Tensor network methods in condensed matter physics

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Targets of tensor network methods

- Lattice models

Localized spin system:

$$\mathcal{H} = \sum_{i,j} J_{ij} S_i S_j$$

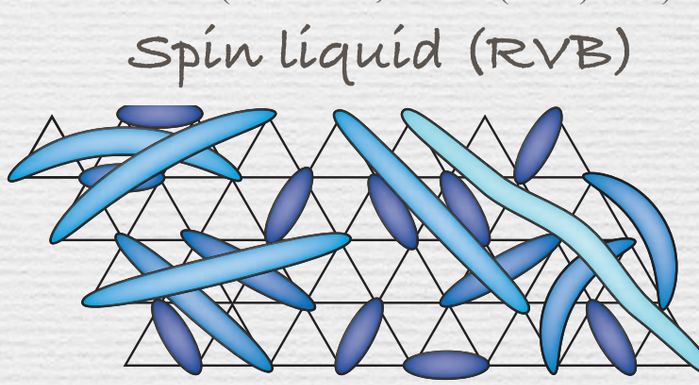
S_i : Spin operator, typically S=1/2

*Spins located on a lattice:
square, triangular, cubic, …

☑ We want to find novel states of the matter

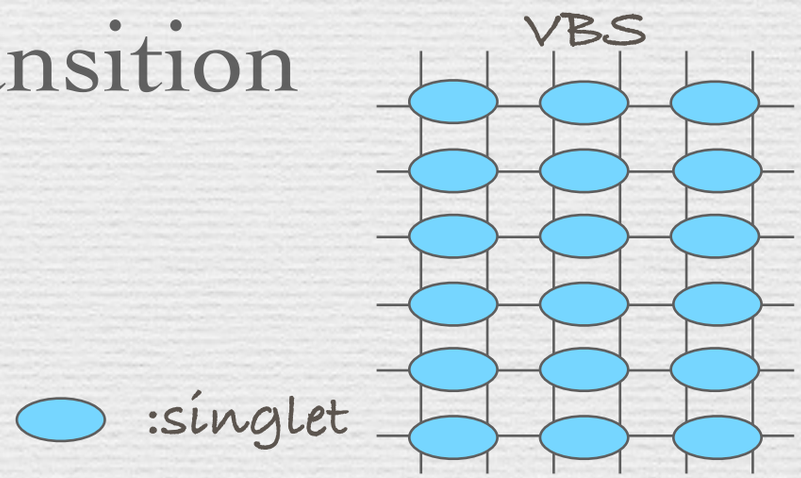
(L. Balents, Nature (2010)より)

- Quantum spin liquids
- Topological phases
- Valence Bond Solids
- …



☑ We want to investigate phase transition

- (Quantum) critical phenomena
- Topological phase transition
- …



Targets of tensor network methods

- Lattice models

Itinerant electron systems: (Hubbard model)

$$\mathcal{H} = \sum_{\langle i,j\rangle,\sigma} t_{i,j}(c^{\dagger}_{i,\sigma}c_{j,\sigma} + \text{H.c.}) + U\sum_{i} n_{i,\uparrow}n_{i,\downarrow}$$

$c^{\dagger}_{i,\sigma}$:creation operator of an electron.

☑ We are interested in

- Super conductivity
- Non-equilibrium phenomena
- …

A lot of interesting things occur
in the Avogadro scale ~ 10

➡ We need large scale calculations.

Numerical methods

☑ Numerical diagonalization

Exact and applicable for any systems, but

S=1/2 spin models ~ 40 sites

Hubbard model ~ 20 sites

→ We need careful extrapolation.
(It is often very difficult.)

☑ Quantum Monte Carlo (QMC)

Within statistical error, solving problem "exactly"!

Easy calculation for

But, Interesting problems are usually suffer from the

☑ Dynamical Mean Field Theory (DMFT)

Kind of mean-field

Temporal quantum fluctuations are treated accurately through a few sites

→ Success in description of metal - insulator phase transition

Numerical methods

☑ Variational method

Assuming a wave-function ansatz with several parameters.
Determining parameters so as to minimize the energy.

