The Density Matrix Renormalization Group

- NRG/real space RG
- Particle in a box
  - Problems with NRG
  - Solutions
  - DMRG for 1 ptle
- Interacting Systems
  - Density Matrix idea
  - DMRG finite system algorithm
  - A few examples from spin chains
- QI perspective: Entanglement and Schmidt Decomposition
- Matrix Product states and Diagrams
  - Periodic BC algorithm

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DMRG (continued)

- Efficiency
  - Efficient H psi
  - Wavefunction transformation
- Errors, extrapolation
- Two dimensions
  - TV scan
  - PEPS
  - Finite size scaling with cylindrical BCs

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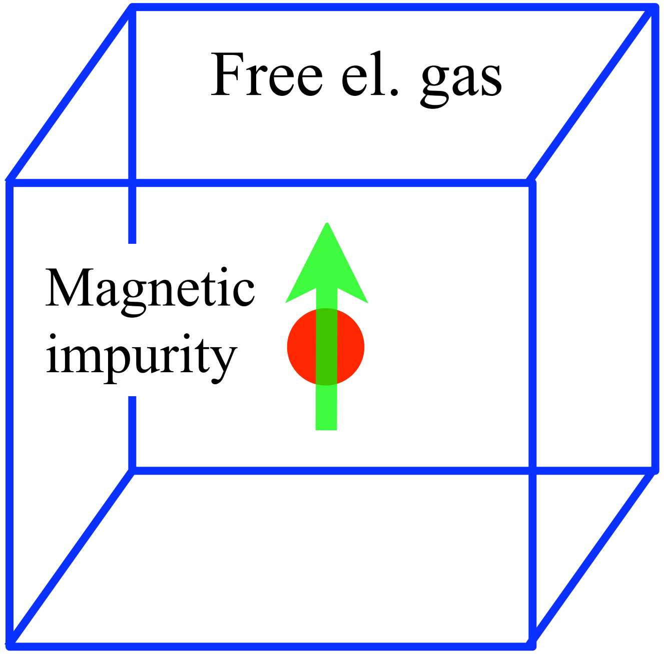
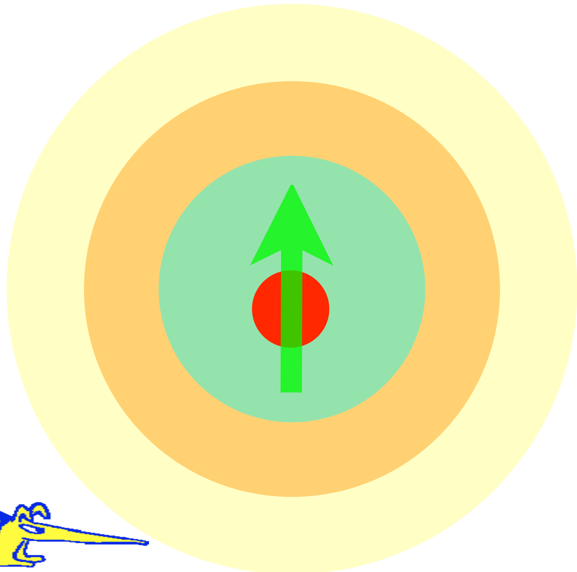
Wilson's numerical RG for a Kondo impurity

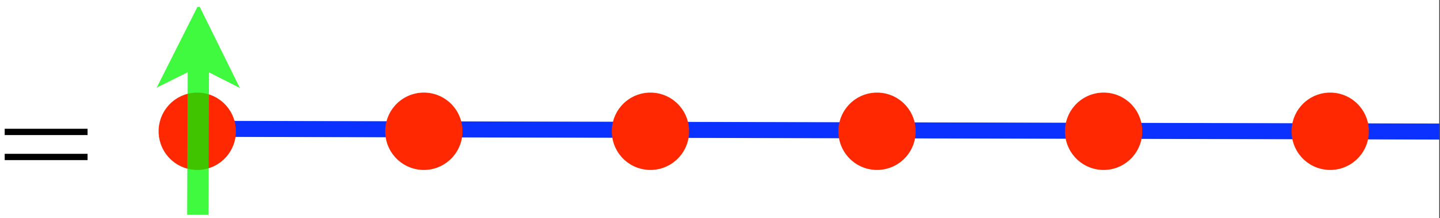


Standard Feynman diagrammatic perturbation approaches failed in the 60's.

Successes:

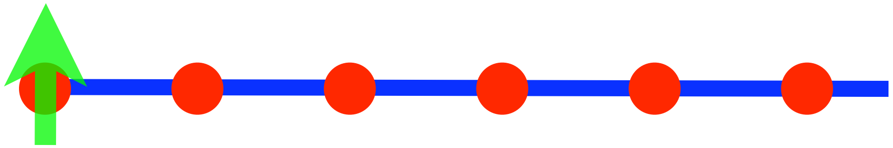
• "Poor man's scaling", Anderson et. al. 1970
•Wilson's NRG, 1975
•Andrei's exact Bethe ansatz solution, 1982

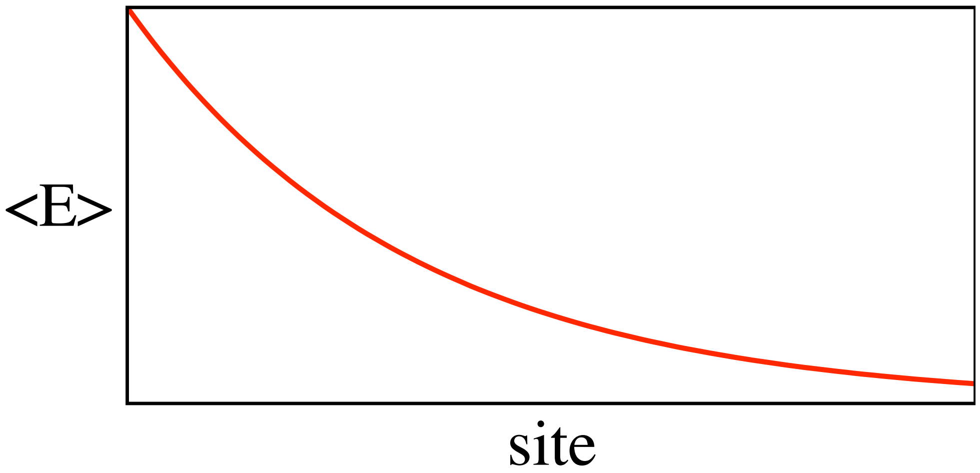




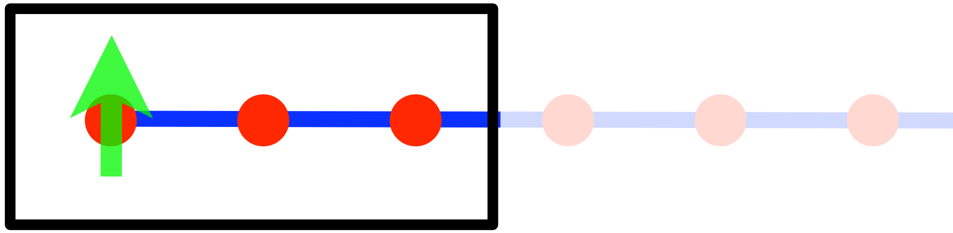
Wilson's logarithmic basis

Wilson's numerical RG

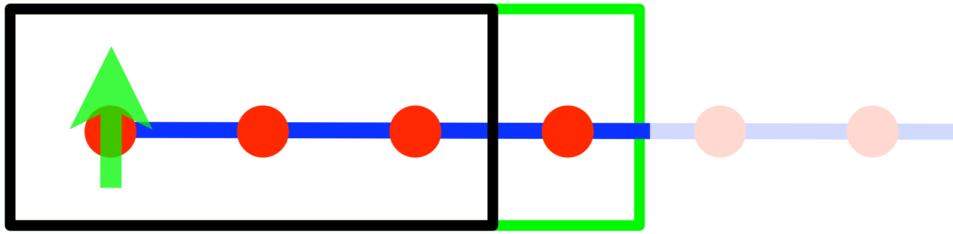




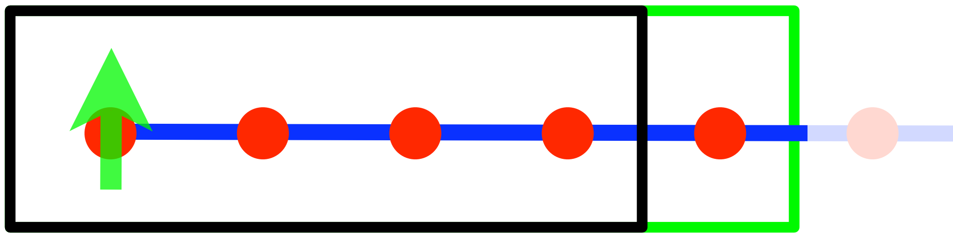
Treat short distance,
high energy scales first



Diagonalize block, keep m lowest energy states

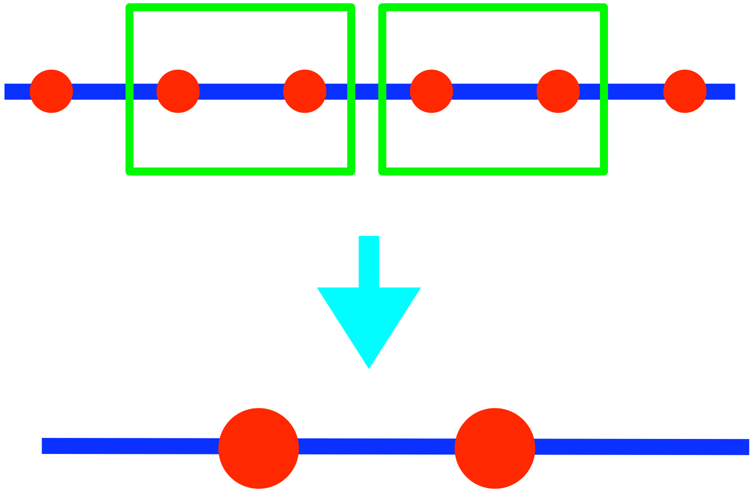


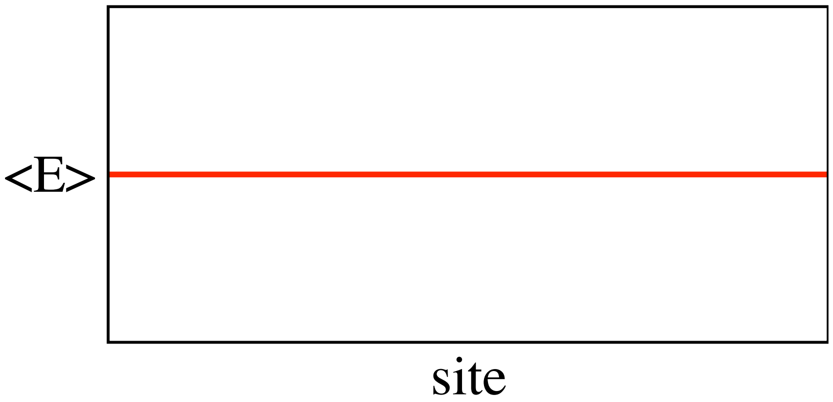
Add one site, diagonalize block Hamiltonian again, keeping m states



