Transformative Research Areas A “Extreme Universe”
Second Annual Meeting @ Kobe Convention Center
2022/12/28 Seminar 7

Search for tree tensor networks matching the entanglement structure of quantum many-body states

Hiroshi Ueda
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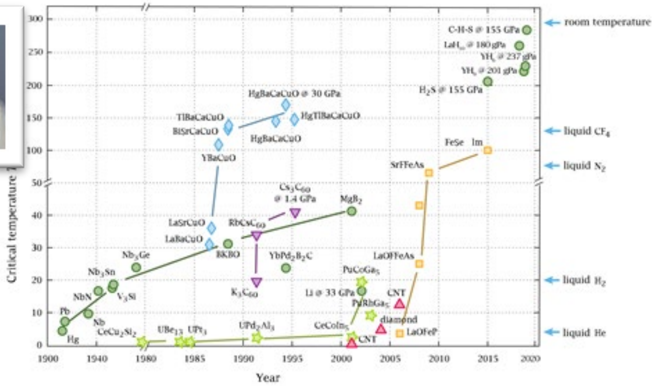
[1] K. Okunishi, **HU**, T. Nishino, arXiv:2210.11741.
[2] T. Hikihara, **HU**, K. Okunishi, K. Harada, T. Nishino, arXiv:2209.03196, to appear in Phys. Rev. Research.

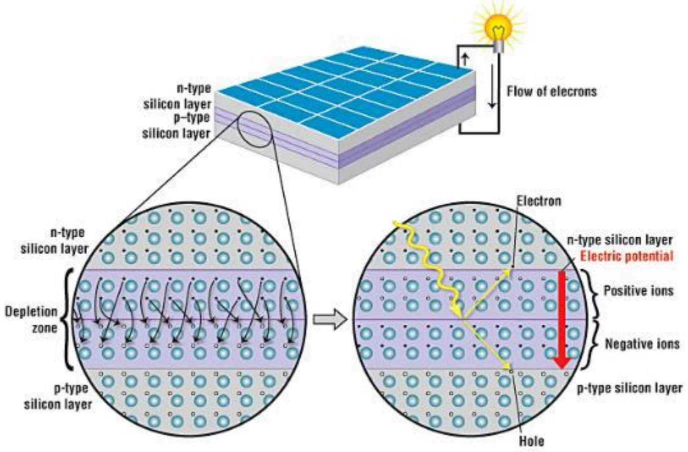
Quantum many-body physics in condensed matter physics

Various applications



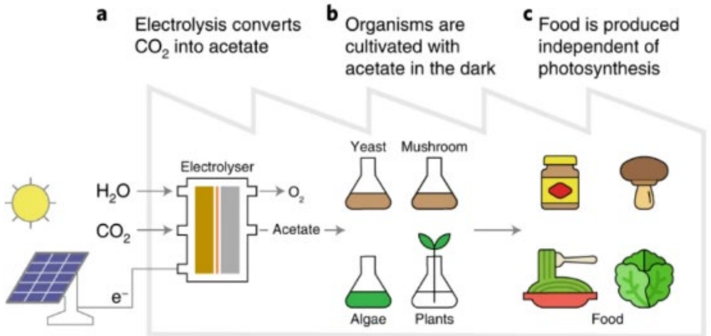
https://www.chemistryworld.com/news/room-temperature-superconductivity-finally-claimed-by-mystery-material/4012591.article

Superconductor



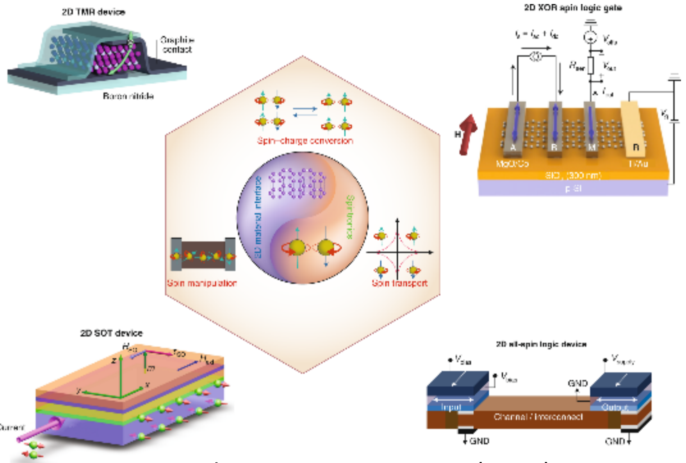
https://www.acs.org/education/resources/highschool/chemmatters/past-issues/archive-2013-2014/how-a-solar-cell-works.html

Solar cell



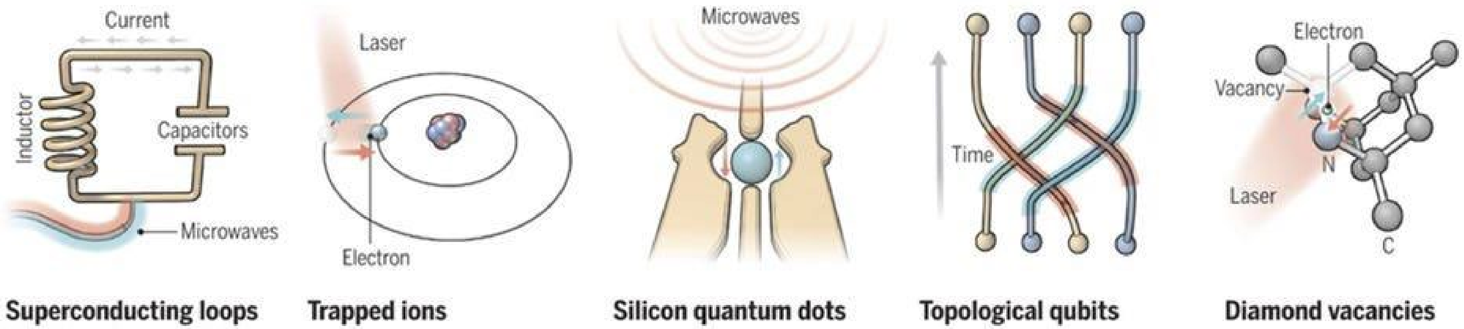
Nature Food **3**, 461–471 (2022).

Artificial photosynthesis



Nature Electronics **2**, 274–283 (2019).

Spintronics



https://www.forbes.com/sites/moorinsights/2019/09/16/quantum-computer-battle-royale-upstart-ions-versus-old-guard-superconductors/?sh=2fcebae32cb8

Quantum computer

Quantum Lattice Model

(Time independent) Schrödinger equation $H|\Psi\rangle = E_\Psi|\Psi\rangle$

- Quantum spin systems（XXZ model)

$$H = \sum_{\langle i,j\rangle}\left[J^{xy}\left(s_i^x s_j^x + s_i^y s_j^y\right) + J^z s_i^z s_j^z\right]$$

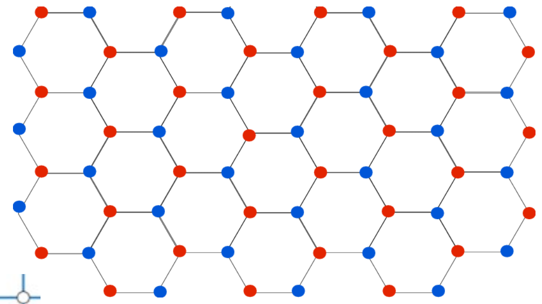
- Hubbard model (Fermion/Boson)

$$H = -t\sum_{\sigma\langle i,j\rangle} c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$

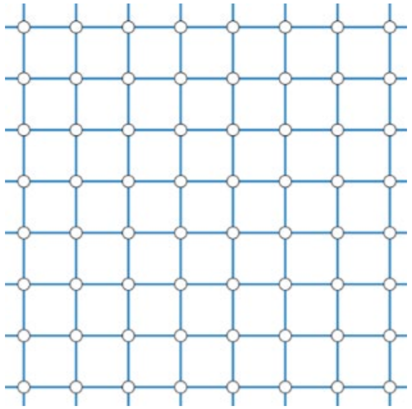
- Kitaev model under the magnetic field

$$H = -\sum_\gamma \sum_{\langle i,j\rangle_\gamma} J_\gamma s_i^\gamma s_j^\gamma - \boldsymbol{h}\cdot\sum_i \boldsymbol{s}_i$$

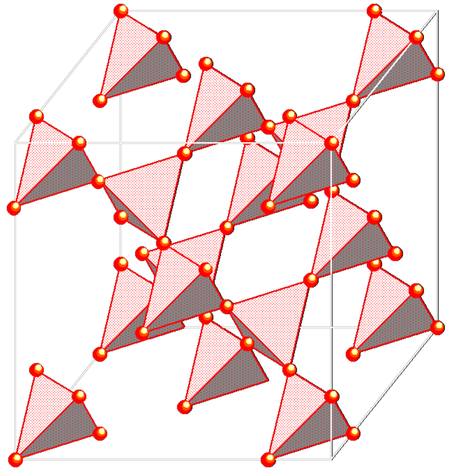
Etc…



Honeycomb Lattice

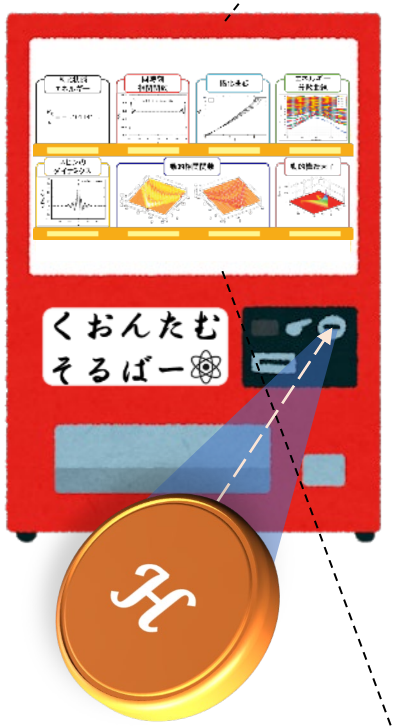


Square Lattice



Pyrochlore Lattice

Ultimate Goal of Quantum Solver (QS)

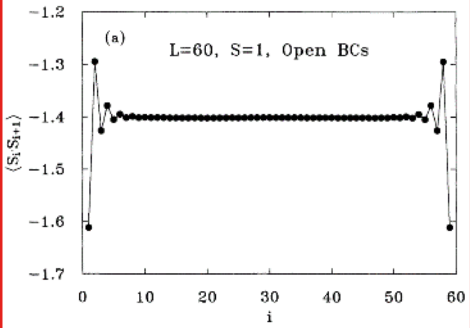


Hamiltonian of $S = 1$ Heisenberg spin chain

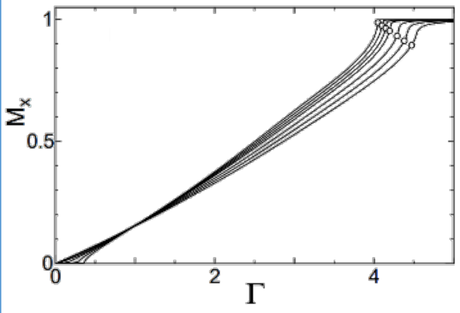
Ground-state energy

$$\frac{E_g}{N} = -1.401484\ldots$$

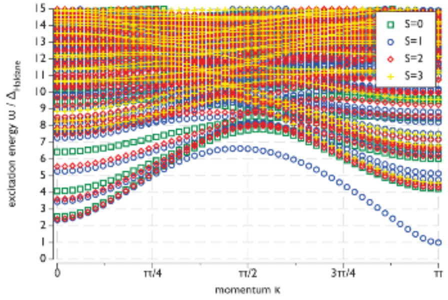
Correlation functions



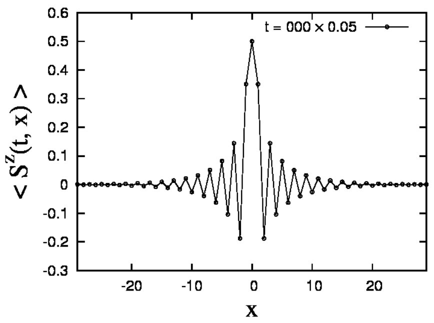
Magnetization curve



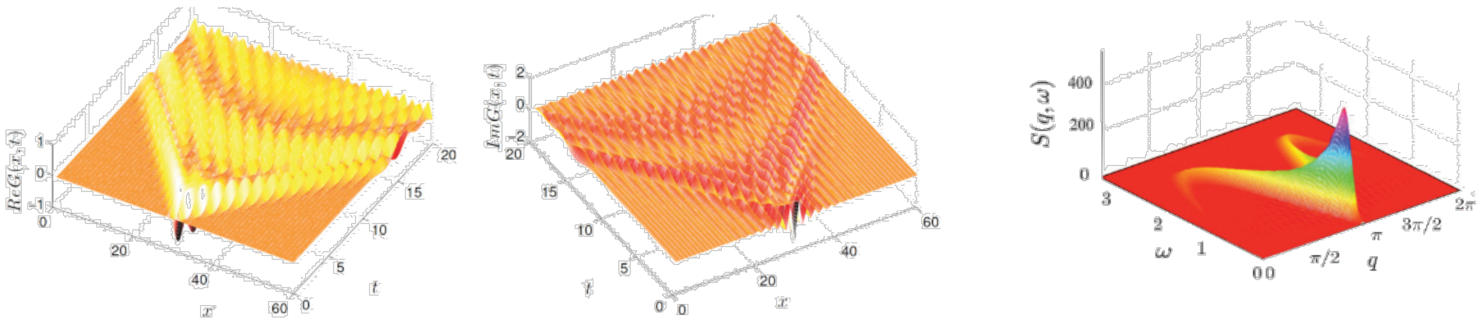
Energy dispersion



Real-time evolution



Dynamical correlation functions / structure factor



Refs. : PRB **48**, 3844 (1993); PRB **48**, 10345 (1993); PRB **64**, 224422 (2001); PRB **85**, 100408(R) (2012); PRB **86**, 245107 (2012).

