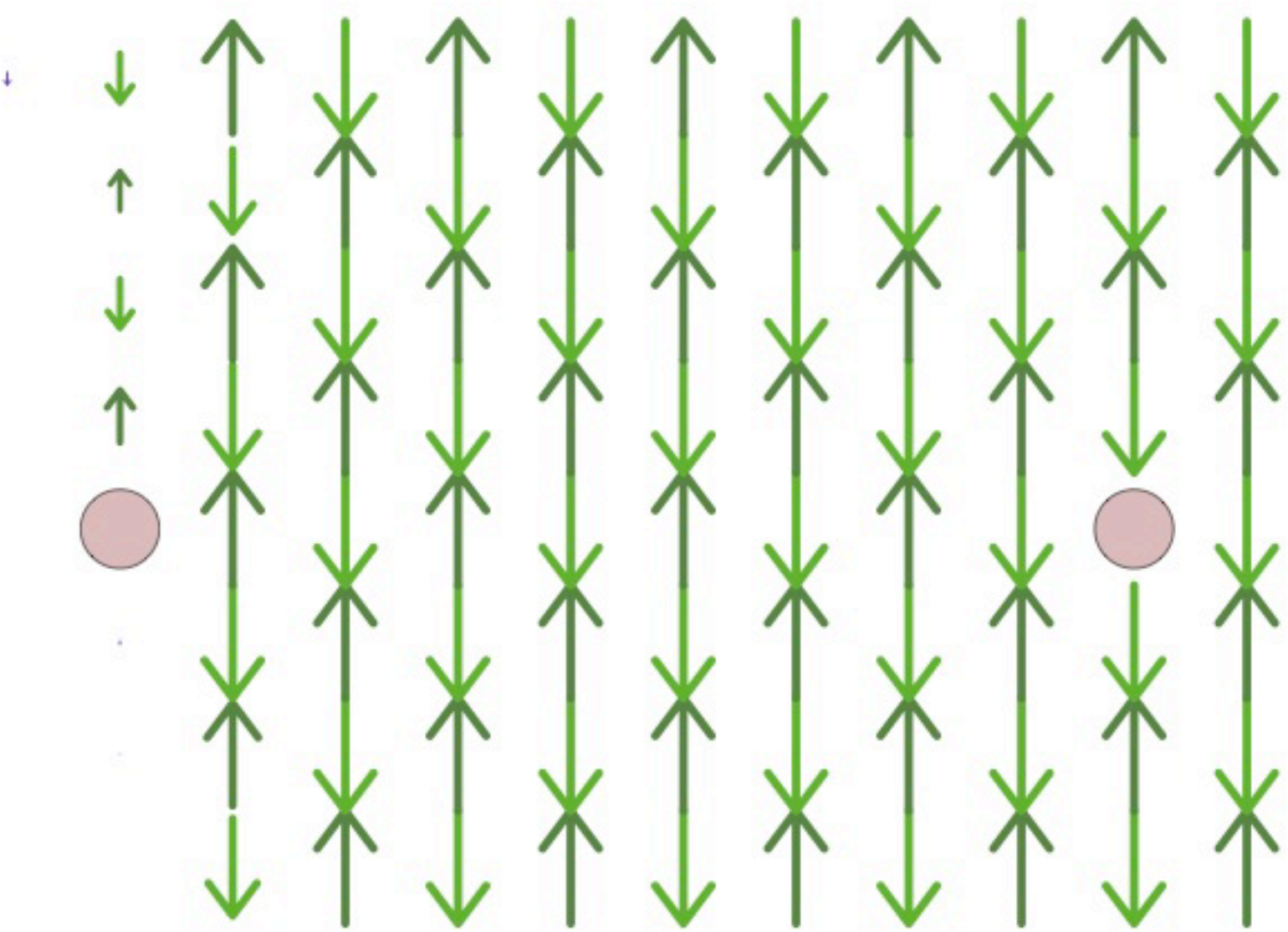
Curved Stripe forms due to open BCs



E = -30.8532 m = 40

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

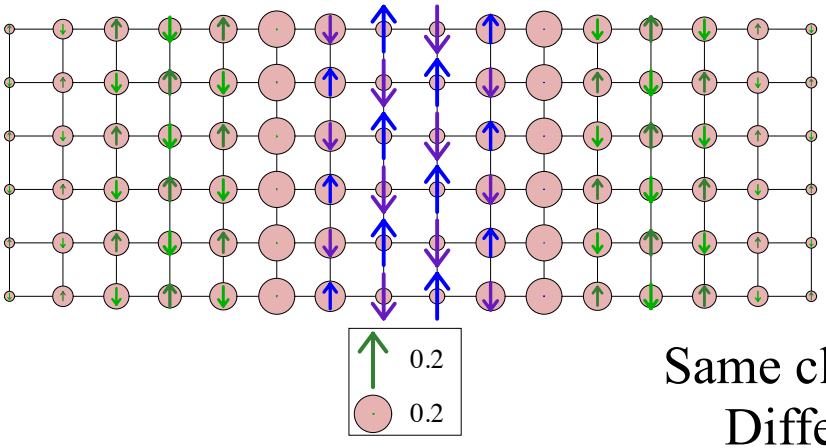
t'=0.3: two holes attract

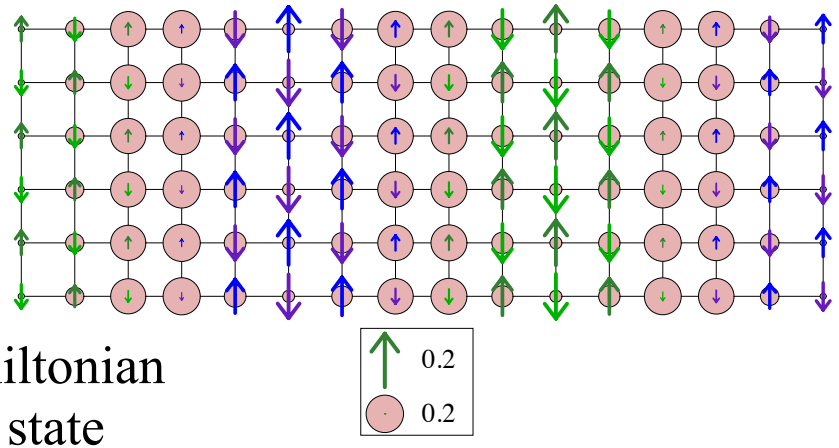


E = -31.0529 m = 40