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

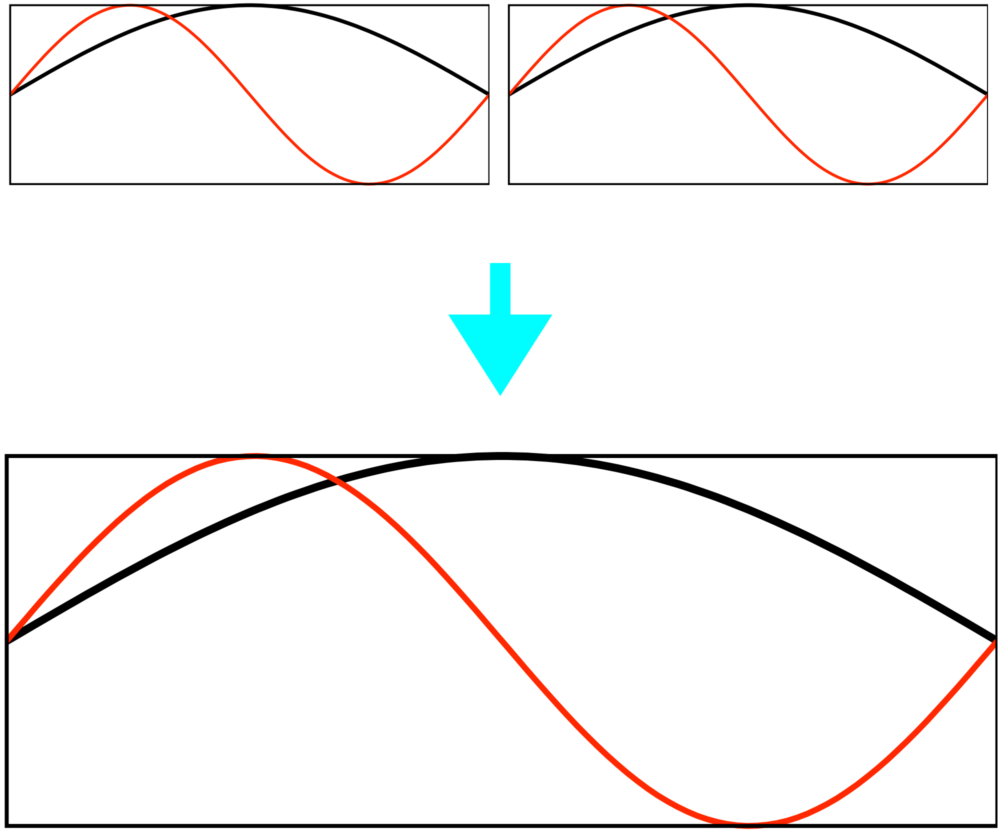
Wilson’s approach applied in real space





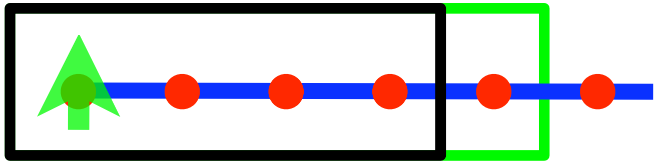
This approach gave qualitatively wrong results.

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



Any truncation yields “kinks” at larger scales.

DMRG Algorithm

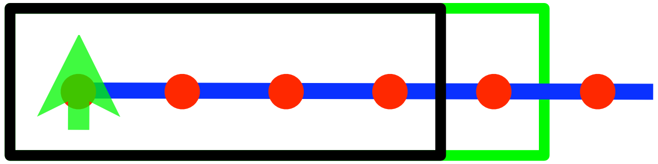


Wilson's algorithm

DMRG sweeps

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

DMRG Algorithm



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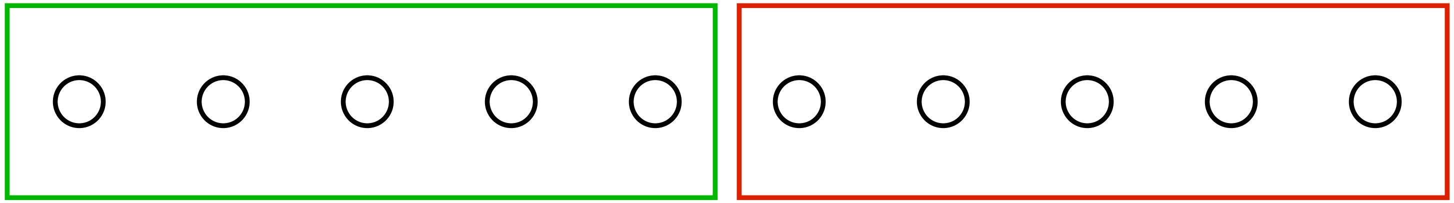

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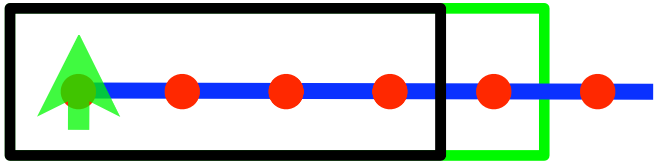

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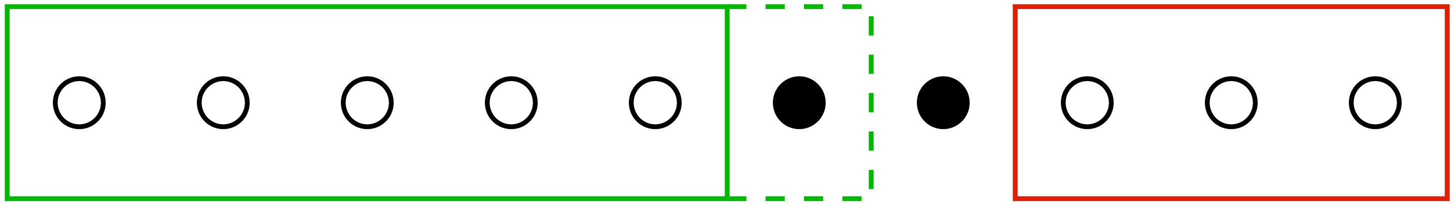

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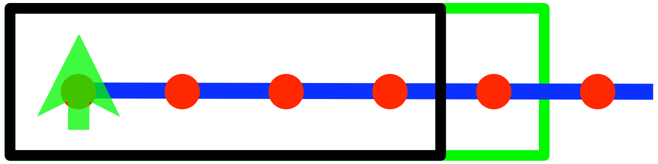

Wilson's algorithm

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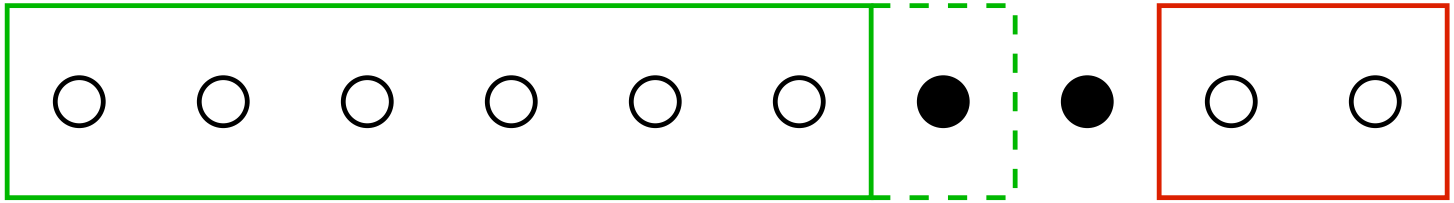

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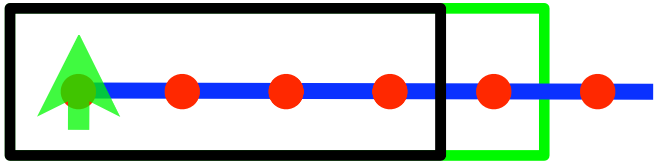
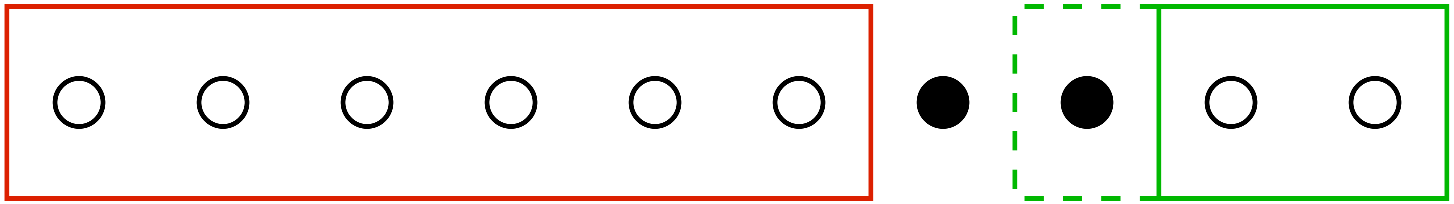


Wilson's algorithm

DMRG sweeps



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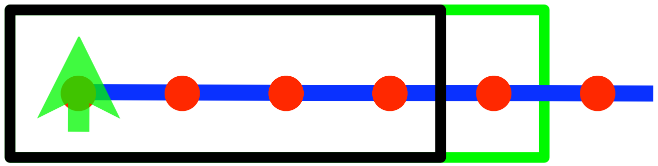
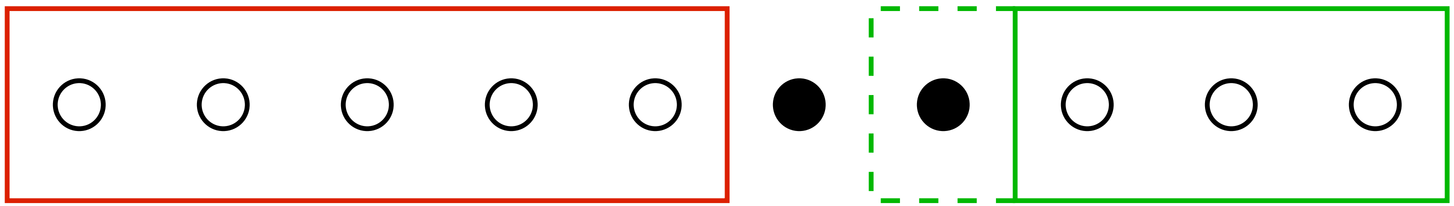


Wilson's algorithm

DMRG sweeps



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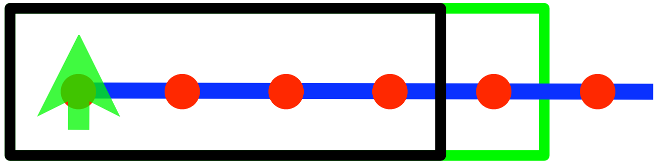

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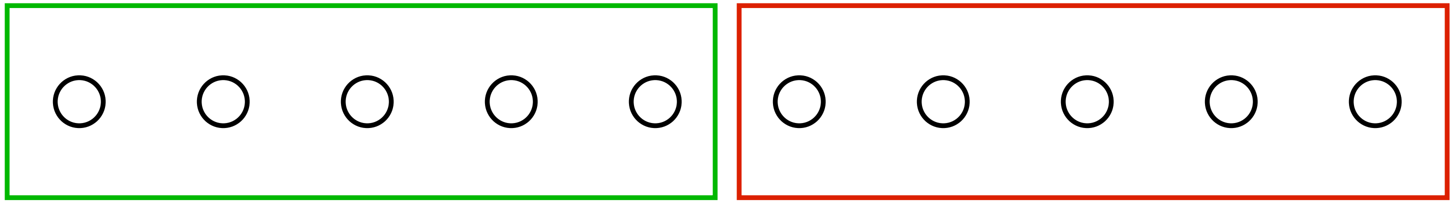

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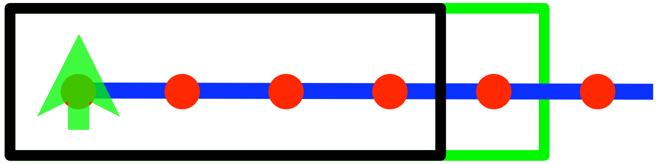