Limitations of Exact solver

Fugaku (RIKEN)

Numerical cost: $\mathcal{O}(\exp(N))$

- Numerical diagonalization

  ~50 spin-1/2 systems @ Sekirei (ISSP)

  A. Wietek and A. M. Läuchli, Phys. Rev. E **98**, 033309 (2018).

  30 spin-1 systems @ Fugaku (RIKEN)

  H. Nakano, et al., J. Phys. Soc. of Jpn. **91**, 074701 (2022).

- State vector simulation

  48-qubit simulation @ K (RIKEN)

  H De Raedt, Comput. Phys. Commun. **237**, 47 (2019).

  Intel Quantum simulator

  G. G. Guerreschi, et al.: Quantum Sci. Technol. **5**, 034007 (2020).

  mpiQulacs for Fugaku

  S. Imamura, et al.: arXiv:2203.16044.

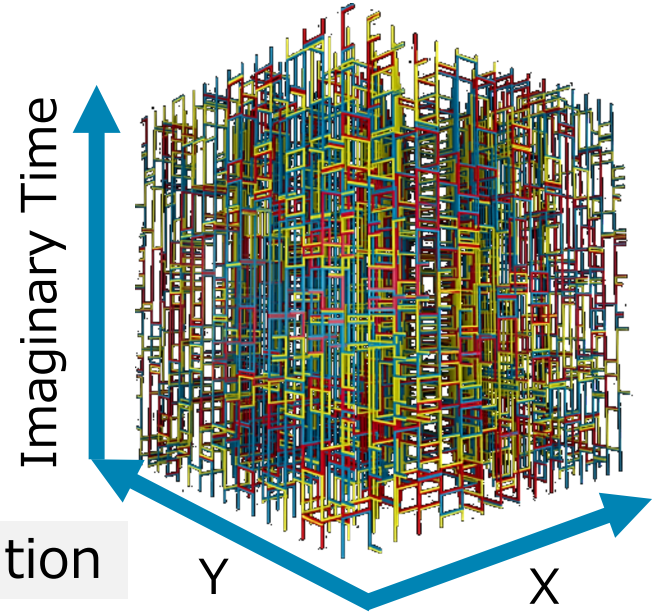
Typical numerical approach

- Quantum Monte Carlo (QMC)

Quantum
D-dim.

↓

Classical
$(D+1)$-dim.



Sampling simulation

https://aics.riken.jp/aicssite/wp-content/uploads/2016/01/3harada.pdf

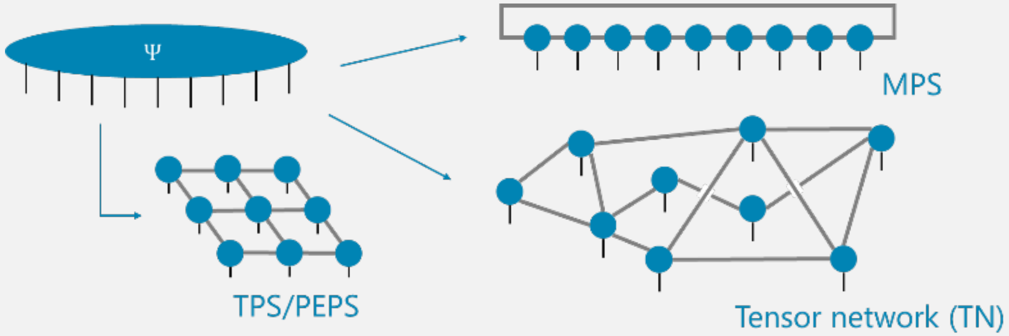
Solving problem “exactly” within stat. error

Sign problem: Frustrated system
Fermion system

- Variational method

Design of wave-function ansatz

- **Tensor network (TN)**



- Variational Monte Carlo (VMC)

$$|\psi\rangle = \mathcal{P}\mathcal{L}|\phi_{\mathrm{Pf}}\rangle$$

- $|\phi_{\mathrm{Pf}}\rangle$: Pair-product part of the WF
- $\mathcal{L}$: Quantum-number projectors
- $\mathcal{P}$: Correlations (Gutzwiller, Jastrow, $\cdots$)

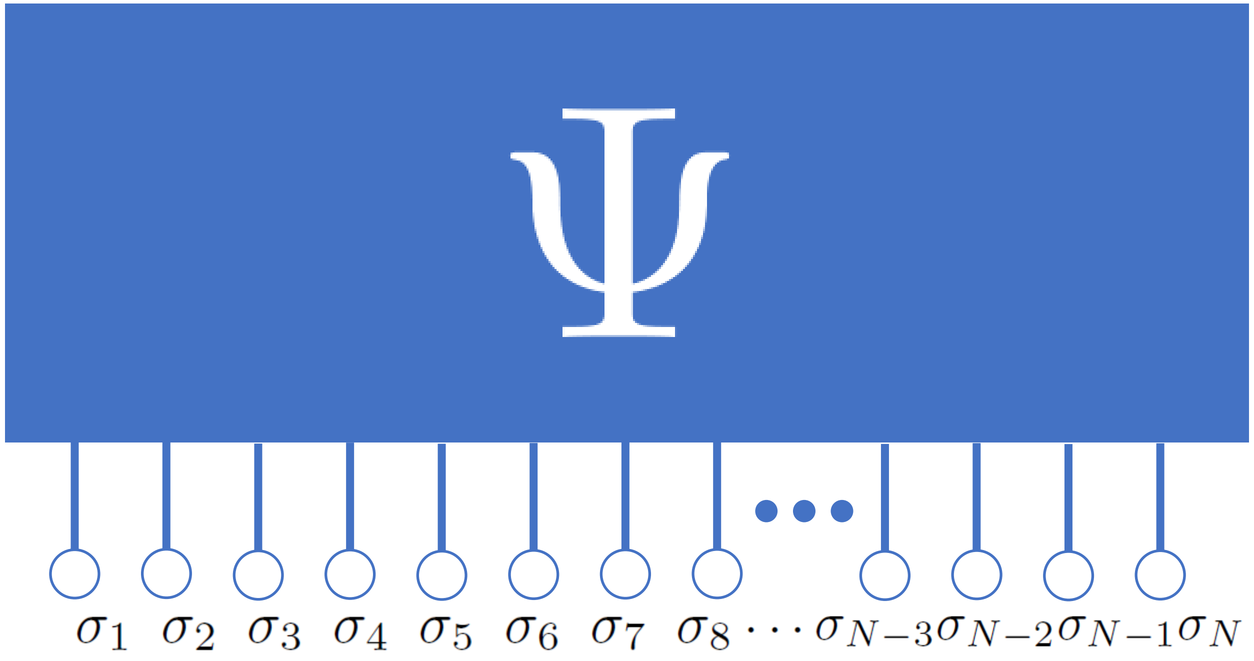
mVMC

T. Misawa et al., Comput. Phys. Commun. **235**, 447 (2019).

Design guidelines for TN

A quantum state on an N-site system: $|\Psi\rangle = \sum_{\sigma_1 \cdots \sigma_N} \Psi_{\sigma_1 \cdots \sigma_N} |\sigma_1 \cdots \sigma_N\rangle \quad \sigma_i = 1, \cdots, d$

$\langle \sigma_1 \cdots \sigma_N | \Psi \rangle =$



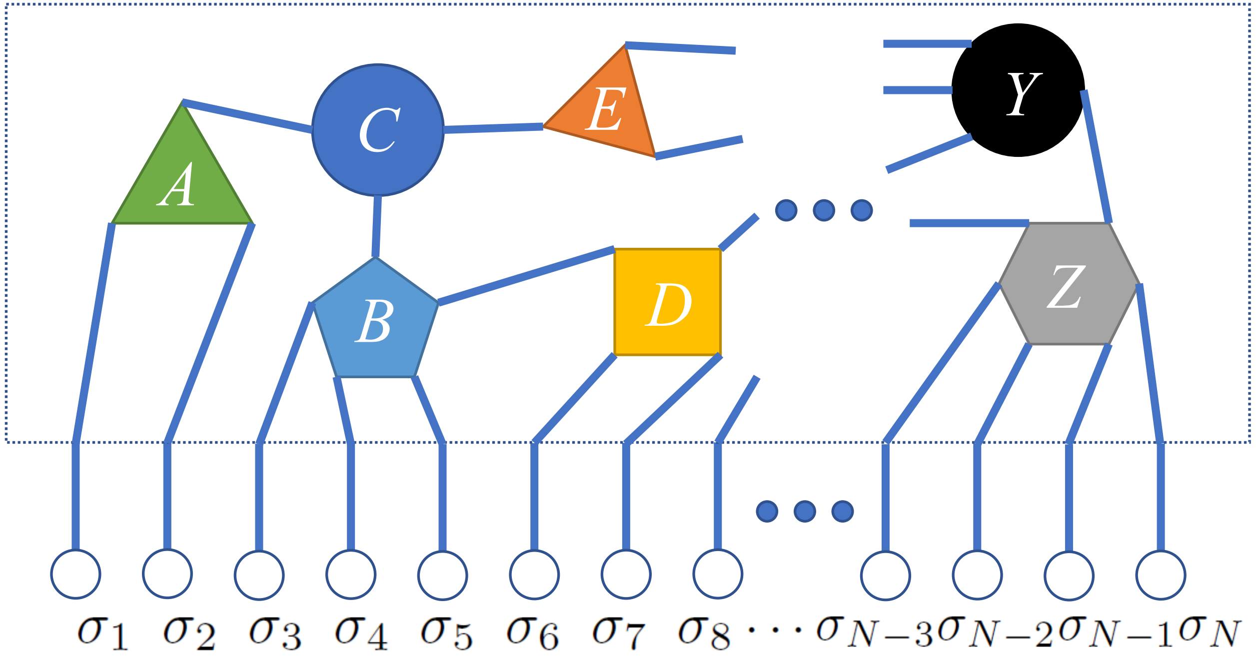
Q. How can we store a d^N-dim. vector approximately in phys. mem. space < d^N ?

Design guidelines for TN

A quantum state on an N-site system: $|\Psi\rangle = \sum_{\sigma_1\cdots\sigma_N} \Psi_{\sigma_1\cdots\sigma_N}|\sigma_1\cdots\sigma_N\rangle$ $\quad \sigma_i = 1,\cdots,d$

$$\sum_{a_1 b_1 b_2 \cdots x_2 y_1} A_{\sigma_1\sigma_2 a_1} B_{\sigma_3\sigma_4\sigma_5 b_1 b_2} C_{a_1 b_1 c_1} D_{b_2\sigma_6\sigma_7 d_1} E_{c_1 e_1 e_2} \cdots Y_{v_1 w_1 x_1 y_1} Z_{x_2 y_1 \sigma_{N-3}\sigma_{N-2}\sigma_{N-1}\sigma_N}$$

$$\langle\sigma_1\cdots\sigma_N|\Psi\rangle =$$



A. Introducing tensor decompositions where each tensor can store in the computer.

Design guidelines for TN

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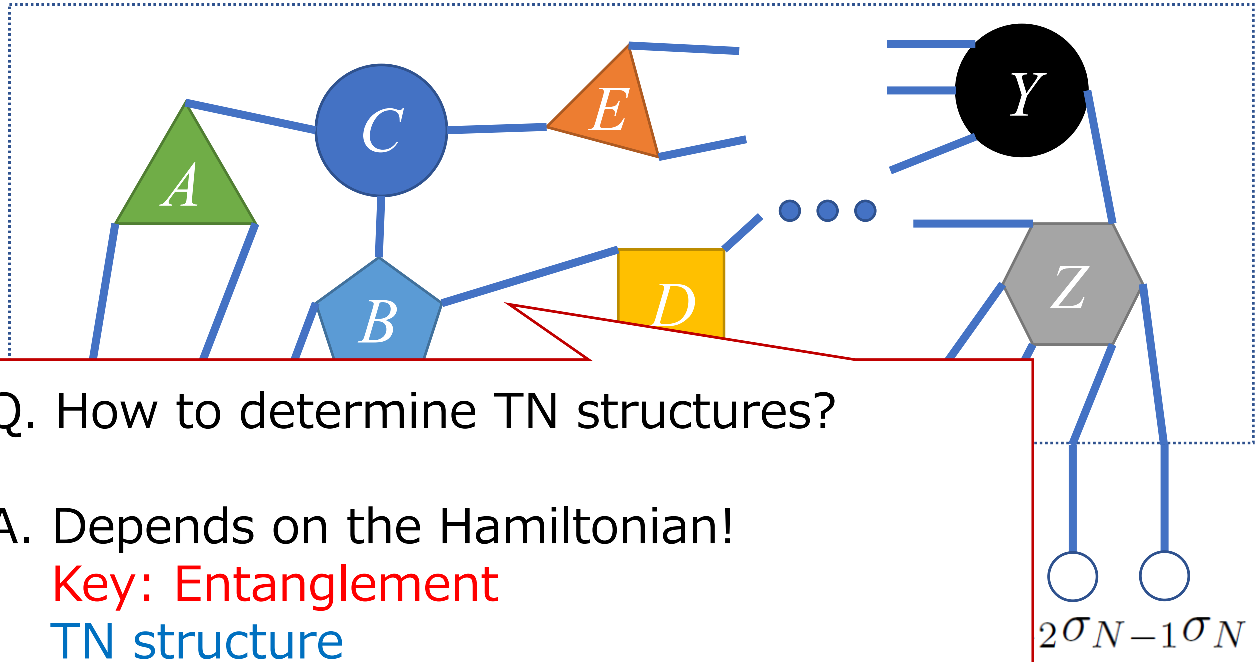

