MERA Study of Quantum Spin Models on Triangular Lattice

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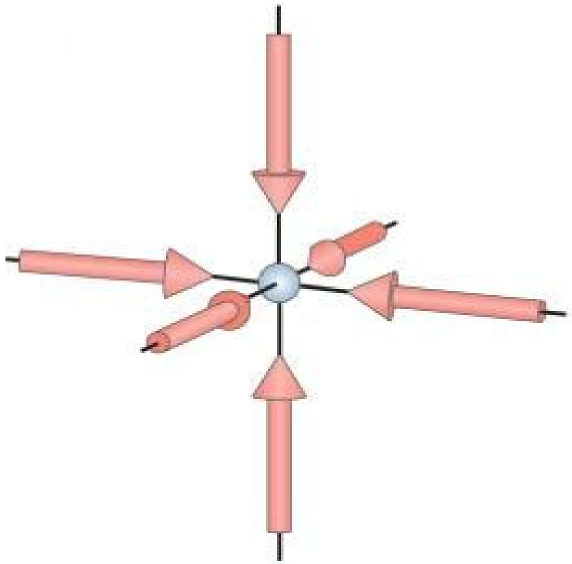
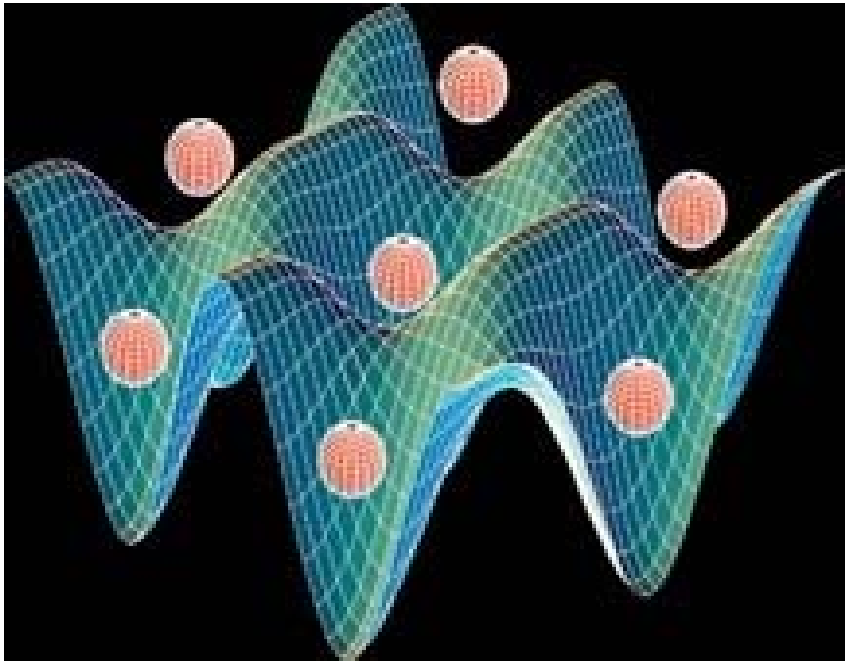
Optical Lattice

Laser beams create a periodic intensity pattern, which acts as a lattice trapping neutral atoms.

quantum computer
and
quantum simulator



Immanuel Bloch, Nature Physics (2005)



M Greiner et al. Nature 415 39

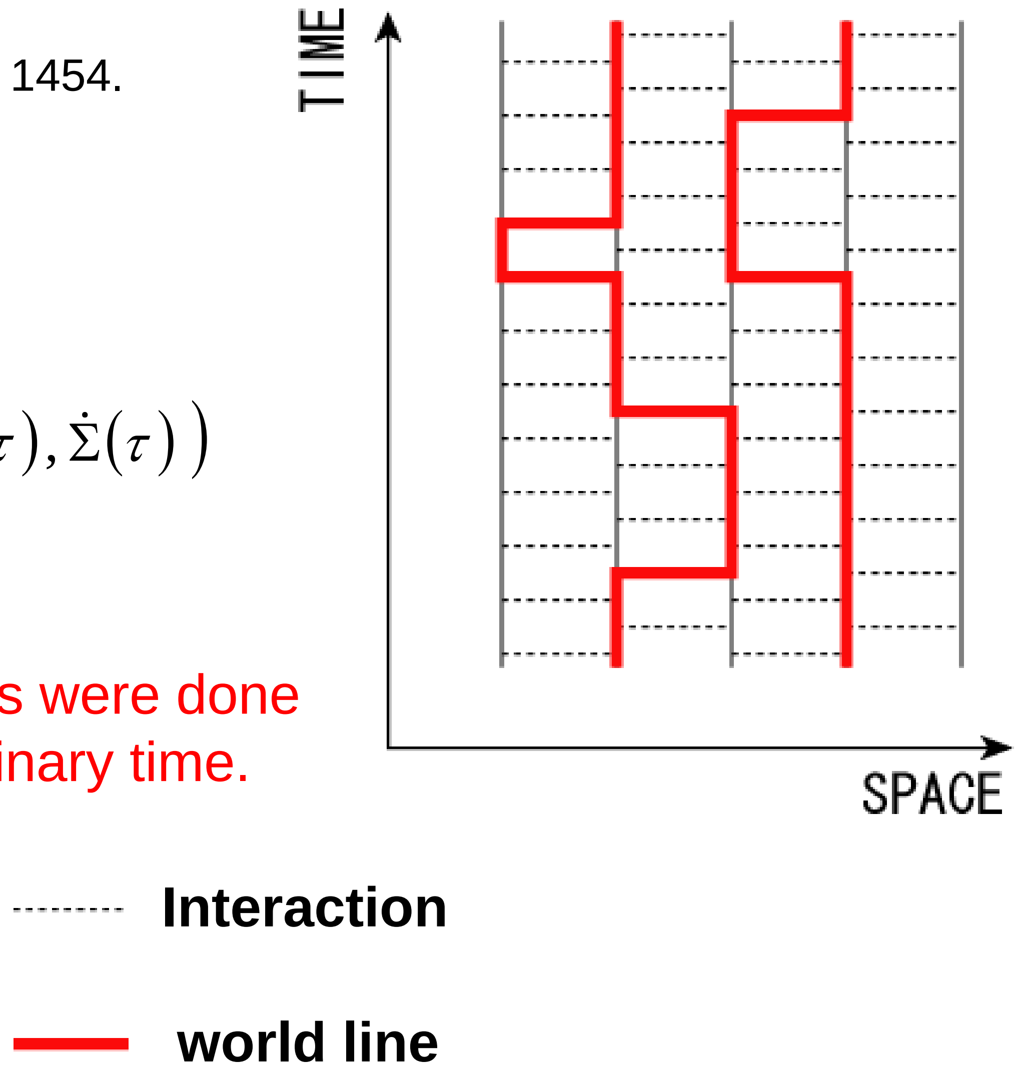
World-Line Monte Carlo

M. Suzuki: Prog. Theor. Phys. 56 (1976) 1454.

$$Z = \sum_{\Sigma} W[\Sigma]$$

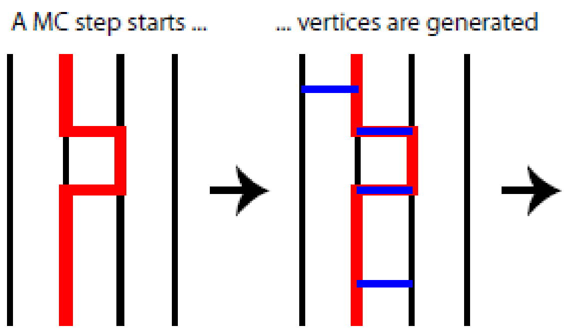
$$W[\Sigma] = e^{-\int_0^\beta d\tau\, L\left(\Sigma(\tau), \dot{\Sigma}(\tau)\right)}$$