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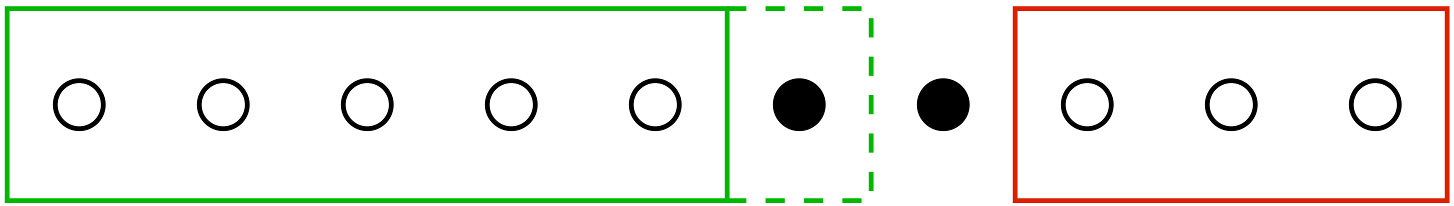
DMRG sweeps



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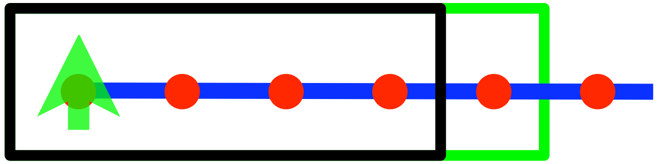

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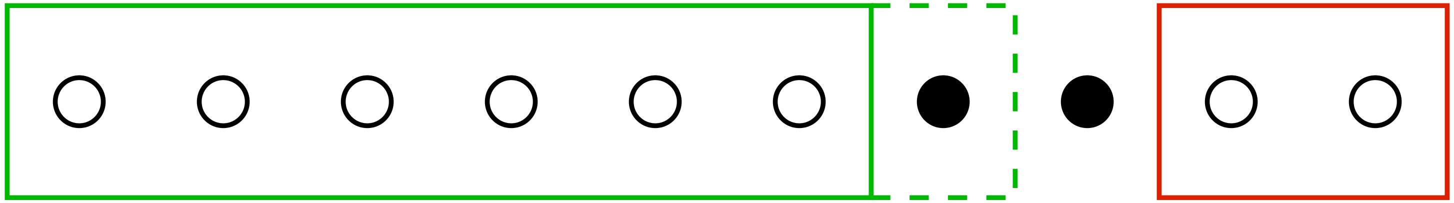

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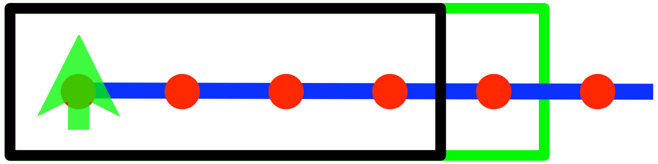

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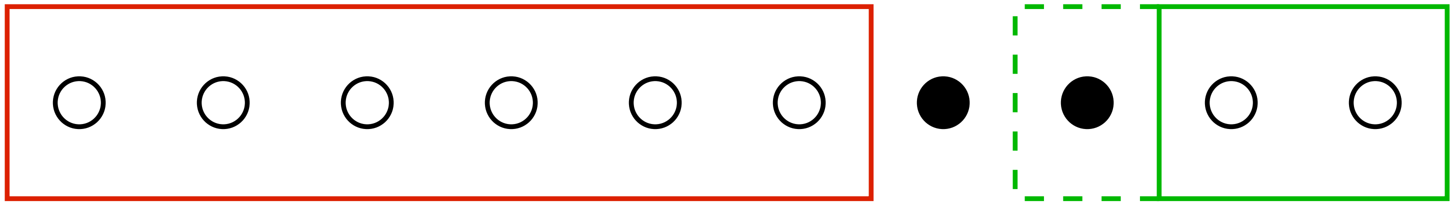
DMRG sweeps



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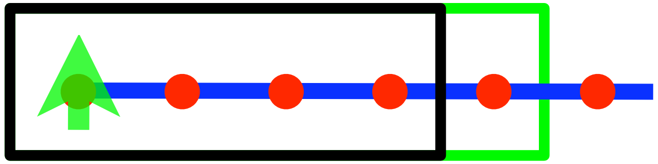

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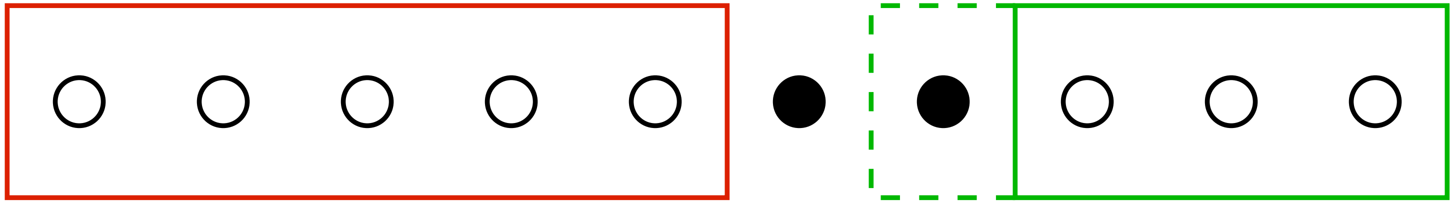
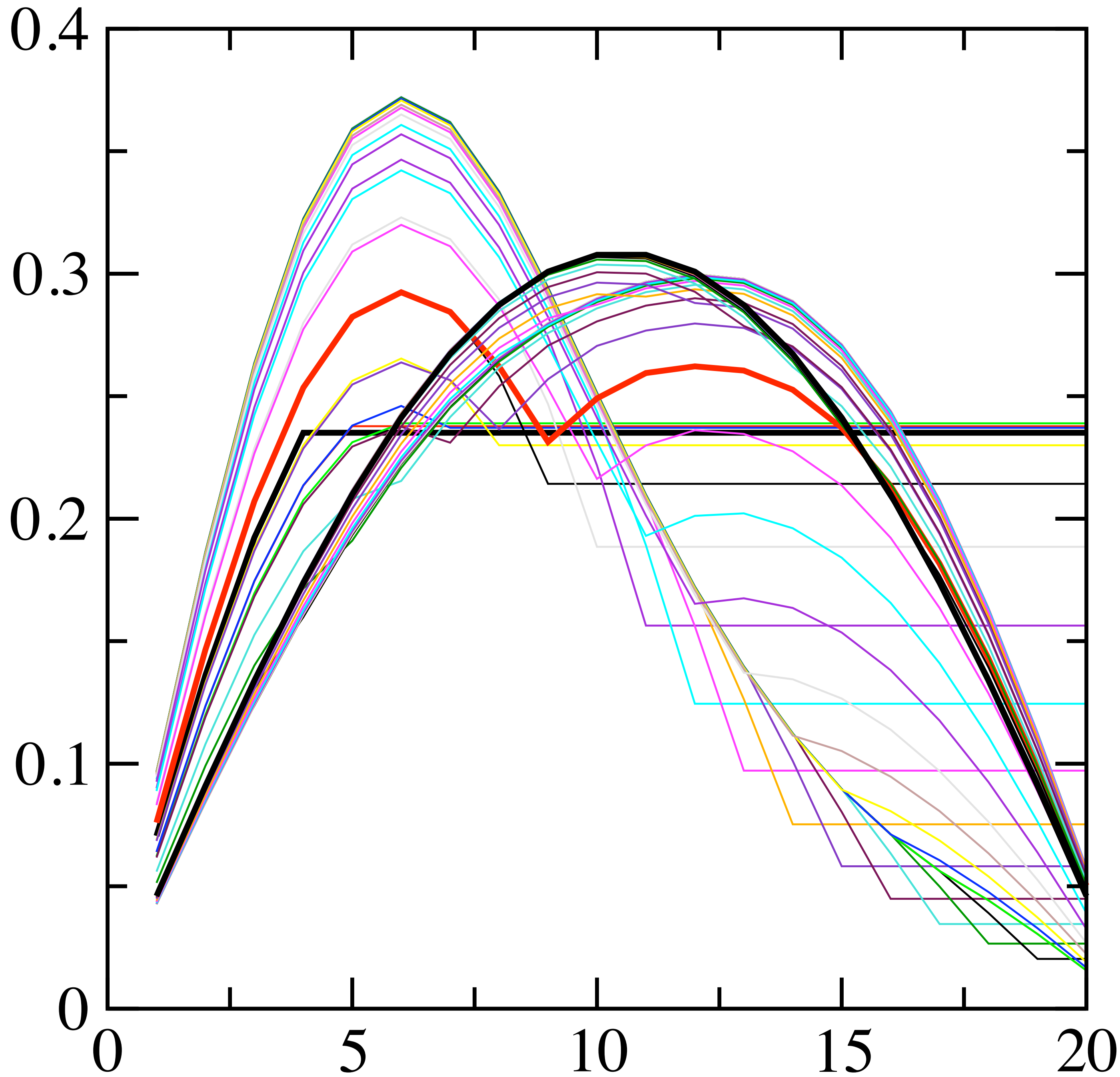
DMRG sweeps



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

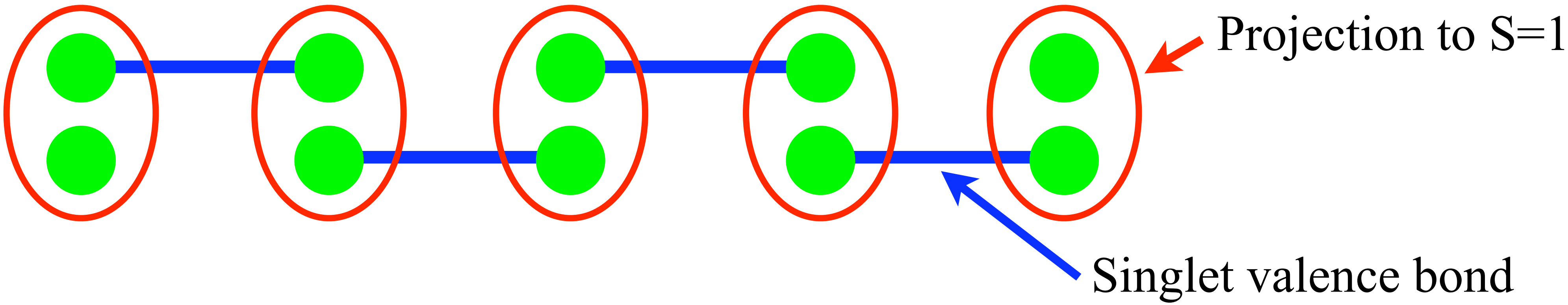
```
    Matrix H(length,length); H = 2.0;
    for(int i = 1; i < n; i++)
        H(i,i+1) = H(i+1,i) = -1.0;
    Vector leftpsi(1), rightpsi(n-3), evals;
    rightpsi = 1.0; leftpsi = 1.0;
// Finite System sweeps
    for(int it = 1; it <= niter; it++)
        {
        for(int i = 1; i <= n-3; i++)
            {
            leftpsi = leftpsi / Norm(leftpsi);
            rightpsi = rightpsi / Norm(rightpsi);
            Matrix Htil(4,4), O(n,4); O = 0.0;
            O.Column(1).SubVector(1,i) = leftpsi;
            O(i+1,2) = O(i+2,3) = 1.0;
            O.Column(4).SubVector(i+3,n) = rightpsi;
            Htil = O.t() * H * O;
            EigenValues(Htil,evals,evecs);
            Vector psitil(evecs.Column(1)), newpsi(n);
            newpsi.SubVector(1,i) = leftpsi * psitil(1);
            newpsi(i+1)  = psitil(2);
            newpsi(i+2)  = psitil(3);
            newpsi.SubVector(i+3,n) = rightpsi * psitil(4);
            if(newpsi(i+1) < 0.0) newpsi *= -1.0;
            cout << "@" << endl;
            for(int j = 1; j <= n; j++)
                cout << j SP newpsi(j) << endl;
            if(i < n-3)
                leftpsi = newpsi.SubVector(1,i+1),
                rightpsi = newpsi.SubVector(i+4,n);
            }
```