- Variational Monte Carlo

  Calculate energy using Monte Carlo sampling

  → No sign problems.

  Larger system size than the diagonalization.

- Tensor network methods (including DMRG)

  Wave-function is represented by

  No sign problems.

  Very large system size (or infinite)

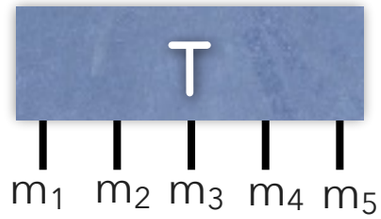
Tensor network method

G.S. wave function: $|\Psi\rangle = \sum_{\{m_i=\uparrow\downarrow\}} T_{m_1,m_2,\cdots,m_N}|m_1,m_2,\cdots,m_N\rangle$

T：N-rank tensor

``Tensor network" decomposition

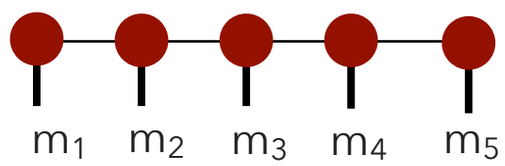
$T_{m_1,m_2,\cdots,m_N}$ =

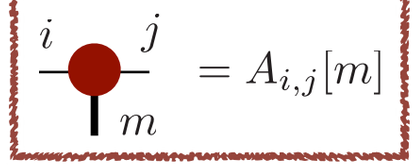


# of Elements＝2^N

- Matrix Product State (MPS)

$A_1[m_1]A_2[m_2]\cdots A_N[m_N]$ =

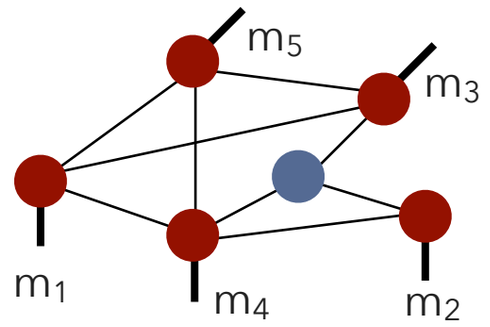


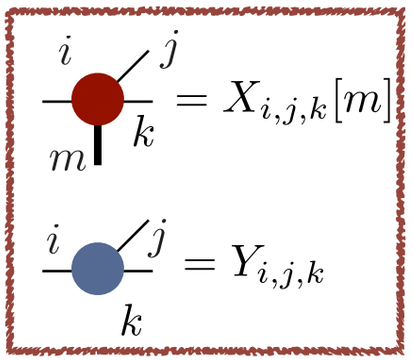


$A[m]$ ：Matrix for state m

- General network

$\mathrm{Tr}X_1[m_1]X_2[m_2]X_3[m_3]X_4[m_4]X_5[m_5]Y$





X,Y : Tensors

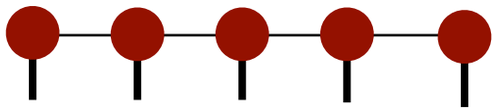
Tr : Tensor network contraction

By choosing a ``good" network, we can express G.S. wave function efficiently.

ex. MPS: # of elements ＝$2ND^2$ D: dimension of the matrix A

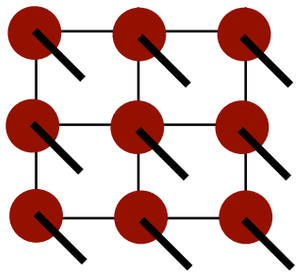
Exponential→ Linear *If D does not depend on N…

Family of tensor network states

MPS: 

