Background of correlated physics

Why tensor network methods?

2022 summer school for physics and tensor-network methods in correlated systems

Yi-Ping Huang [a,b]

[a] National Tsing Hua University, Taiwan

[b] Institute of Physics, Academia Sinica, Taipei 115, Taiwan

注意事項

- 保證金 ： 除曠課及罰金外，全勤學員於課程結束當天(8月31日)全額退還保證金。

- 《防疫提醒》
  1. 若為確診者、居隔者，及接觸前述狀況者，請來電請假，並請在家好好休息。
  2.上課期間，請務必佩戴好口罩，提醒口鼻勿外露。

Mind set

- The purpose of summer school is to help you learning. So don't be afraid to ask questions!
  - Ask the lecturer (to help you learn)
  - Ask YOURSELVES! (to develop your own way of thinking!)
- Discuss with people, to be confused in an efficient way.
- If you got an answer that you are not satisfied, ask yourselves: how to make the answer better? Then, you can share your answer!

Mind set

- Don’t be afraid to make mistake or to show your ignorance. That is just a process of learning.
- “一個人只有顛覆了「自己認為自己已經知道了」這件事之後，學習才真正地開始。換言之，掙扎於不能理解的閱讀過程，正是構成教育與學習的起點。”
- 如何顛覆「自己認為自己已經知道了」？
  - 教自己的研究夥伴
  - 挑戰自己用不同的角度理解一個問題
    - 比方說寫個程式…

Mind set

- Learning by doing - the hands on tutorial sections.
- Writing a program is an important way to check whether you really understand the concept.

Outline

- Tensor network method
  - for nontrivial correlations
    - for quantum systems — quantum entanglement
    - for classical statistical mechanics
  - for quantum dynamics of correlated many-body system

Non-trivial correlations in many-body systems

- Classical correlations : correlations <u>not</u> related to entanglement
- Quantum correlations : correlations related to <u>entanglement</u>

- Classical statistical mechanics (covered in most lectures)

$$P(\xi) = \frac{1}{Z} e^{-\beta H(\xi)}$$

- Quantum many-body system

$$P(a) = |\langle \psi | a \rangle|^2$$

Tensor networks for <u>quantum systems:</u>
Ground state and time-evolution

What is quantum entanglement?

From the superposition principle⋯

- Quantum bit（q-bit)
  - Linear superposition

$$|\psi\rangle = |\uparrow\rangle + |\downarrow\rangle$$

Sometimes people said the state is simultaneously spin up and spin down. That is not a correct description.

  - Superposition with a complex phase

$$|\psi\rangle = |\uparrow\rangle + e^{i\theta}|\downarrow\rangle$$

What is quantum entanglement?

- Quantum bit （q-bit)
  - Linear superposition

$$|\psi\rangle = |\uparrow\rangle + |\downarrow\rangle$$

  - Superposition with a complex phase

$$|\psi\rangle = |\uparrow\rangle + e^{i\theta} |\downarrow\rangle$$

Axioms of quantum mechanics：

1. A system is described by a quantum state.
2. The time evolution of the state is described by the Schödinger equation.
3. The distribution of the measurement is described by the modulo square of the projection to the measurement basis.
4. The Hilbert space of a composite system is formed by the tensor product of sub Hilbert spaces.

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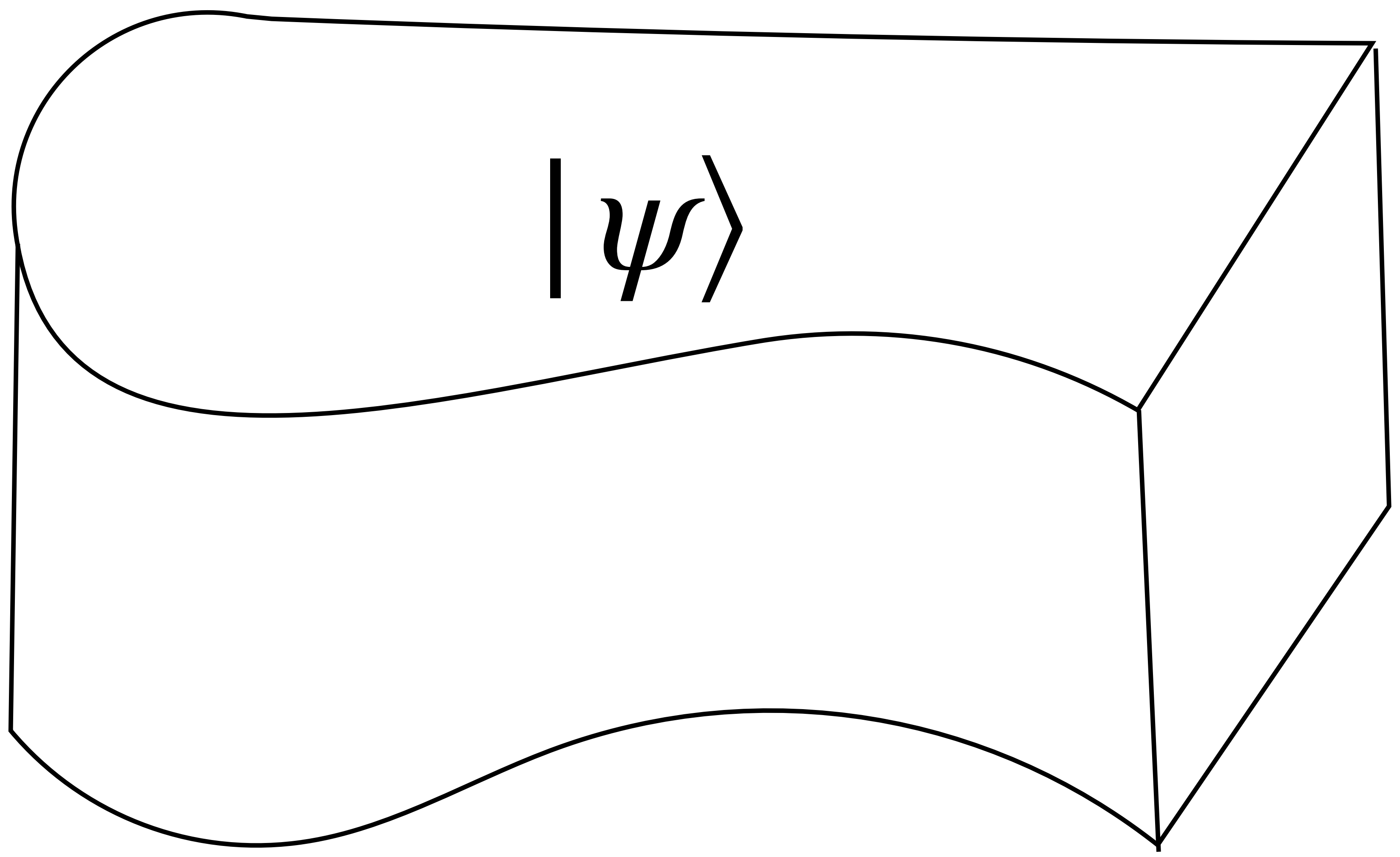
$$|\psi\rangle \in \mathscr{H}$$