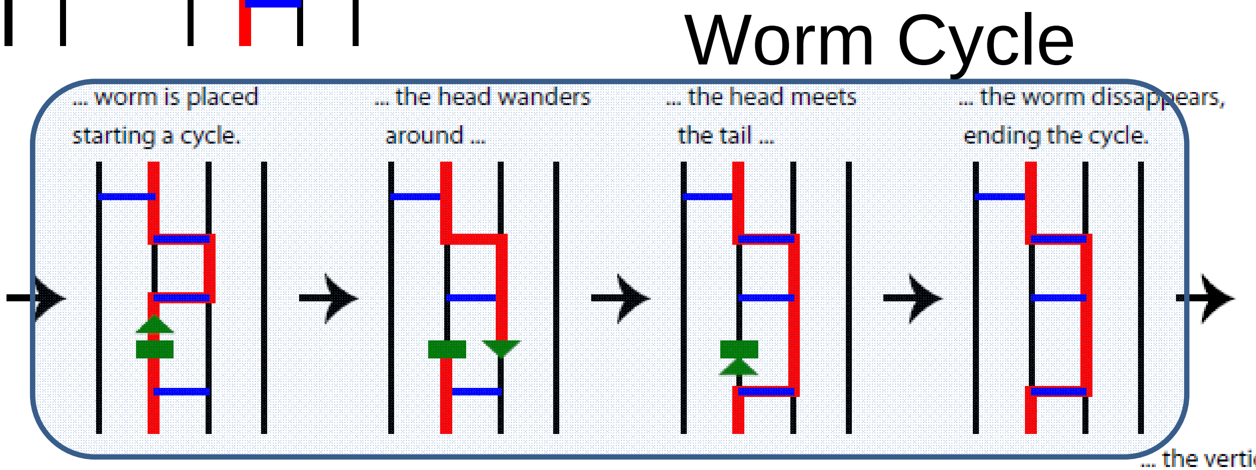
Before 1995, simulations were done with discretized imaginary time.

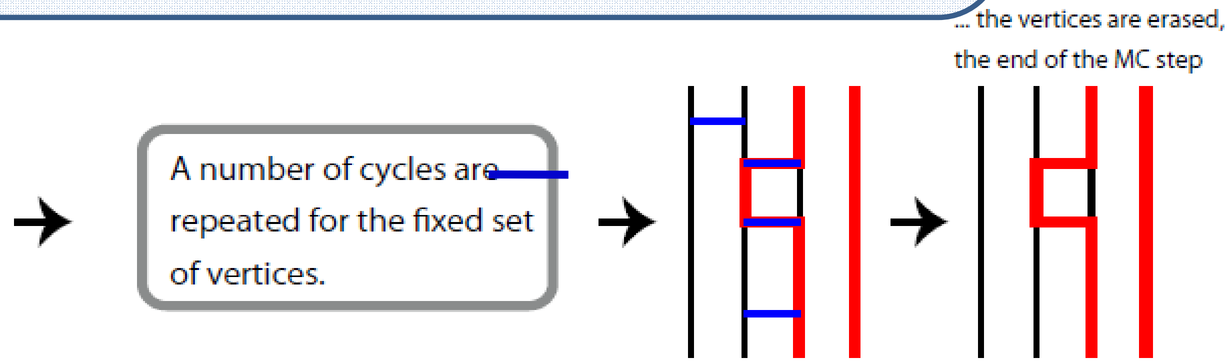


DLA (Directed-Loop Algorithm)