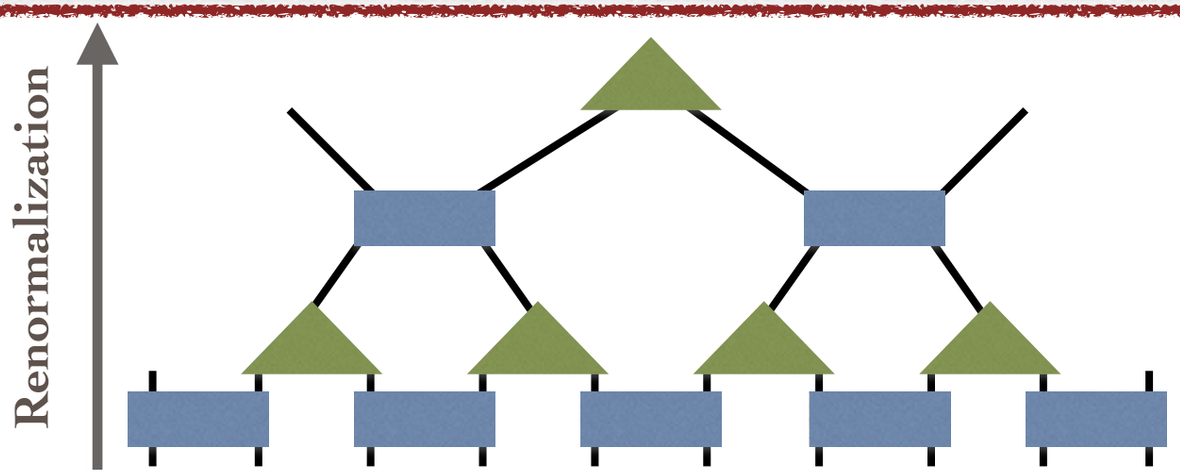
Work well in one-dimensional systems

DMRG, TEBD, …

PEPS,TPS: 

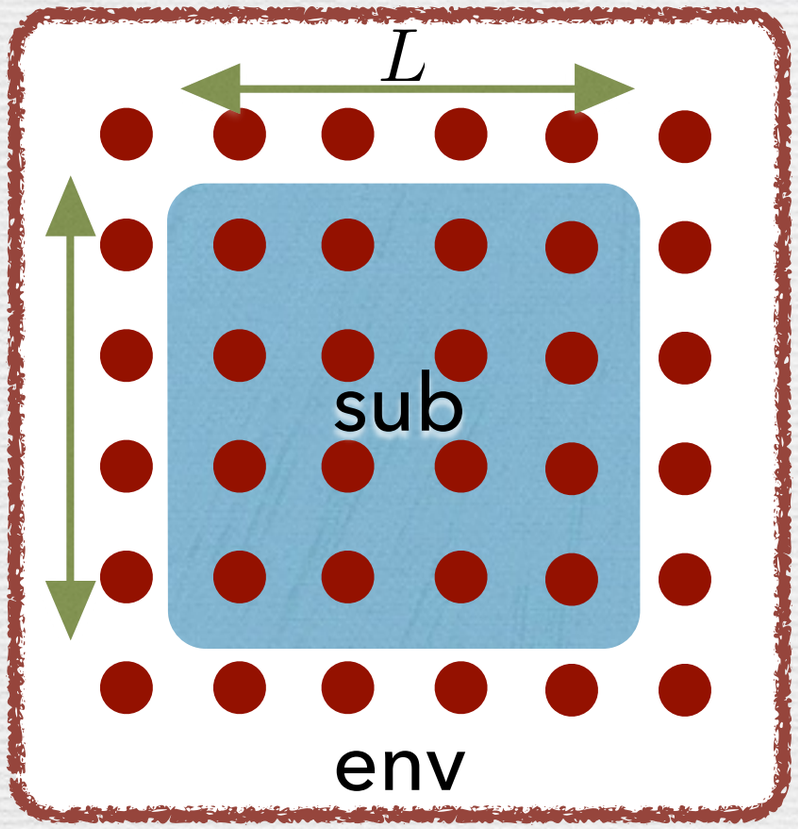
two or higher dimensional systems

generalization of MPS

MERA: 

Suitable for a
scale invariant states

Quantum Entanglement



Reduced density matrix of the subsystem.

$$\rho_{\rm sub} \equiv {\rm Tr}_{\rm env} |\Psi\rangle\langle\Psi|$$

Entanglement entropy

$$S_{\rm sub} \equiv -{\rm Tr}(\rho_{\rm sub} \log \rho_{\rm sub})$$

general states: $S_{\rm sub} \sim L^d$:Volume low

L: boundary length

A lot of ground state

$S_{\rm sub} \sim L^{d-1}$:Area low

1-dimensional gapless system: $S_{\rm sub} \sim \log L$

Metallic system : $S_{\rm sub} \sim L^{d-1} \log L$

Entanglement entropy of MPS and PEPS

- Entanglement entropy of MPS

  Sub-system connected to the environment
  through only two bonds.