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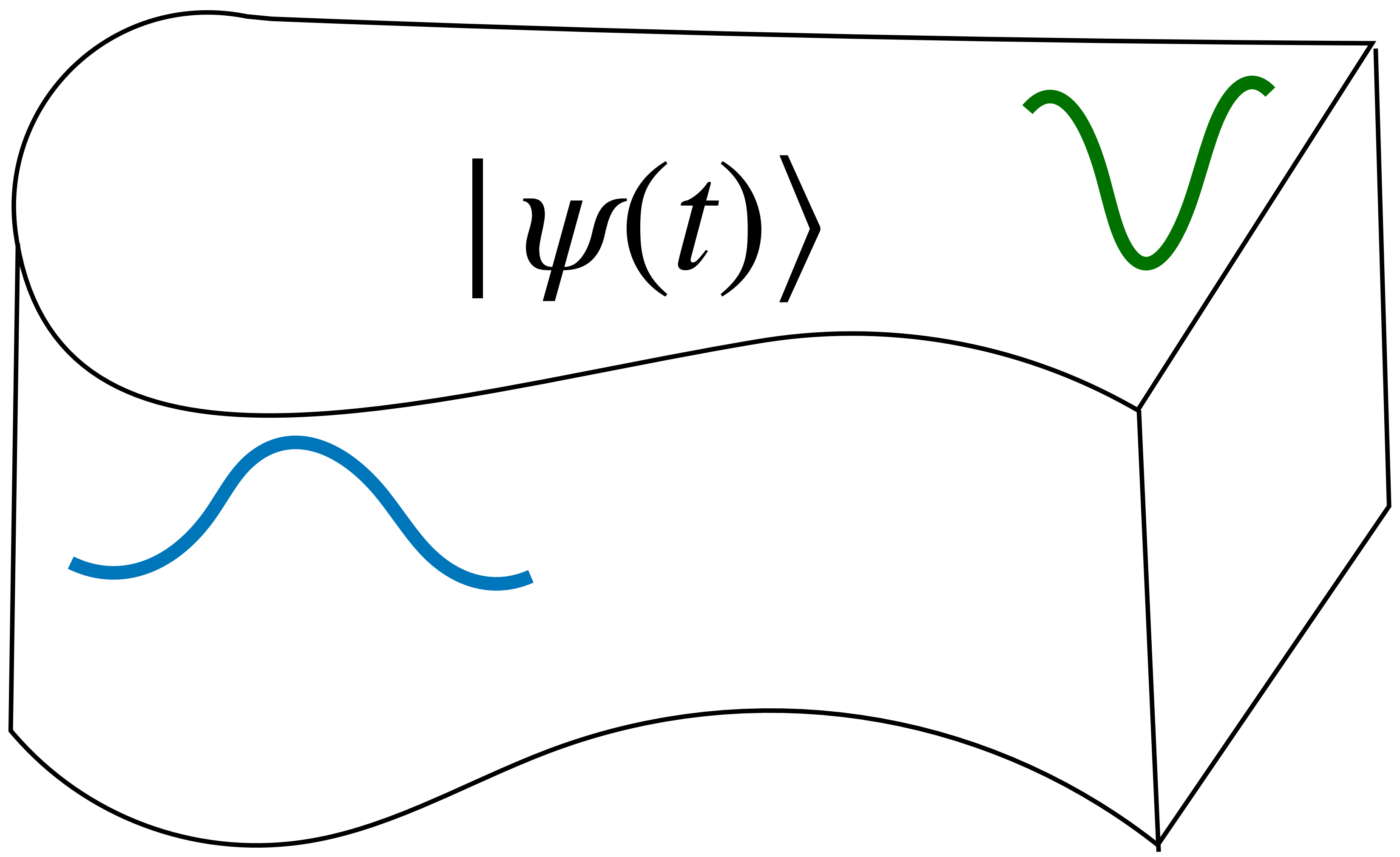

$$i\hbar\partial_t|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

$$\hat{A} : \{\, |a\rangle \,\} \qquad P(a) = |\langle \psi | a \rangle|^2$$

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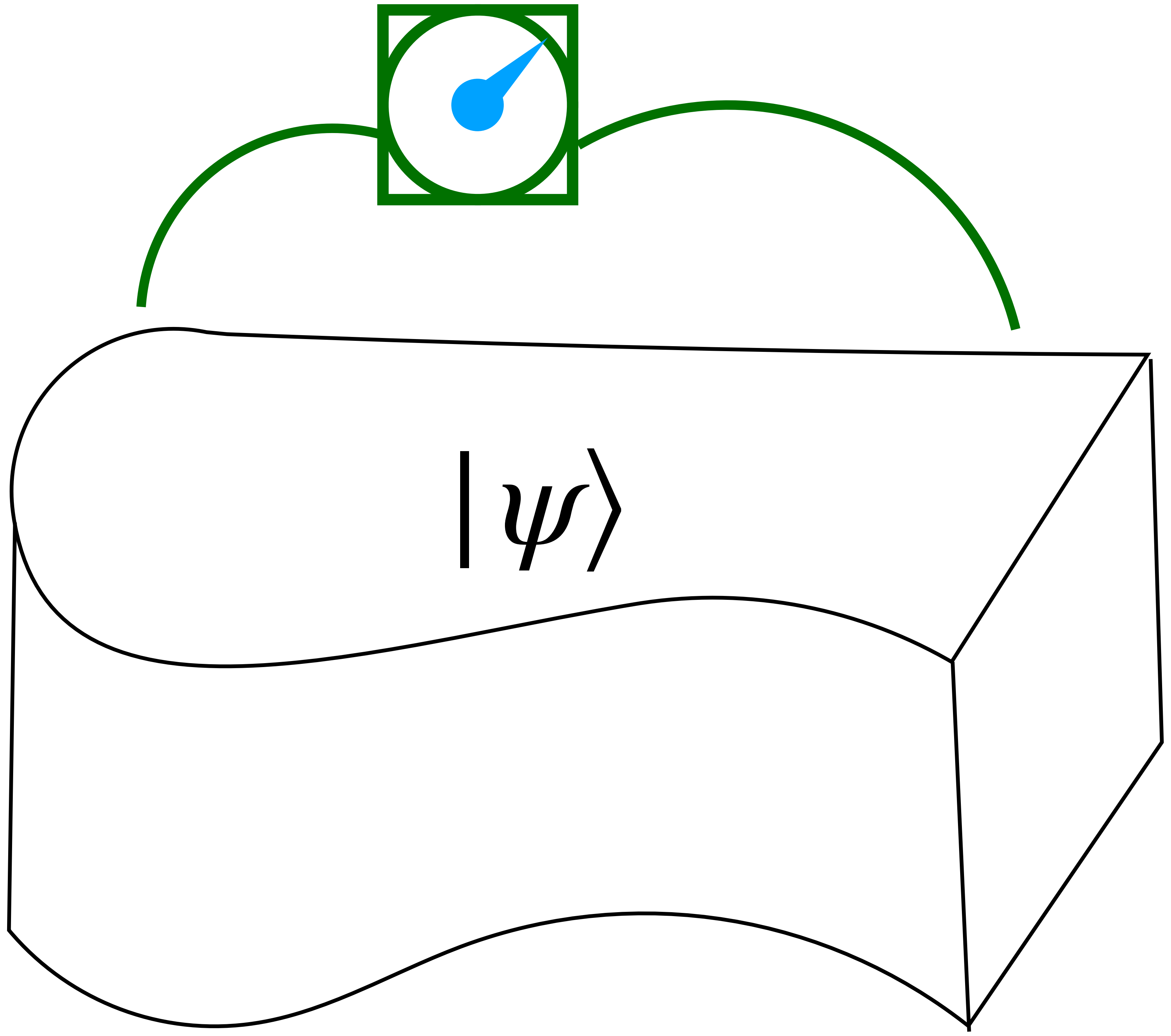

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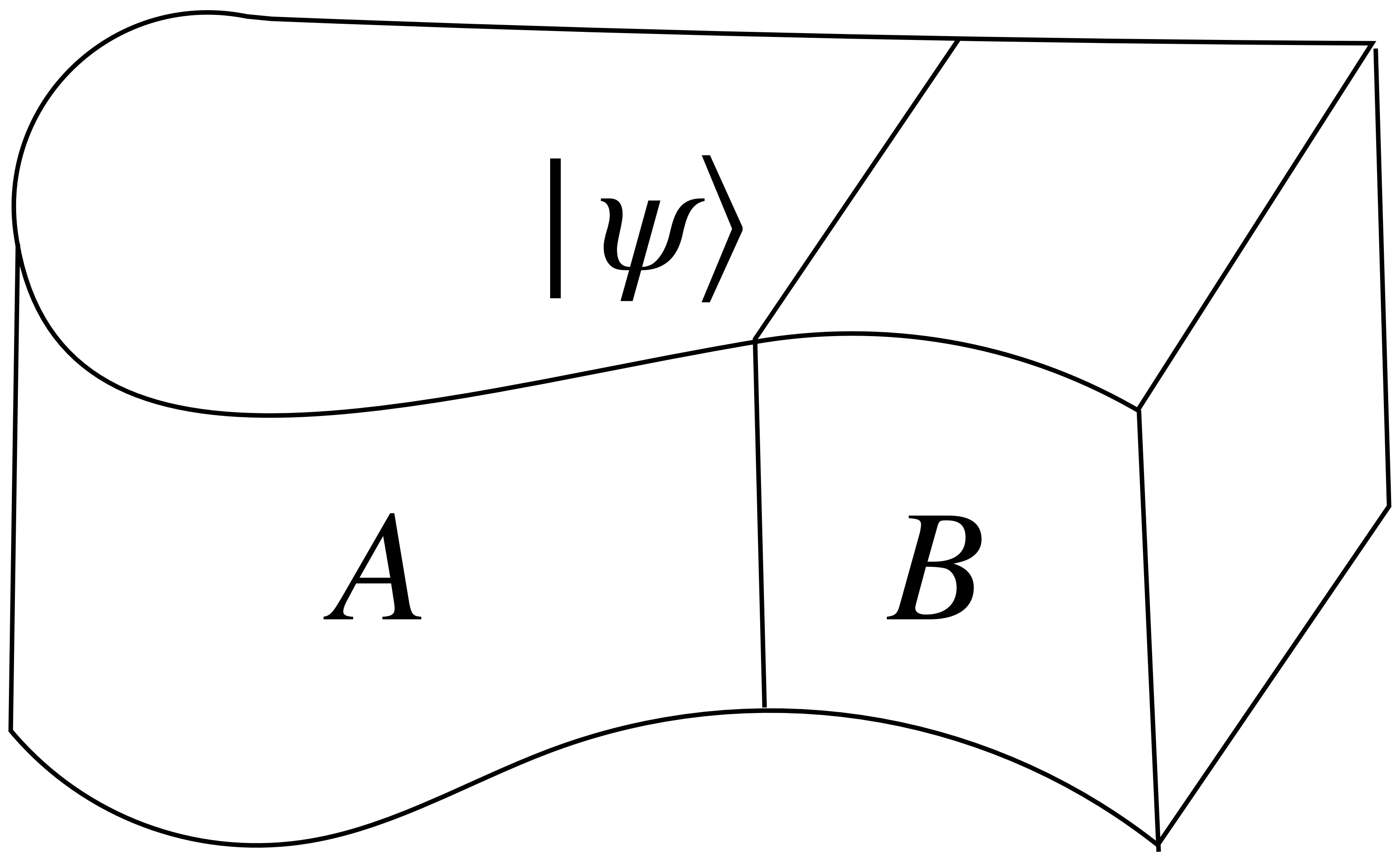
$$|\psi\rangle \in \mathscr{H} = \mathscr{H}_A \otimes \mathscr{H}_B$$



What is quantum entanglement?