O. F. Syljuasen, A. W. Sandvik:
Phys. Rev. E 66, 046701(2002)

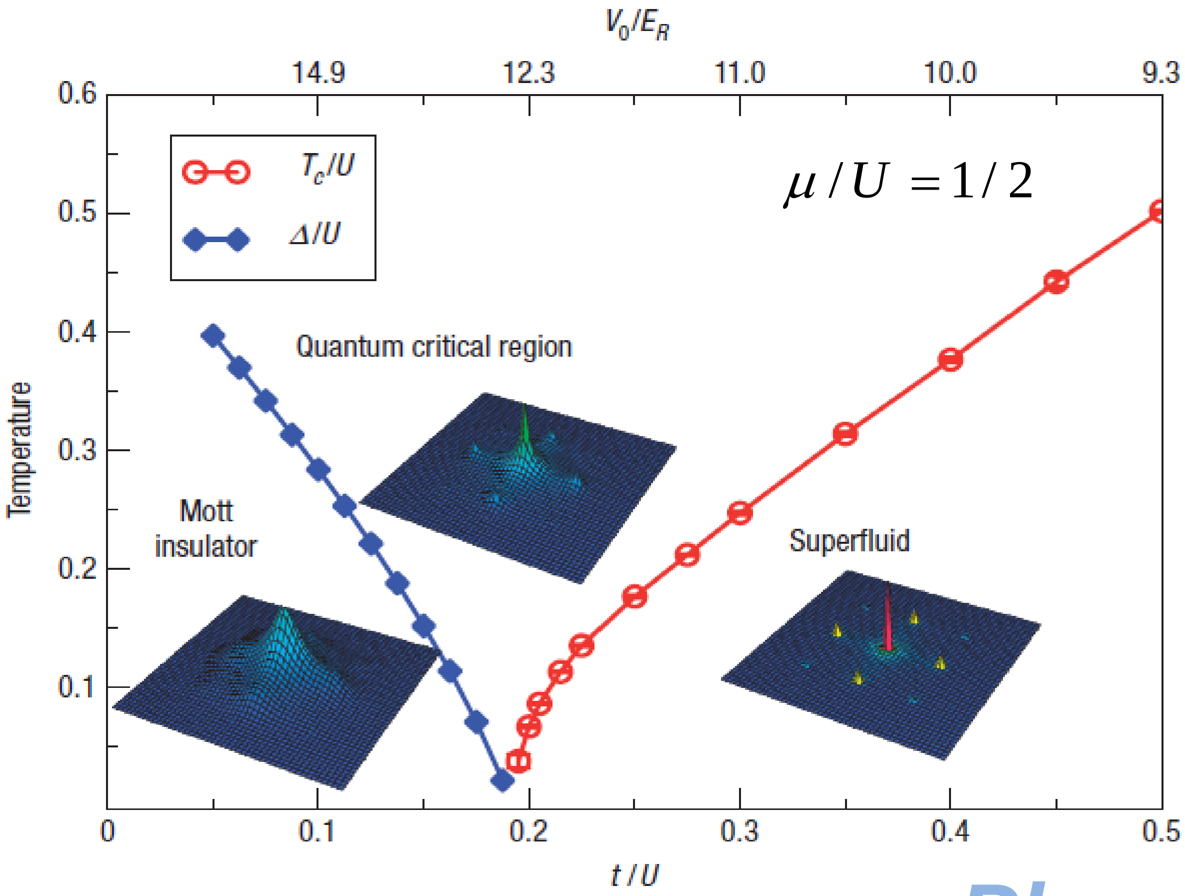


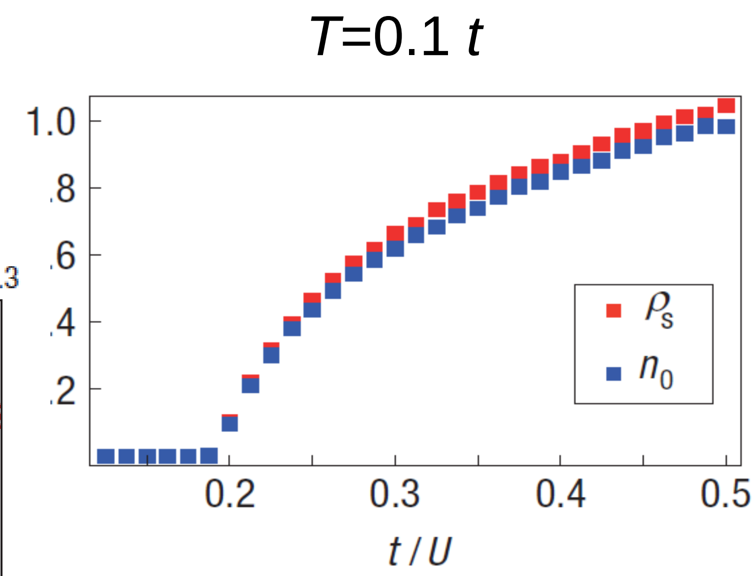




Directed Loop Algorithm

Generic Finite-T Phase Diagram

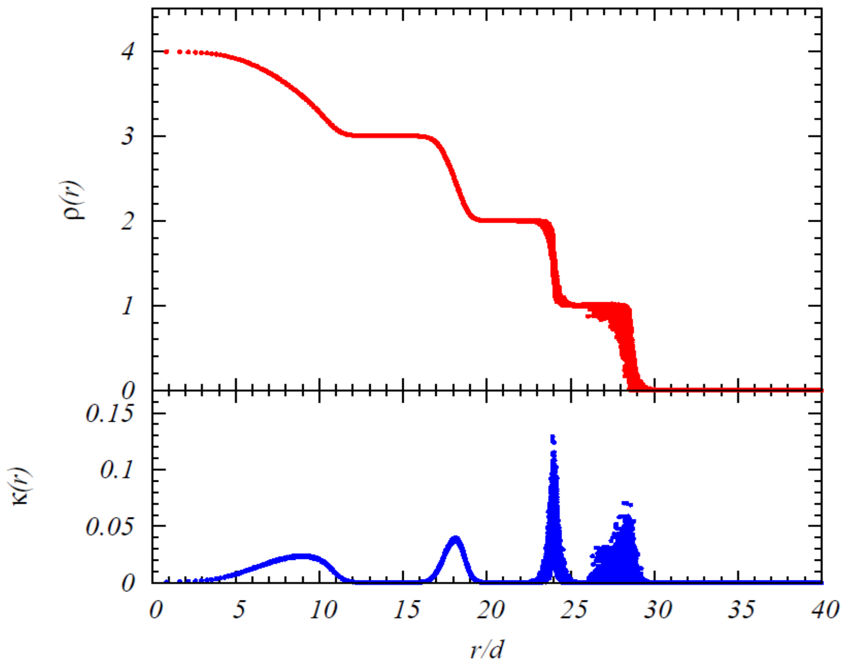


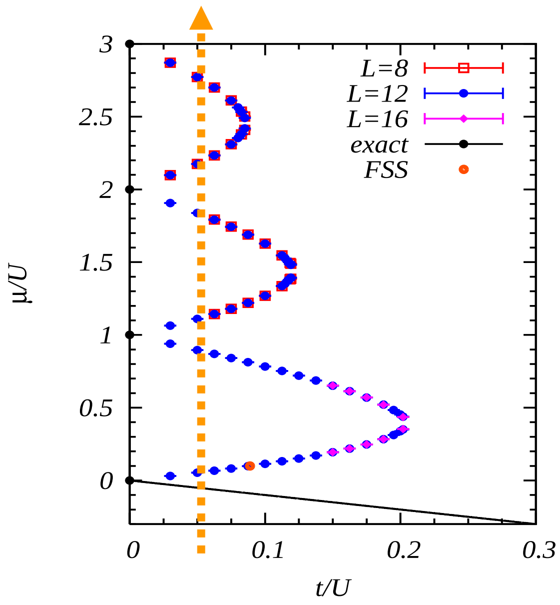


Kato, Zhou, N.K., and Trivedi, Nature Physics 4 617 (2008)

"Big wedding cake"

$$t/U = 0.05,\quad \mu_0/U = 3.3,\quad \Omega/U = 0.08,$$
$$(L/a)^3 = 64^3 \sim 2.6\times10^5,\quad \beta t = 5.0.$$





The number of bosons

$$N = 0.6936(1)\times 64^3,$$
$$\sim 1.8\times10^5.$$

cf: $2.0\text{x}10^5$ (Bloch's group experiment 2005)

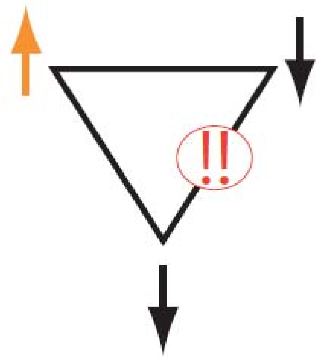
We have reached the system size comparable to experiments.

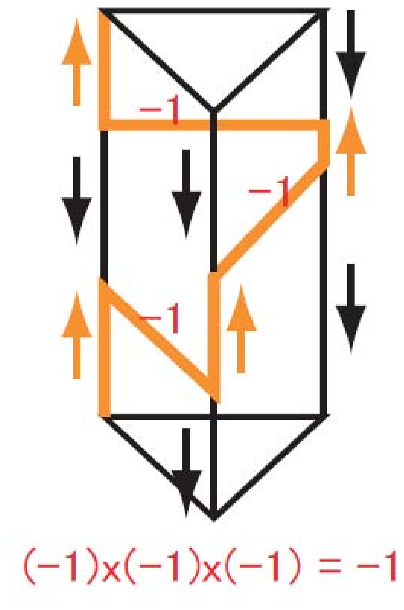
Negative Sign Problem

$$Z = \sum_{\Sigma} W[\Sigma] \; (\Sigma : \text{Feynman path})$$

$W[\Sigma]$ can be negative in general.

$$H = J\left(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 + \boldsymbol{S}_2 \cdot \boldsymbol{S}_3 + \boldsymbol{S}_3 \cdot \boldsymbol{S}_1\right)$$





Odd loops cause
frustration and negative sign.

Netative Sign Problem

If it is just occasional appearance of negative terms, it would've been OK. But in fact, it is more like ...

$$
\begin{aligned}
&(3-2)^{10} \\
&= 3^{10} - 10\cdot 3^{9}\cdot 2 + 45\cdot 3^{8}\cdot 2^{2} - \cdots + 2^{10} \\
&= 590490 - 10\times 39336 + 45\times 26244 - \cdots + 1024 \\
&= 1
\end{aligned}
$$

To this day, we've been needing to be lucky for being able to compute anything about massive quantum systems.

... absence of negative sign,

and/or

small finite-size corrections

We need REAL tools for REAL quantum systems (i.e., ones with frustration and fermion signs.)

Limited Variety of Tools for Frustrated Quantum Many-body Systems

- Quantum Monte Carlo
  - >> negative sign problem
- Exact diagonalization
  - >> only for small systems
- Series expansion
  - >> difficult reach beyond singularities
- Density matrix renormalization group (DMRG)
  - >> effective mainly for 1D systems
- Tensor network wave function
  - ✔ Tree network
    - >> incapable to express states with large entanglement
  - ✔ **Projected entangled pair state (PEPS)**
    - **>> exponential growth of computational time for exact contraction**
  - ✔ **Multi-scale entanglement renormalization ansatz (MERA)**
    - **>> no obvious drawback, so far.**

Ground State Calculation

Variational Wave Function:

$$|\psi\rangle = \sum_{x_1, x_2, \cdots, x_N} A_{x_1 x_2 \cdots x_N} |x_1\rangle \otimes |x_2\rangle \otimes \cdots \otimes |x_N\rangle$$

$$A_{x_1 x_2 \cdots x_N} = [\text{Contractio n of tensor network leaving } x_1, x_2, \cdots, x_N \text{ alive}]$$

$$(e.g.\ \ A_{x_1 x_2 \cdots x_N} = P^{y_1}_{x_1 x_2} Q^{y_2}_{x_3 x_4} \cdots R^{y_{N/2}}_{x_{N-1} x_N} S^{z_1}_{y_1 y_2} T^{z_2}_{y_1 y_2} \cdots)$$

Our task is to find ...

(1) the structure of the network,

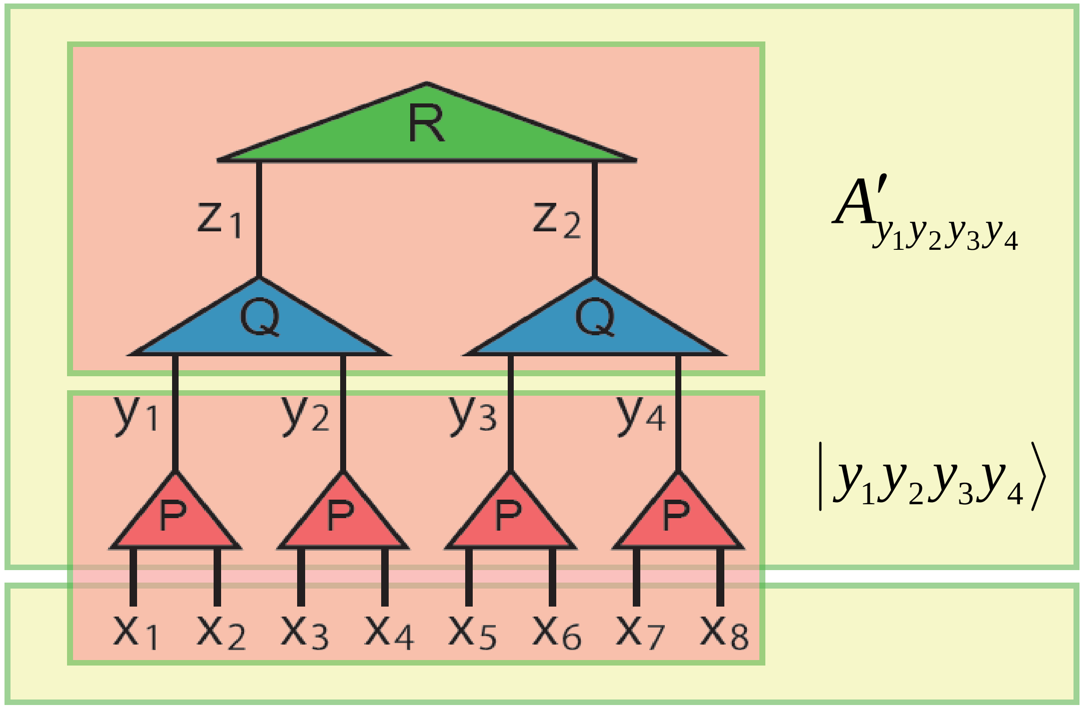
(2) the dimension of each index, and

(3) the elements of each tensor.