0.4
0.3
0.2
0.1
0
0
5
10
15
20

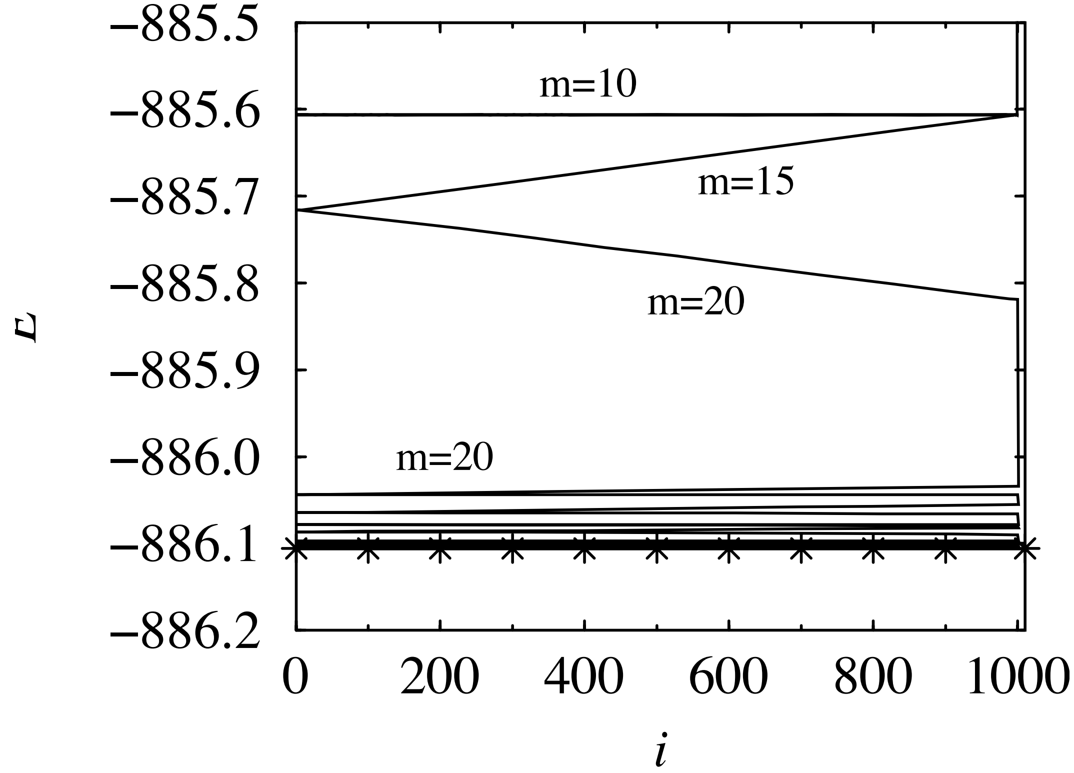
S=1 Heisenberg Chain

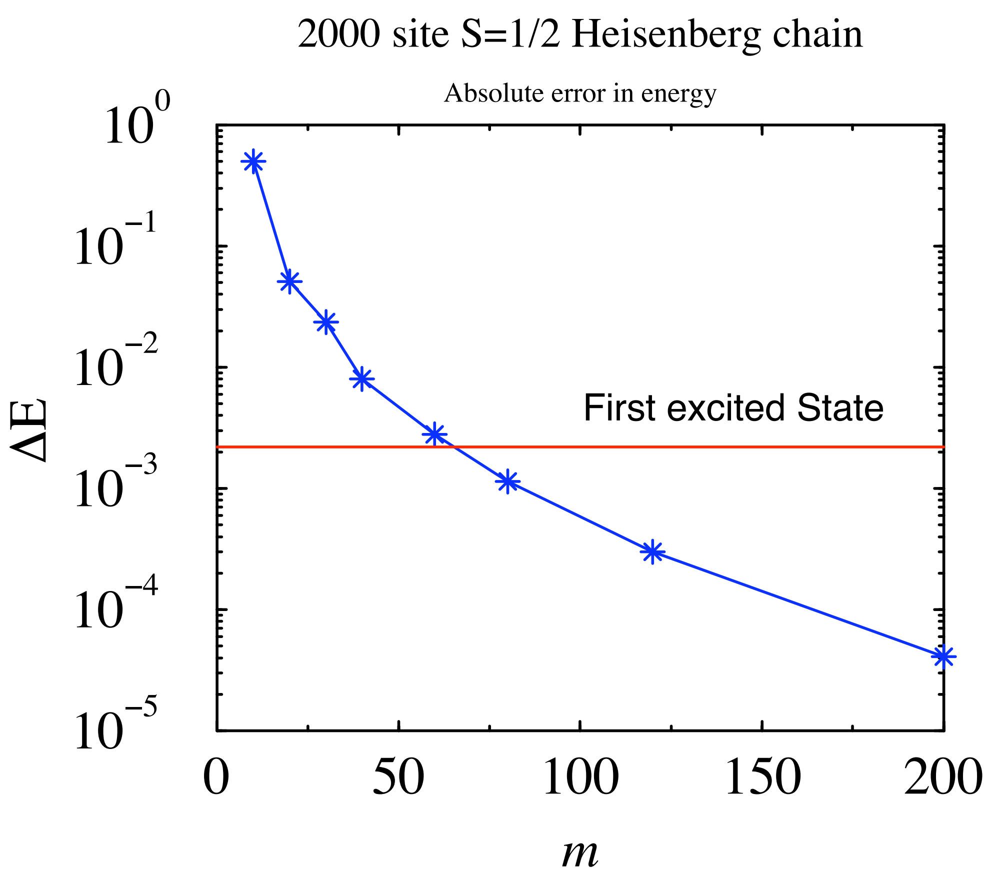
- Disordered, Haldane gap, finite ξ
- Good picture: Affleck-Kennedy-Lieb-Tasaki state



- AKLT is a matrix product state with m=2 !
- S=1 magnon excitations
- S=1/2 free end spins

Convergence for S=1/2 chain





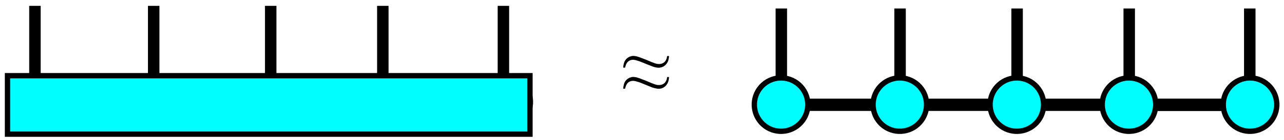
Comparison with Bethe Ansatz

Matrix Product States (Ostlund and Rommer, 1995)

- Insert density matrix/Schmidt eigenstates between all pairs of sites

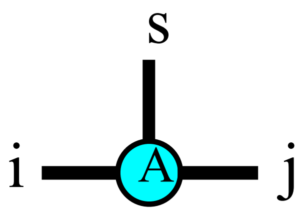
Matrix Product State: $\Psi(s_1, s_2, .. s_N) \approx A^1[s_1]\, A^2[s_2] \,...\, A^N[s_N]$

2^N

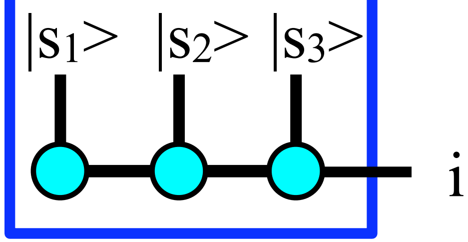


$N\, m^2$

Basic Unit: tensor/matrix A^s_{ij} =

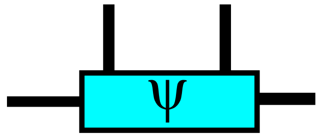


DMRG Blocks = set of basis states:

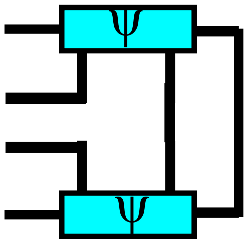


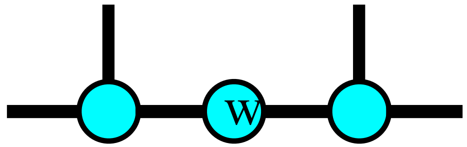
= { | i > }

DMRG versus MPS: blocks and bases versus variational states

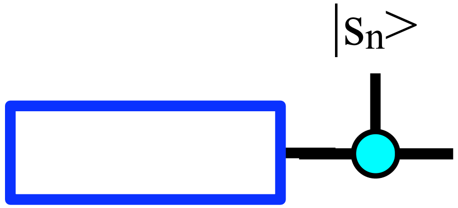
DMRG wavefunction: 

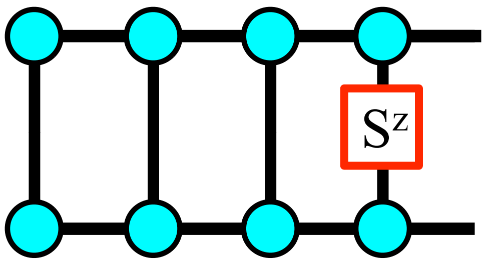
$= \psi(l,s,t,r)$

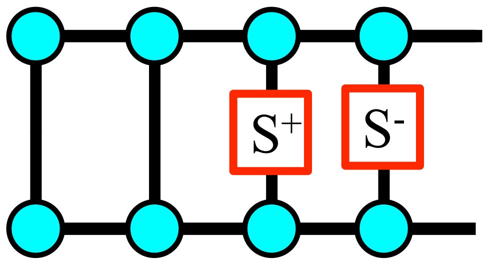
Density Matrix: 

$=$ 

Diagonalized form

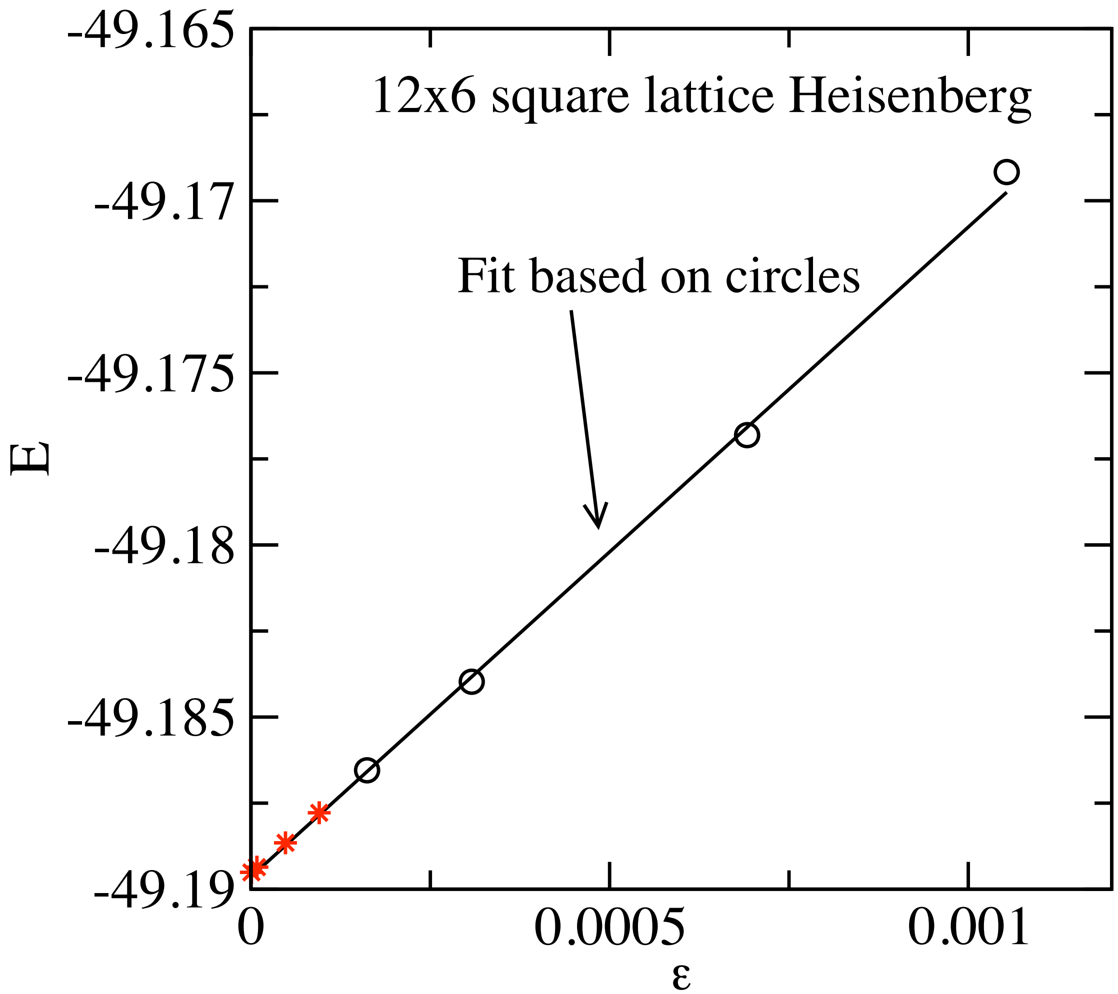
New block: 