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

t-J model: stripes on width 6 cylinders

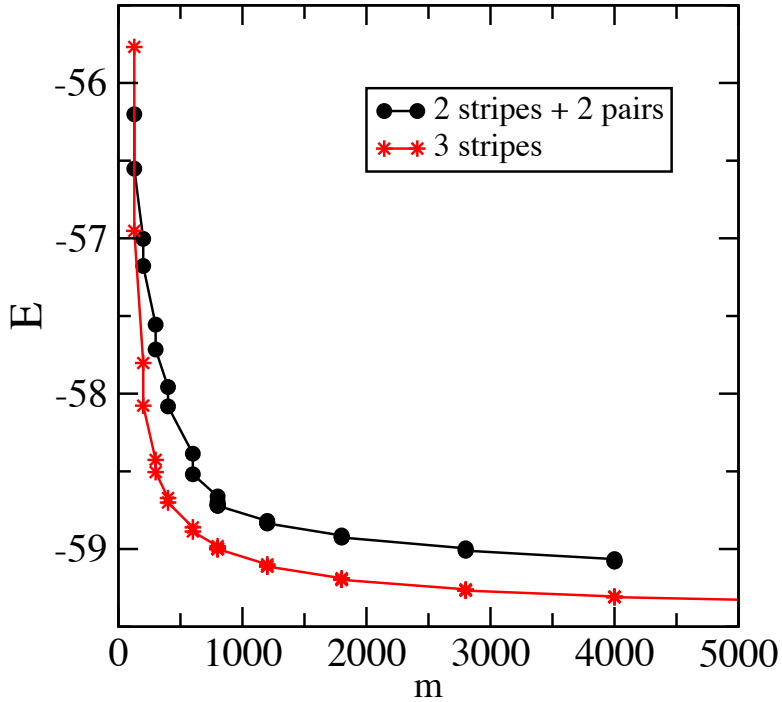




Same cluster, Hamiltonian
Different initial state

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

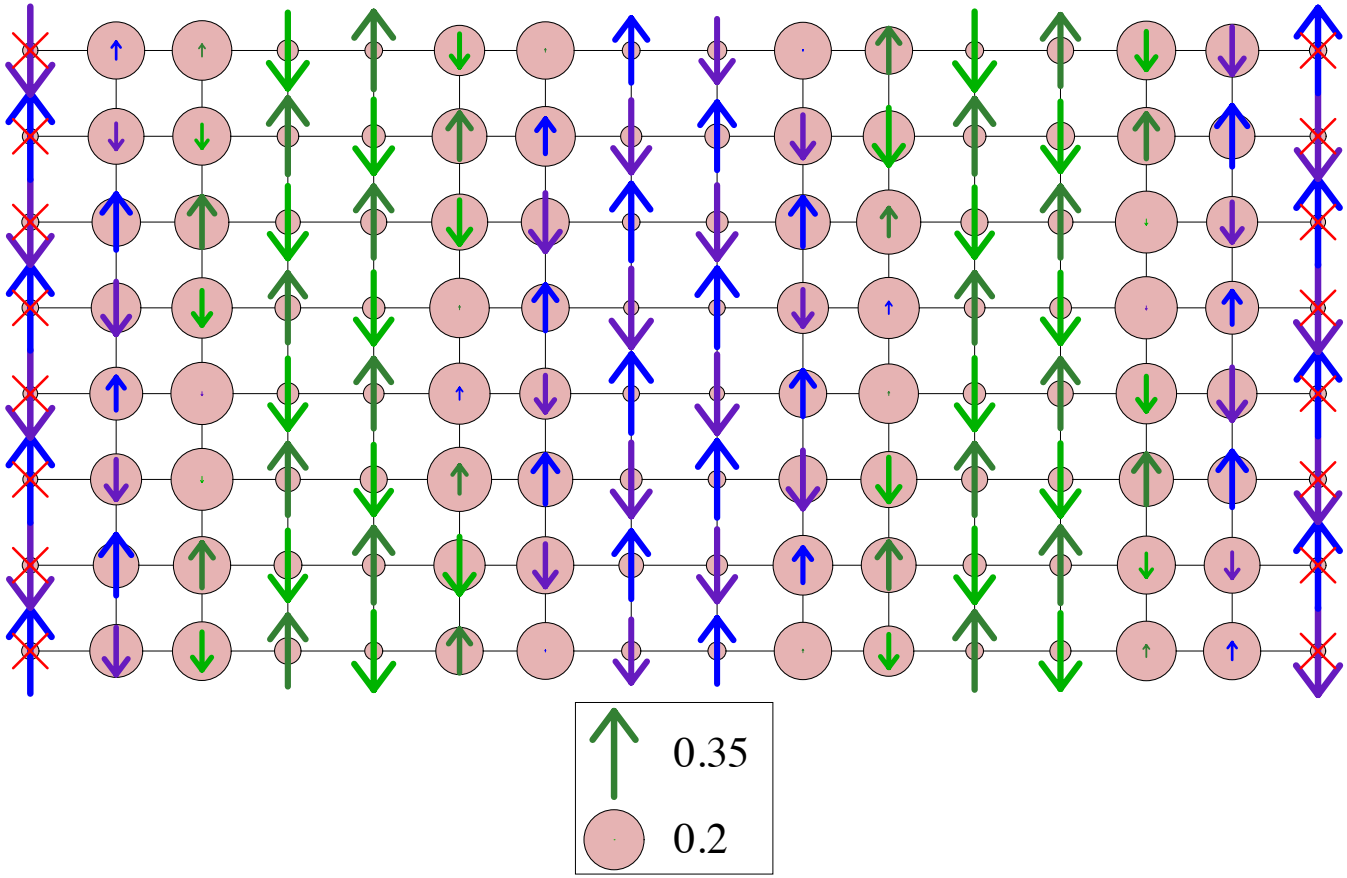
16 x 6 system, Vertical PBC's
J/t = 0.35, 12 holes