... so many things to play with.

Tensor Network gives a natural framework for numerical renormalization group

$$A_{x_1x_2x_3x_4x_5x_6x_7x_8} = R_{z_1z_2}\,Q^{z_1}_{y_1y_2}\,Q^{z_2}_{y_3y_4}\,P^{y_1}_{x_1x_2}\,P^{y_2}_{x_3x_4}\,P^{y_3}_{x_5x_6}\,P^{y_4}_{x_1x_2}$$



$A_{x_1x_2x_3x_4x_5x_6x_7x_8}$

$|x_1x_2x_3x_4x_5x_6x_7x_8\rangle$

$$|\psi\rangle = \sum_{x_1,x_2,\cdots,x_8} A_{x_1x_2\cdots x_8}\,|x_1x_2\cdots x_8\rangle = \sum_{y_1,y_2,y_3,y_4} A'_{y_1y_2y_3y_4}\,|y_1y_2y_3y_4\rangle$$

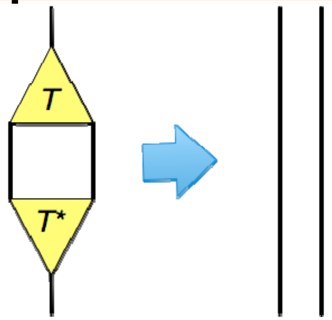
Cost of MERA Computations

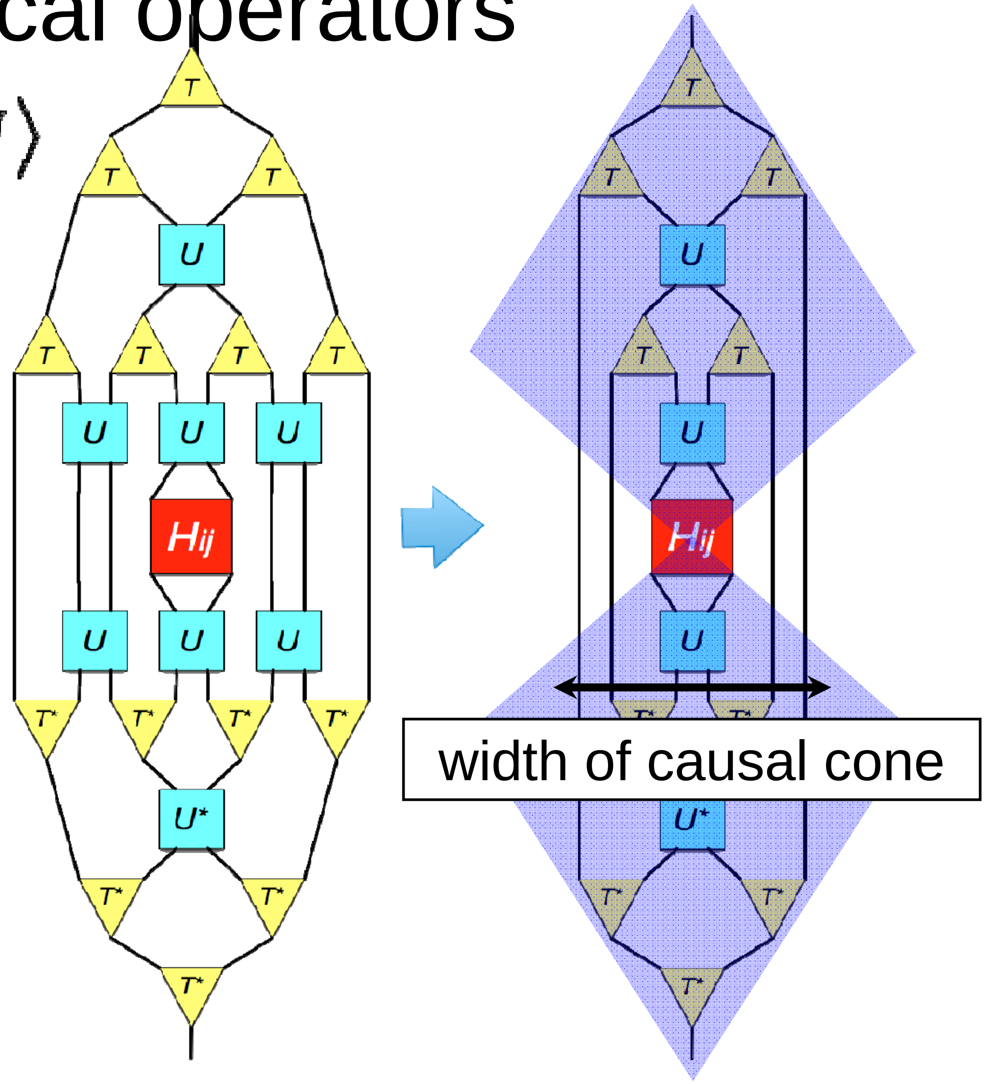
Expectation value of local operators

e.g., $E_{ij} \equiv \langle\Psi|H_{ij}|\Psi\rangle$

Isometricity simplifies

Isometricity





computational cost

$$O(m^{2w+k})$$

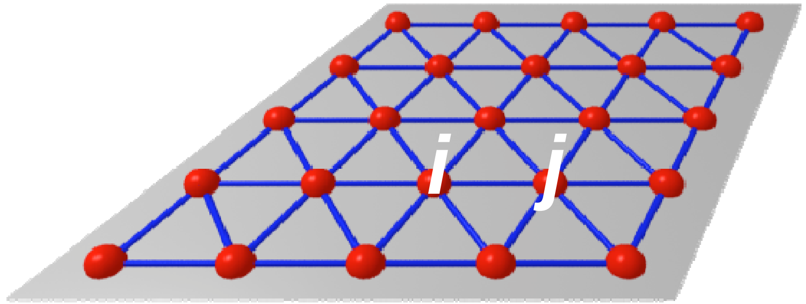
m : Dimension of indexes of tensors

w: The width of the causal cone

Triangular Lattice Antiferromagnet

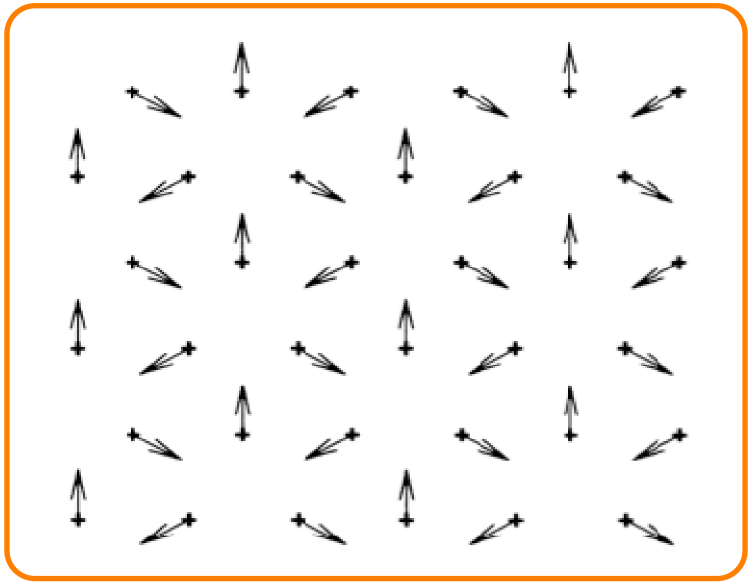
- Hamiltonian

$$H = 2\sum_{\langle ij\rangle} S_i \cdot S_j$$



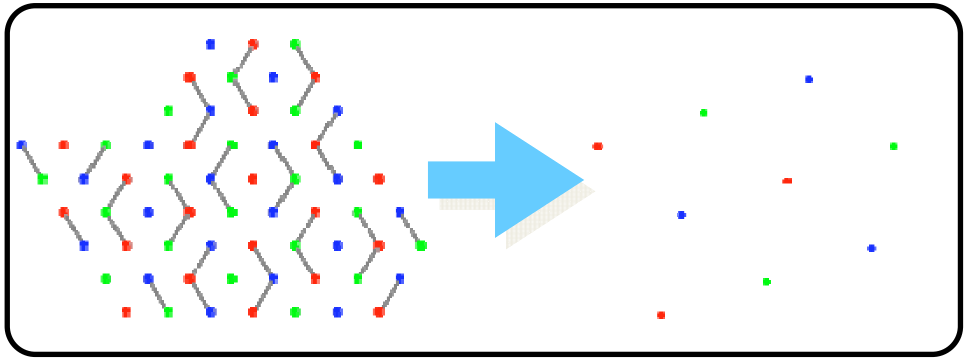
- Previous results
  - Three-sublattice Néel order
  - Exact diaogonalization
  - (B.Bernu, et al. 1994)