Q. How to determine TN structures?

A. Depends on the Hamiltonian!
Key: Entanglement
TN structure
⇔ Limitation of Ent. in variational states.

A. Introducing tensor decompositions where each tensor can store in the computer.

Design guidelines for TN

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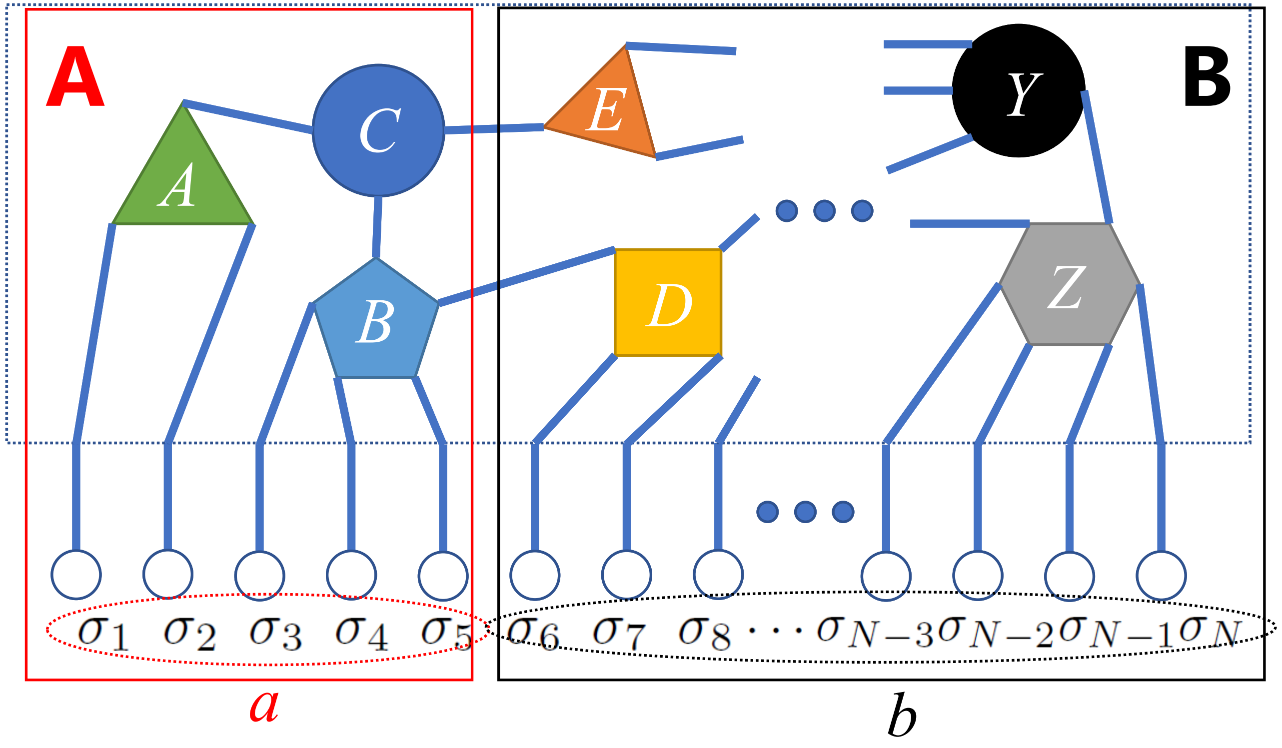
$$\sum_{a_1 b_1 b_2 \cdots x_2 y_1} A_{\sigma_1 \sigma_2 a_1} B_{\sigma_3 \sigma_4 \sigma_5 b_1 b_2} C_{a_1 b_1 c_1} D_{b_2 \sigma_6 \sigma_7 d_1} E_{c_1 e_1 e_2} \cdots Y_{v_1 w_1 x_1 y_1} Z_{x_2 y_1 \sigma_{N-3} \sigma_{N-2} \sigma_{N-1} \sigma_N}$$

$\langle \sigma_1 \cdots \sigma_N | \Psi \rangle =$



Design guidelines for TN

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$$\sum_{a_1 b_1 b_2 \cdots x_2 y_1} A_{\sigma_1\sigma_2 a_1} B_{\sigma_3\sigma_4\sigma_5 b_1 b_2} C_{a_1 b_1 c_1} D_{b_2\sigma_6\sigma_7 d_1} E_{c_1 e_1 e_2} \cdots Y_{v_1 w_1 x_1 y_1} Z_{x_2 y_1 \sigma_{N-3}\sigma_{N-2}\sigma_{N-1}\sigma_N}$$

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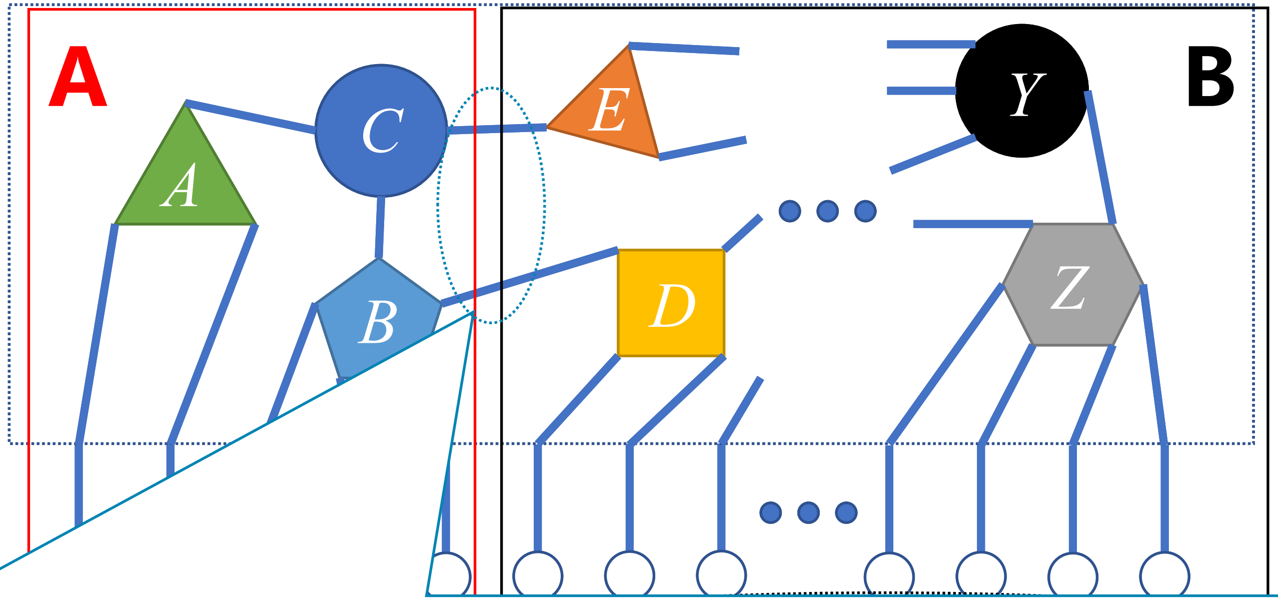

Maximum Ent. Ent. = log(Schmidt rank of the matrix Ψ_{ab})

Sufficiently large area A and B ➔ log(Direct prod. dim. of tensor leg across A and B)

Example of this slide: max EE = log[max($b_2 c_1$)]

Design guidelines for TN

A quantum state on an N-site system: $|\Psi\rangle = \sum_{\sigma_1\cdots\sigma_N} \Psi_{\sigma_1\cdots\sigma_N} |\sigma_1\cdots\sigma_N\rangle \quad \sigma_i = 1,\cdots,d$

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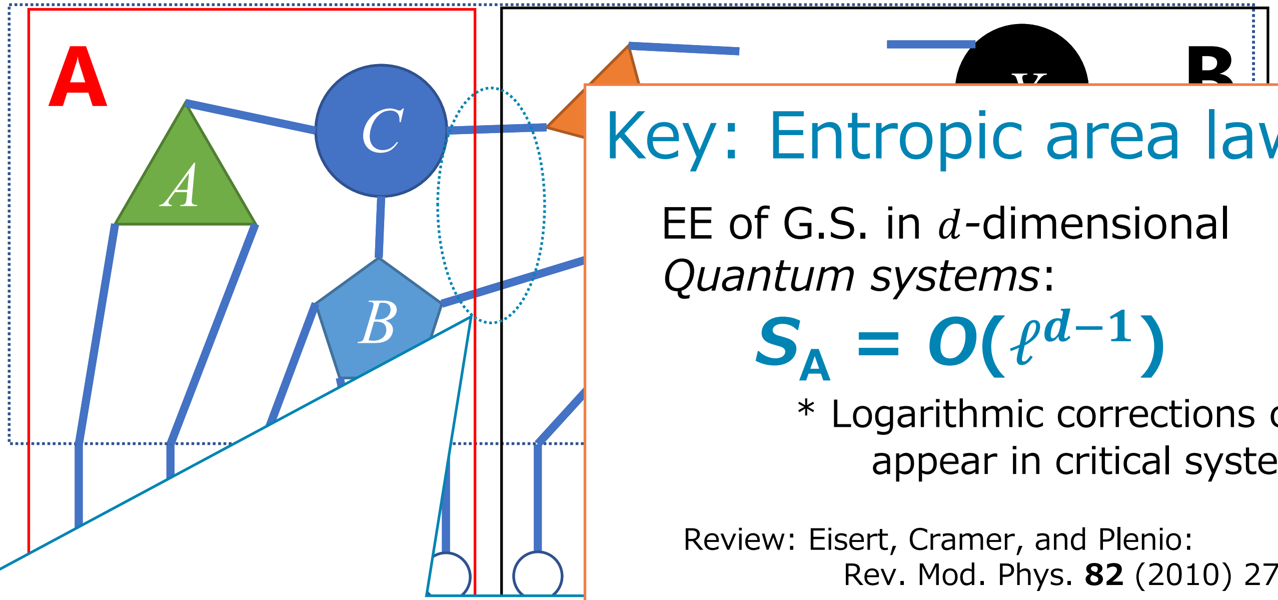
$$\langle\sigma_1\cdots\sigma_N|\Psi\rangle =$$



Key: Entropic area law

EE of G.S. in d-dimensional *Quantum systems*:

$$S_A = O(\ell^{d-1})$$

* Logarithmic corrections can appear in critical systems

Review: Eisert, Cramer, and Plenio: Rev. Mod. Phys. **82** (2010) 277.

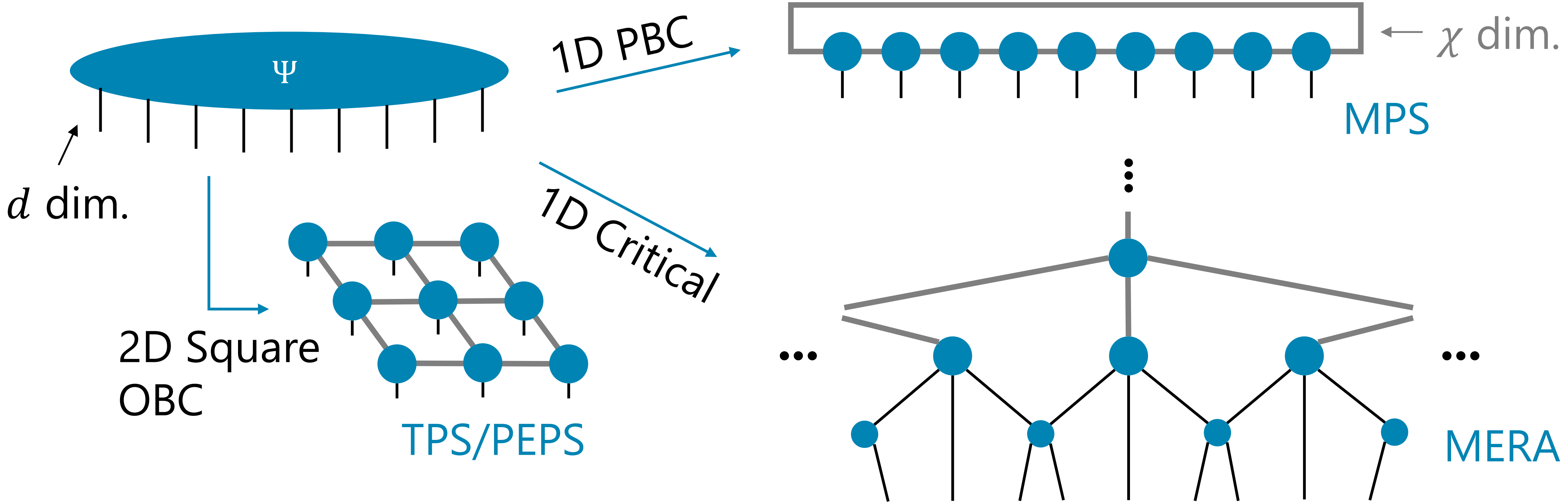
Maximum Ent. Ent. = log(Schmidt rank of the matrix Ψ_{ab})

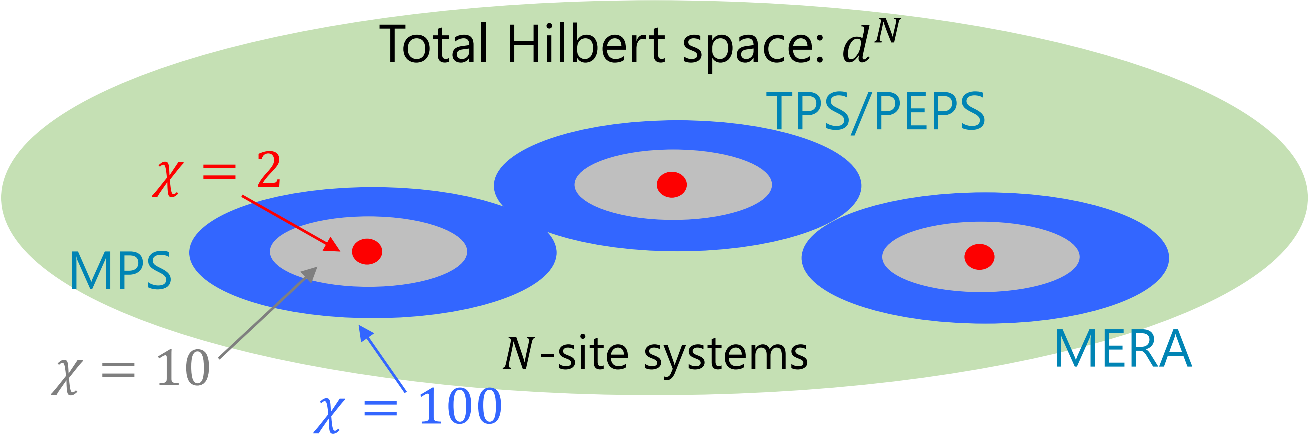
Sufficiently large area A and B ➔ log(Direct prod. dim. of tensor leg across A and B)

Example of this slide: max EE = log[max($b_2 c_1$)]

Established TNs

Review: R. Orus, Ann.Phys. **349**, 117 (2014).