  For matrix dimension D:

$$S_{\text{sub}} \leq 2 \log D$$

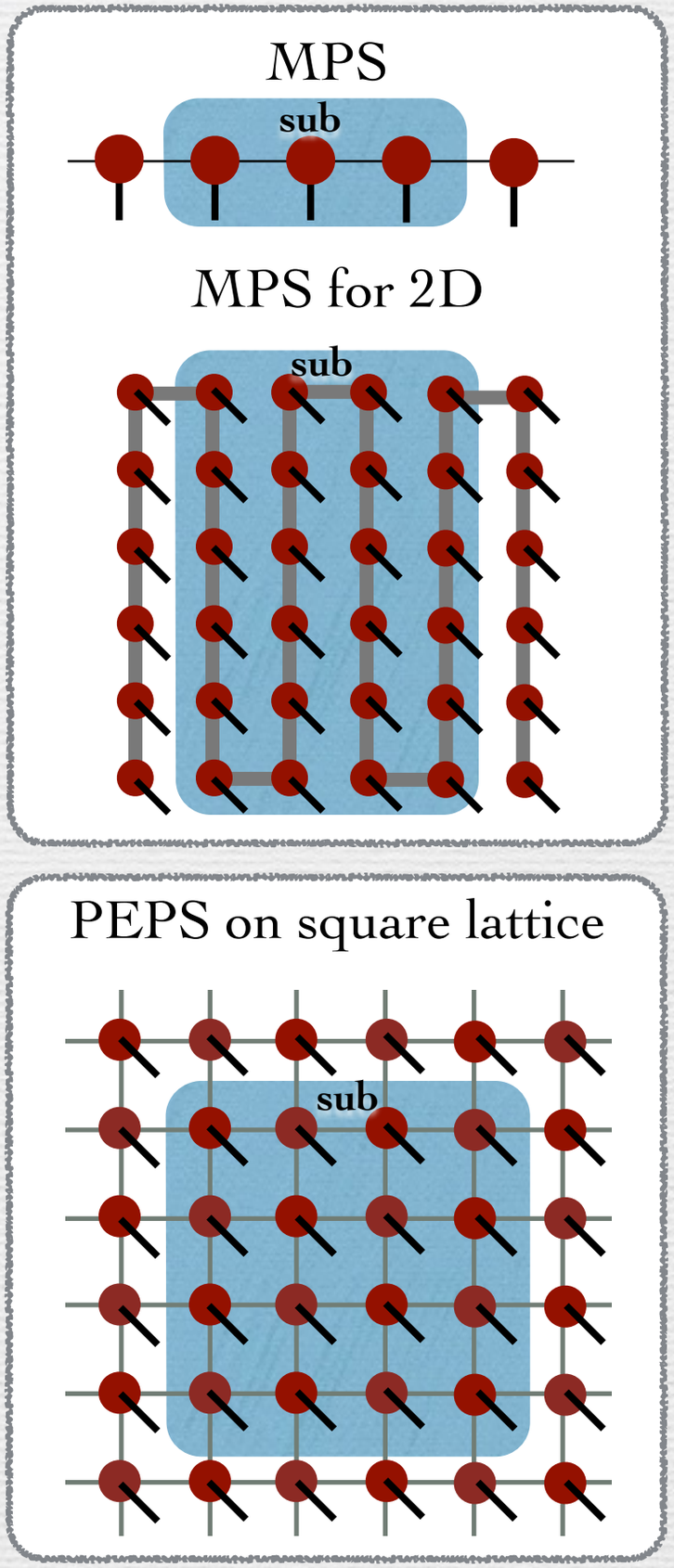
  In order to represent the entanglement entropy,
  we need exponentially large matrix dimension
  for two and higher dimensions.

- Entanglement entropy of PEPS

  For tensor dimension D:

$$S_{\text{sub}} \leq L^{d-1} \log D$$

  For sufficiently large, but finite, D,
  a lot of ground states of very large
  (infinite) system can be represented
  by PEPS!