Convergence to metastable state: excellent

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

Stripes on 8 leg ladders



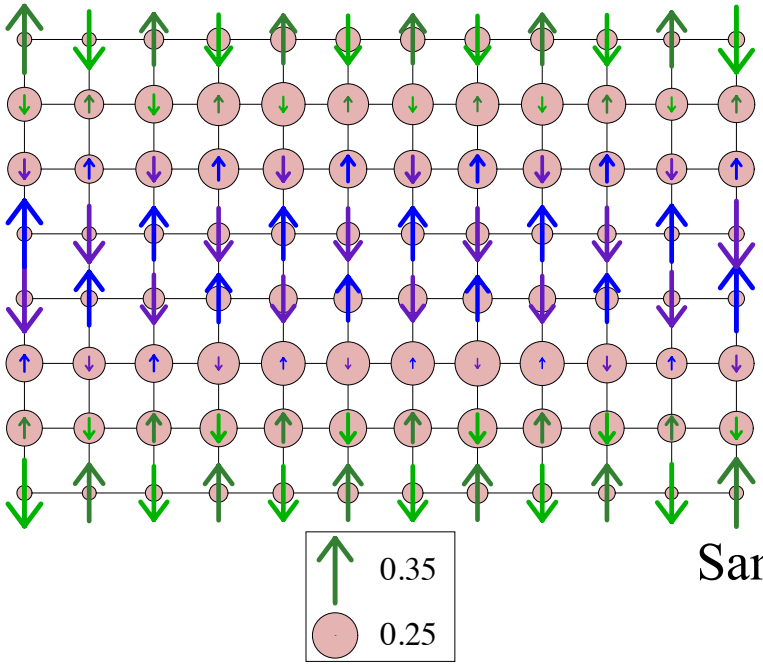
16 x 8 system, Vertical PBC's

J/t = 0.35, 16 holes

White and Scalapino,PRL '98

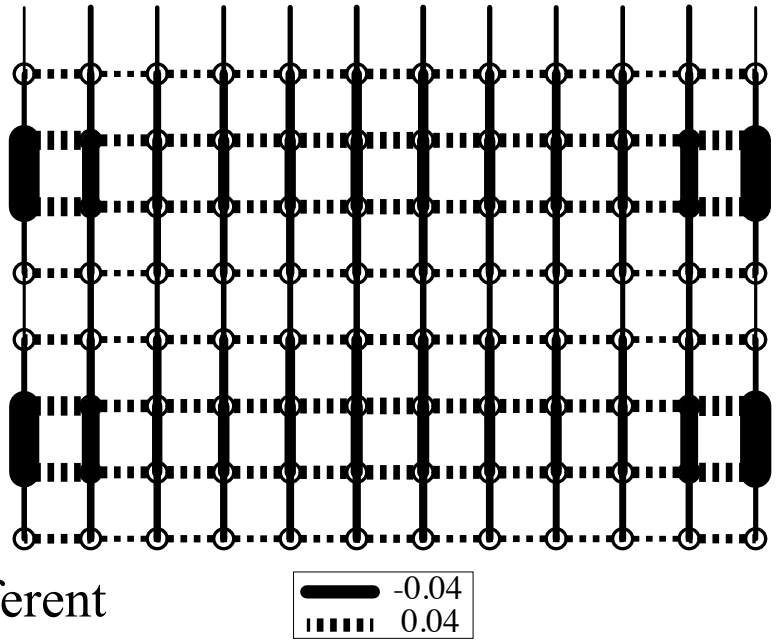
m ~ 2000 → m ~ 10000-15000 still striped

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

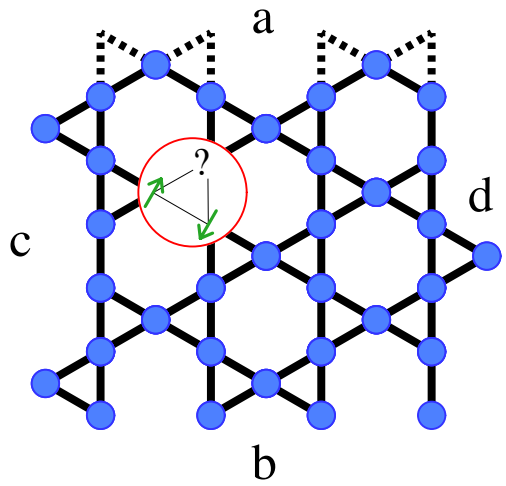


12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

Bond thickness shows pairing strength (dashed = negative)

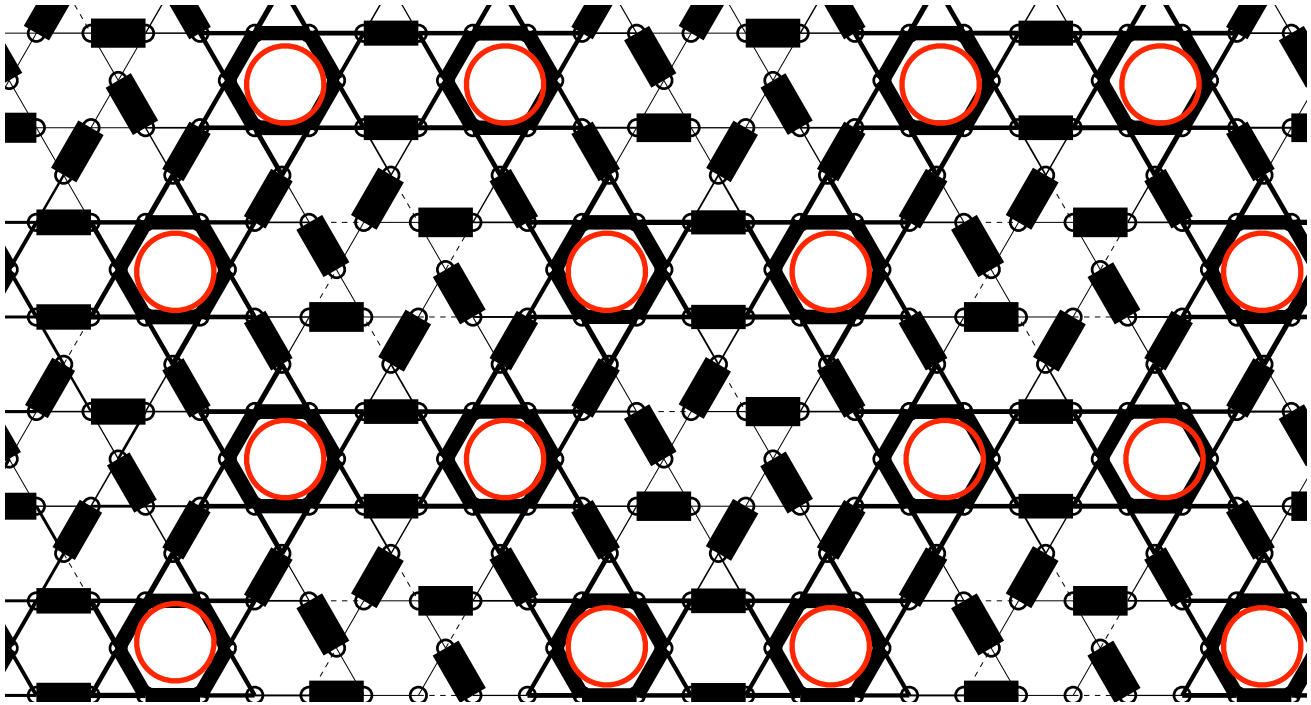
- To orient the stripes longitudinally, we use Jx>Jy.
- Larger J gives stronger pairing.
- Local measurements of response converge much more quickly than correlations, especially for pairing.