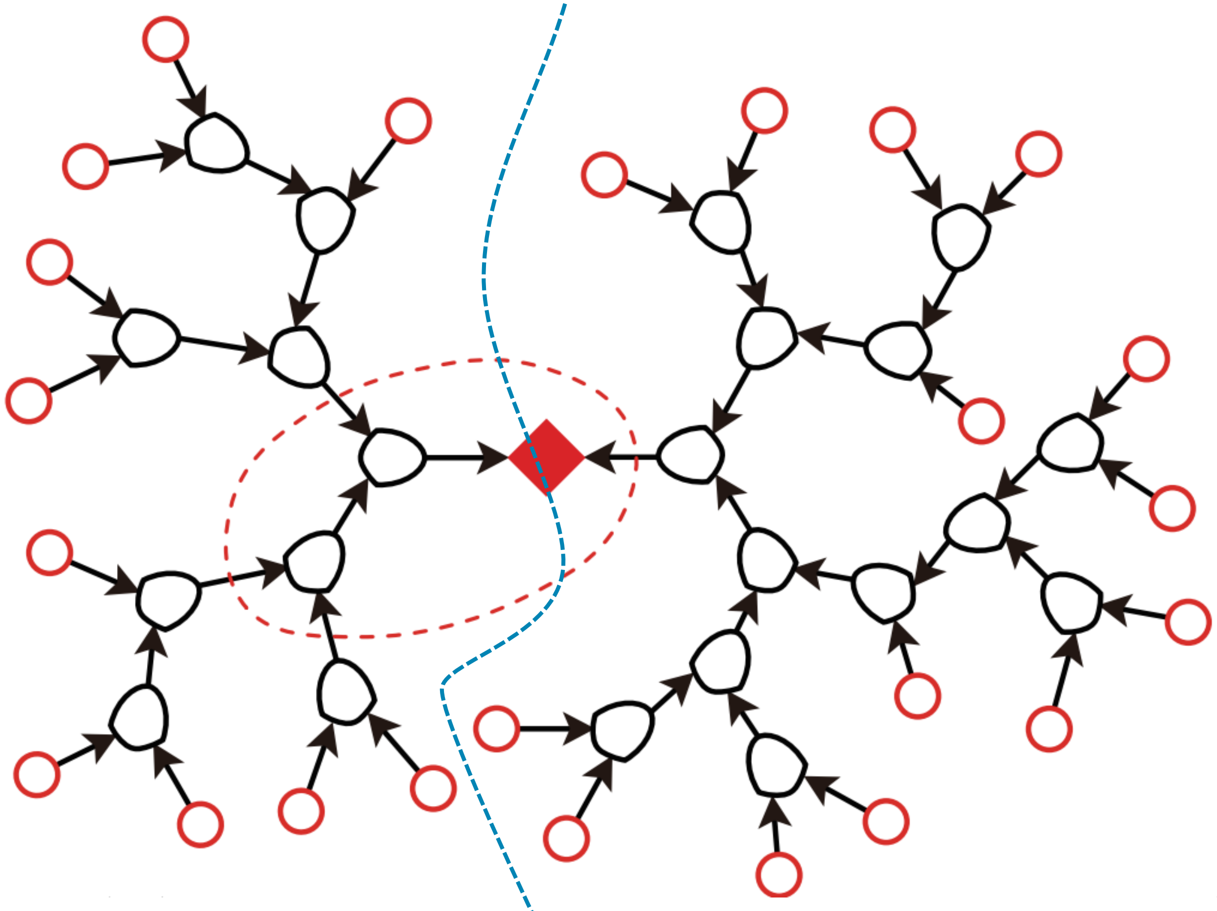


Good TN ⟺ Good approximation of target quantum states with small χ

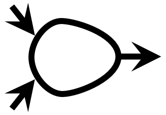
How can we design TNs in inhomogeneous systems?

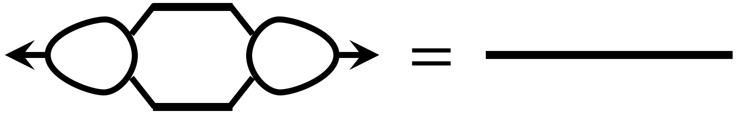
A definition of "Optimal" TN

Today's target: Tree TN (TTN)

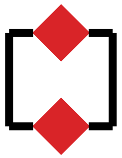


○ : Physical d degrees of freedom


: Isometry



: Schmidt coefficient (≥ 0)



Schmidt decomposition

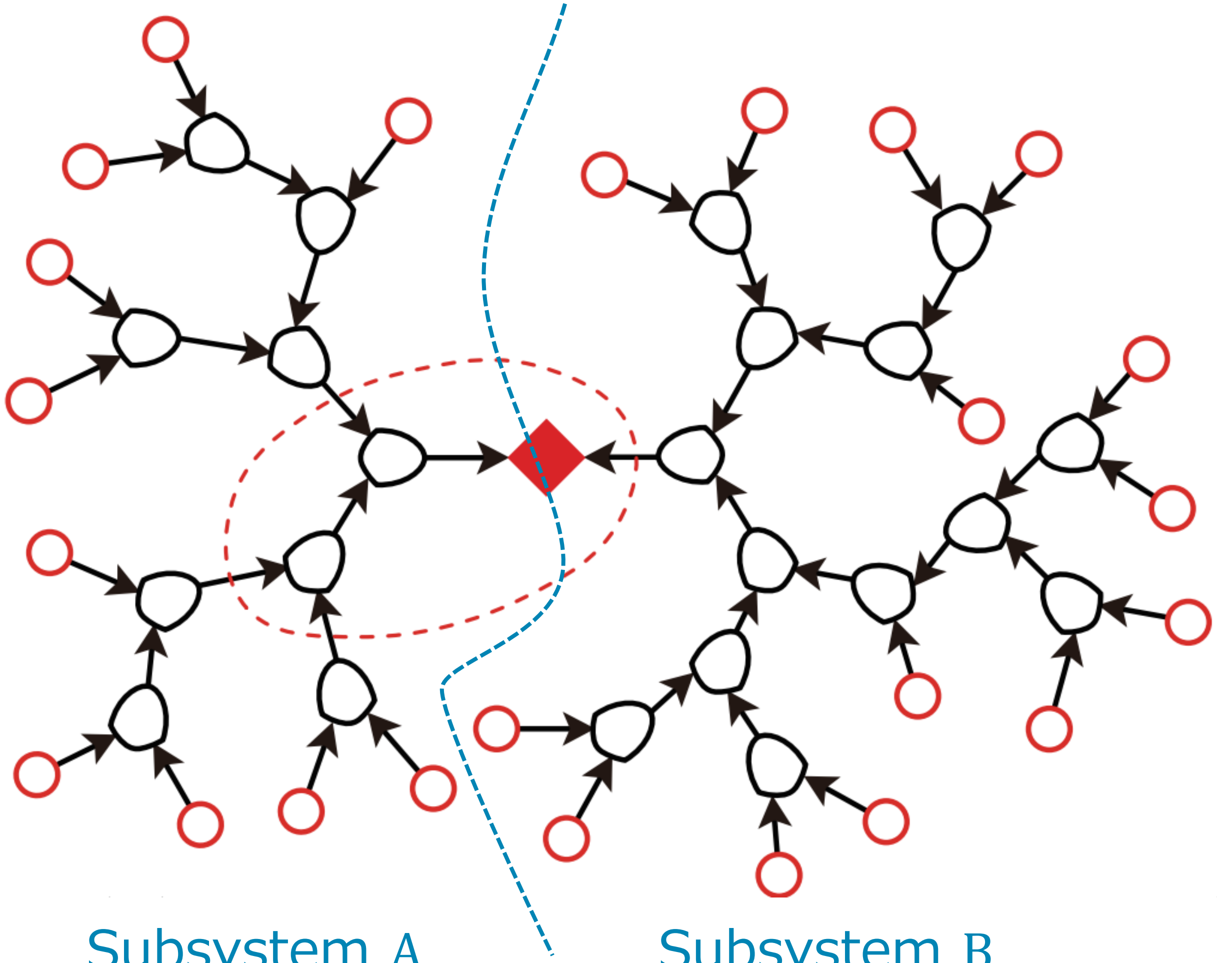
$$|\Psi\rangle = \sum_{ij} \Psi_{ij} |i\rangle_\mathrm{A} |j\rangle_\mathrm{B}$$

$$\overset{\text{SVD}}{=} \sum_{ij\alpha} U_{i\alpha} \Lambda_\alpha V^*_{j\alpha} |i\rangle_\mathrm{A} |j\rangle_\mathrm{B}$$

$$= \sum_\alpha \Lambda_\alpha |\alpha\rangle_\mathrm{A} |\alpha\rangle_\mathrm{B}$$

A definition of "Optimal" TN

Today's target: Tree TN (TTN)



Entanglement entropy (EE)

$$S_{\mathrm{EE}}(A) = -\sum_\alpha \Lambda_\alpha^2 \log \Lambda_\alpha^2$$

Min. # of $\chi \sim e^{S_{\mathrm{EE}}}$

Total # of TTN patterns: $(2N-5)\,!!$

Ex) $2^{16} = 65536$
$27\,!! = 213458046676875$

Too large!!

"Optimal" decomposition of 1st step

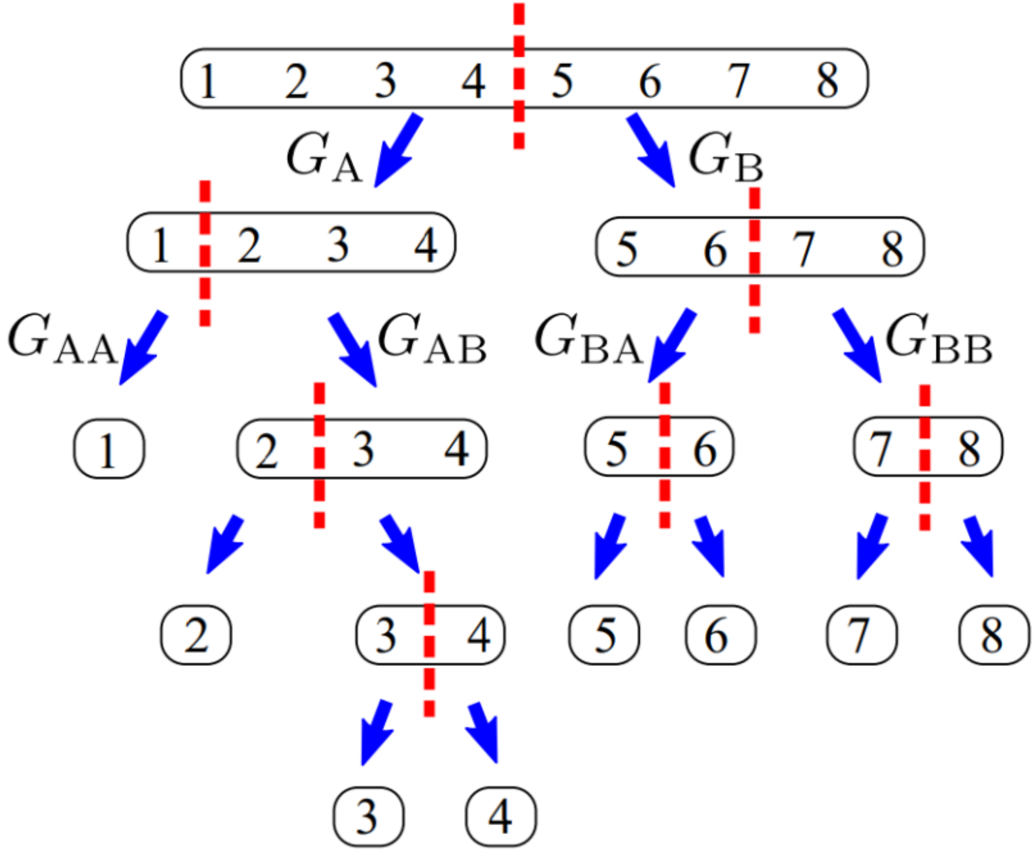
$$\mathrm{A} \in \mathrm{argmin}_{\mathrm{A}'}\, S_{\mathrm{EE}}(\mathrm{A}')$$

Total # of bipartite patterns: $O(2^N)$

A definition of “Optimal” TTN

“Optimal” TTN: Recursive “optimal” decomposition

K. Okunishi, HU, T. Nishino, arXiv:2210.11741.



“Optimal” decomposition for $n+1$ generation

$$\mathrm{Q}_n = \overbrace{\mathrm{AB}\cdots\mathrm{A}}^{n}$$

$$f_{\mathtt{MMX}} \equiv \mathtt{max}\big(S(G_{\mathrm{Q}_n\mathrm{A}}), S(G_{\mathrm{Q}_n\mathrm{B}})\big)$$

MMX: minimization of the maximum loss

Const. in TTN

$$f_{\mathtt{MMI}} \equiv S(G_{\mathrm{Q}_n\mathrm{A}}) + S(G_{\mathrm{Q}_n\mathrm{B}}) - \boxed{S(G_{\mathrm{Q}_n\mathrm{A}} \cup G_{\mathrm{Q}_n\mathrm{B}})}$$

MMI: minimization of mutual information

$$\mathrm{Q}_n\mathrm{A} \in \mathrm{argmin}_{\mathrm{A}'}\, f_{\mathrm{MMX/I}}(\mathrm{Q}_n\mathrm{A}')$$