- two q-bits（Simplest non-trivial example)
  - Hilbert space : $\mathscr{H}_1 \otimes \mathscr{H}_2$
  - not entangled states (product states)

    $|\psi_a\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2$

    $|\psi_b\rangle \propto |\uparrow\rangle_1 |\uparrow\rangle_2 + |\downarrow\rangle_1 |\downarrow\rangle_2 + |\downarrow\rangle_1 |\uparrow\rangle_2 + |\uparrow\rangle_1 |\downarrow\rangle_2$

    $|\psi_b\rangle \propto (|\uparrow\rangle_1 + |\downarrow\rangle_1) \otimes (|\uparrow\rangle_2 + |\downarrow\rangle_2)$

  - entangled states

    $|\psi_e\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2 \nrightarrow |\Phi\rangle_1 \otimes |\Psi\rangle_2$

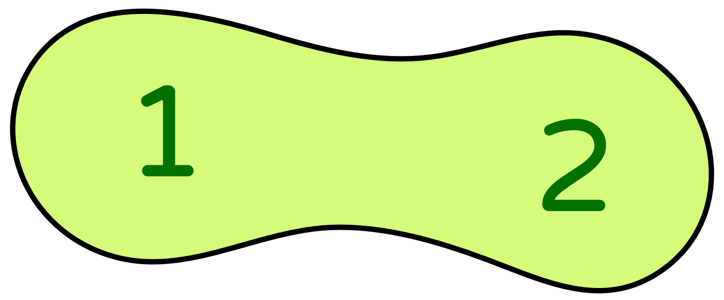
- not entangled states (product states) : Just like we put two system together “classically”.

$$|\psi_a\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2$$

$$|\psi_b\rangle \propto (|\uparrow\rangle_1 + |\downarrow\rangle_1) \otimes (|\uparrow\rangle_2 + |\downarrow\rangle_2) \propto |\rightarrow\rangle_1 \otimes |\rightarrow\rangle_2$$

- entangled states : No classical analogy!

$$|\psi_e\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2 - |\downarrow\rangle_1 |\uparrow\rangle_2 \nrightarrow |\Phi\rangle_1 \otimes |\Psi\rangle_2$$



Why entanglement pattern is important?

The product state, a state that could have classical analogy. ↔ The entangled state, a state that has no classical analogy.

↓

Can be used to develop new technique! Quantum computing!

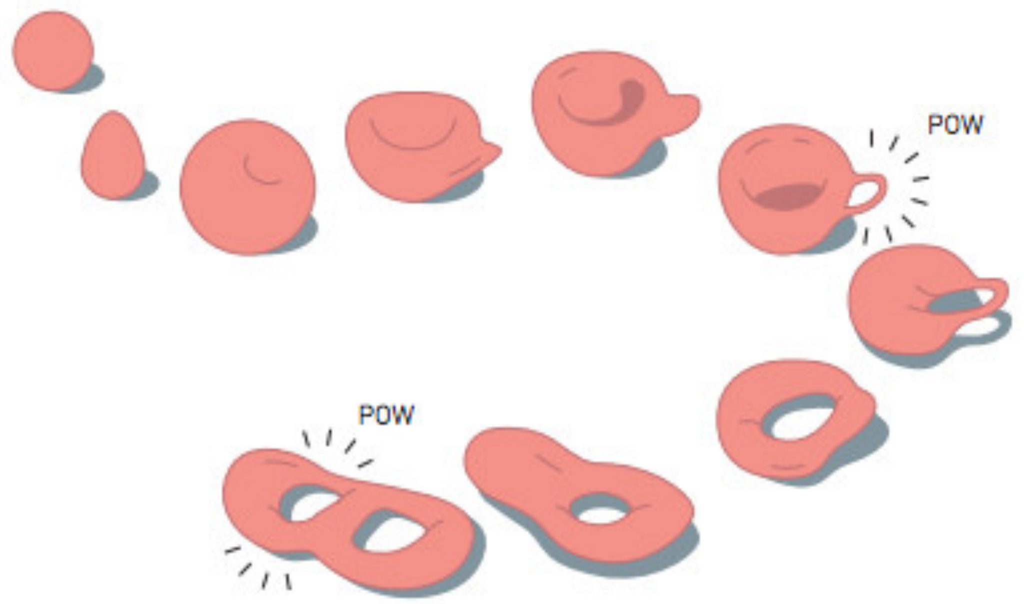
Entanglement pattern?

- Why understanding entanglement pattern is useful/cool?
- Can we understand entangled many-body wave functions in a systematic way?
  - Gapped quantum phases are more well understood⋯
- What kind of entanglement pattern can be robust/useful/cool?
- How to detect the entanglement pattern?
- ⋯ Need a good tool to describe entanglement!

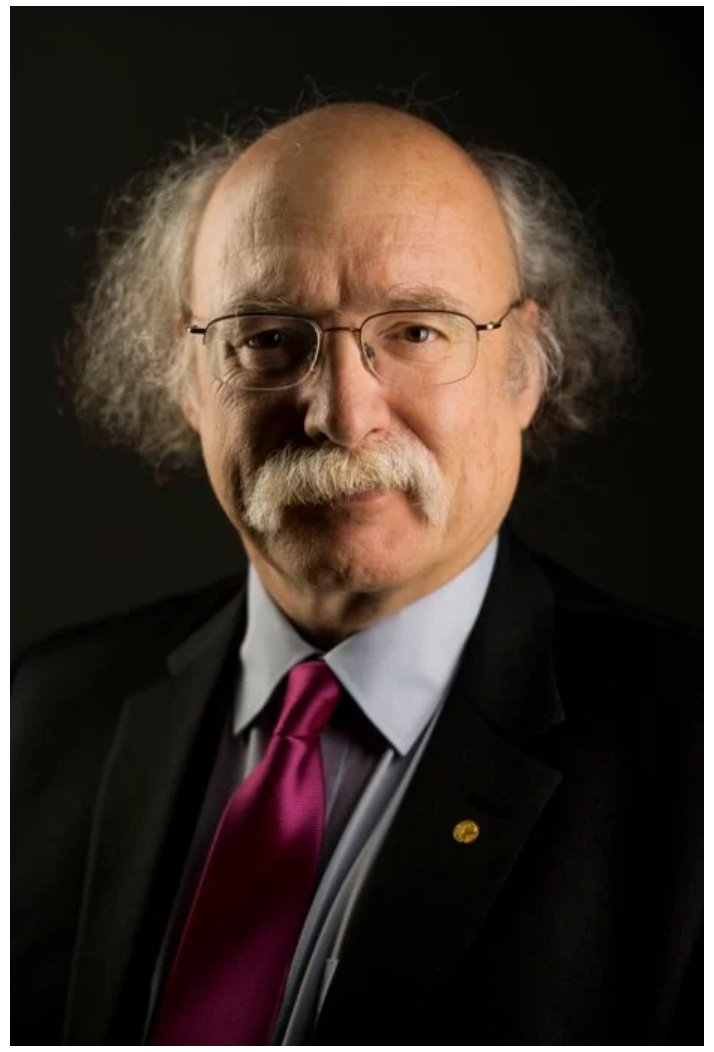
Tensor network approach!