Operators: 

J/2 

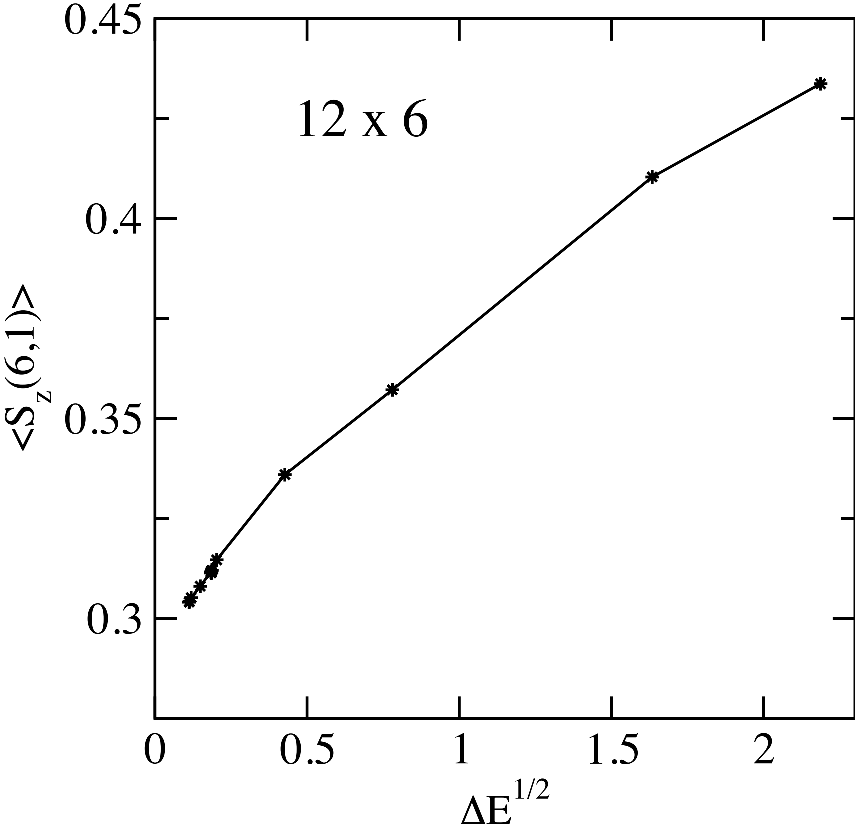
$+ \quad \ldots \quad = H_{block}$

Energy extrapolation



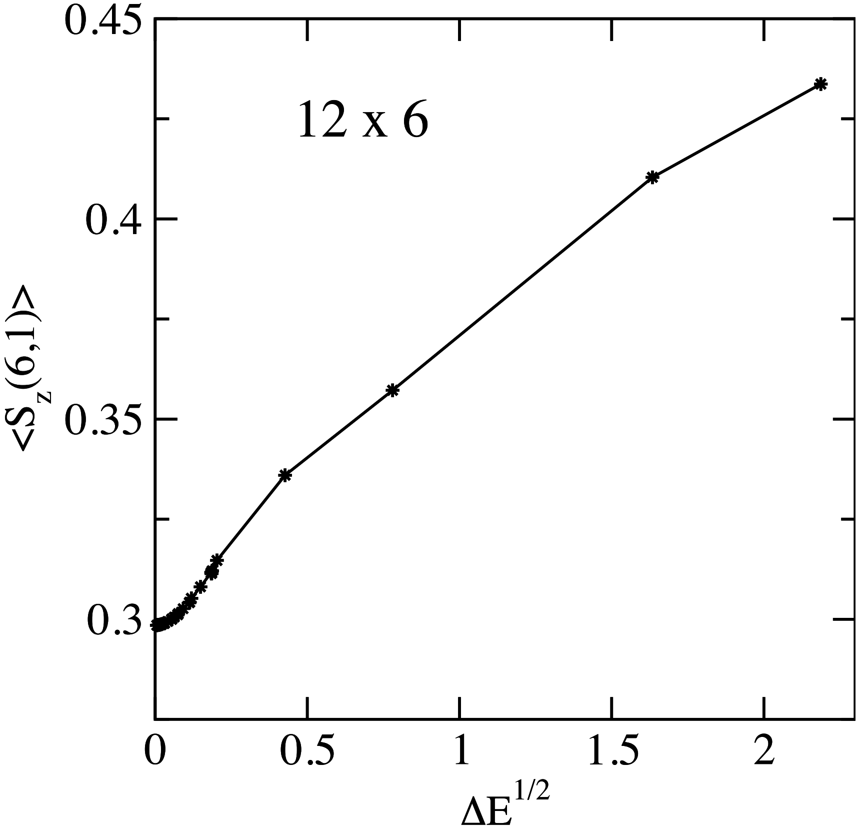
Probability of states thrown away

Typical extrapolation of magnetization



Pinning AF fields applied to edges, cylindrical BCs

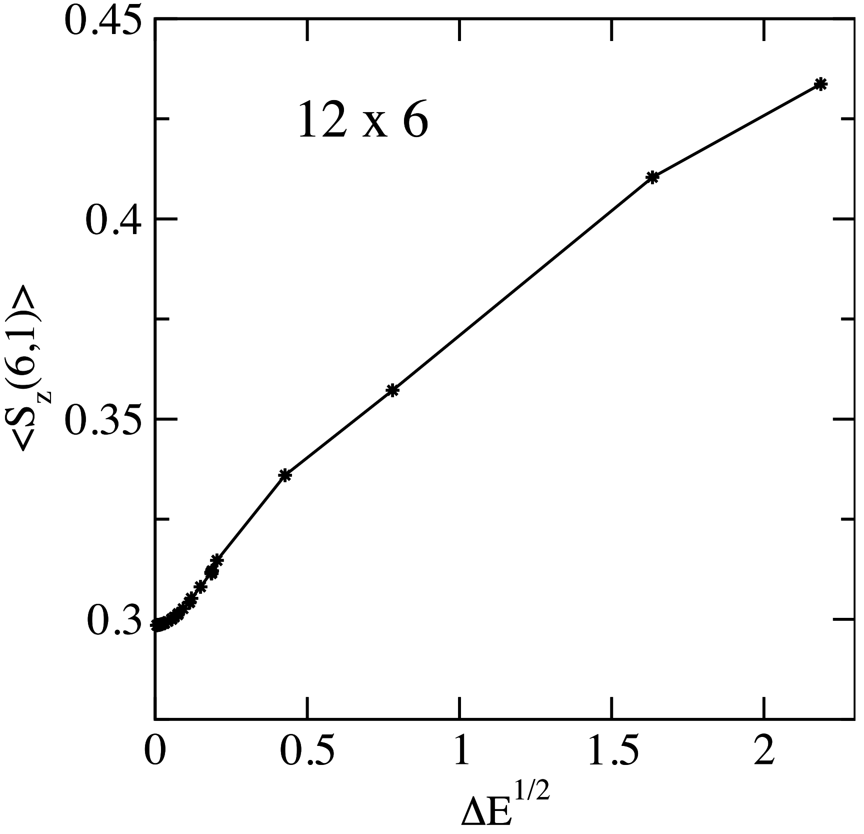
Typical extrapolation of magnetization

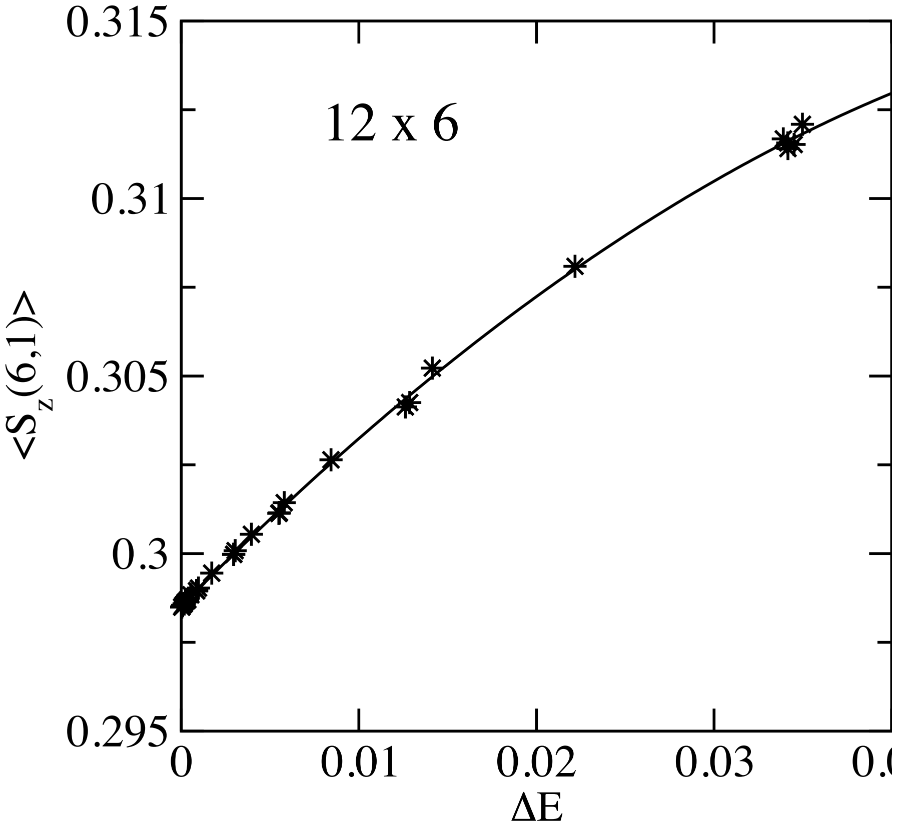


High accuracy points indicate quadratic approach!