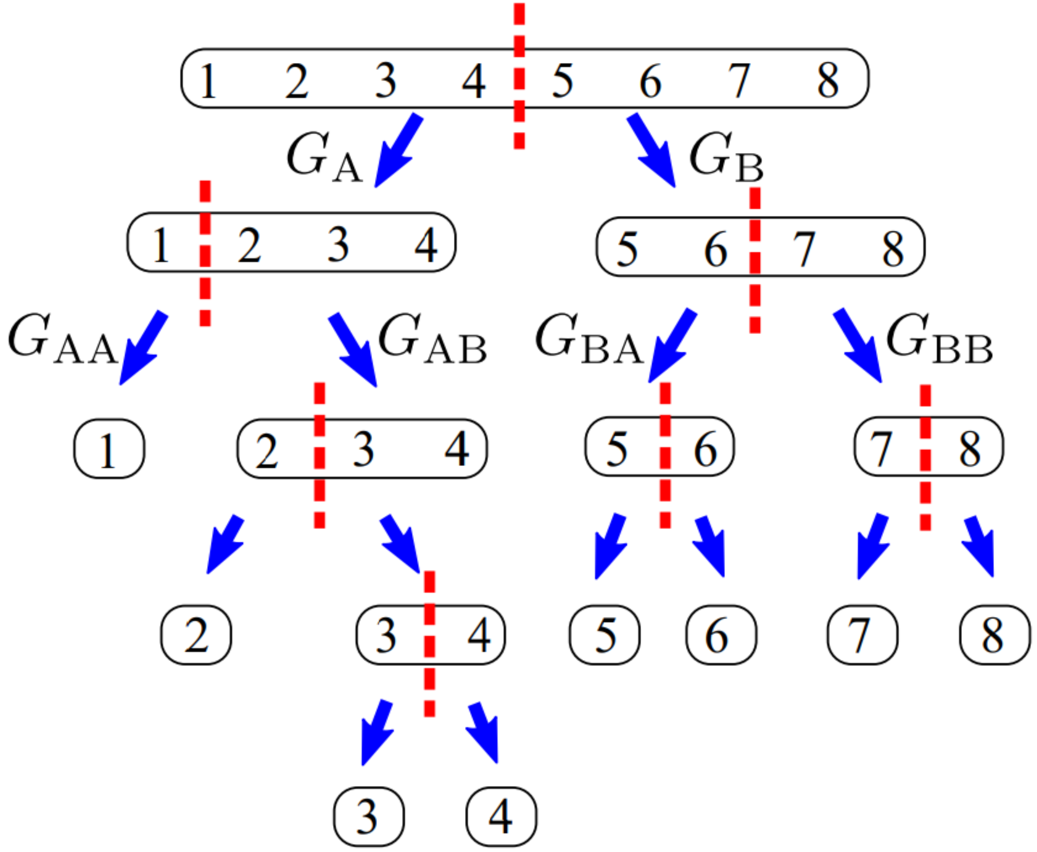
Total # of bipartite patterns: $O(2^{N_{Q_n}})$

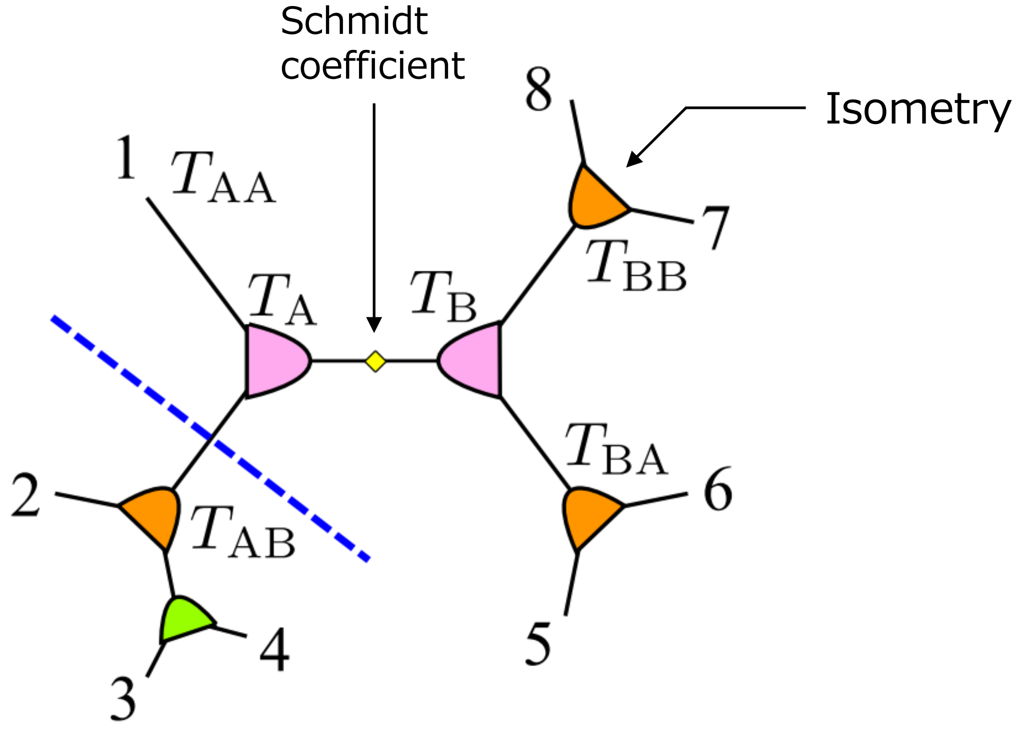
Top-down approach（N is up to 16.)

A definition of “Optimal” TTN

“Optimal” TTN: Recursive “optimal” decomposition

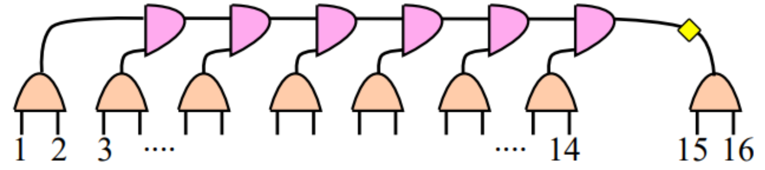
K. Okunishi, HU, T. Nishino, arXiv:2210.11741.





Top-down & deterministic approach (*N* is up to 16.)

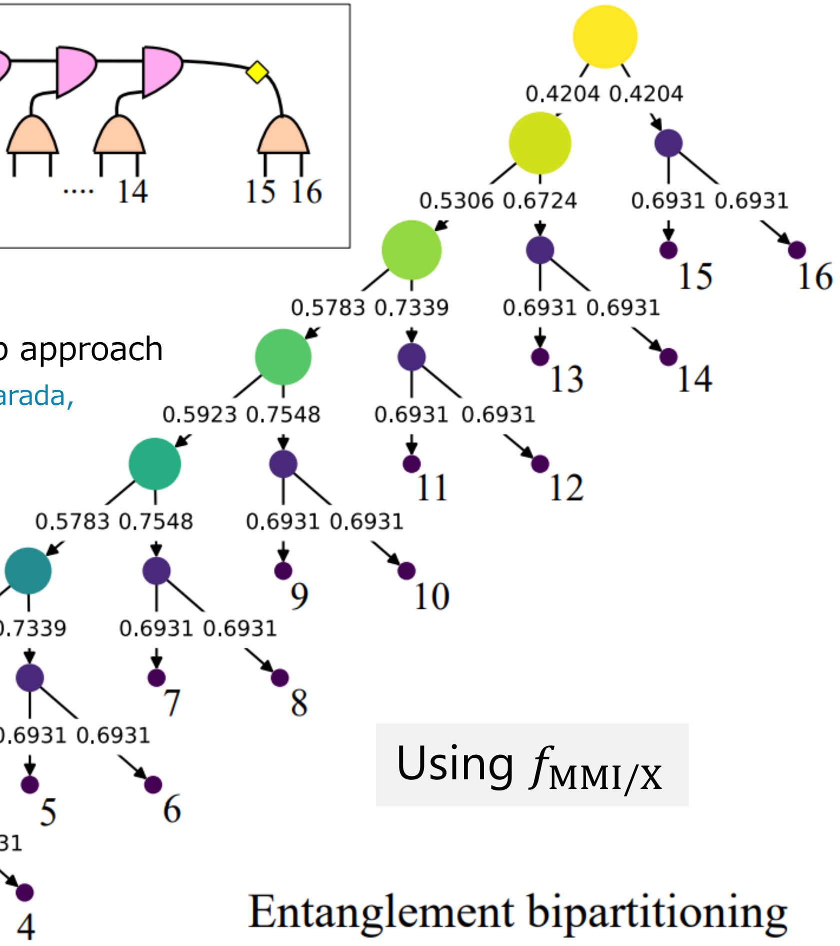
$S = 1/2$ antiferromagnetic Heisenberg (AFHB) chain w/ OBC



dimer MPS

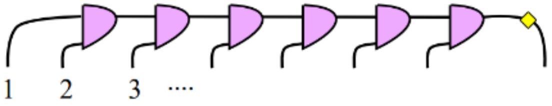
Consistent w/ our bottom-up approach

T. Hikihara, HU, K. Okunishi, K. Harada, T. Nishino, arXiv:2209.03196.

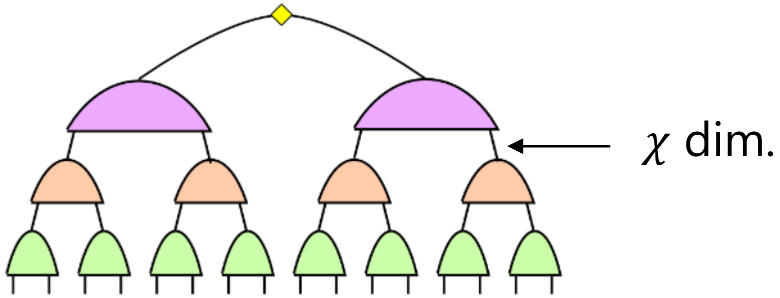


Using $f_{\mathrm{MMI/X}}$

Entanglement bipartitioning



Uniform MPS [Typical TN]



Perfect-binary TTN (1D) [Typical TN]

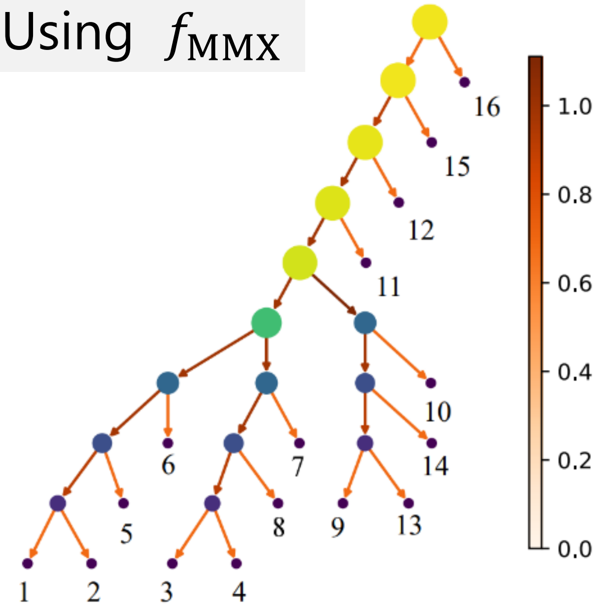
	E	ΔE
Exact	-6.911737146···	—
dimer MPS	-6.911614696	0.00122
uniform MPS	-6.911558558	0.00179
pbTTN	-6.891960394	0.01977

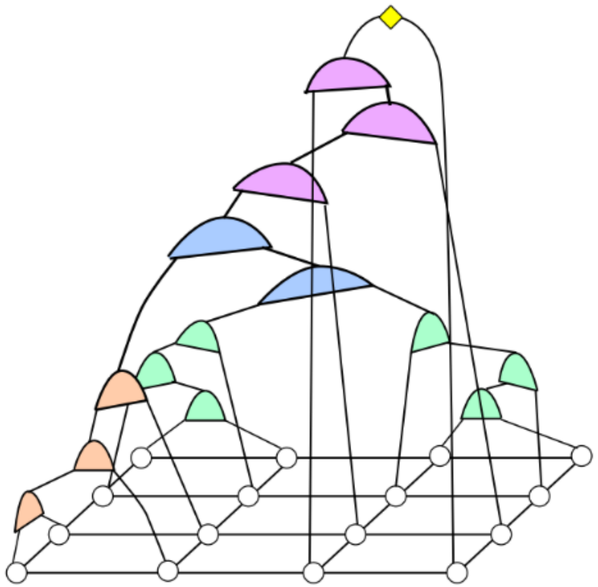
$\chi = 8$

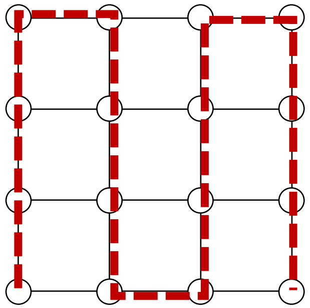
Results and Variational Optimization

$S = 1/2$ AFHB model on the square lattice w/ OBC

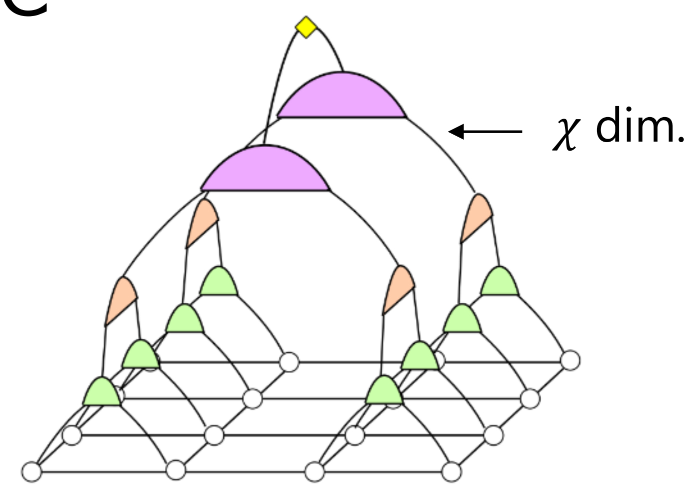
Using f_{MMX}







Snake MPS
[Typical TN]



Perfect-binary TTN (2D)
[Typical TN]