物質態（phases of matter）

- 2016: Topological phase transitions and topological phases of matter
→拓墣相變與物質的拓墣態




David J. Thouless


F. Duncan M. Haldane

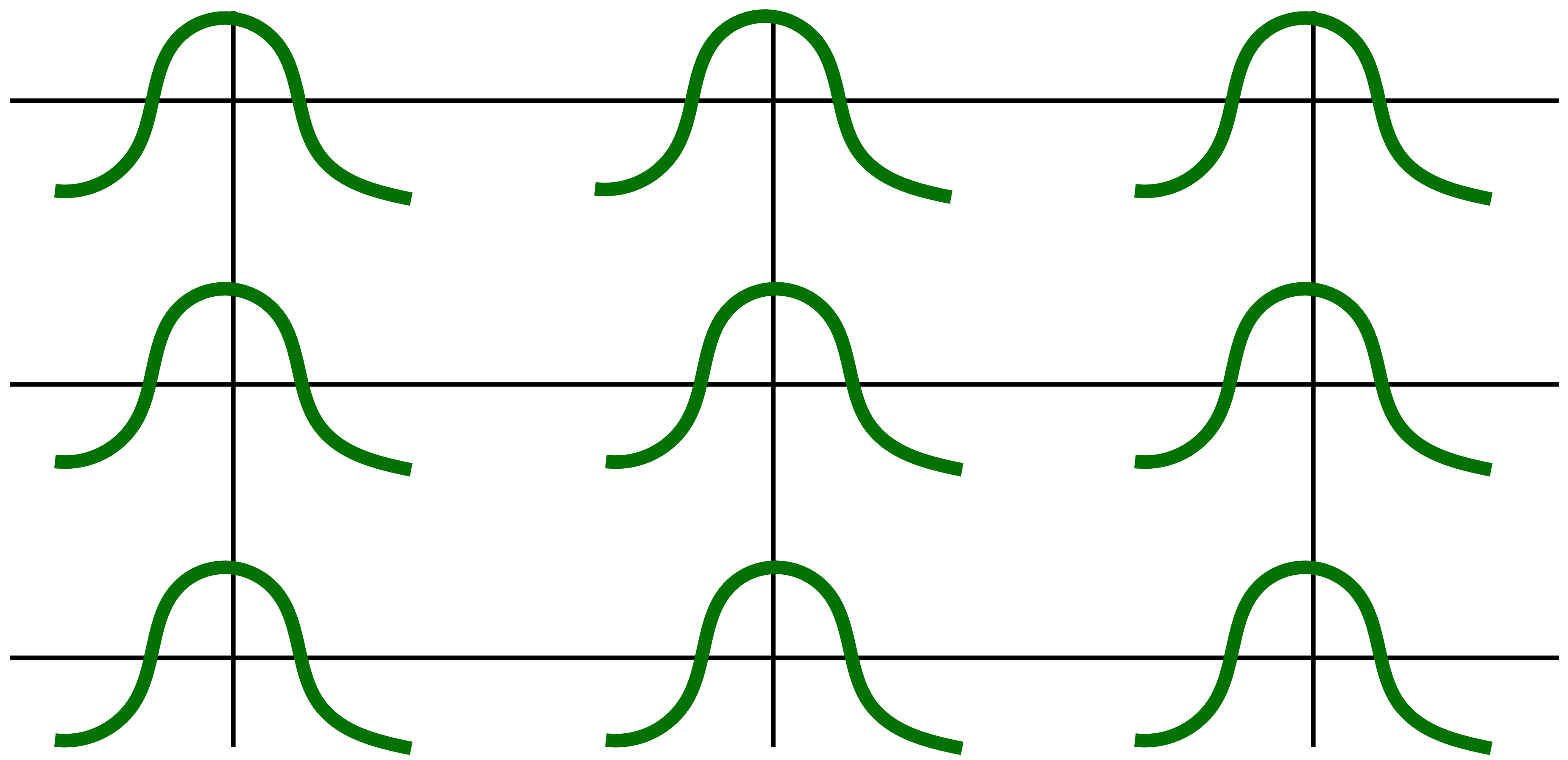

J. Michael Kosterlitz

What kind of entanglement pattern is out there?

- The product state is special, because it is the boring state from the entanglement point of view.
- Important simple examples with non-trivial entanglement?
  - Haldane phase (related to the idea of Symmetry Protected Topological phases (SPTs))
  - Eigenstates for toric code model (related to the idea of Symmetry Enriched Topological order (SETs))
  - What are the matrix product state representations of these states?

Gapped quantum phases — from the boring one

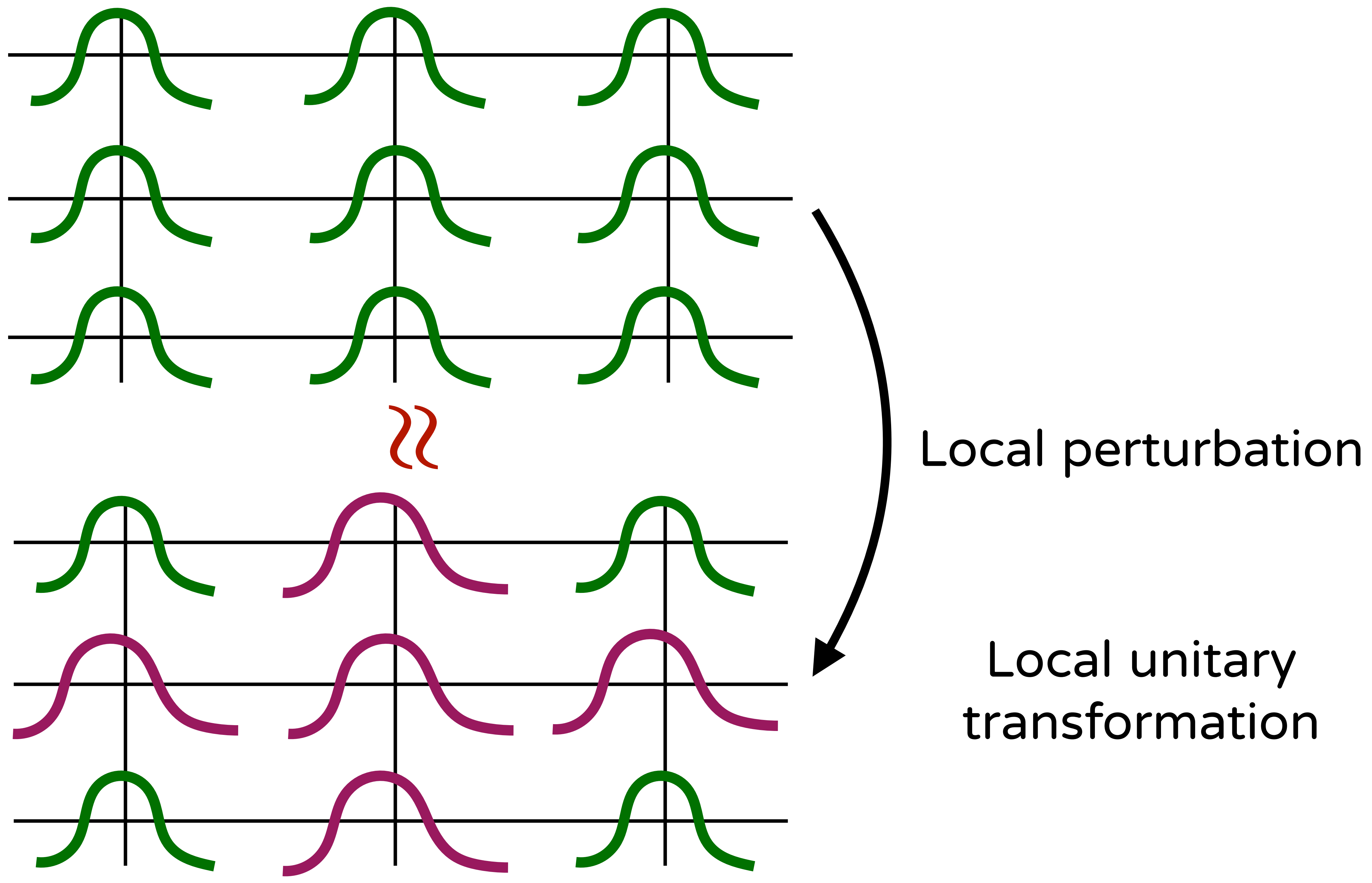
- The product state is special, because it is the boring state from the entanglement point of view.