Kagome Basics



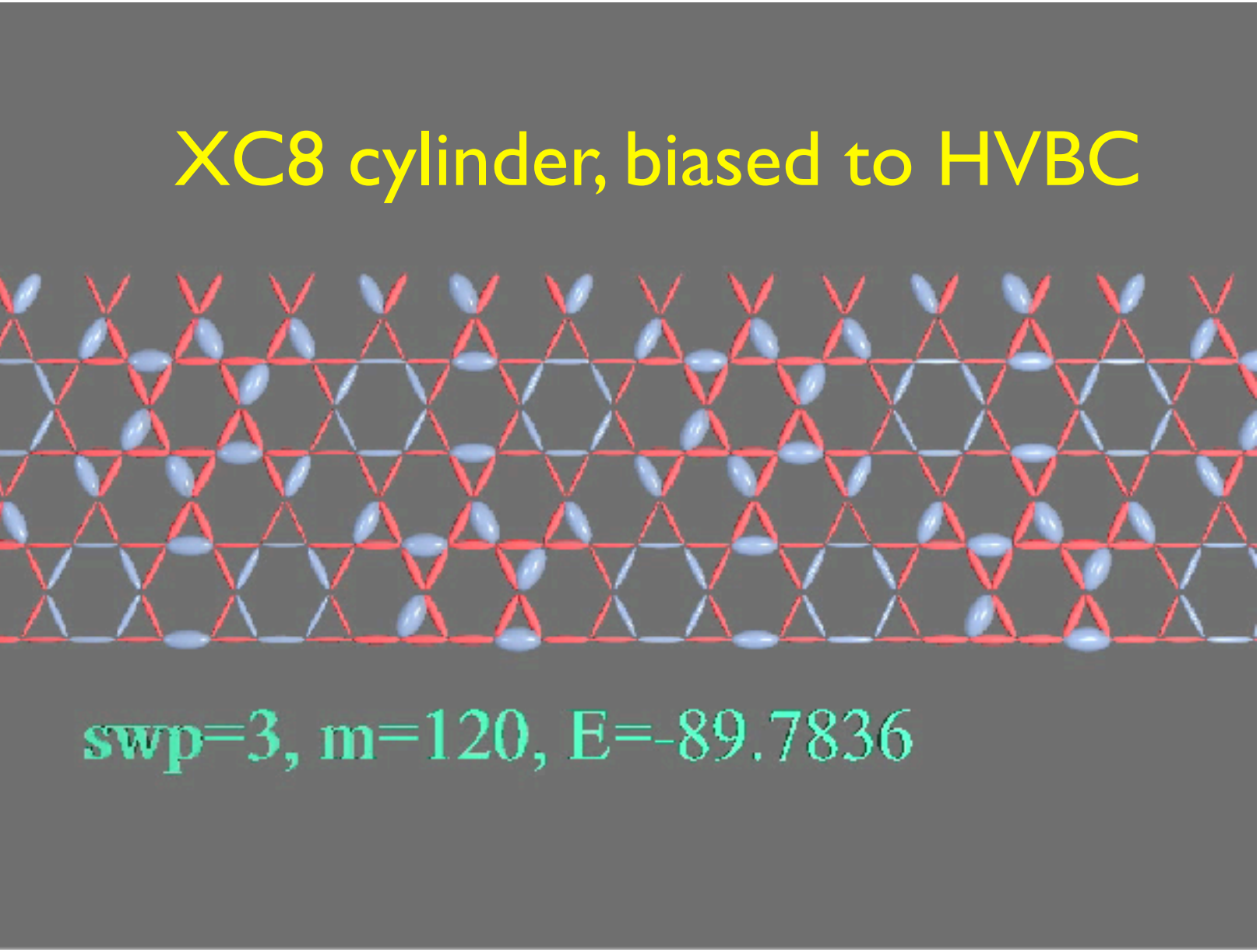
- The Heisenberg model on the kagome lattice is one of the most frustrated systems
  - Proposed as a possible spin liquid in late 80's, support from field theory (Z_2...)(Sachdev, Read)

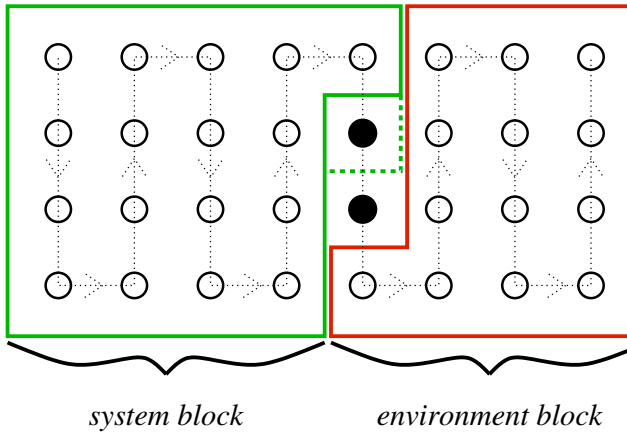
But is it instead a valence bond crystal??