$$2\langle S_i \cdot S_j\rangle_\infty = -0.363$$

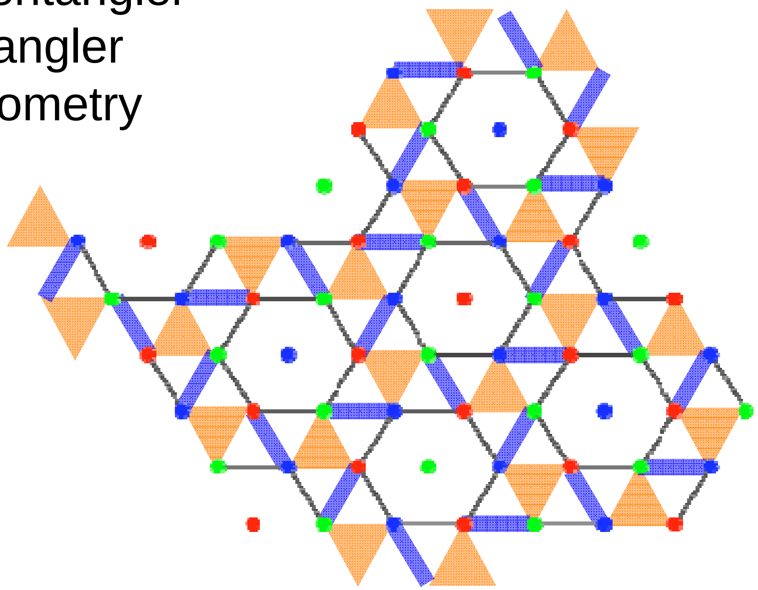


(Max N=36, periodic cond.)

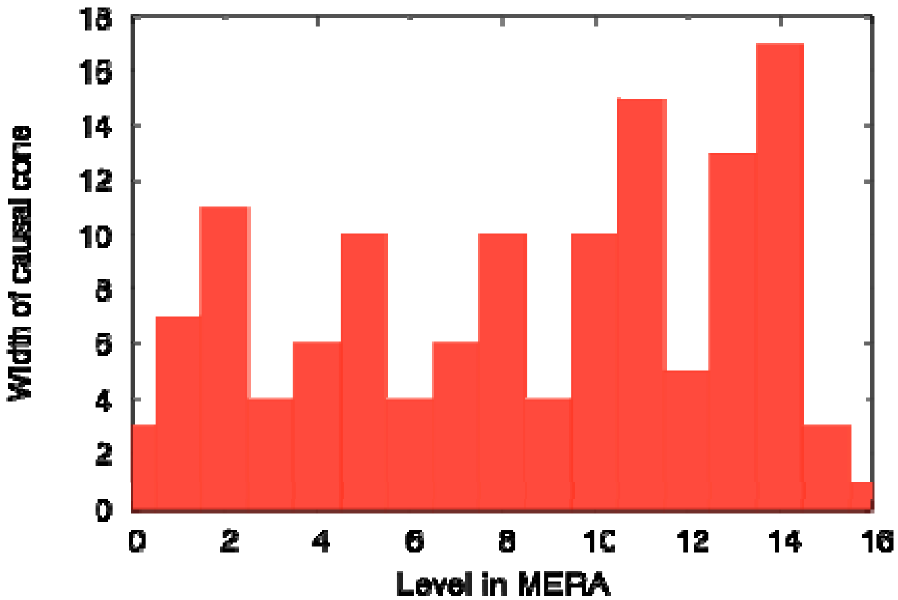
Network structure is important



Entanglement renormalization (ER)
1. Orange disentangler
2. Blue disentangler
3. Hexagon Isometry



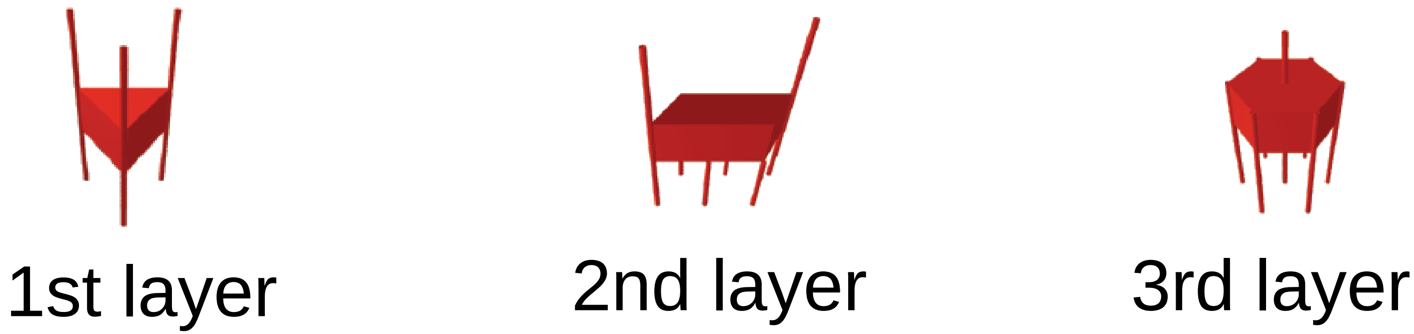
- Width of causal cone



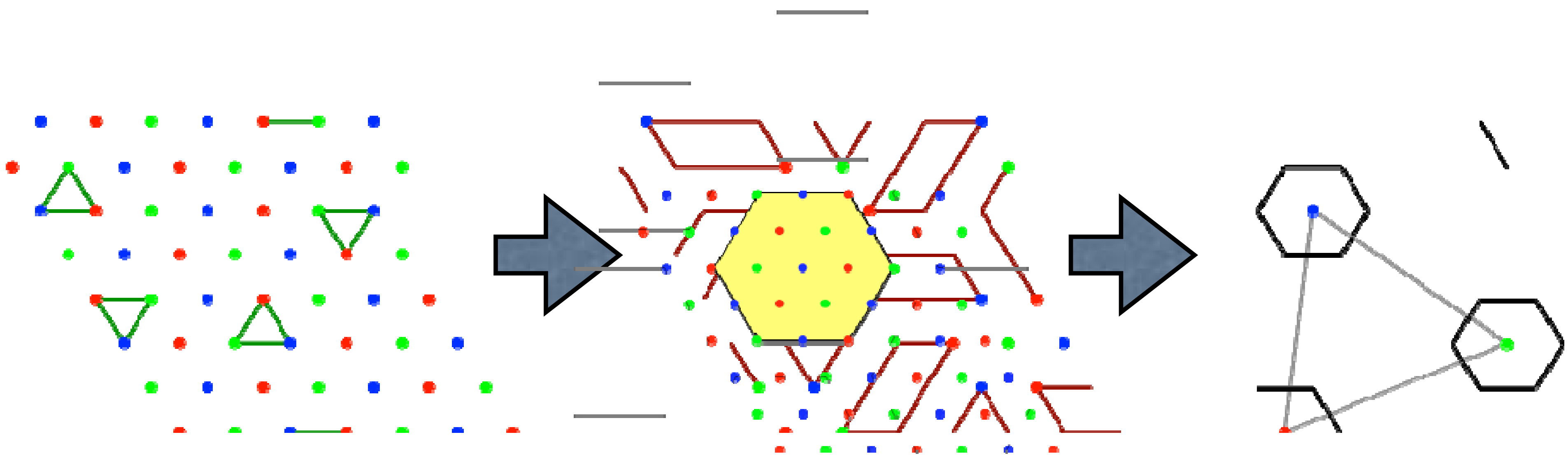
$$w = 17$$

Very large !