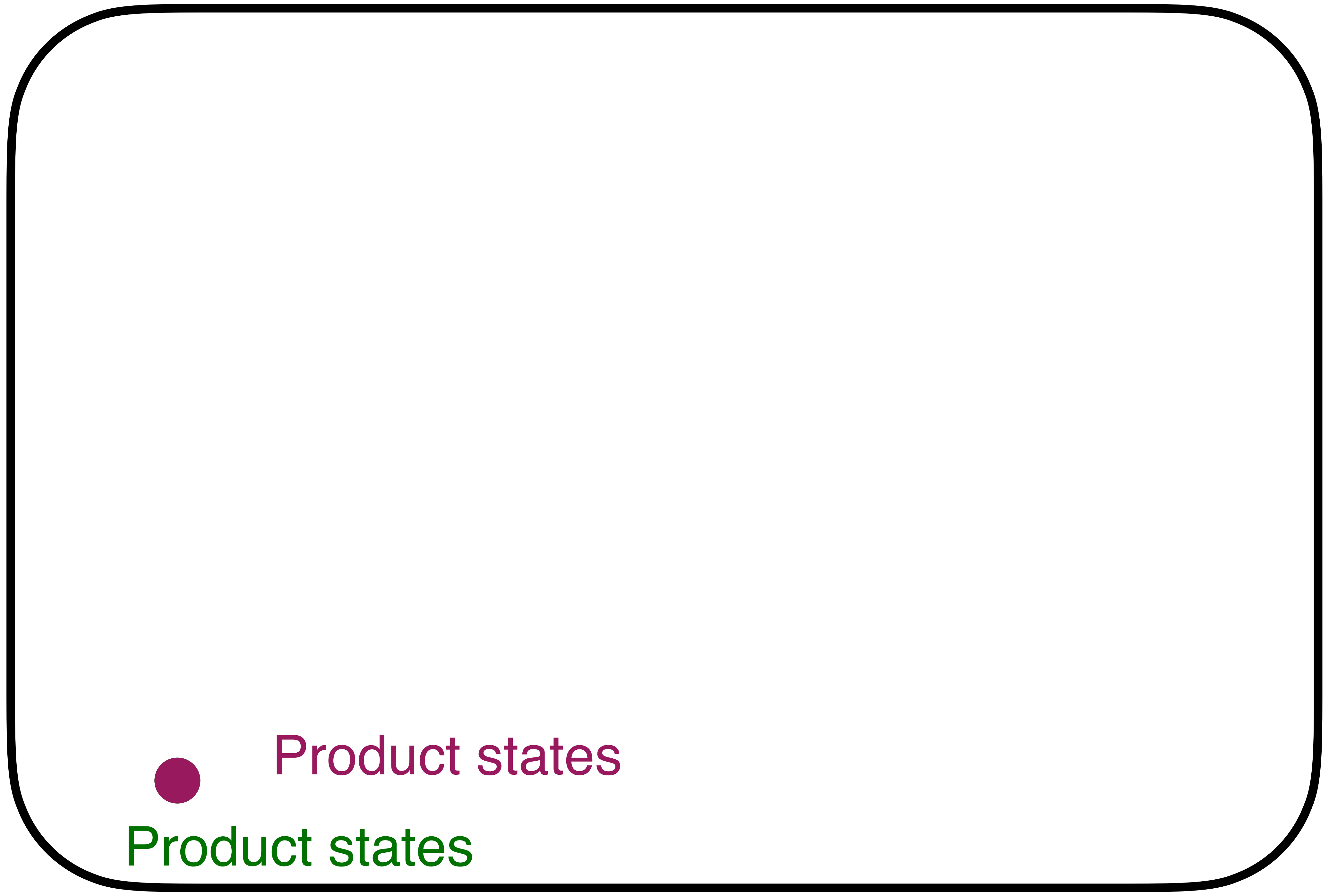


T=0 many-body Hilbert space (2D, gapped)

Why energy gap?

Many-body energy gap → possible to define local perturbation



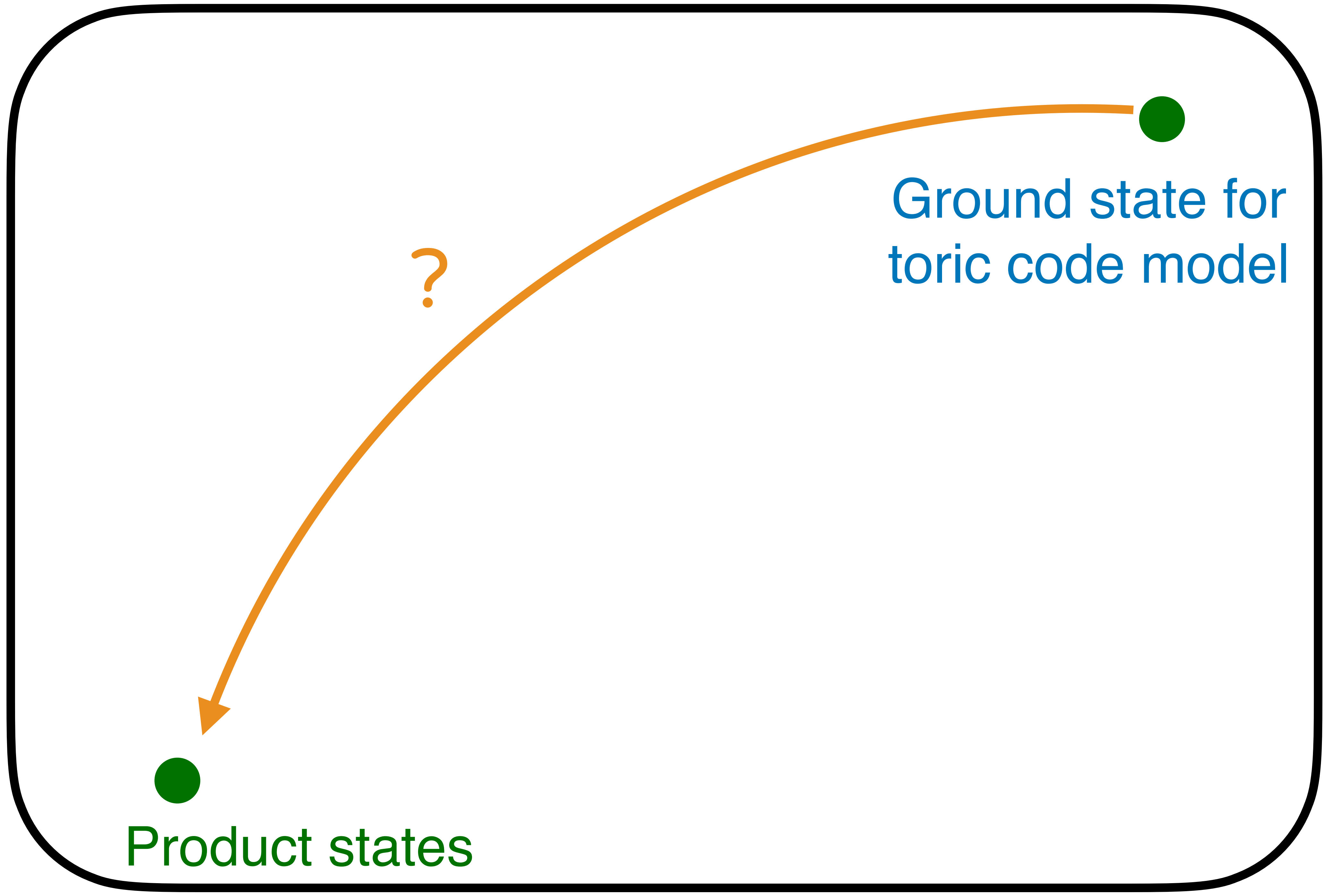


T=0 many-body Hilbert space (2D, gapped)

Are there gapped quantum phases with non-trivial entanglement pattern?

YES! Many of them…
e.g. The toric code model (Z_2 quantum spin liquid)

Can we deform toric code ground state to a product state with a path that the energy gap remains open?



T=0 many-body Hilbert space (2D, gapped)

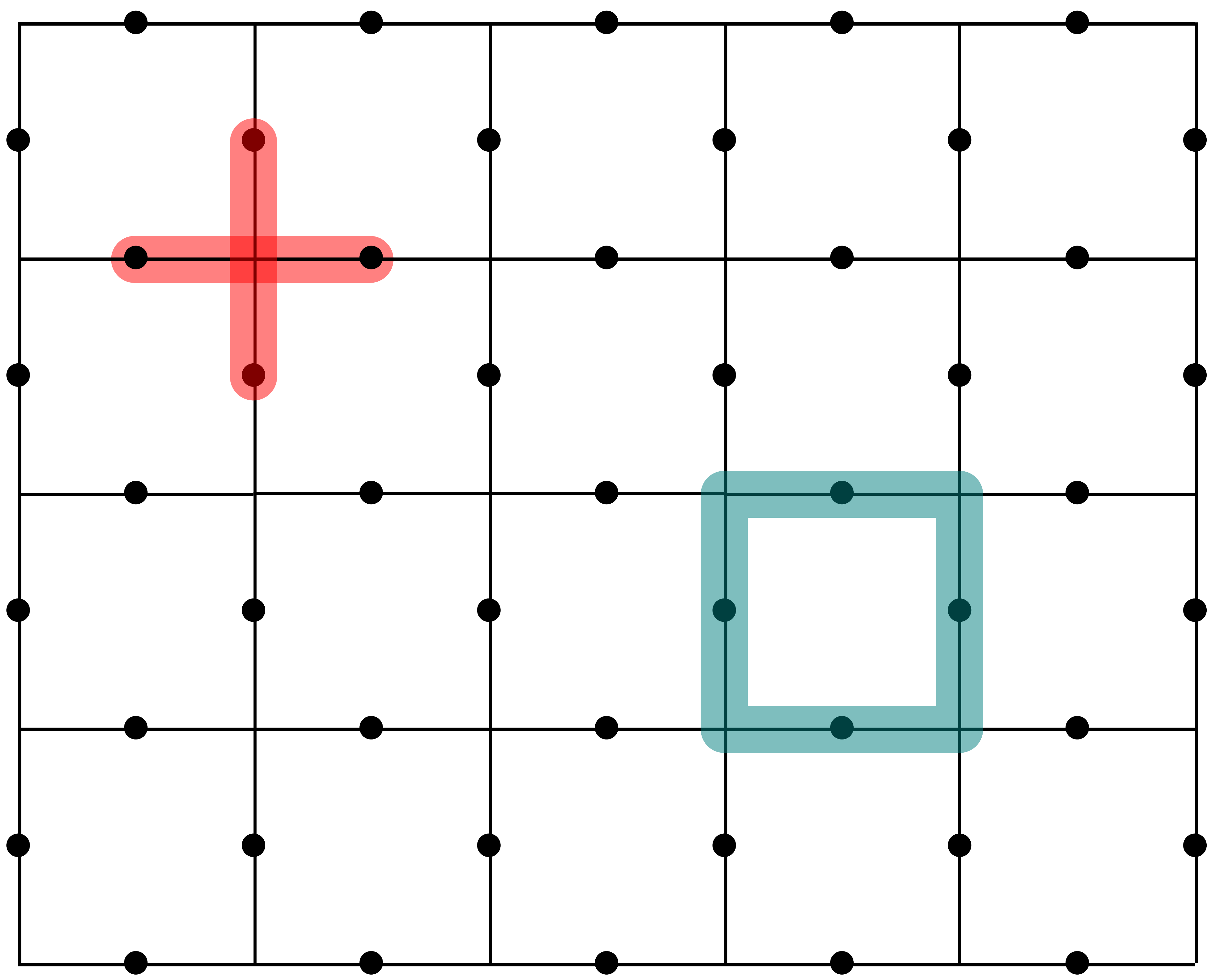
A.Yu. Kitaev O. Hirota, A.S. Holevo, C.M. Caves (Eds.), Quantum Communication, Computing and Measurement, Plenum, New York (1997)