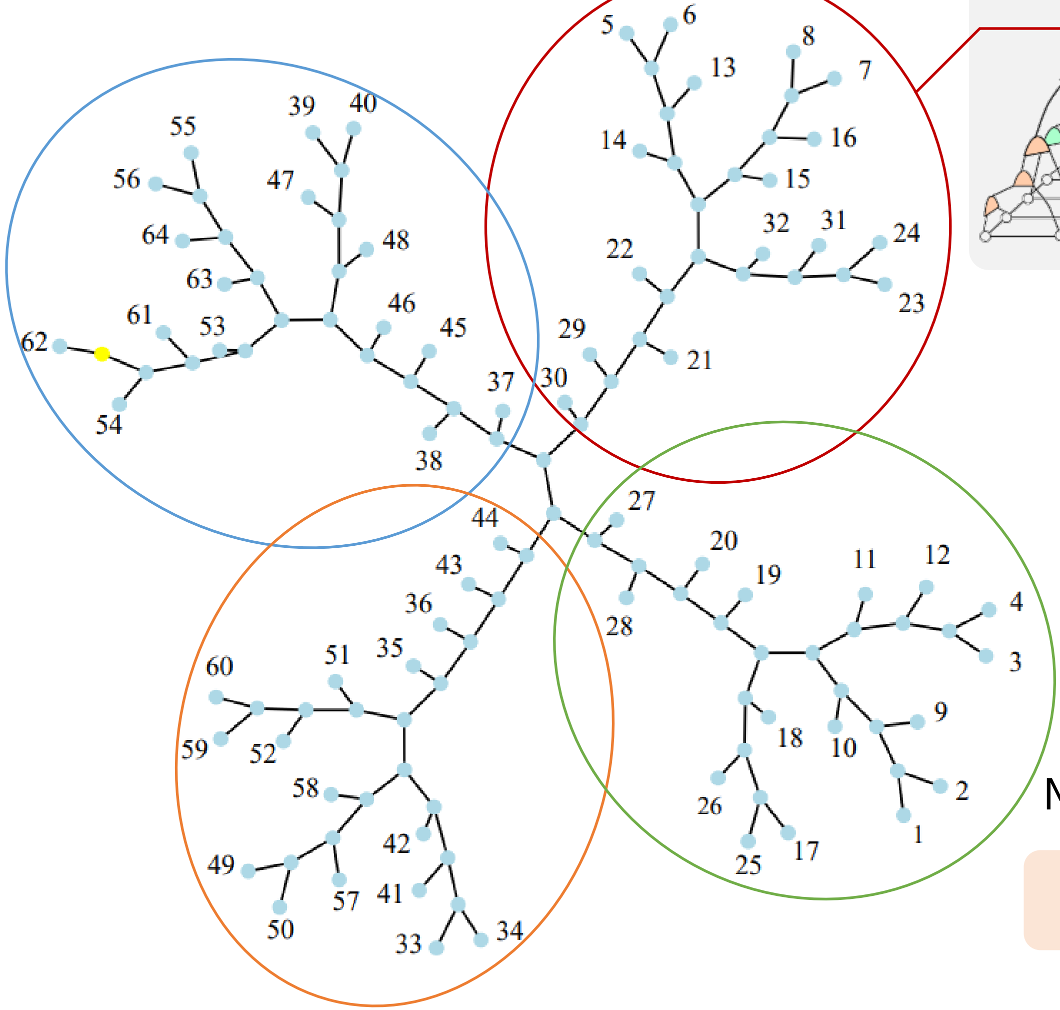
	E	ΔE
Exact	-9.189207···	—
MMX	-9.052564	0.136643
MMI	-8.980623	0.208584
pbTTN	-9.052564	0.136643
snake MPS	-8.760211	0.428996

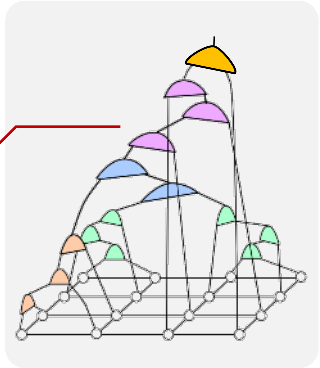
$\chi = 8$

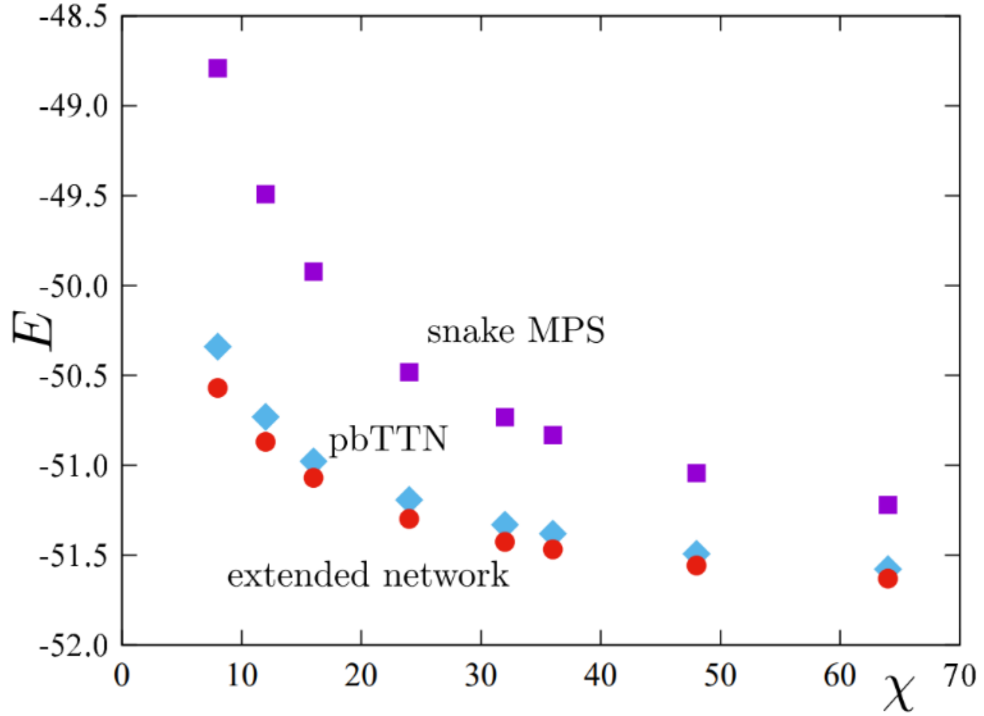
Good guiding principle

minimizing the maximum loss of the EE due to the truncation

64-site systems







E(Snake MPS w/ $\chi = 64$) $\simeq$ E(ext. TTN w/ $\chi = 20$)

Mem. Cost (Single-site): $d\chi^2 = 8192 \quad \simeq \quad \chi^3 = 8000$

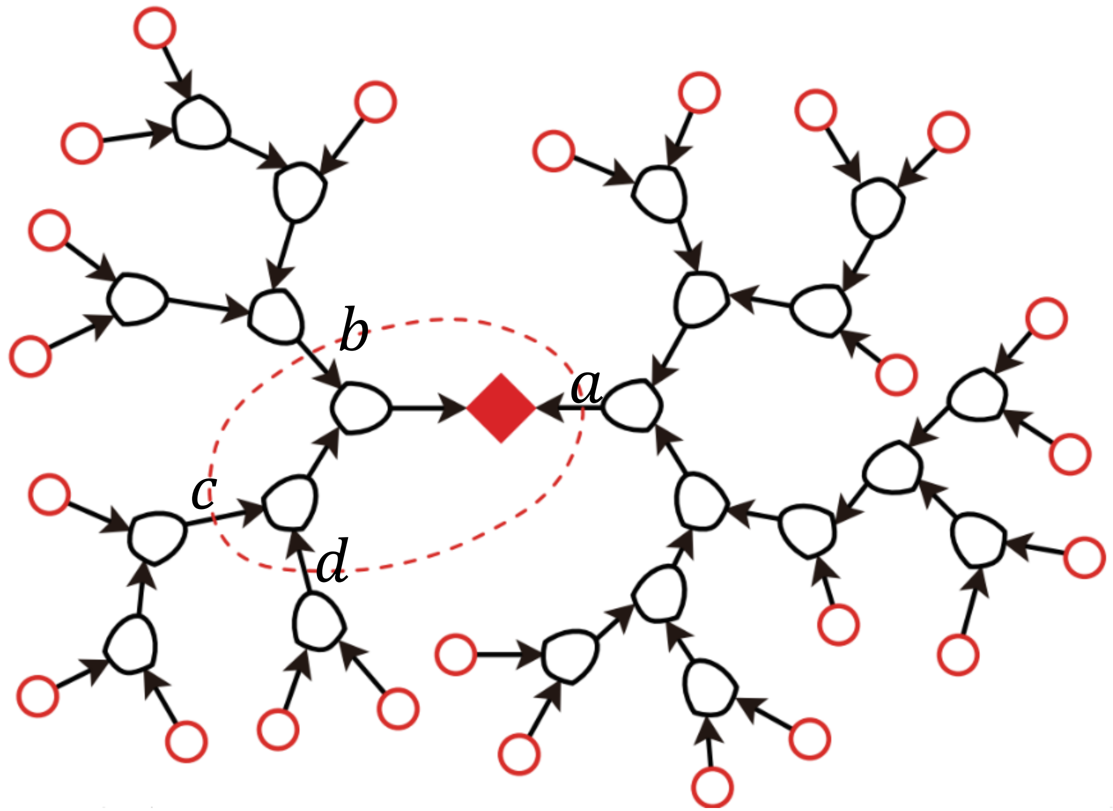
Calc. Cost (Single-site): $d\chi^3 \sim 5.2 \times 10^5 \quad > \quad \chi^4 \sim 1.6 \times 10^5$

Automatic optimization of TN structure

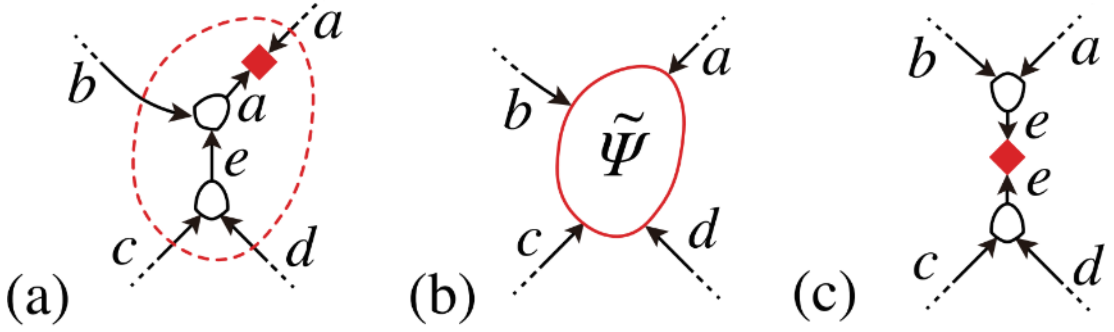
T. Hikihara, HU, K. Okunishi, K. Harada, T. Nishino, arXiv:2209.03196, to appear in Phys. Rev. Research.

Target: large-scale TN structure

Up-date scheme: Finite-size DMRG & Local reconnection



Typical update process:



(a) Prepare an initial wave function Ψ_{abcd}

(b) Diag. effective Ham. $\tilde{H}_{abcd,a'b'c'd'}$

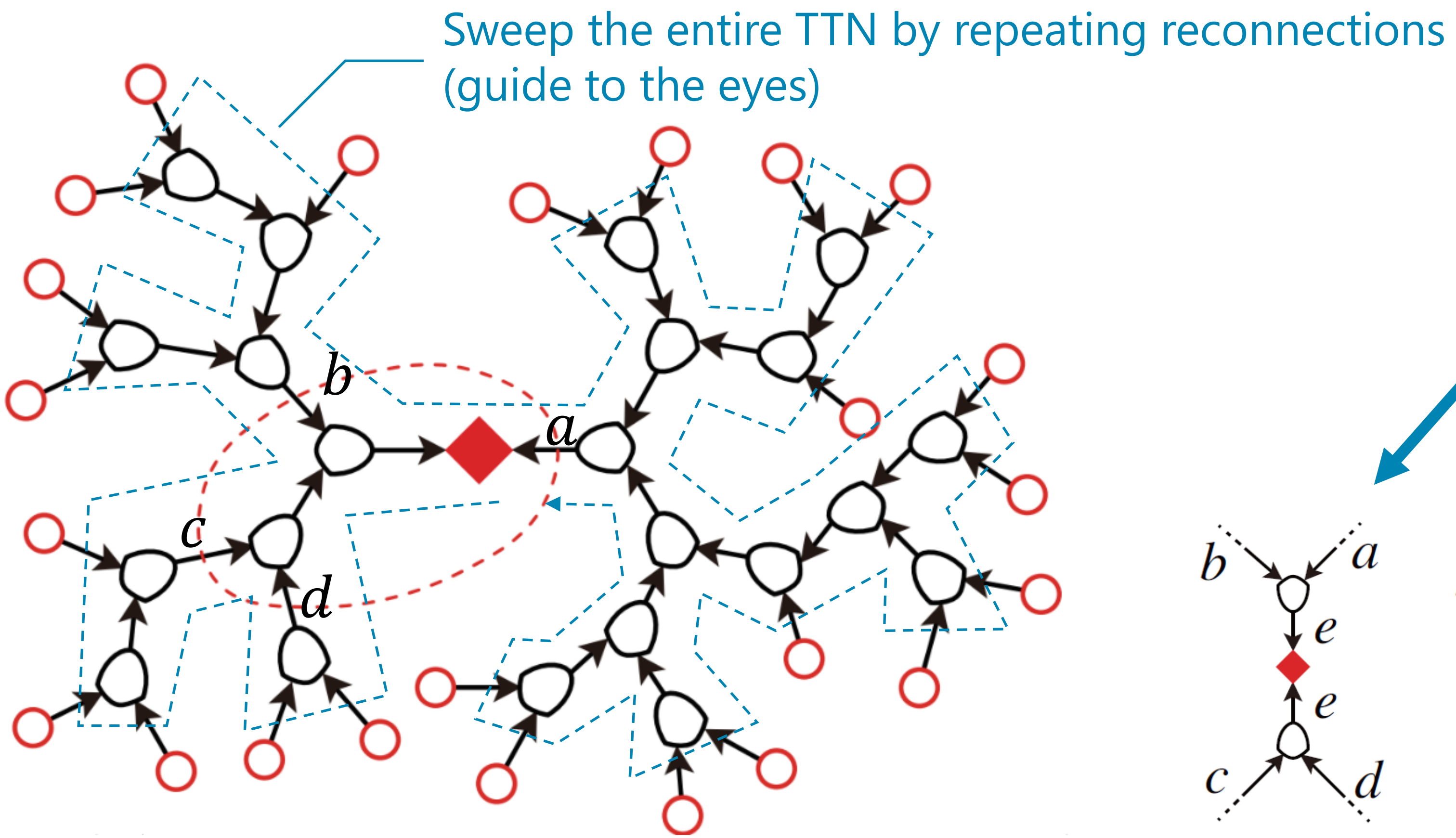
G.S. of $\tilde{H}$: $\tilde{\Psi}_{abcd}$