Pinning AF fields applied to edges, cylindrical BCs

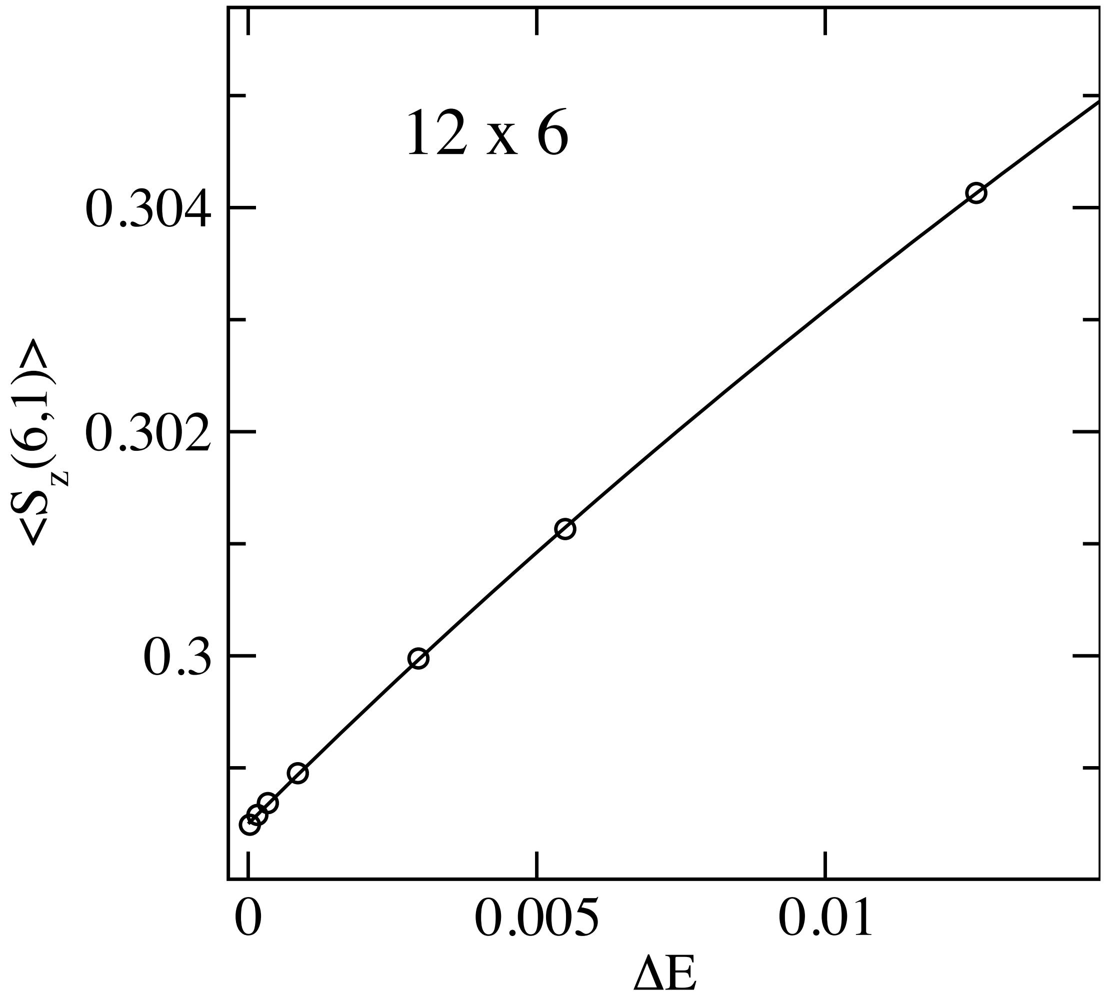
Typical extrapolation of magnetization



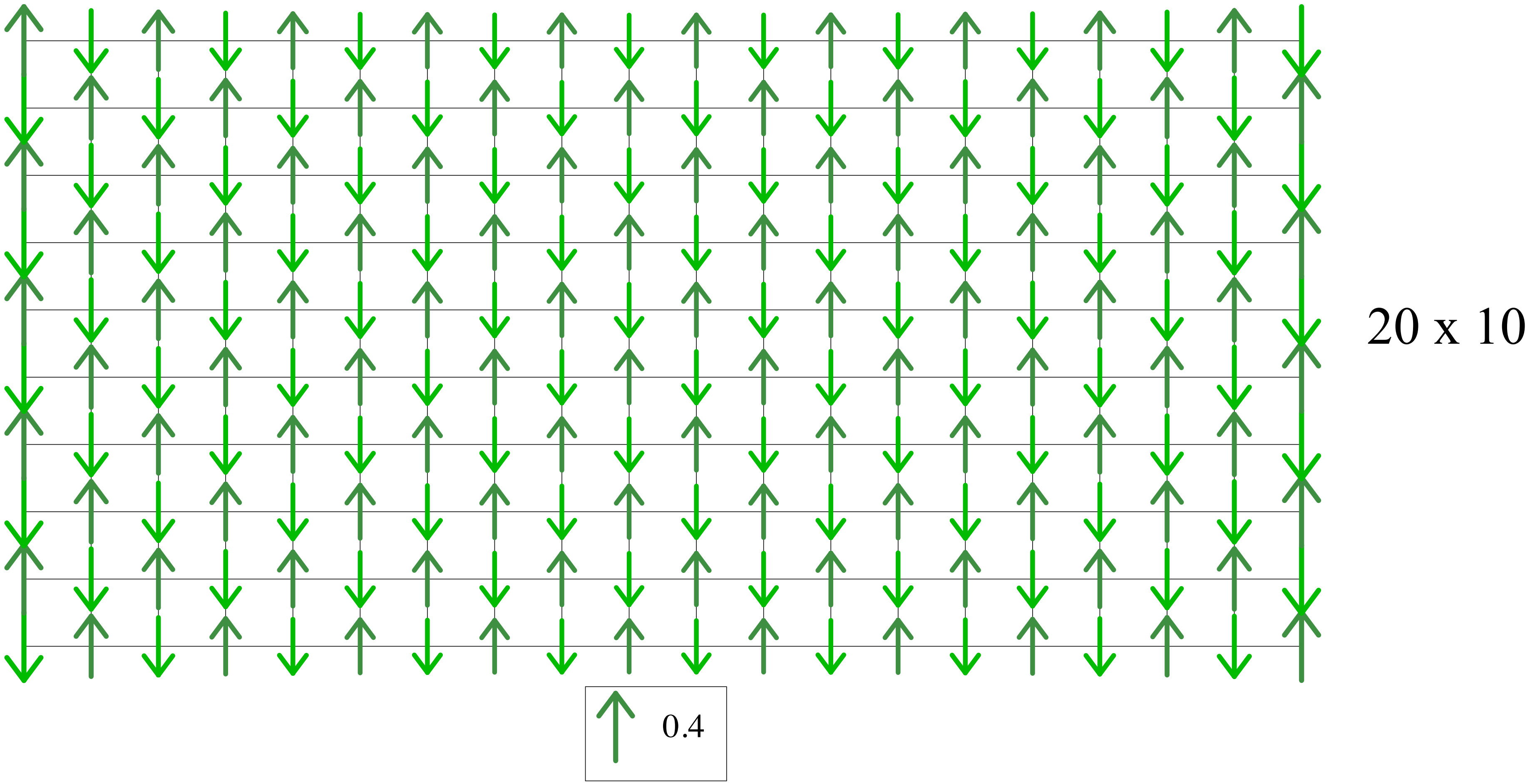


Pinning AF fields applied to edges, cylindrical BCs

Cubic fit to well-converged measurements

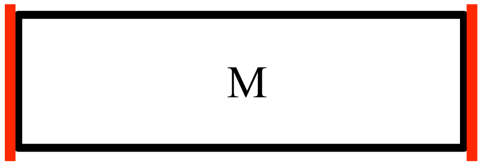


Square lattice: benchmark against QMC

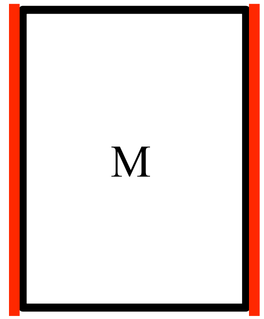


- Cylindrical BCs: periodic in y, open in x
- Strong AF pinning fields on left and right edges
- 21 sweeps, up to m=3200 states, 80 hours