The toric code model

- Exact solvable model (Full spectrum)
  - Ground state : superposition of closed loops.
  - Topological excitations (e, m, ε)
  - Gapped topological order with robust entanglement pattern.
  - The close loop constraint forbidden the deformation into product states → non-trivial entanglement.

Pauli spin operators

$$H_{TC} = -\sum_s K_e(s)\left(\prod_{i\in +}\tau_i^x\right) - \sum_p K_m(p)\left(\prod_{i\in \square}\tau_i^z\right)$$



The toric code model

- Assume
  $K_e(s) = K_e, K_m(p) = K_m; K_e, K_m > 0$

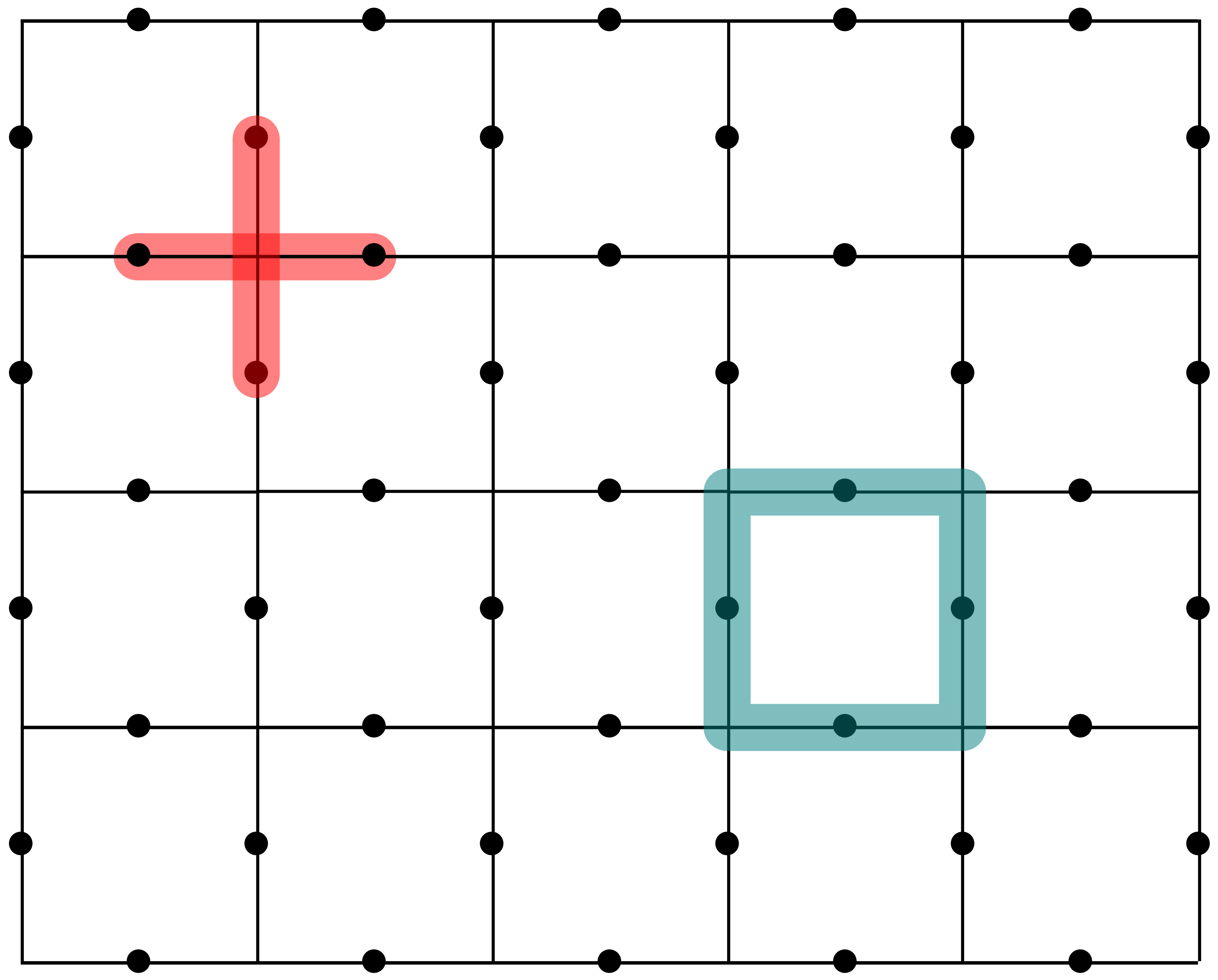
- $[H_{TC}, A_s] = [H_{TC}, B_p] = [A_s, B_p] = 0$
  $[A_s, A_{s'}] = [B_p, B_{p'}] = 0$
  (Can you show that?)

- Ground state satisfy $A_s = B_p = +1$. How to have a wave function that can minimize both terms simultaneously?

$$H_{TC} = -\sum_s K_e(s)A_s - \sum_p K_m(p)B_p$$

$$A_s = \left(\prod_{i\in +} \tau_i^x\right); B_p = \left(\prod_{i\in \square} \tau_i^z\right)$$

Pauli spin operators on the links.



The toric code model

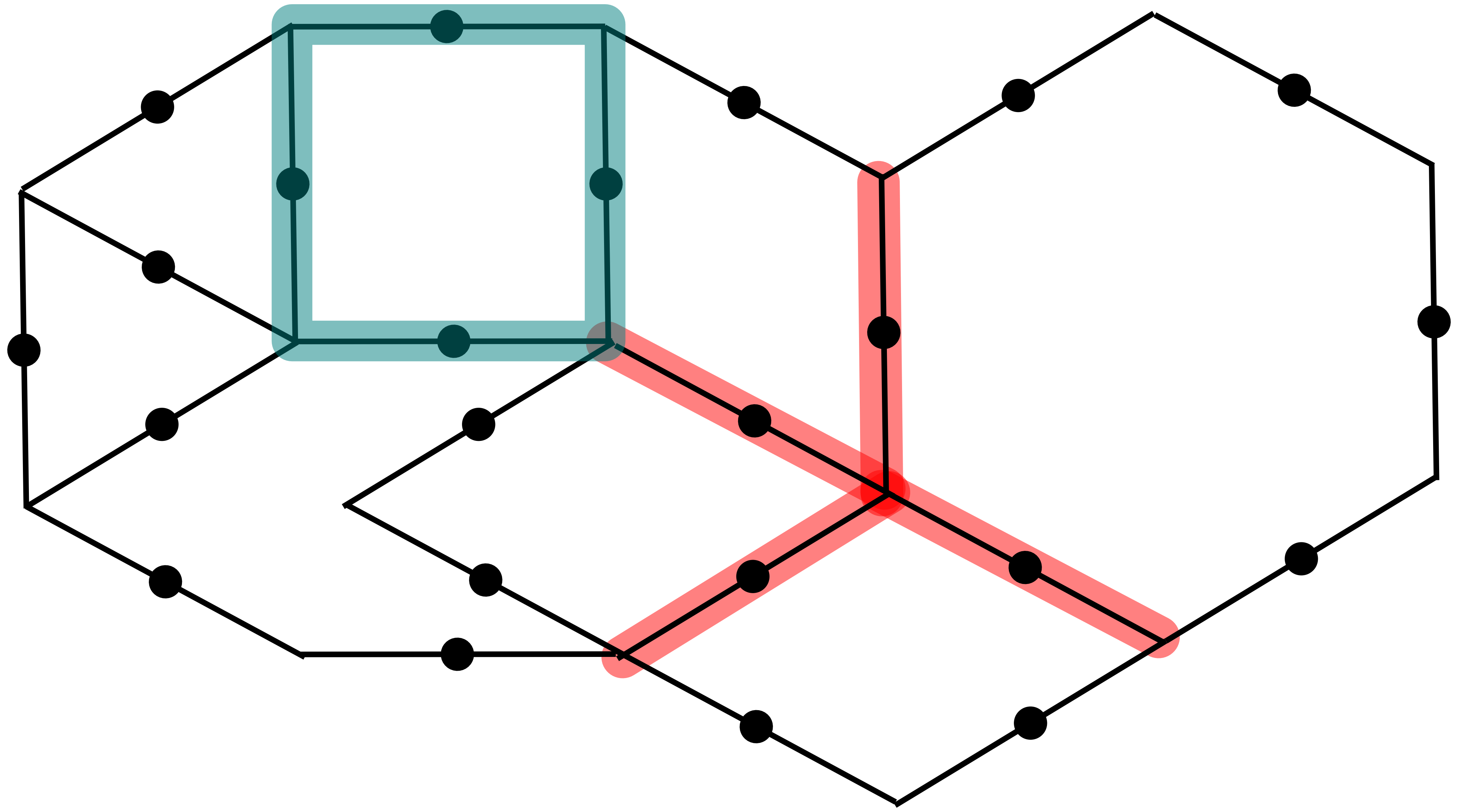
$$H_{TC} = -\sum_s K_e(s) A_s - \sum_p K_m(p) B_p$$