MERA on a triangular lattice

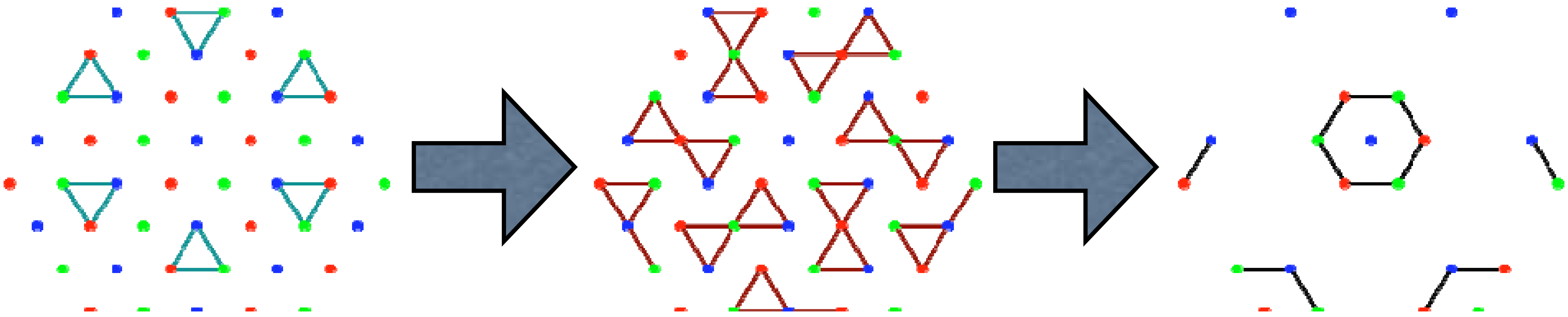


1 ER operation renormalizes 19 sites into 1



Evenbly-Vidal's MERA on a Triangular Lattice

ER for 16 sites (arXiv:0904.3383v1)



E/N= − 0.363

infinite-size method

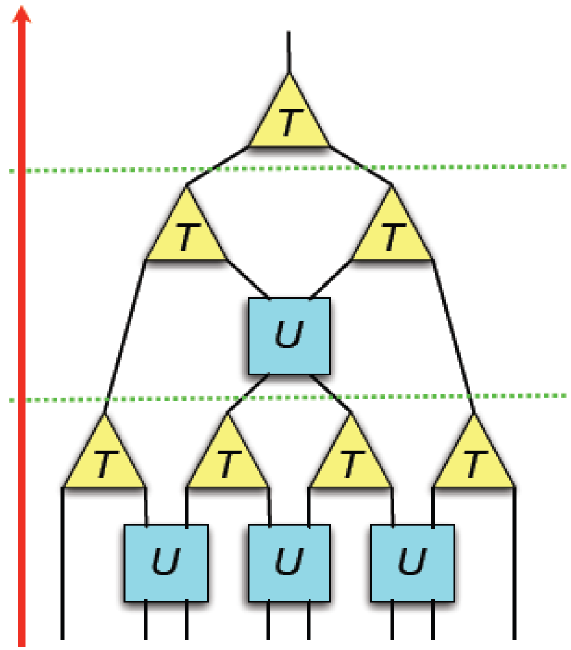
Various MERA Schemes

Evenbly-Vidal

✔Translationally Invariant Scheme

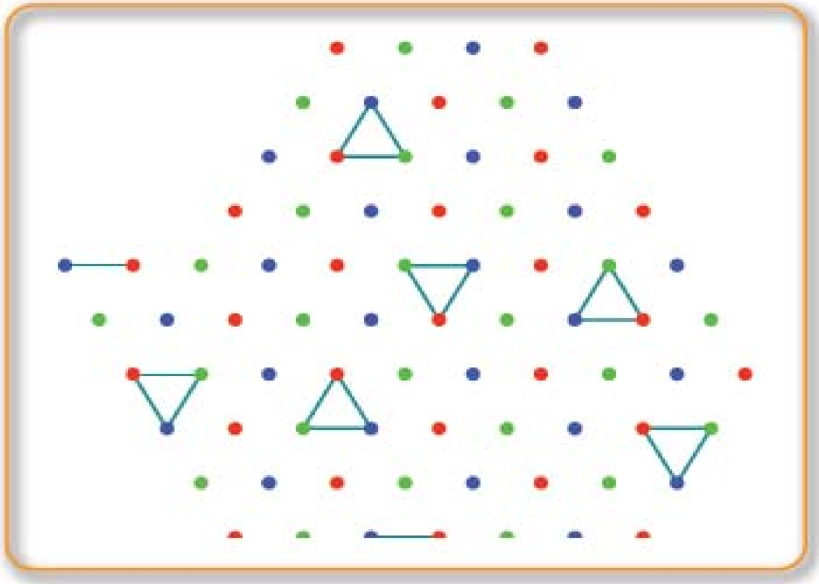
✔Scale Invariant Scheme

✔Excitated State Scheme
(The dimension of a top leg > 1)



Details of Computation

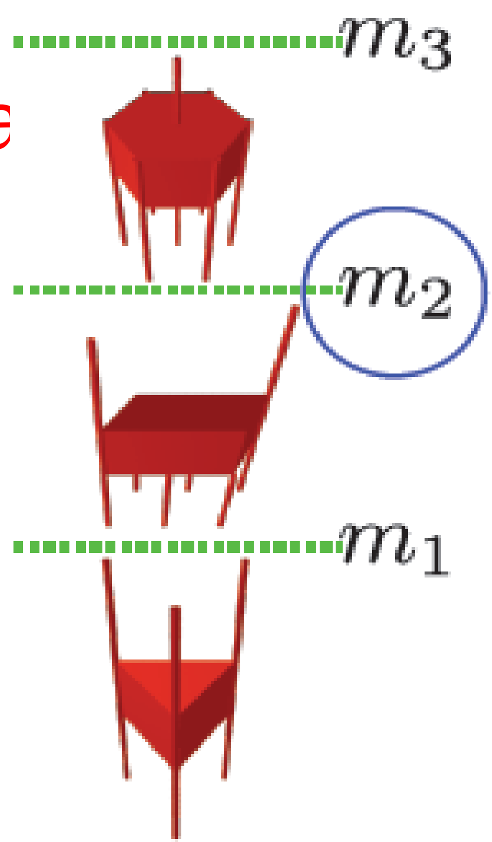
- **MERA Network**
  - >> The width of the causal cone = 6
  - >> CUP time $O(m^{14})$
  - >> Memory $O(m^{12})$



- **Lattice**
  - >> Triangular Lattice
  - >> 1 Generation : 76 (=4x19) sites
  - >> 2 Generations : 1444 (=76x19) sites
  - >> Periodic Boundary Condition

Optimization of Tensor Elements

Candidates: variants of steepest decent, projection method, etc.
Here we used the standard singular va
decomposition (SVD)