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



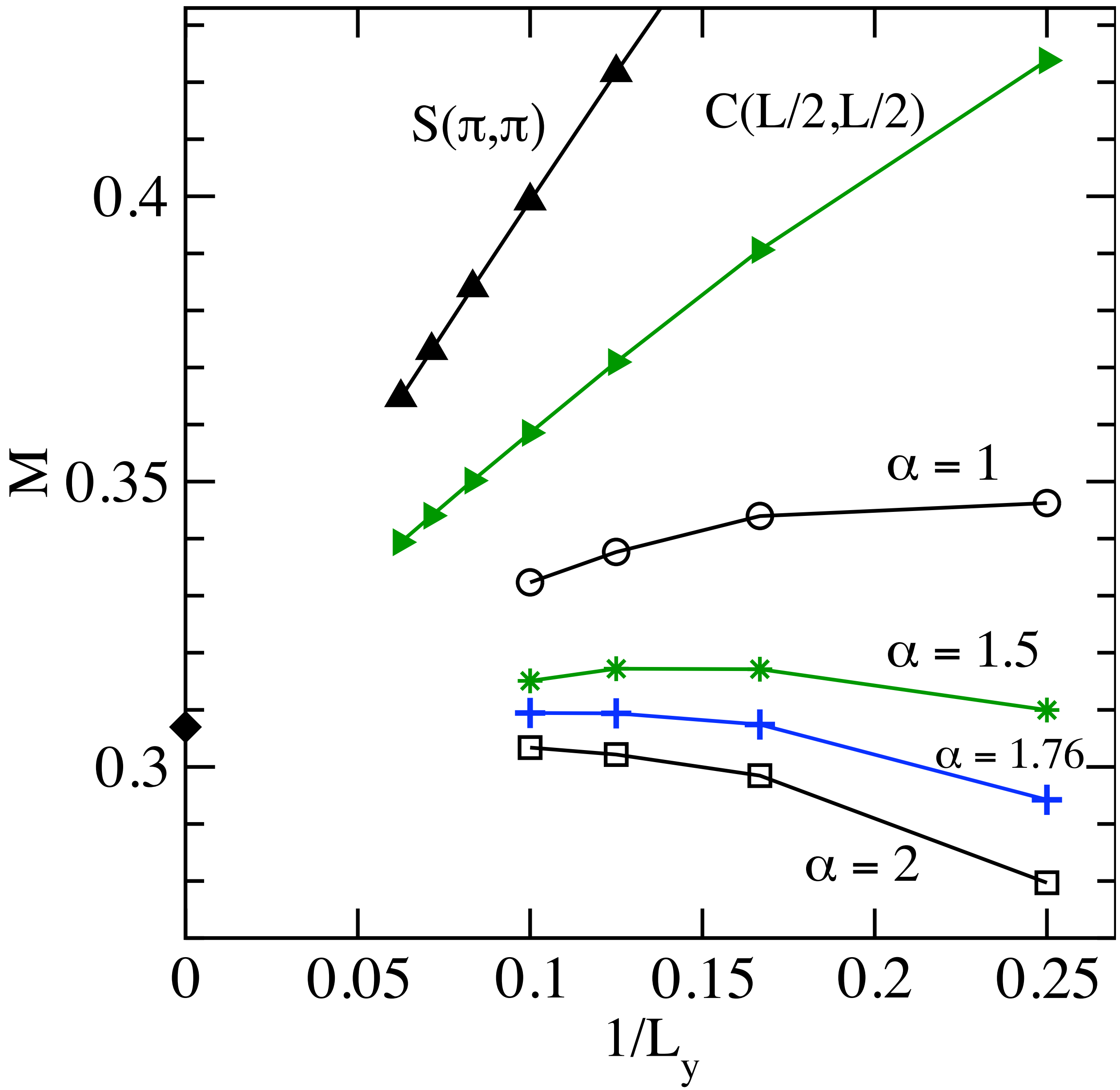
Long: 1D makes M small



Short: proximity to strong pinning makes M large

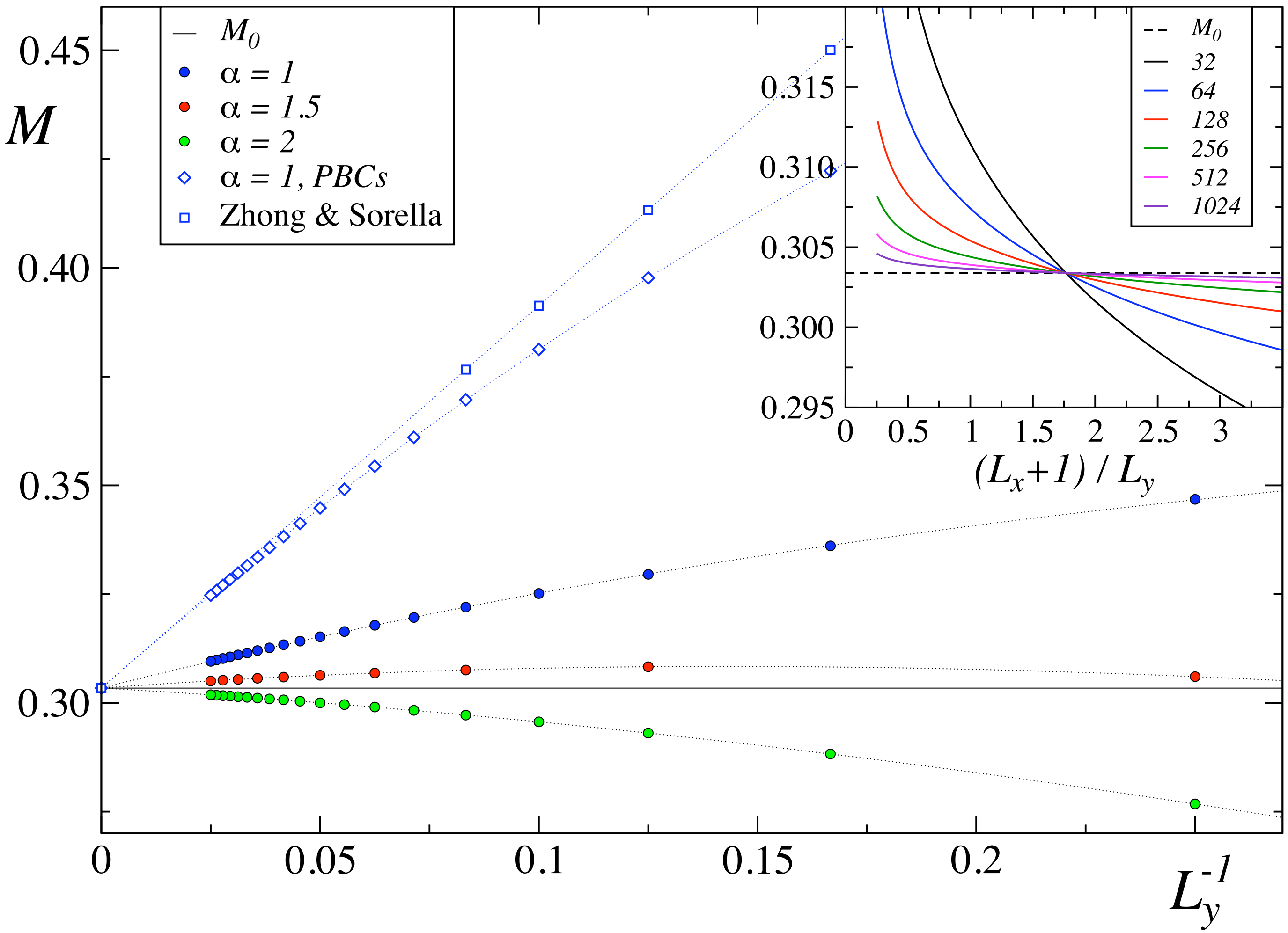
- “Standard” measurements in QMC estimate M^2 using correlation functions and have large finite size effects $O(1/L_y)$
- Can one choose a special aspect ratio to eliminate $O(1/L_y)$ term?
- What is behavior at large length scales? Use finite system spin wave theory as a guide.

Square lattice



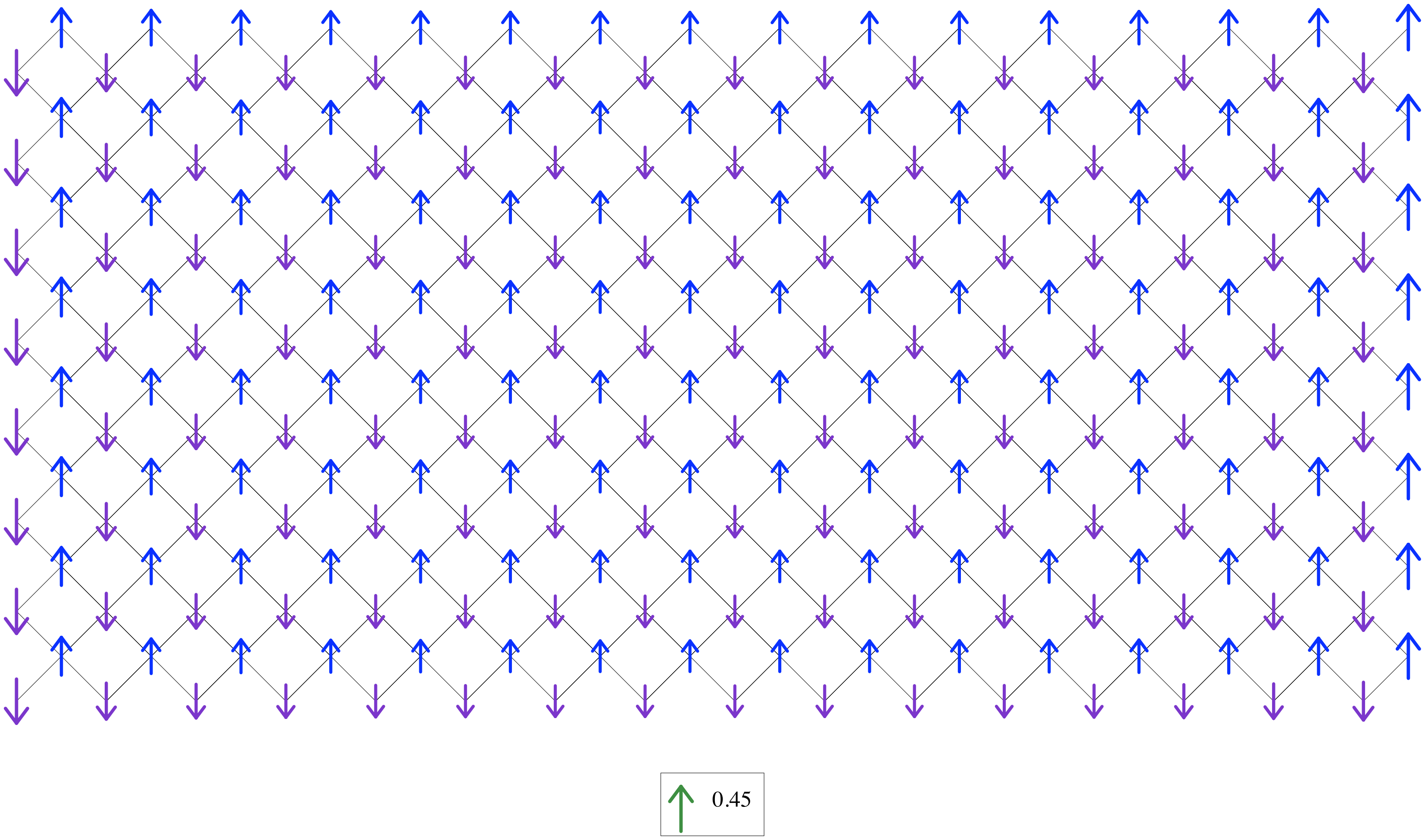
$$\alpha = L_x / L_y$$

Finite size spin wave theory



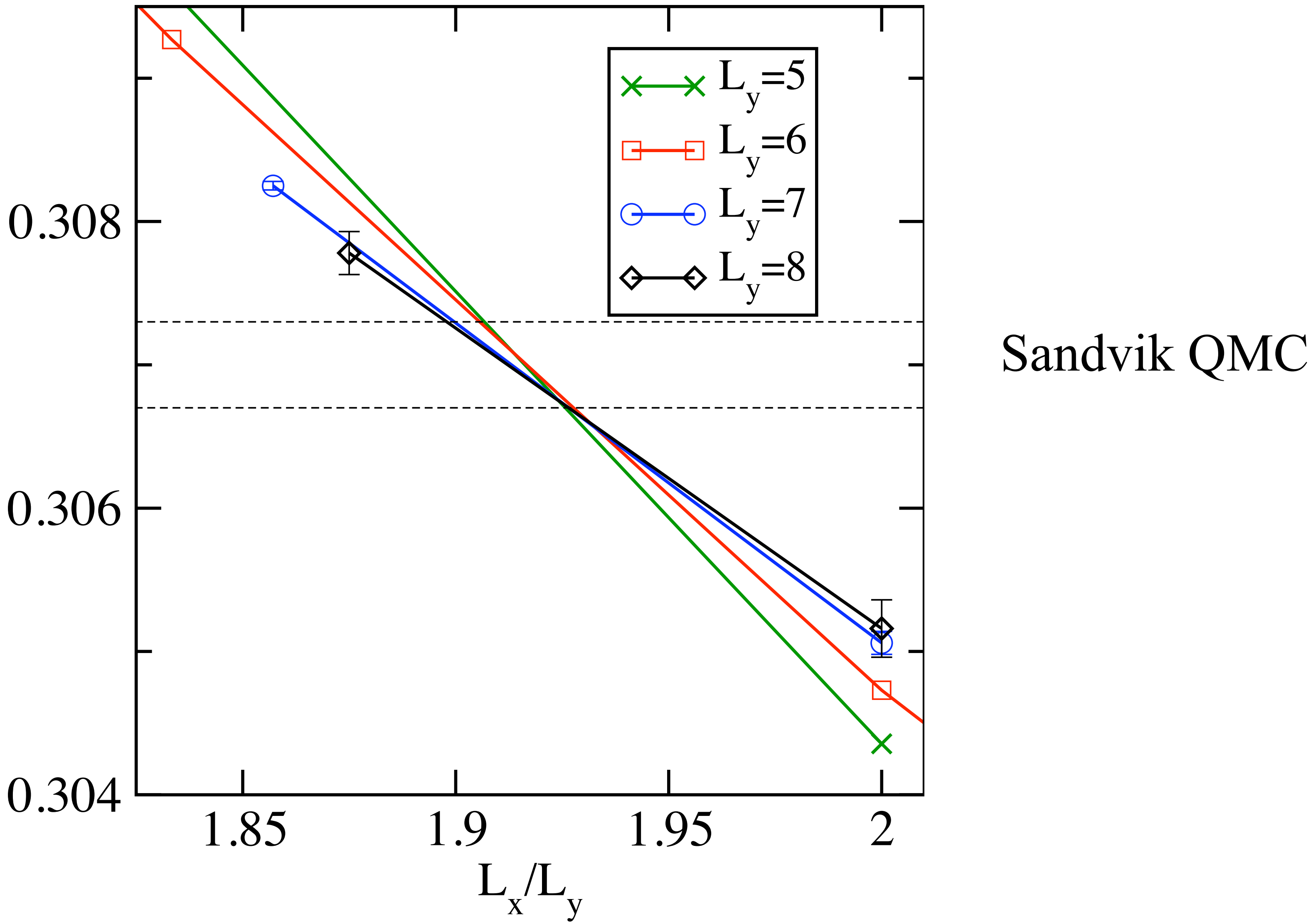
- Optimal choice $\alpha = 1.764$ eliminates linear term
- Even $\alpha = 1$ has much smaller finite size effects