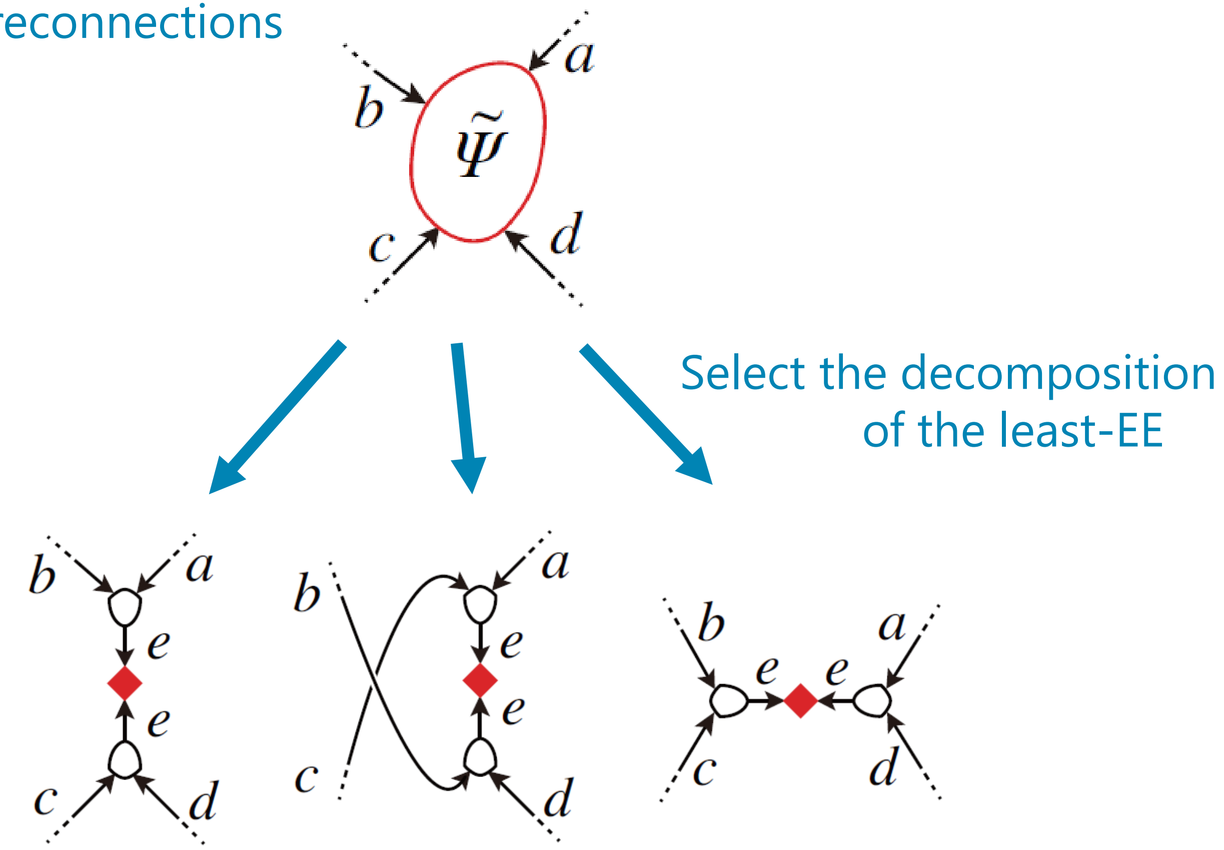
(c) SVD: $\tilde{\Psi}_{abcd} = \sum_e U_{ab,e} \Lambda_e V^*_{cd,e}$

Automatic optimization of TN structure

Target: large-scale TN structure

Up-date scheme: Finite-size DMRG & Local reconnection





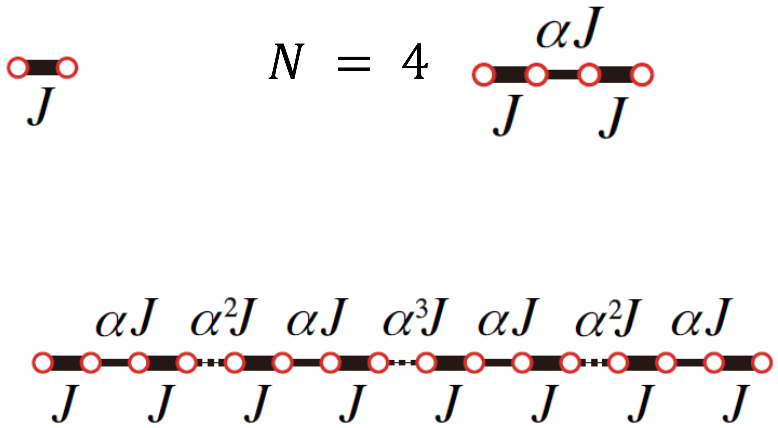
Bottom-up & deterministic approach

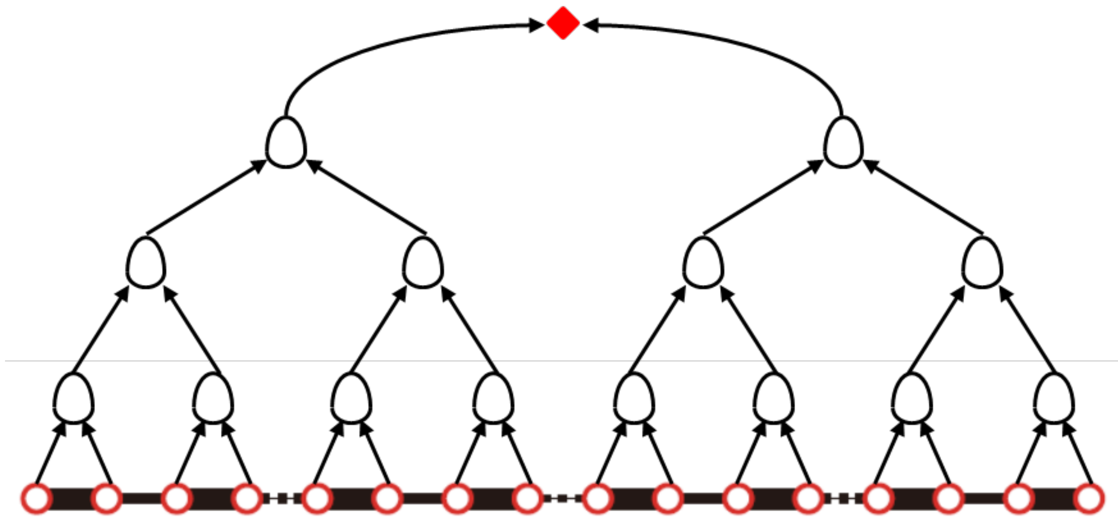
Numerical Results

Hierarchical AFHB chain

$$\mathcal{H} = \sum_i J_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$$

$N = 2$ $N = 4$ $N = 16$



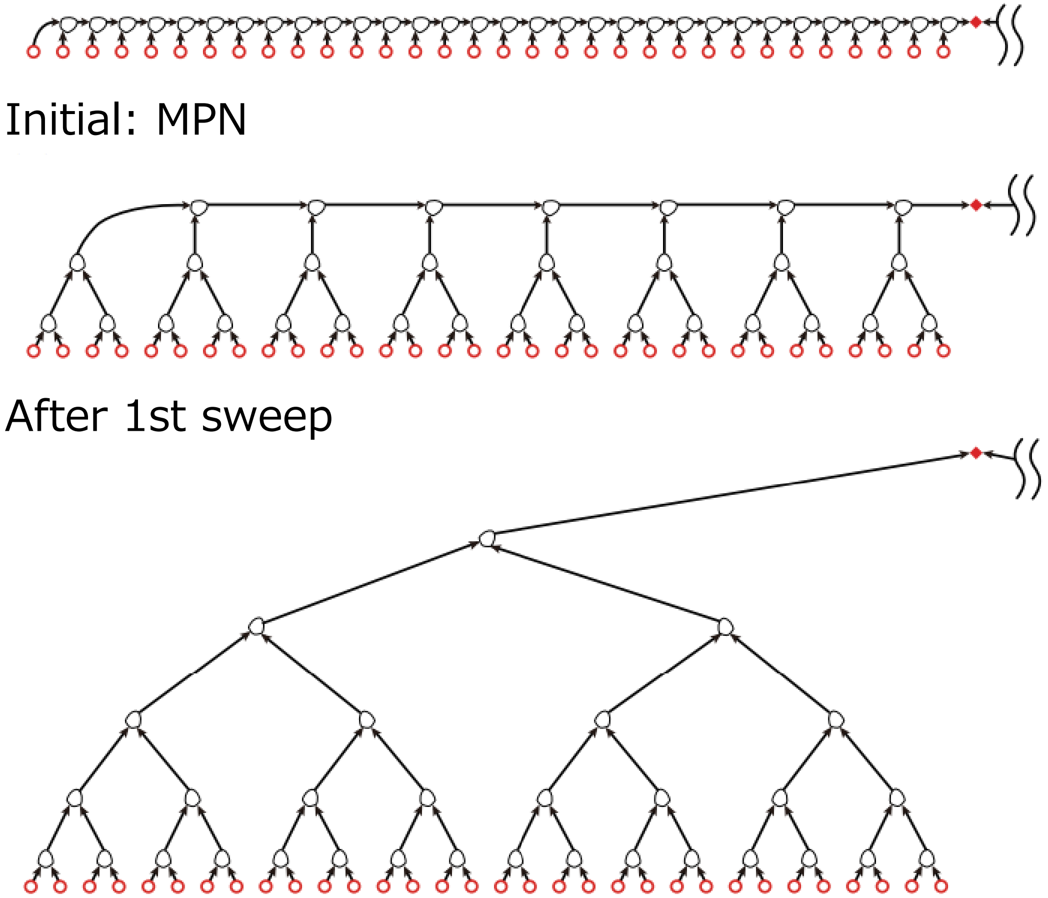


Connect two 2^n-site units via exchange $\alpha^n J$ to form 2^{n+1}-site unit.

The recursive RG procedure yields the pbTTN as long as the alpha is sufficiently small.

Numerical Results

$\alpha = 0.5,\ N = 64,\ \chi_{\max} = 26$

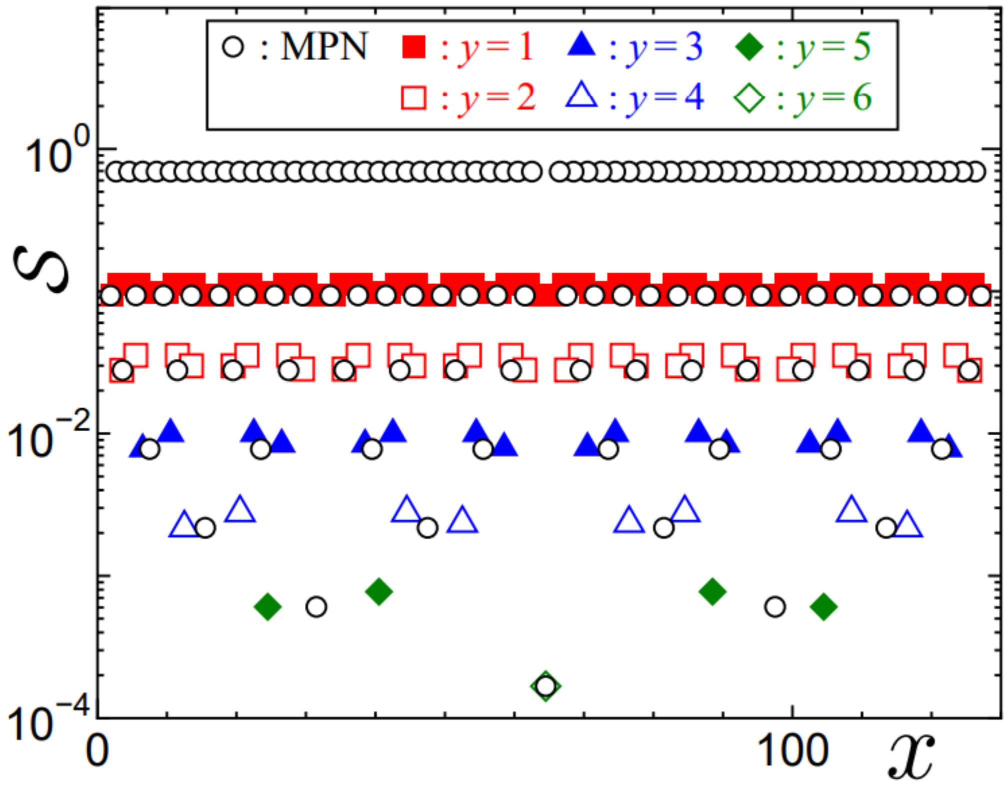


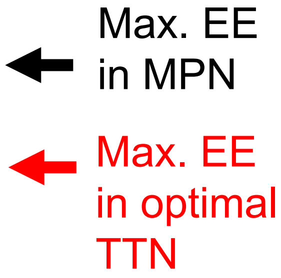
Initial: MPN

After 1st sweep

After 2nd sweep

Consistent with the TN w/ the recursive RG



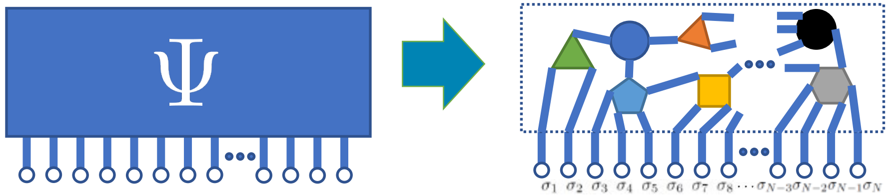


Type	Maximun	Average
optimized TTN ($N = 64$)	0.1110	0.0640
optimized TTN ($N = 128$)	0.1110	0.0625
MPN ($N = 64$)	0.6935	0.3697
MPN ($N = 128$)	0.6935	0.3719