Advantage of tensor network method

☑ Efficient representation of the ground state

MPS (for d=1) and PEPS (for 2 > d) can represent
the ground state wave-function for very large system efficiently.

Finite tensor-dimension

☑ Applicable to any system

No sign problems!

☑ Small bias

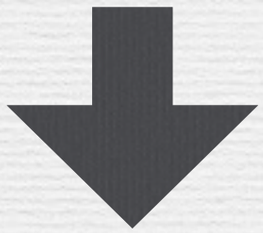
- Assumed wave-function contains large # of elements.
- The shapes of MPS and PEPS reflect only underlying lattice geometry.

Difficulties

1. High computational costs for contraction of the network

For PEPS:

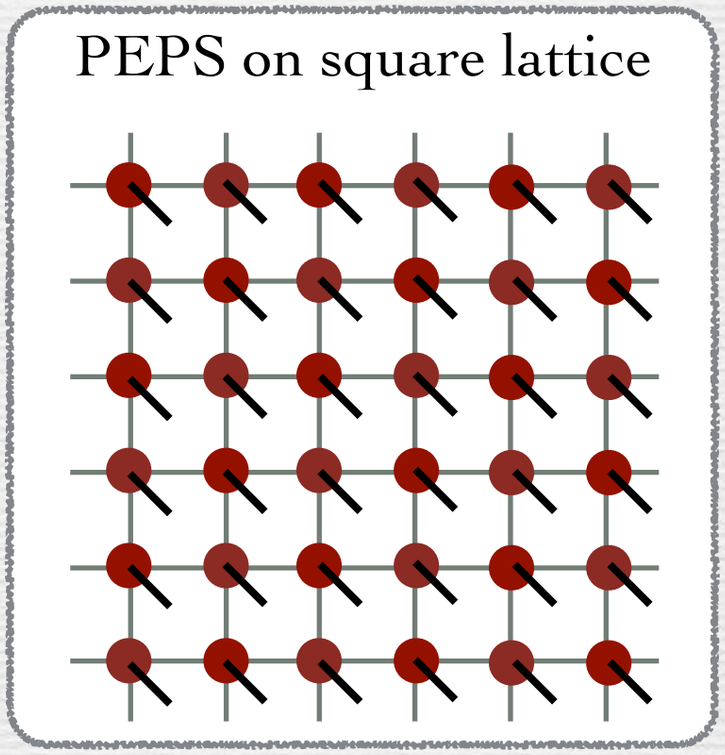
Calculation of the entire tensor products need exponentially large costs



We use

But, still very high cost.

2D- PEPS: O(D  MPS: O(D



For two or higher dimensions, tensor dimensions are limited:
D~10

Difficulties

2. Fermionic system with fermi surface (metal, semi-metal)

Entanglement entropy has a

$$S_{\mathrm{sub}} \sim L^{d-1} \log L$$

PEPS need

- Another tensor network states: branching MERA?
- Combination with variational Monte Carlo ?
- ….

Challenging problem!