- Ground state satisfy $A_s = B_p = +1$. How to have a wave function that can minimize both terms simultaneously?

$$|\Psi_g\rangle = \left[\prod_s \frac{1}{\sqrt{2}}\left(1 + A_s\right)\right] |\{\tau_i^z = 1\}\rangle$$

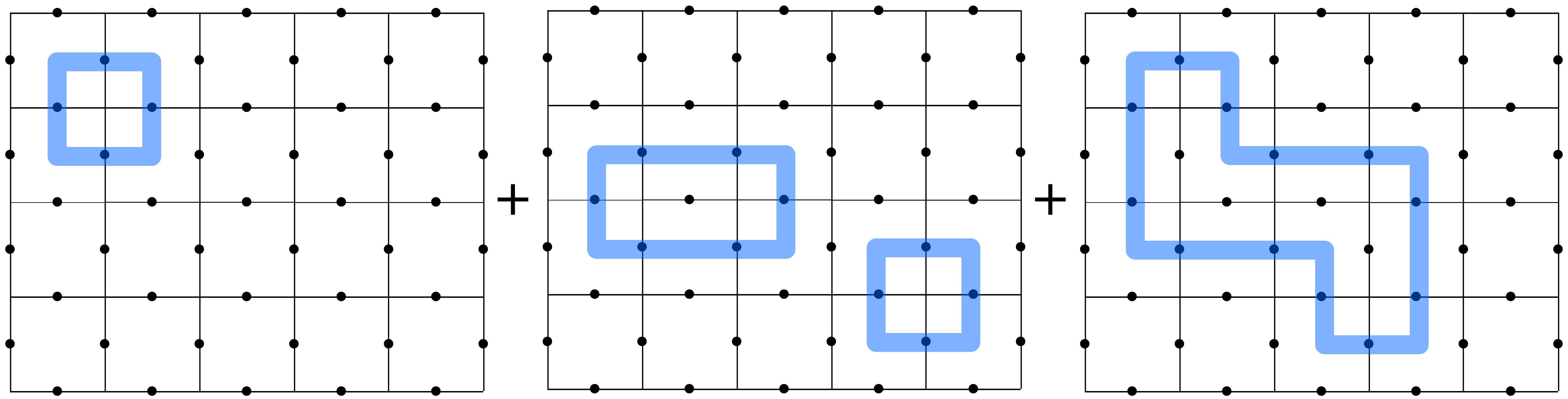
- Can you show that the two terms are minimized by this wave function?

- The assumption $K_e(s), K_m(p)$ is homogeneous is not important.



Why toric code ground state cannot be deformed into product states when gap remains open?

$|\Psi_g\rangle \propto$



$+\dots$

τ^z basis, background $\tau^z = +1$

$$|\Psi_g\rangle = \left[\prod_s \frac{1}{\sqrt{2}}\left(1 + A_s\right)\right] |\{\tau_i^z = 1\}\rangle$$

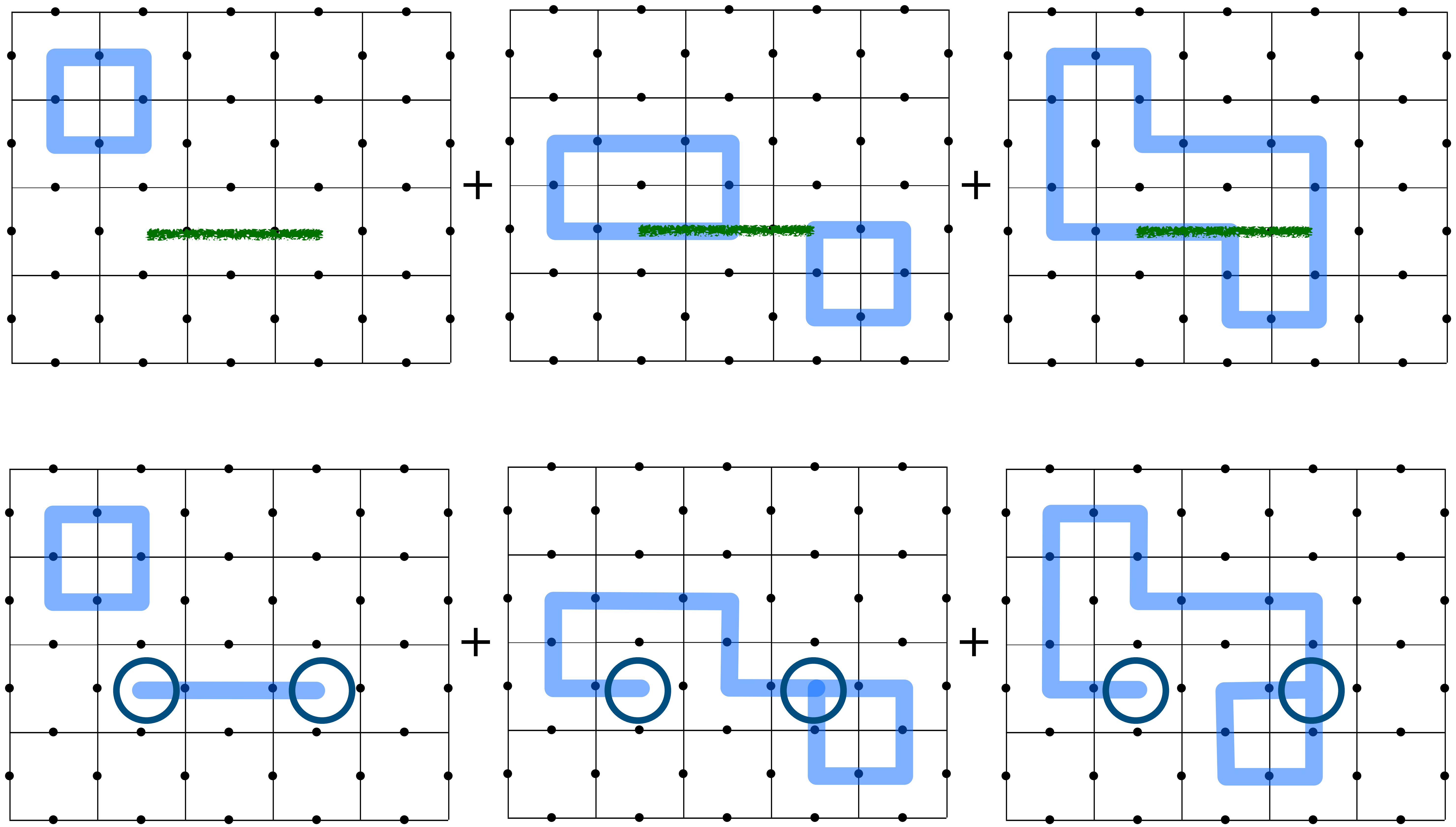
$$A_s = \left(\prod_{i\in +} \tau_i^x\right); B_p = \left(\prod_{i\in\square} \tau_i^z\right)$$

Why toric code ground state cannot be deformed into product states when gap remains open?

$|\Psi_g\rangle \propto$ ... $+$ ... $+$ ... $+\ldots$

τ^z basis, background $\tau^z = +1$

$\hat{O}_m = \otimes_{i \perp m-string}\, \tau_i^x$



$|\Psi_m\rangle \propto \hat{O}_m |\Psi_g\rangle \propto$ ... $+$ ... $+$ ...

Separated by an energy gap!

- Can you show that $|\Psi_m\rangle$ is an eigenstate? What if m-string form a loop?

Why toric code ground state cannot be deformed into product states when gap remains open?