Summary

Search for TTN matching the entanglement structure of quantum many-body states

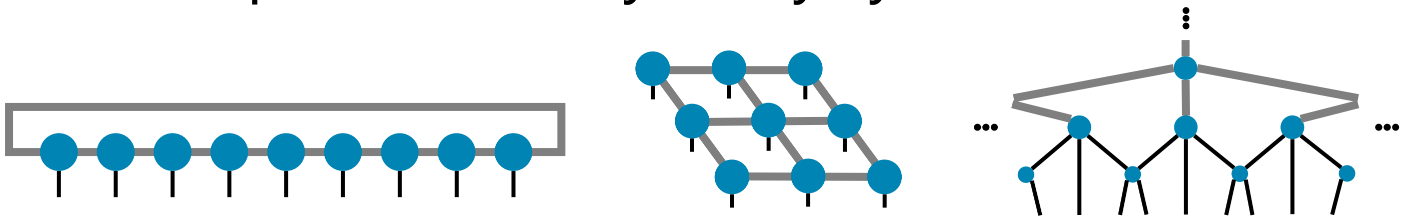
- TN: pattern of tensor decomposition



- Accuracy of numerical simulation of quantum many-body systems

⬍ **Entanglement**

Geometric structure of TN



- Searching algorithm for “optimal” TTN

Top-down Minimizing the maximum loss of the EE (MMX) due to the truncation

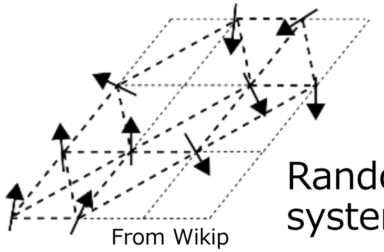
K. Okunishi, HU, T. Nishino, arXiv:2210.11741.

Bottom-up DMRG + Local reconnection of TN according to the MMX principle

T. Hikihara, HU, K. Okunishi, K. Harada, T. Nishino, arXiv:2209.03196, to appear in Phys. Rev. Research.

Possibilities for new collaborative research between different disciplines

- Variational optimization problem for non-uniform systems

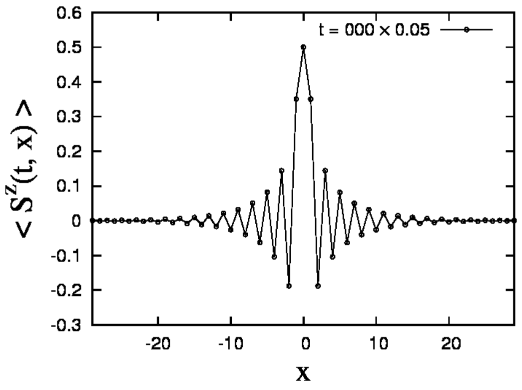


From Wikipedia

Random spin systems

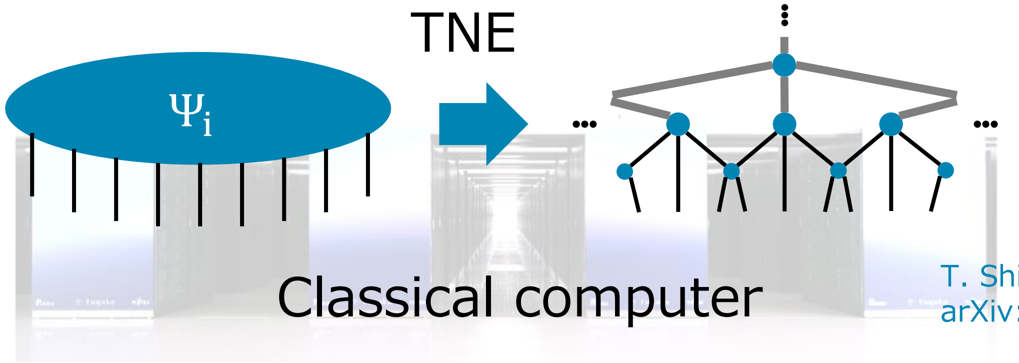
Nature Reviews Chemistry **4**, 490 (2020).

Quantum chemistry

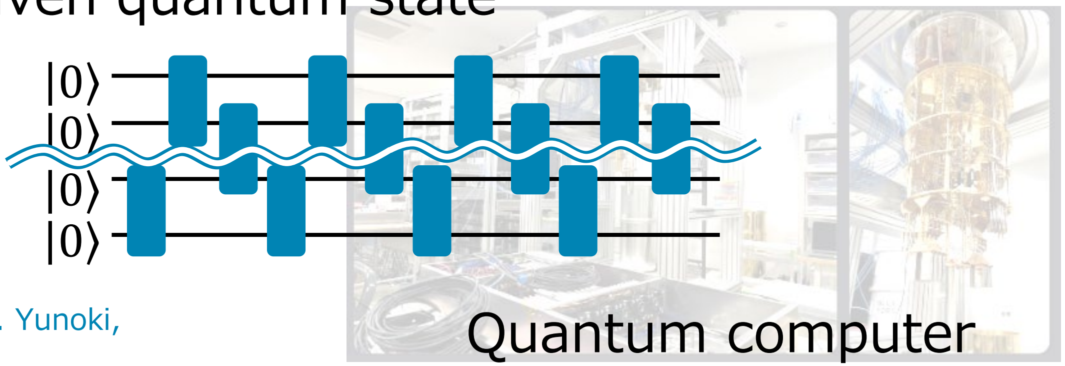


Real-time evolution

- Efficient quantum circuit encoding (QCE) of a given quantum state



QCE



T. Shirakawa, HU, S. Yunoki, arXiv:2112.14524.

- Network geometry of a discrete system ⟷ Geometry in the corresponding continuous system

"Optimal" TN ⟷ ???

Ex) Gauge-gravity correspondence

Supplement: Kitaev materials

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Kitaev materials

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A R T I C L E I N F O

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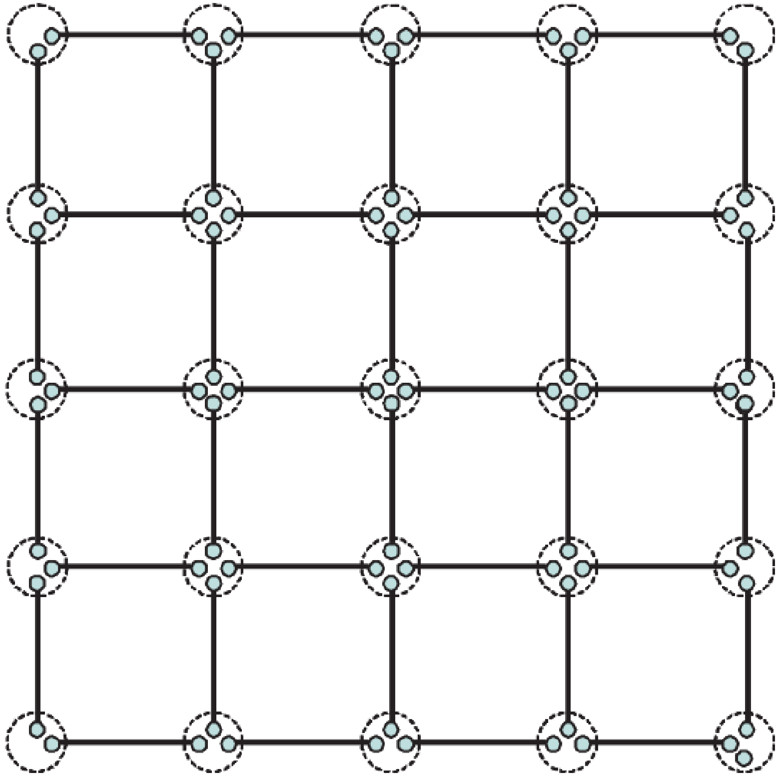
A B S T R A C T

In transition-metal compounds with partially filled 4*d* and 5*d* shells spin–orbit entanglement, electronic correlations, and crystal-field effects conspire to give rise to a variety of novel forms of topological quantum matter. This includes Kitaev materials — a family of spin–orbit assisted Mott insulators, in which local, spin–orbit entangled $j = 1/2$ moments form that are subject to dominant bond-directional Ising exchange interactions. On a conceptual level, Kitaev materials attract much interest for their potential for unconventional forms of magnetism, such as spin liquid physics in two- and three-dimensional lattice geometries or the formation of non-trivial spin textures. Experimentally, a number of Kitaev materials have been synthesized, which includes the honeycomb materials Na_2IrO_3, α-Li_2IrO_3, $H_3LiIr_2O_6$, and, most prominently, α-$RuCl_3$, the triangular materials $Ba_3Ir_xTi_{3-x}O_9$, as well as the three-dimensional hyper-honeycomb and stripy-honeycomb materials β-Li_2IrO_3 and γ-Li_2IrO_3. We provide a short review of the current status of the theoretical and experimental exploration of these Kitaev materials.

Supplement: TPS/PEPS results

F. Verstraete, J. I. Cirac, arXiv:cond-mat/0407066



the algorithm is polynomial in N and D.

We have first considered a 4×4 lattice on which the imaginary time evolution can be determined exactly. In Fig. 2, we plotted the exact evolution versus the one where the evolution is approximated variationally within the PEPS with bonds of dimension $D = 2, 3$ ($D = 4$ cannot be distinguished from the exact result). We used the same Trotter approximation for the exact and variational simulations with $\delta t = -3i/100$. It is remarkable that even for $D = 3$ we obtain a very good approximations, both regarding time evolution and ground state energy. The algorithm clearly converges to the ground state, and the difference between the exact ground state energy and the one obtained with our scalable algorithm rapidly decreases with D[17]; more specifically, $1 - E_{var}/E_{exact}$ is given by $.35, .02; .004; 0.0008$ for $D = 1, 2; 3; 4$ (note that the trivial situation $D = 1$ corresponds to the Néel state).

Ref.) Opt TTN / pbTTN with $\chi = 8$: $1 - 9.05/9.19 \sim 0.015$
$\Leftrightarrow$ TPS/PEPS $D \sim 2$

Supplement: Intermediate structures

T. Hikihara, HU, K. Okunishi, K. Harada, T. Nishino, arXiv:2209.03196, to appear in Phys. Rev. Research.

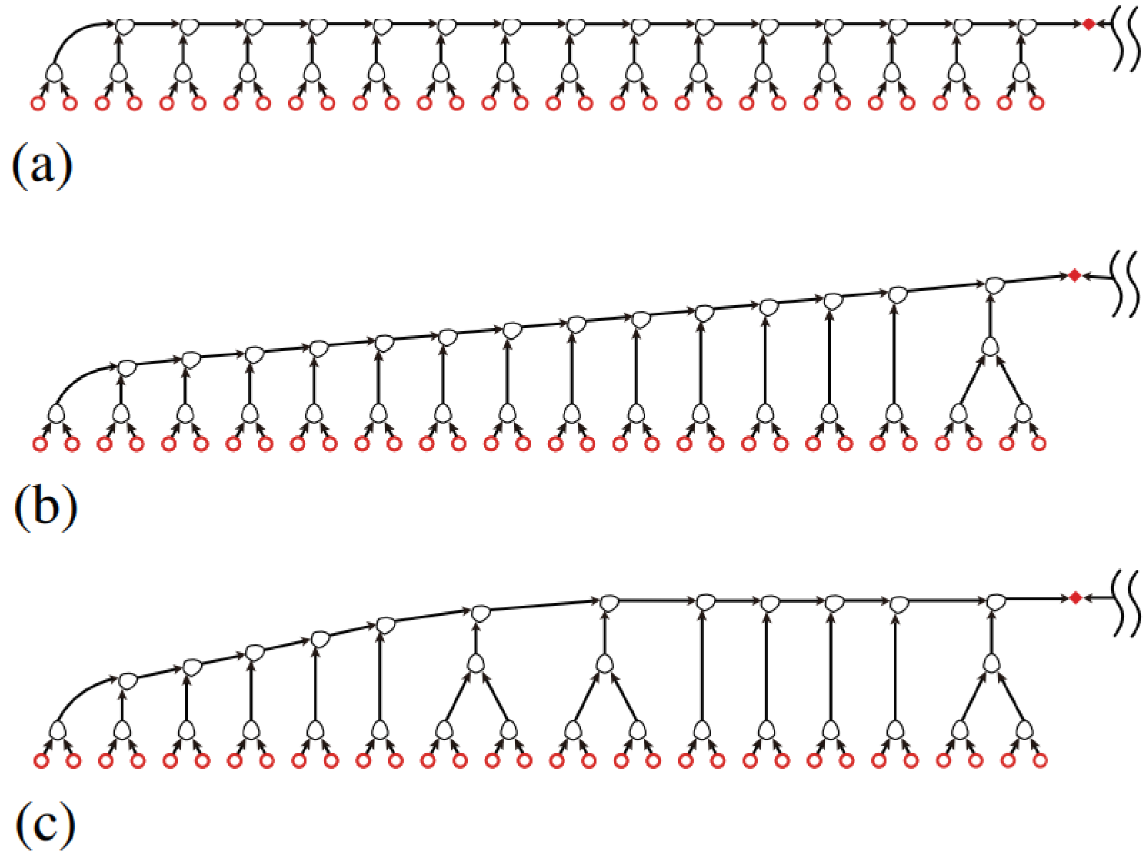


FIG. 10. Optimal structures for (a) $\alpha = 1.00$, (b) $\alpha = 0.80$, and (c) $\alpha = 0.75$. The system size is $N = 64$. Only the left half of the TTN is presented while the right half is symmetric with respect to the center of the system.