Tilted square lattice



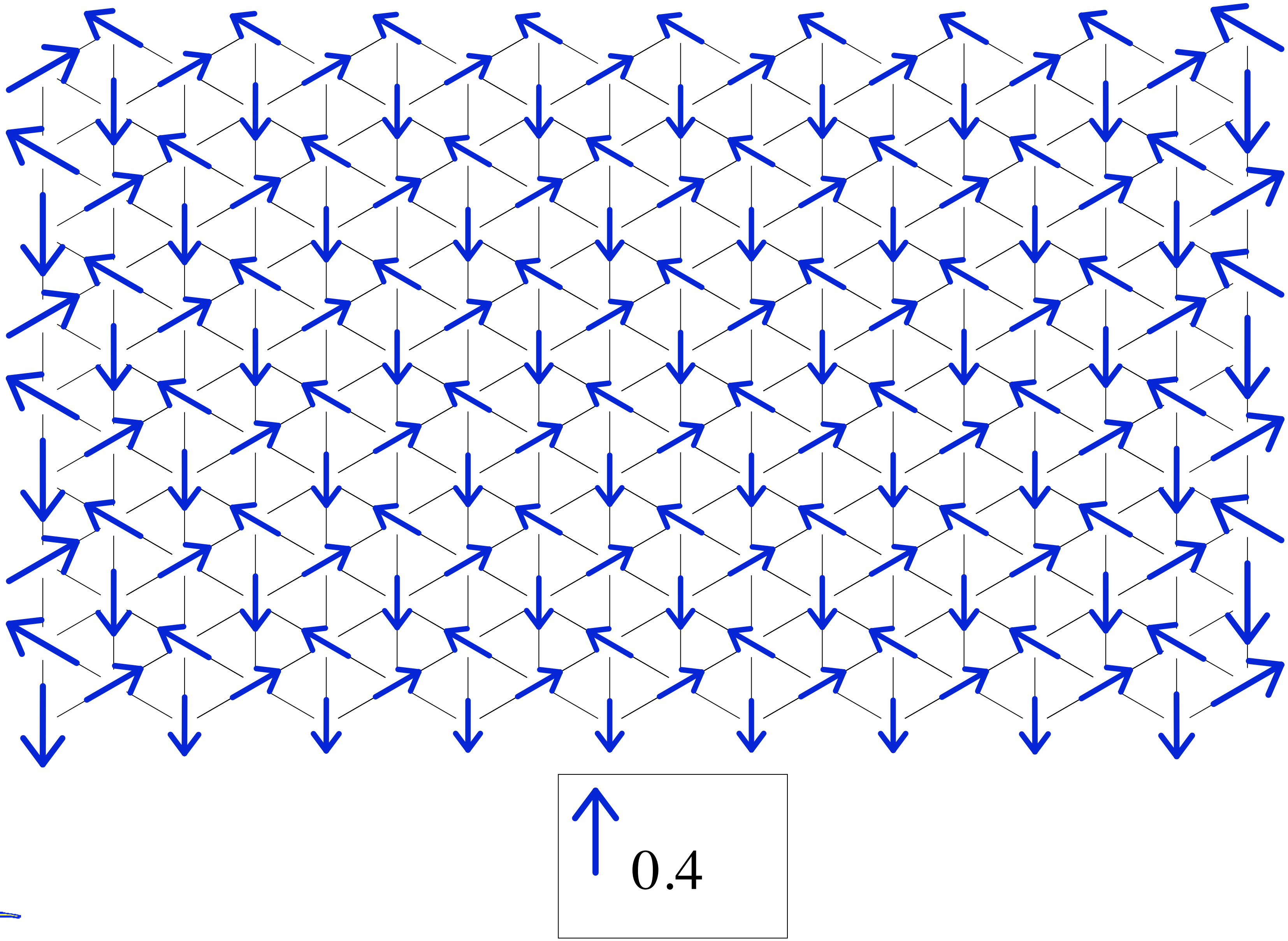
- Tilted lattice has smaller DMRG errors for its width
- For this “32x8” obtain M = 0.3052(4)

Tilted square lattice

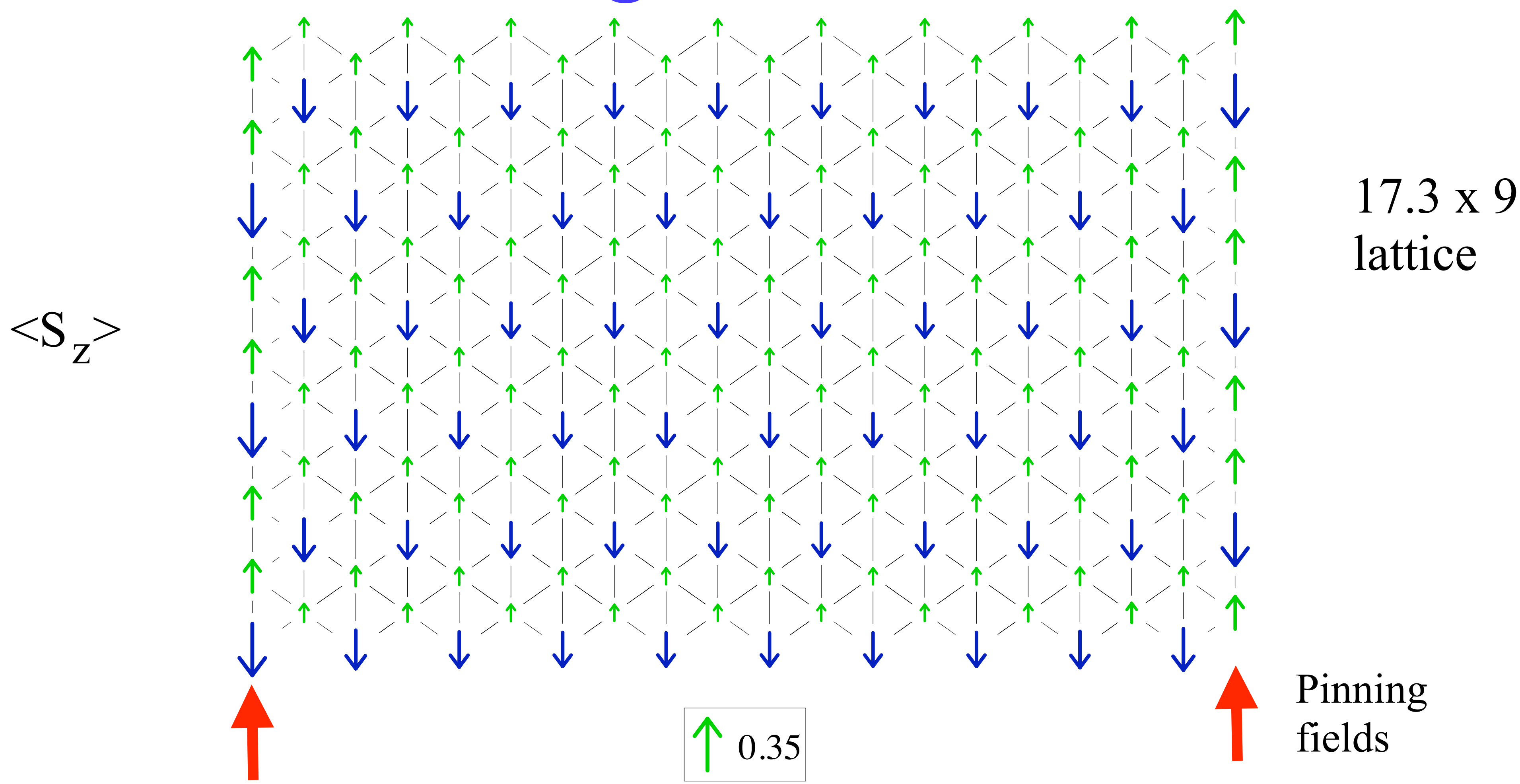


- Results are consistent with and with comparable accuracy to QMC!

Results with Sz conservation turned off

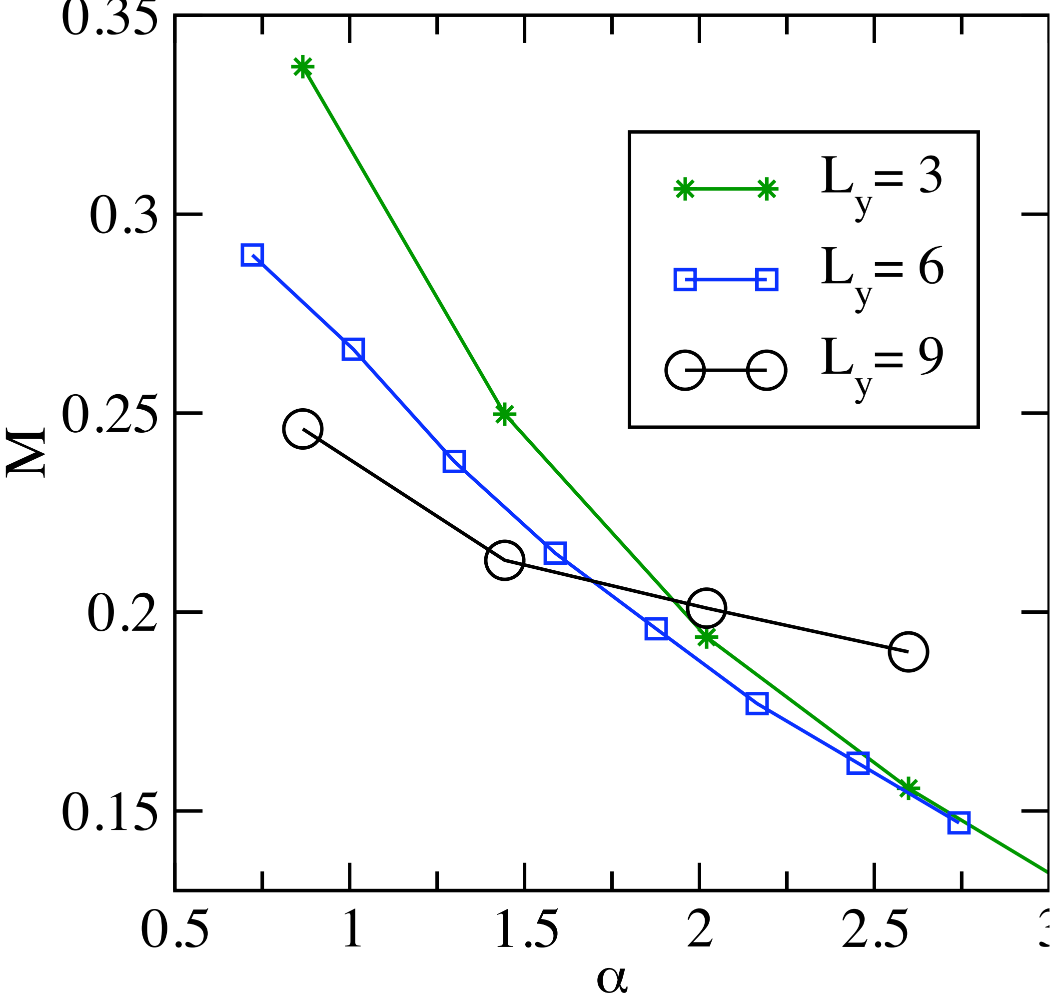


Triangular Lattice



- Only one sublattice pinned, other two rotate in a cone
- Other two have z component -M/2
- Here only have L_y= 3, 6, 9, ...

Triangular lattice, Scaled Data



What is the best α for the triangular lattice? With limited number of widths and finite size effects, could use analytic help...

If α is within range 1.5 - 2, width 9 data has a range of 0.195 - 0.22, consistent with GFMC and series expansions (but not SWT).

Preliminary Results--Triangular lattice

- Current result: M = 0.205(15)
- Consistent with Series, GFMC
- SWT not nearly as accurate as for square lattice

Method	Ref.	N	E_0/N	M
Series	this work	∞	$-0.5502(4)$	0.19(2)
ED	5,68	12	-0.6103	
		36	-0.5604	0.40
GFQMC	41	∞	$-0.5458(1)$	0.205(10)
SWT+1/S	42	∞	-0.5466	0.2497
SWT+1/S	43	∞		0.266
Coupled cluster	53	∞		0.2134