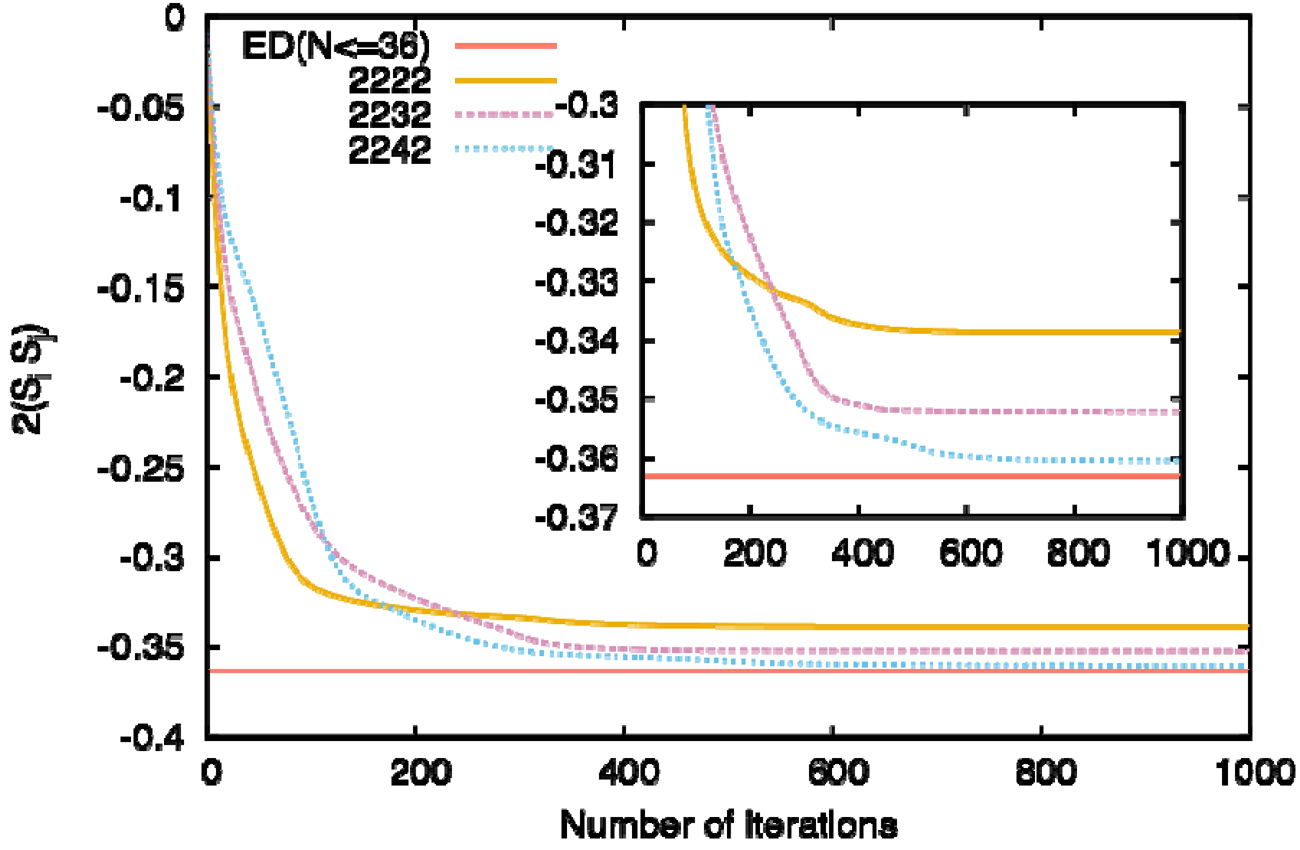
m_1=m_3=2 (fixed)