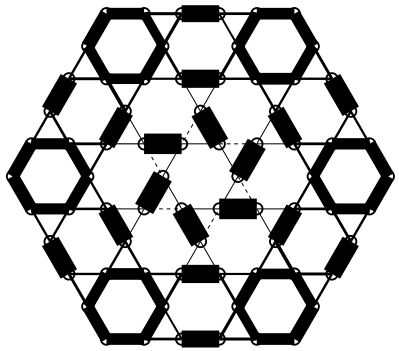


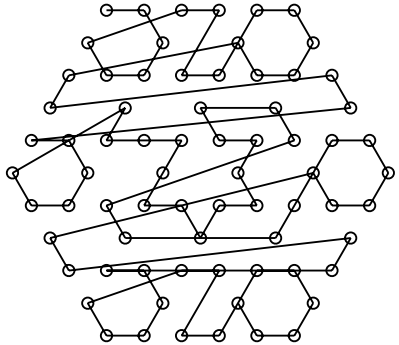
Honeycomb VB crystal: maximizes 6 site (hexagon) resonance configurations

Sample DMRG simulation on Kagome









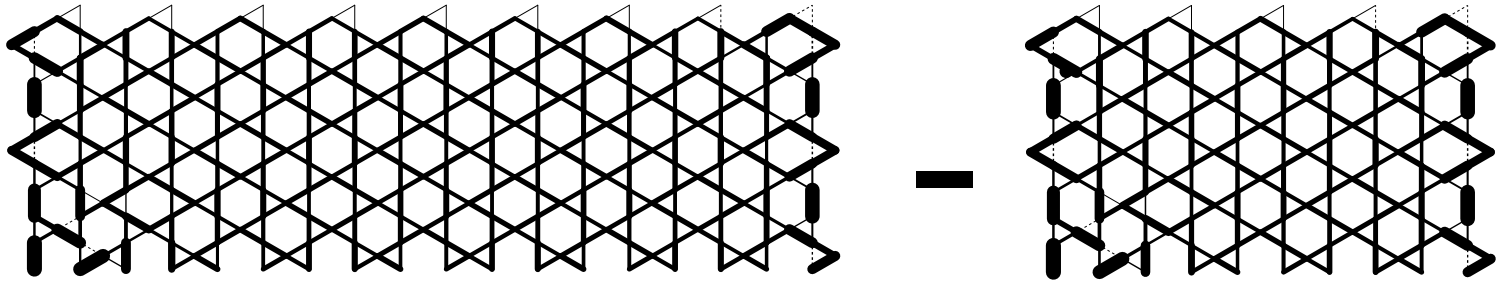
Density matrix renormalization group = energy minimization method over matrix product states