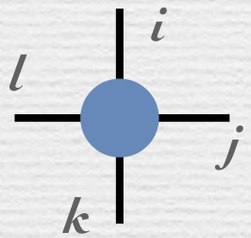
Partition function representation

Partition function: $Z = \mathrm{Tr}\exp(-\beta\mathcal{H})$

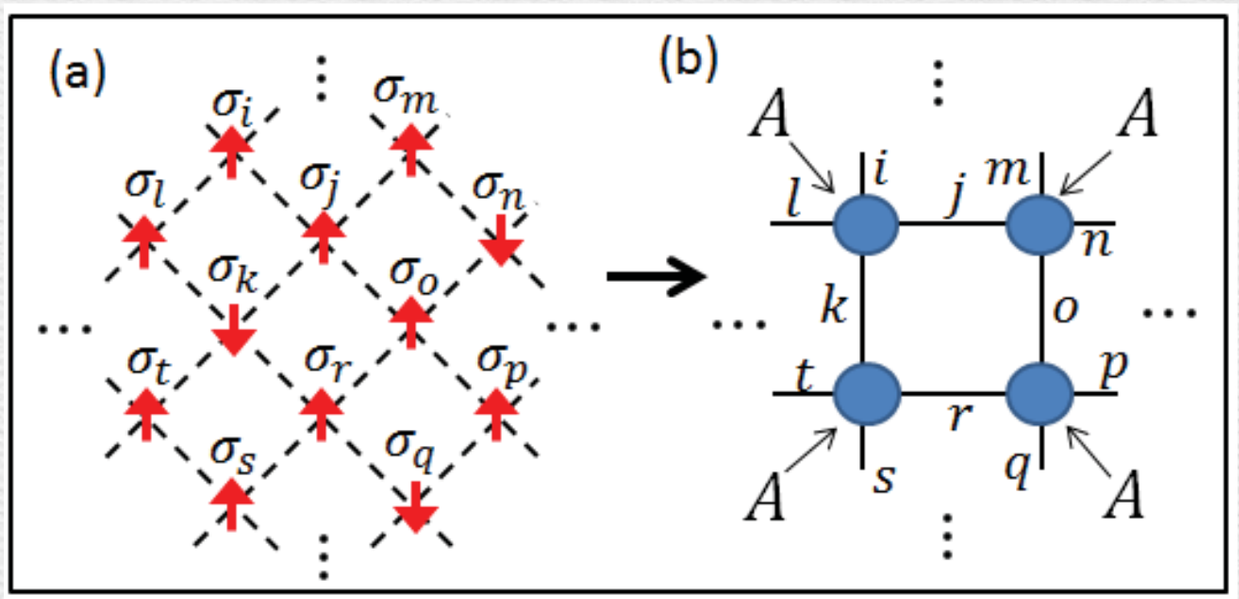
Z can be represented by

Example: classical Ising model on the

$$A_{i,j,k,l} = e^{(\sigma_i\sigma_j+\sigma_j\sigma_k+\sigma_k\sigma_l+\sigma_l\sigma_i)/T}$$



$$\sigma_i = \pm 1 = \uparrow, \downarrow$$



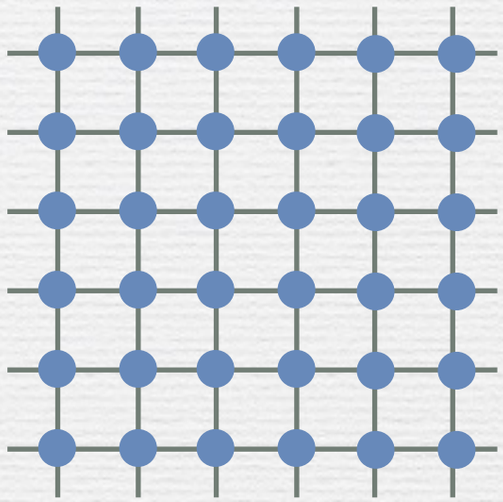
from G. Evenbly and G. Vidal, arXiv:1412.0732

*For quantum system:

Path integral representation ➡ 1+d dimensional tensor network

Contraction and renormalization

$$Z = \mathrm{Tr}\exp(-\beta\mathcal{H}) \quad =$$

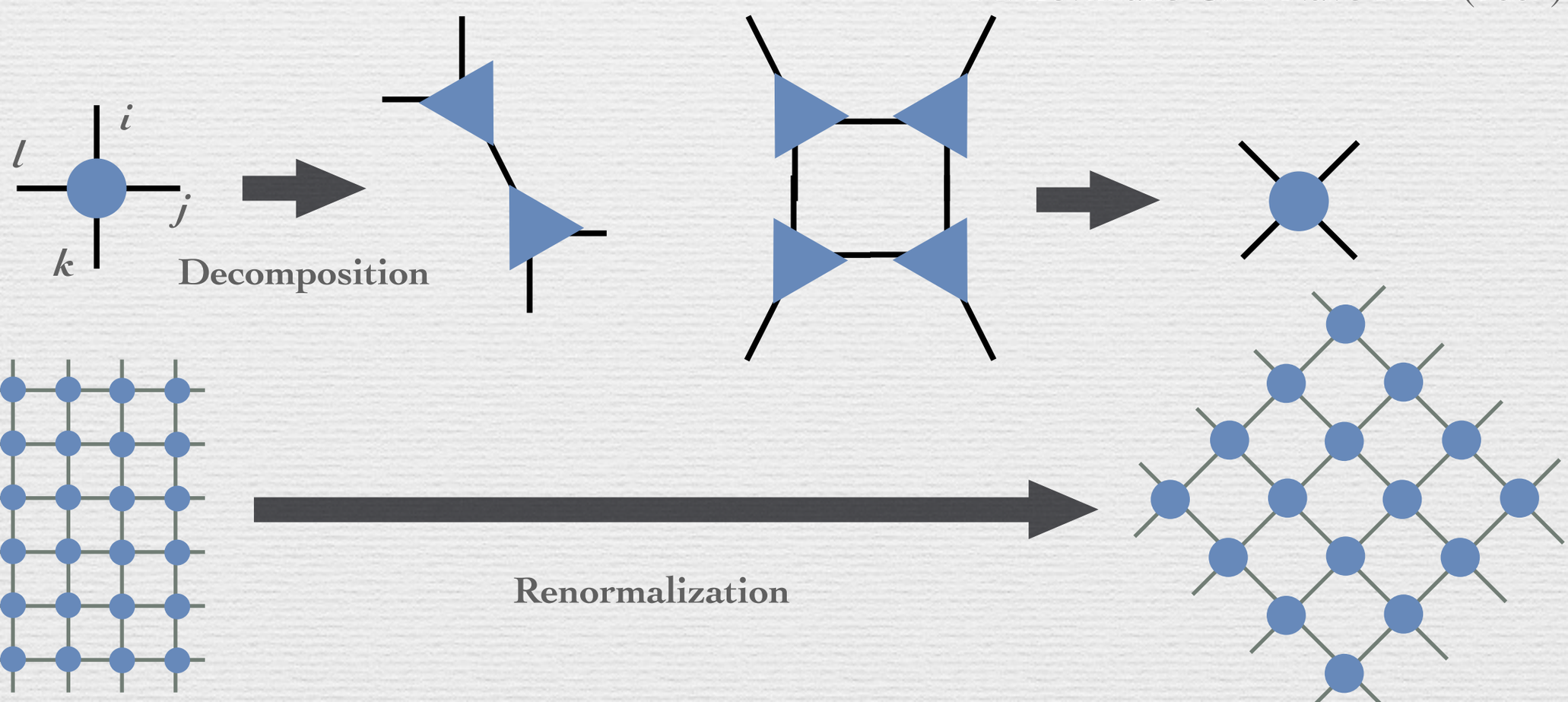


Contraction: exponentially large cost

Approximation: Using real space renormalization

Tensor Renormalization Groupe (TRG)