	m_2=2	m_2=3	m_2=4
# of param.	576	3556	17472
memory	85K	170M	920M

Single Generation Calculation

Translationally Invariant MERA

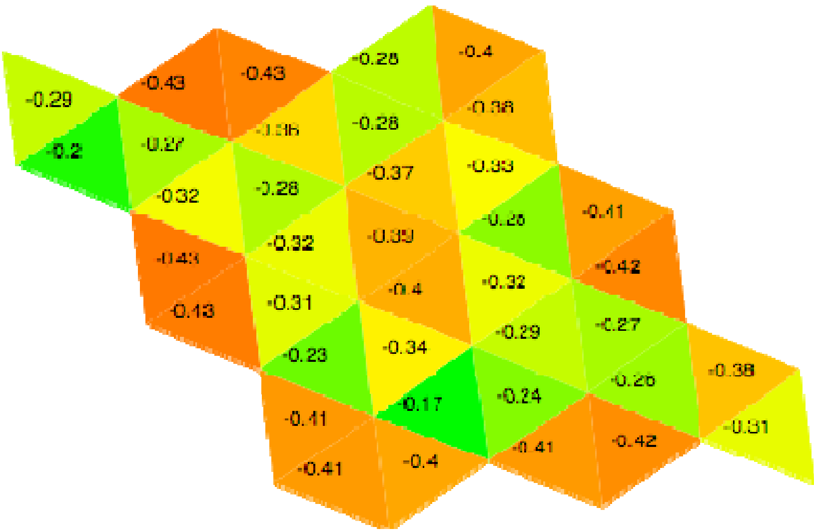
N=76



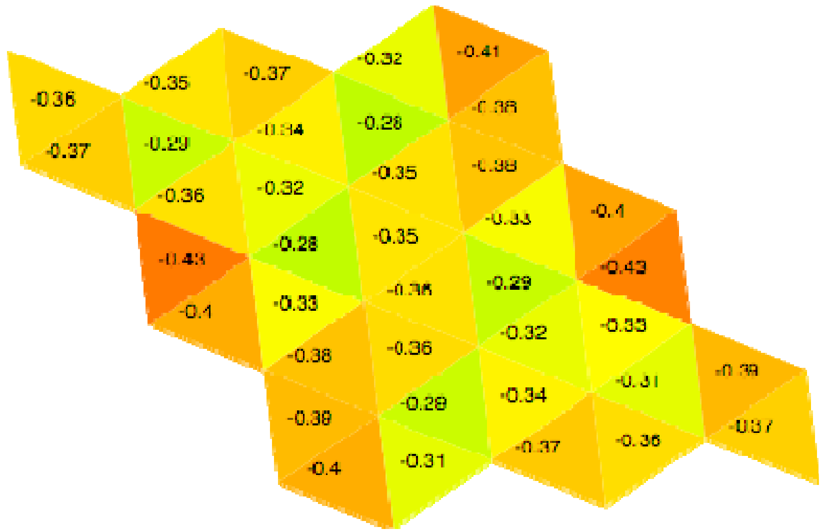
Network capability is sensitive to m_2

Quality of Wave Function

m=2



m=3

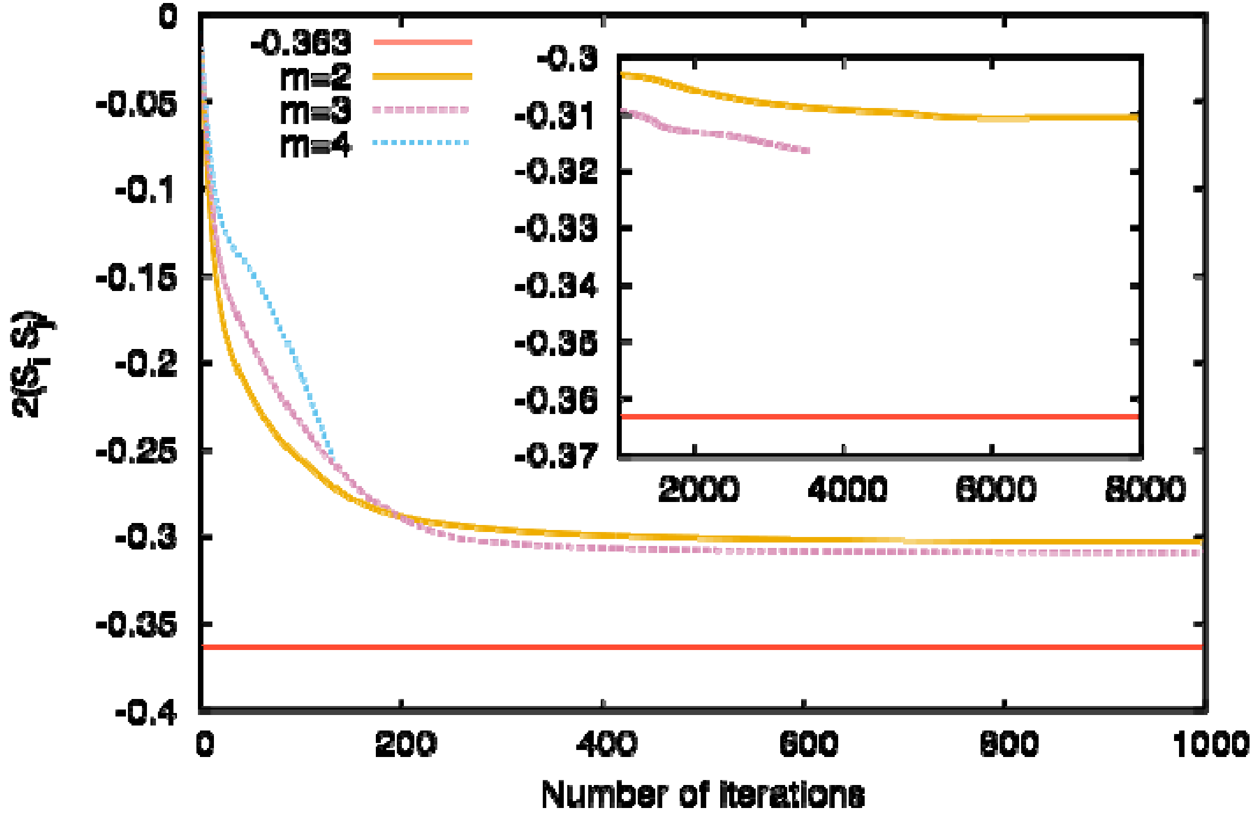


More homogeneous for larger m

Two-Generation Calculation

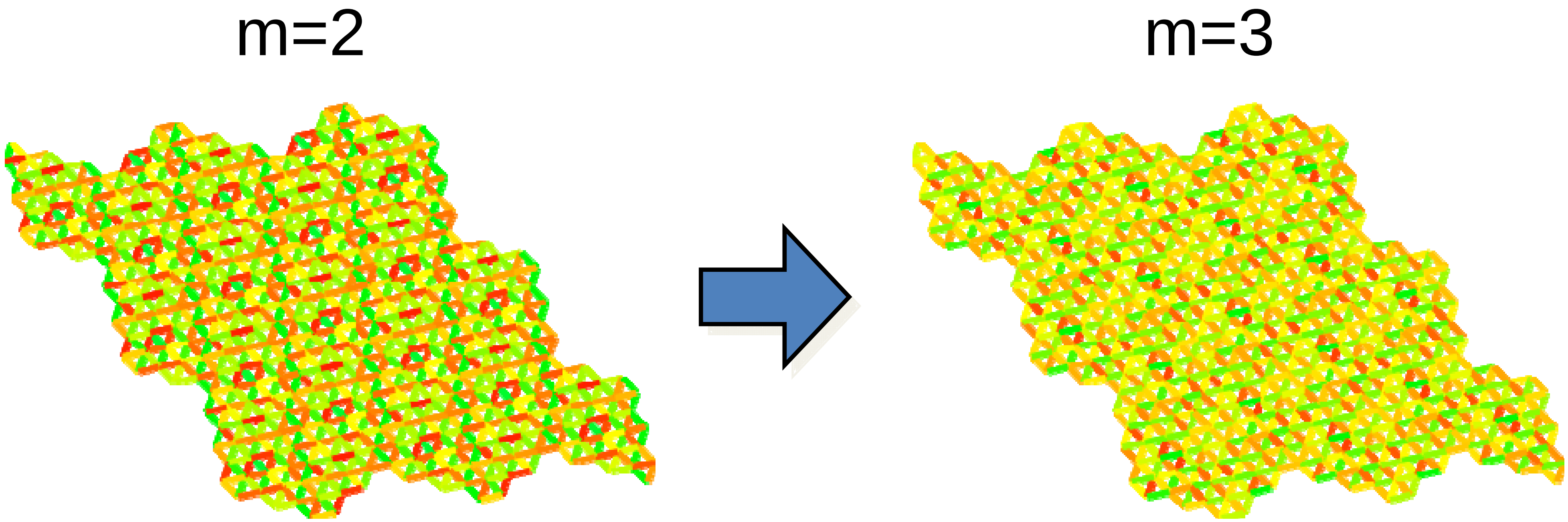
Translationally Invariant MERA

N=1444



Slow!

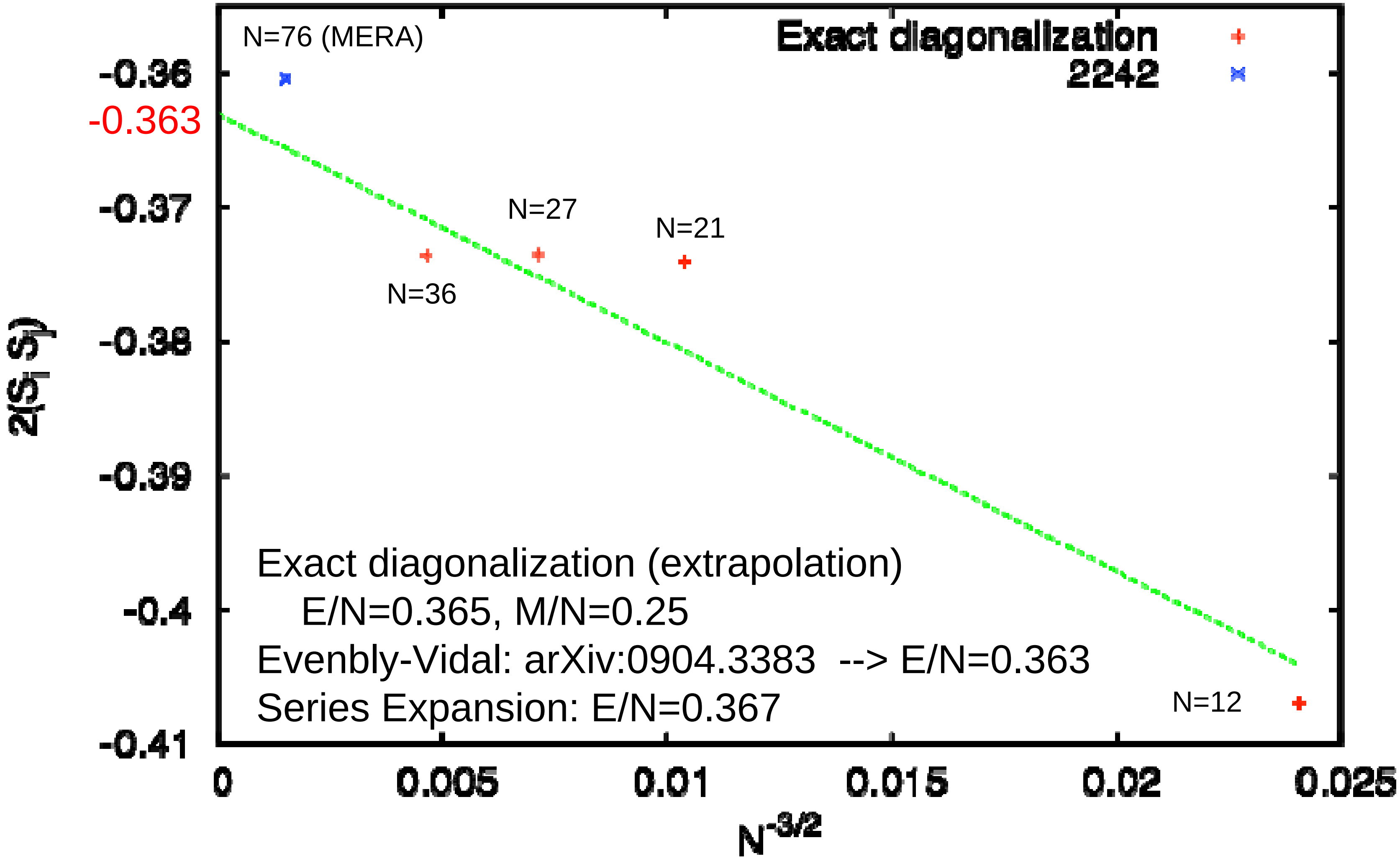
Quality of Wave Function (2 gen.)



Looks like a pachwork made of the single-gen. result.
The second generation doesn't improve much (yet).

With results of exact diagonalization

B.Bernu, et al., PRB **50** (1994) 10048



Magnetization

$$E_\infty = \langle 2\mathbf{S}_i \cdot \mathbf{S}_j \rangle = -0.365 \text{ and } M_\infty = 0.25.$$ (Bernu)

The results Kenji got this morning:

$$\boldsymbol{m}_{\mathrm{A}} = \left\langle \sum_{i \in A} \boldsymbol{S}_i \right\rangle , \quad C_{\mathrm{AB}} = \boldsymbol{m}_{\mathrm{A}} \cdot \boldsymbol{m}_{\mathrm{B}}$$

$$m_{\mathrm{A}} = \sqrt{C_{\mathrm{AA}}} = |\boldsymbol{m}_{\mathrm{A}}| , \quad x_{\mathrm{AB}} = \frac{C_{\mathrm{AB}}}{\sqrt{C_{\mathrm{AA}} C_{\mathrm{BB}}}} = \cos\theta_{\mathrm{AB}}$$

m2	mA	mB	mC	xAB	xBC	xCA
2	0.301	0.266	0.264	-0.549	-0.414	-0.533
3	0.244	0.264	0.241	-0.538	-0.547	-0.411
4	0.238	0.269	0.255	-0.482	-0.534	-0.484

Summary

● Variational principle calculation with MERA network variaional function.

● Applied to the Heisenberg antiferromagnet on the triangular lattice.

● Single generation caculation converges and m2 is important for expressing the correct ground state.

● Two generation caculation is slow to converge.

● The method is starting to breaking records!