Highly biased path

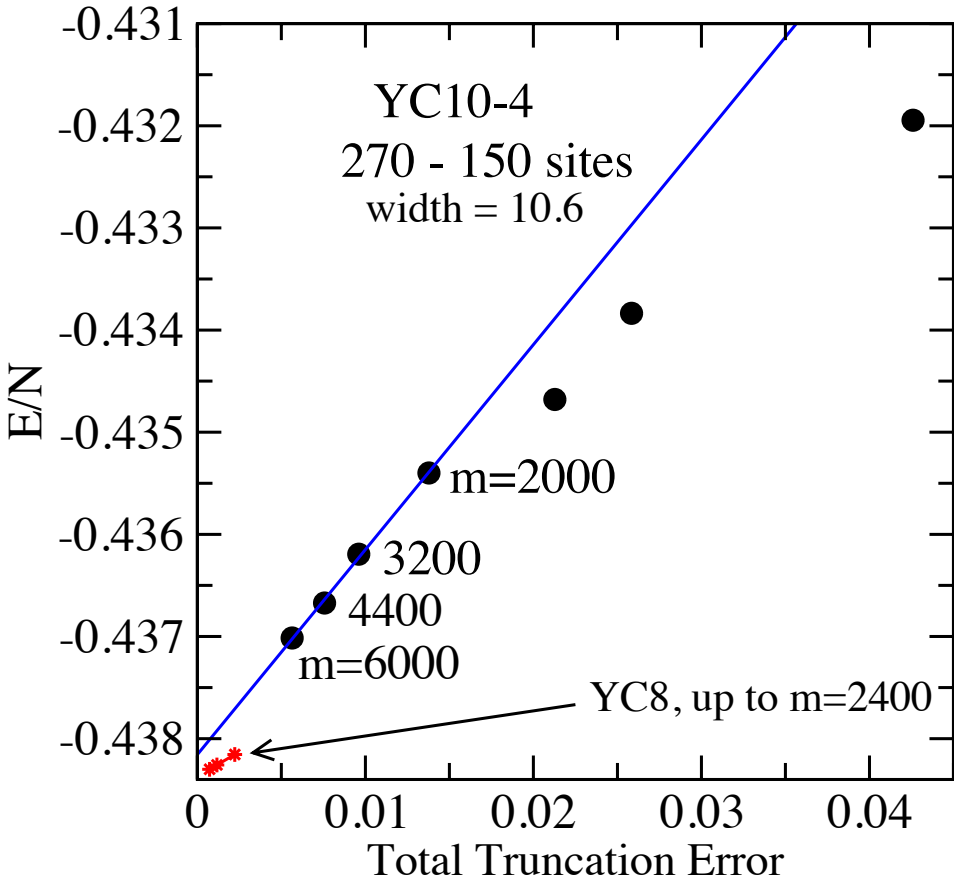
Practical Issues for Kagome

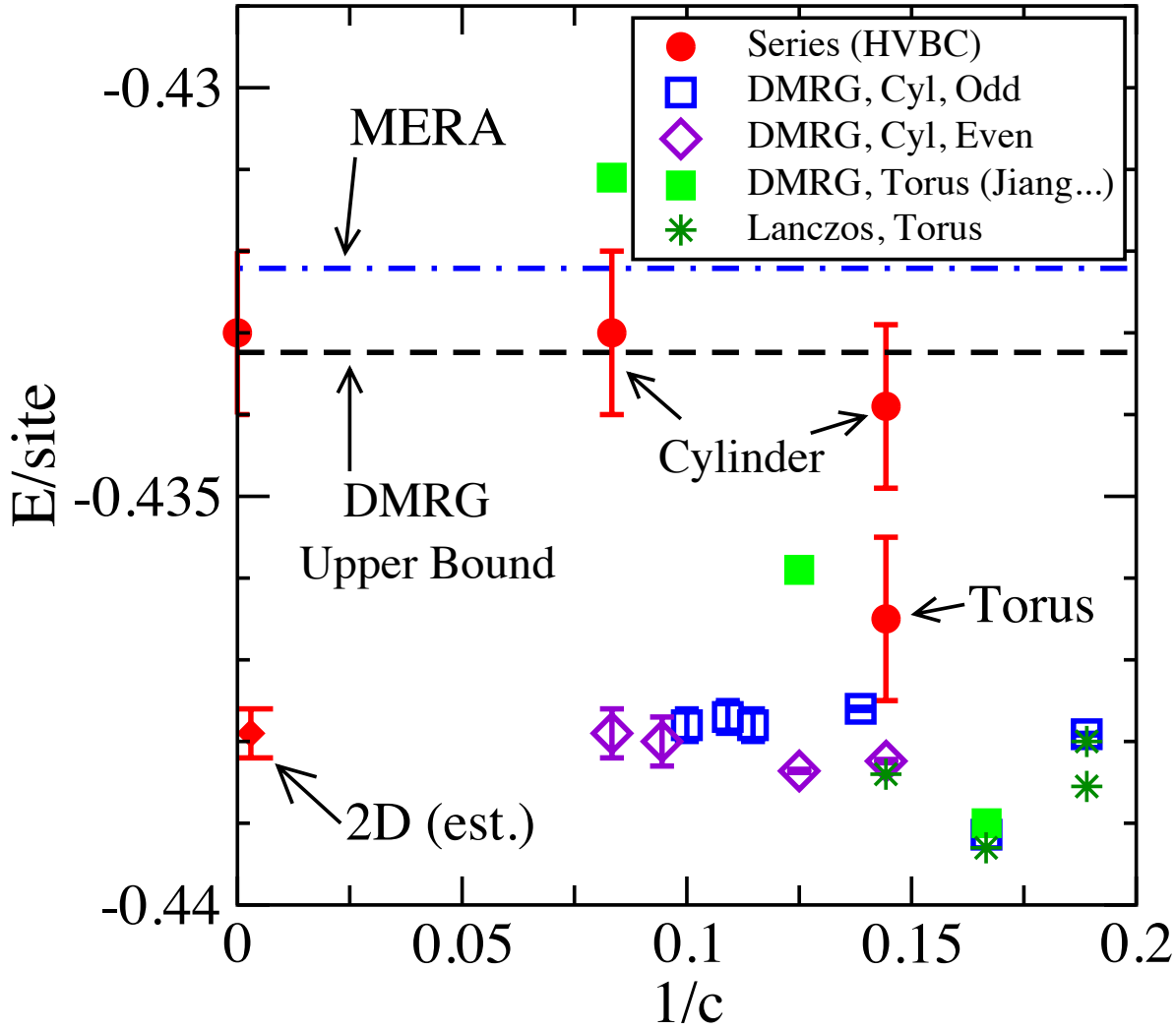
1. Metastability: getting stuck in a higher energy state (usually an issue only on wider cylinders)
   - Need to understand system and find a simple state close to the ground state to initialize DMRG
2. Strong dependence on width (and shift) of cylinders
   - Need to do many cylinders and understand patterns of behavior
3. Open edges--obtaining bulk cylinder behavior
   - This is a minor problem for this system
   - Open ends useful for pinning, selecting different topological sectors...

Total Energy comparisons



Cylinders--
subtract to
get bulk
energy



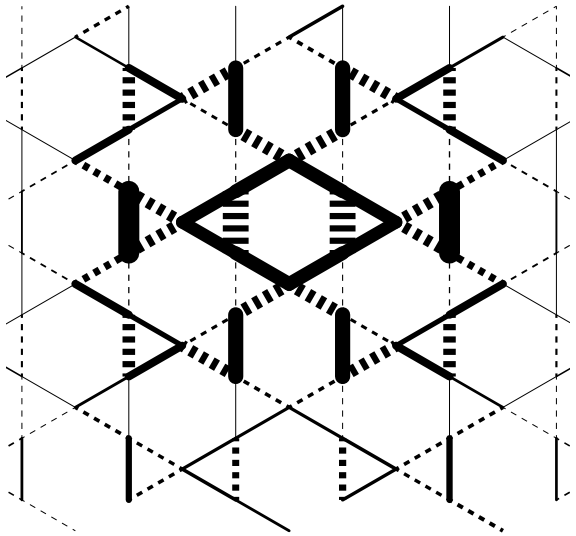


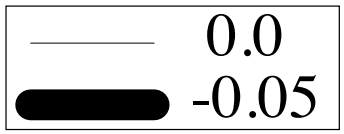
The Kagome spin liquid ground state: questions:

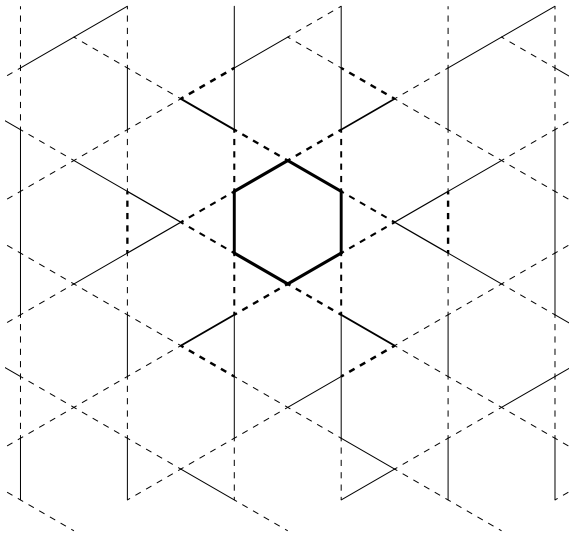
- Does it have a gap? What type of SL? Can we see topological degeneracies?
- Is it close to a particular VBC? (a "melted" VBC)
- If an RVB description applies, what are the key resonances?
- What are the excitations? statistics?
- What is the extended phase diagram (J_2, ...)
- How does it compare to experiments? (Herbertsmithite)
  - Both spin liquids!! But Herbertsmithite first appeared gapless(??) Later, experiments flipped, and now gapped, but small gap. But now new DMRG/theoretical pointing back towards gapless or small gap (He et al Phys. Rev. X 7, 031020 (2017)

Response to small bond perturbations

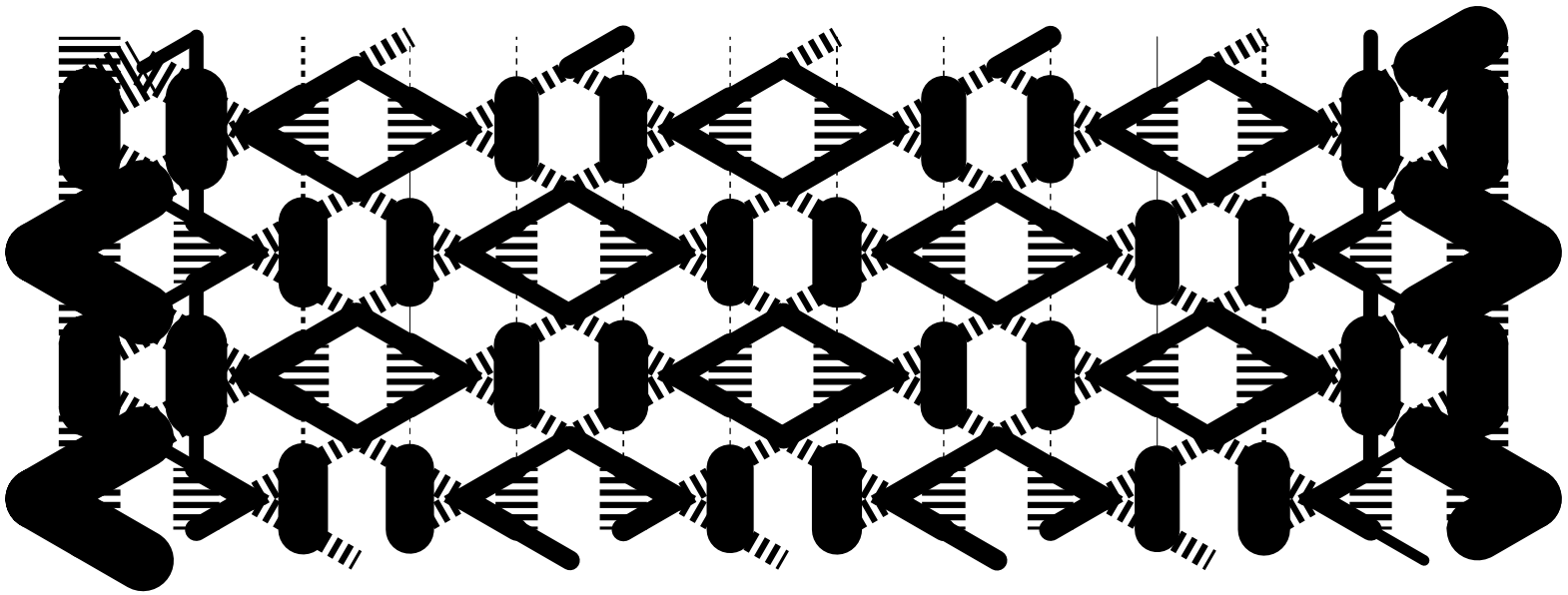
Response to 1% increase in J on one diamond