M. Levin and C. P. Nave PRL (2007)



Improved renormalization method

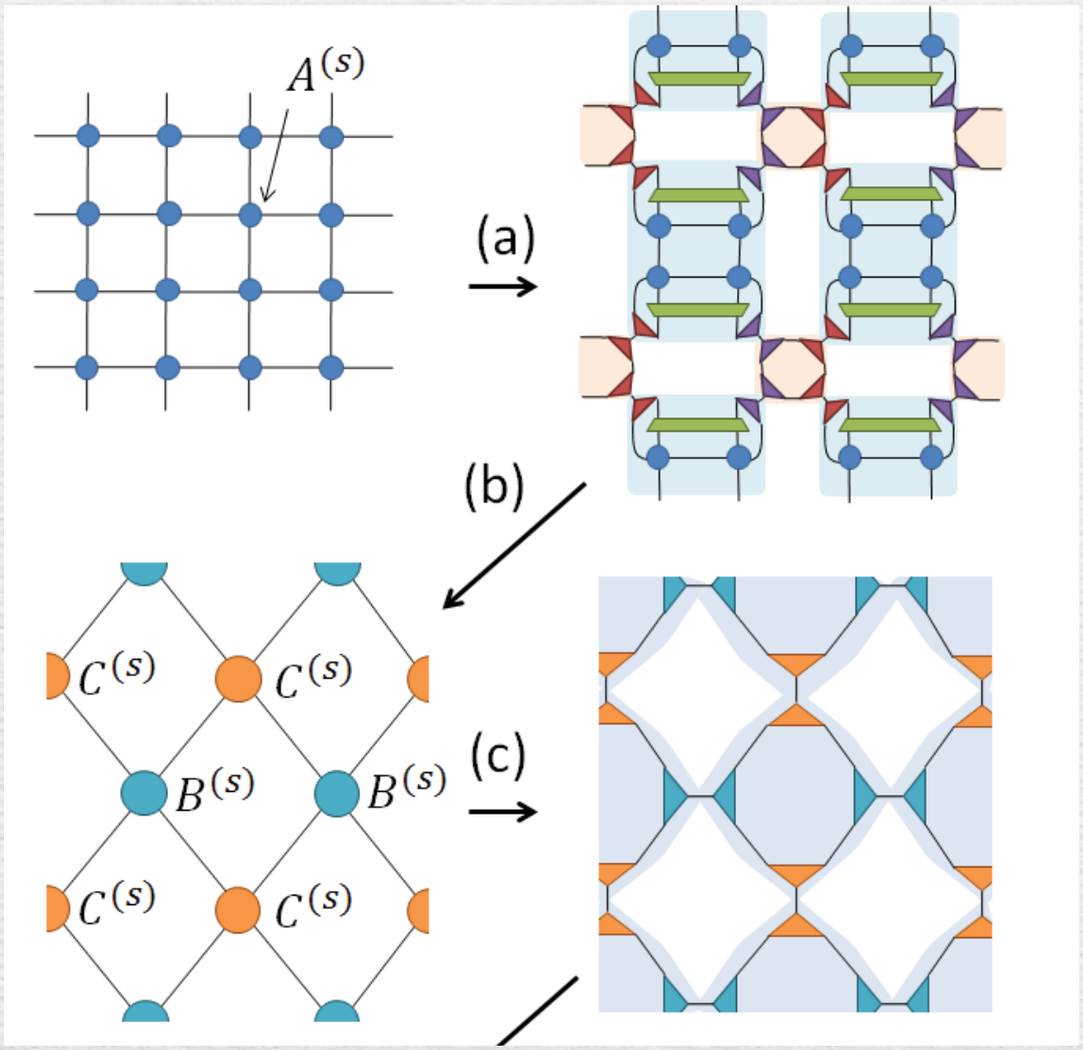
Problems in TRG: TRG does not represent

Especially,

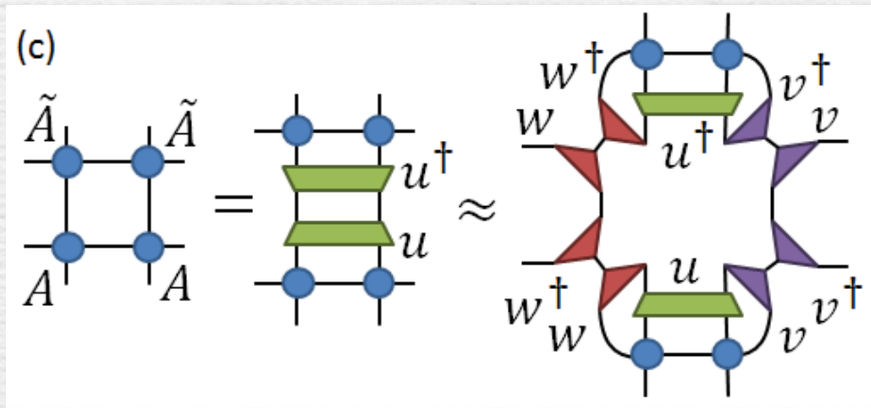
New renormalization methods: **Tensor Network Renormalization (TNR)**

G. Evenbly and G. Vidal, arXiv:1412.0732.

arXiv:1502.05385.



Point



Insertion of disentangler

efficient renormalization of short range correlation

TNR can produce renormalization flow to the physical fixed point!

Summary

- Tensor network methods are efficient tools to investigate condensed matter physics
  - As the ansatz of variational wave-functions
  - As a tool for efficient Real space renormalization