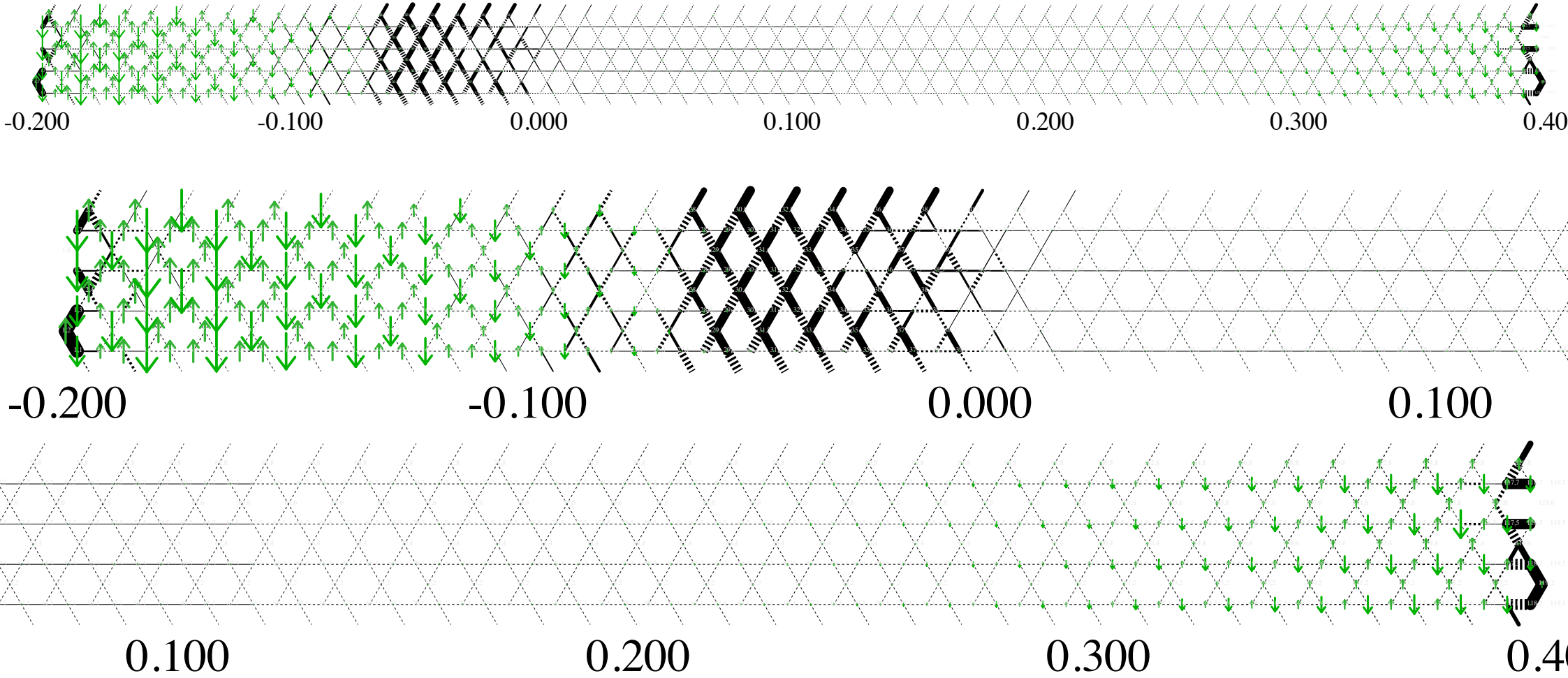


Response to 1% increase in J on one hexagon

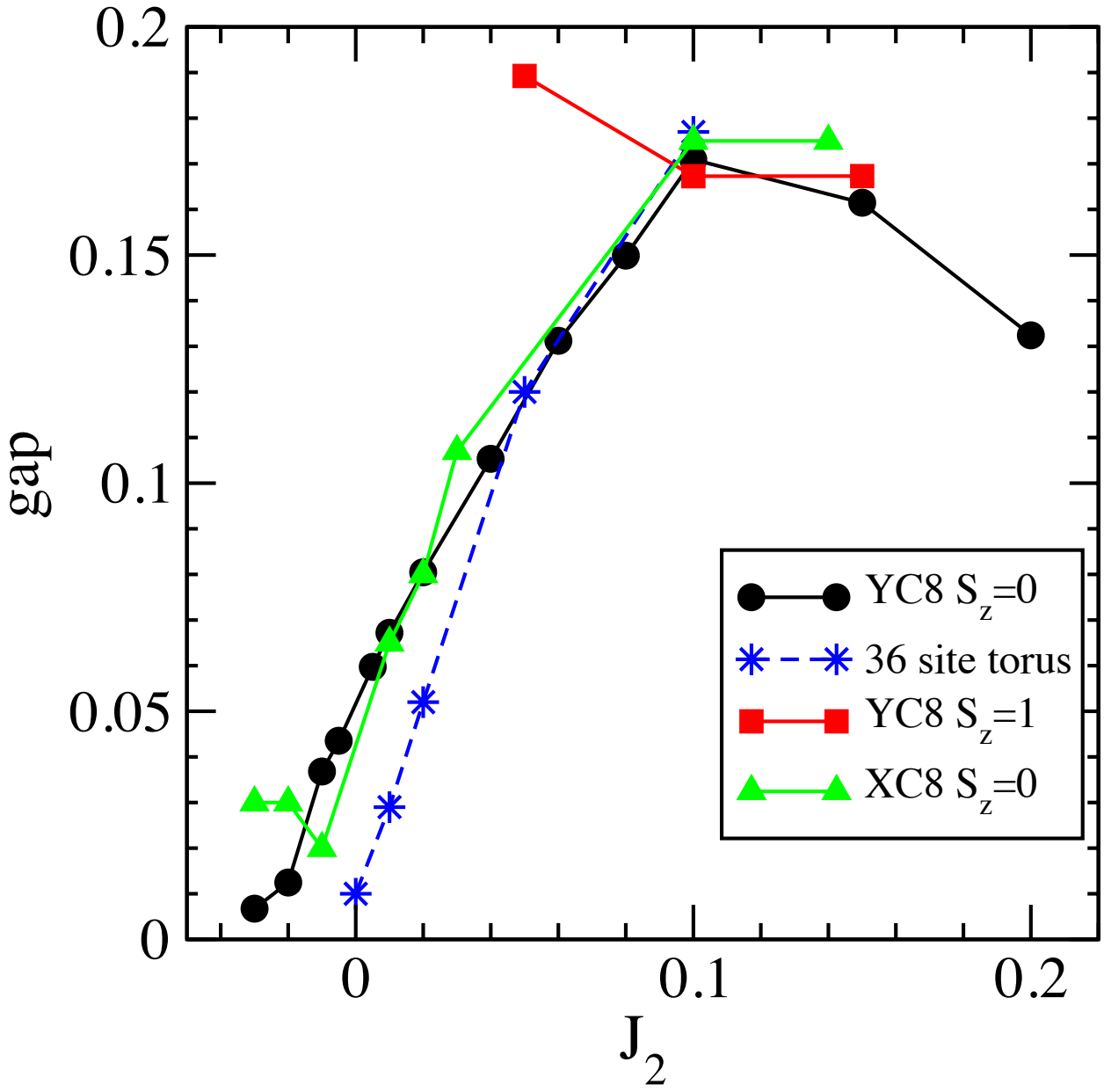


Response to 0.5% increase/decrease in J on fat vertical bonds: the "diamond pattern", which fits only on the even cylinders

Varying J_2 with x coordinate



Next nearest neighbor J_2



36 site exact diagonalization: Sindzingre and Lhuillier

The finite size shift of the phase boundary explains the many low lying states in ED.

Note: no sign of 4-fold degeneracy for torus

Tips for DMRG on hard/2D systems

- Use simulations first as a way of intuitively understanding the system. Perform many numerical experiments with different initial states, different sizes, and different boundary conditions. Plot local observables as a function of sweeps to understand how the system lowers its energy. Compare results with theoretical predictions and "cartoon" descriptions of the system.
- Start with small diameter cylinders, with nearly exact treatments, then do bigger cylinders.
- Explore the broader phase diagram
- Extrapolate in the truncation error.
- Measure local properties rather than correlation functions.