Entangled states

$|\Psi_g\rangle$: configuration with **close loops** only.

$|\Psi_m\rangle$: configuration with **pairs** of open ends

Product states

$|\Psi\rangle$: All possible configurations, arbitrary number of open ends.

e.g. $\otimes_i (|\uparrow\rangle_i + |\downarrow\rangle_i)$

As long as the energy of the excited states and the ground state energy are different, the two states cannot form a linear superposition

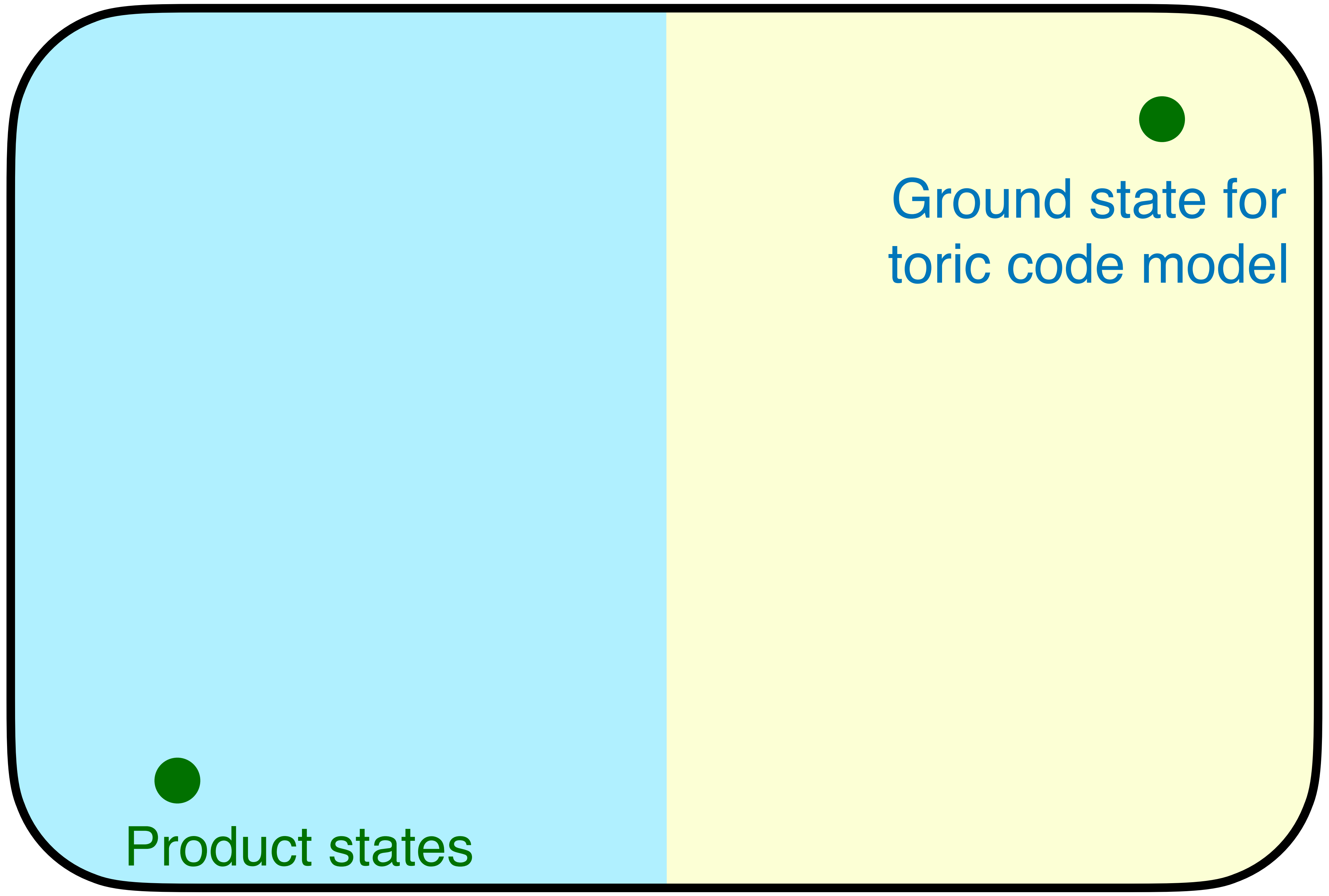
$\rightarrow$ Cannot relax the nontrivial constraints

$\rightarrow$ Cannot be a product state (No knowledge of what's going on after certain length scale)

The entanglement pattern for gapped quantum matter

Are there other ways to restrict the allowed deformation of entanglement pattern?

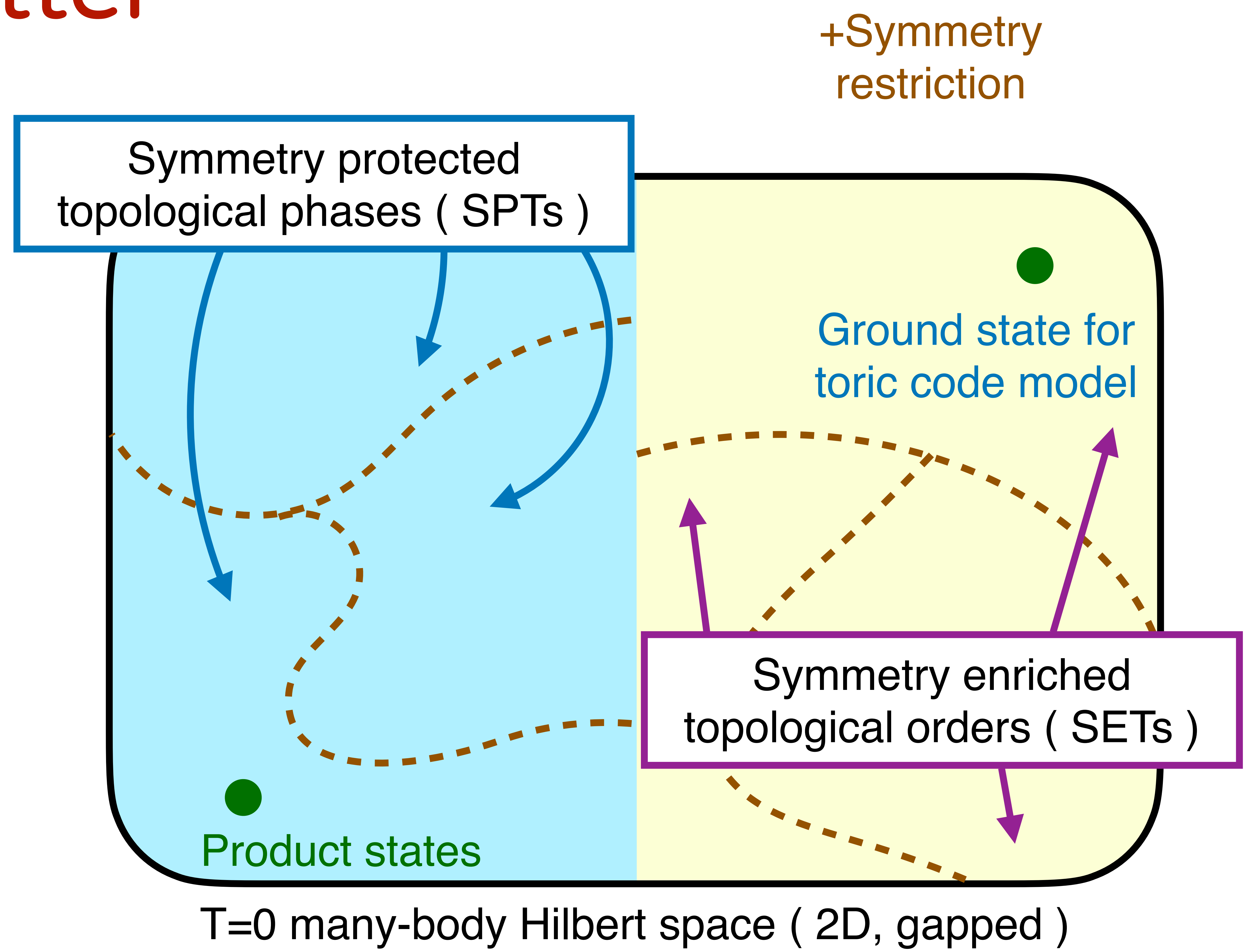
Yes, symmetry! How a quantum many-body state transform under symmetry?



T=0 many-body Hilbert space (2D, gapped)

The entanglement pattern for gapped quantum matter

- How tensor network helps us to understand entanglement pattern for more general cases?
- Detecting topological order from tensor network method, Prof. Ching-Yu Huang
- Projected Entangled Pair States, topological order, and topological spin liquids, Prof. Norbert Schuch's



M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010)
T. Senthil, Ann. Rev. Cond. Matt. (2015),
X. G. Wen, Rev. Mod. Phys. 89, 41004 (2017)

X. G. Wen, Phys. Rev., B65, 165113 (2002)
A. Essin and M. Hermele, Phys. Rev. B **87**, 104406 (2013)

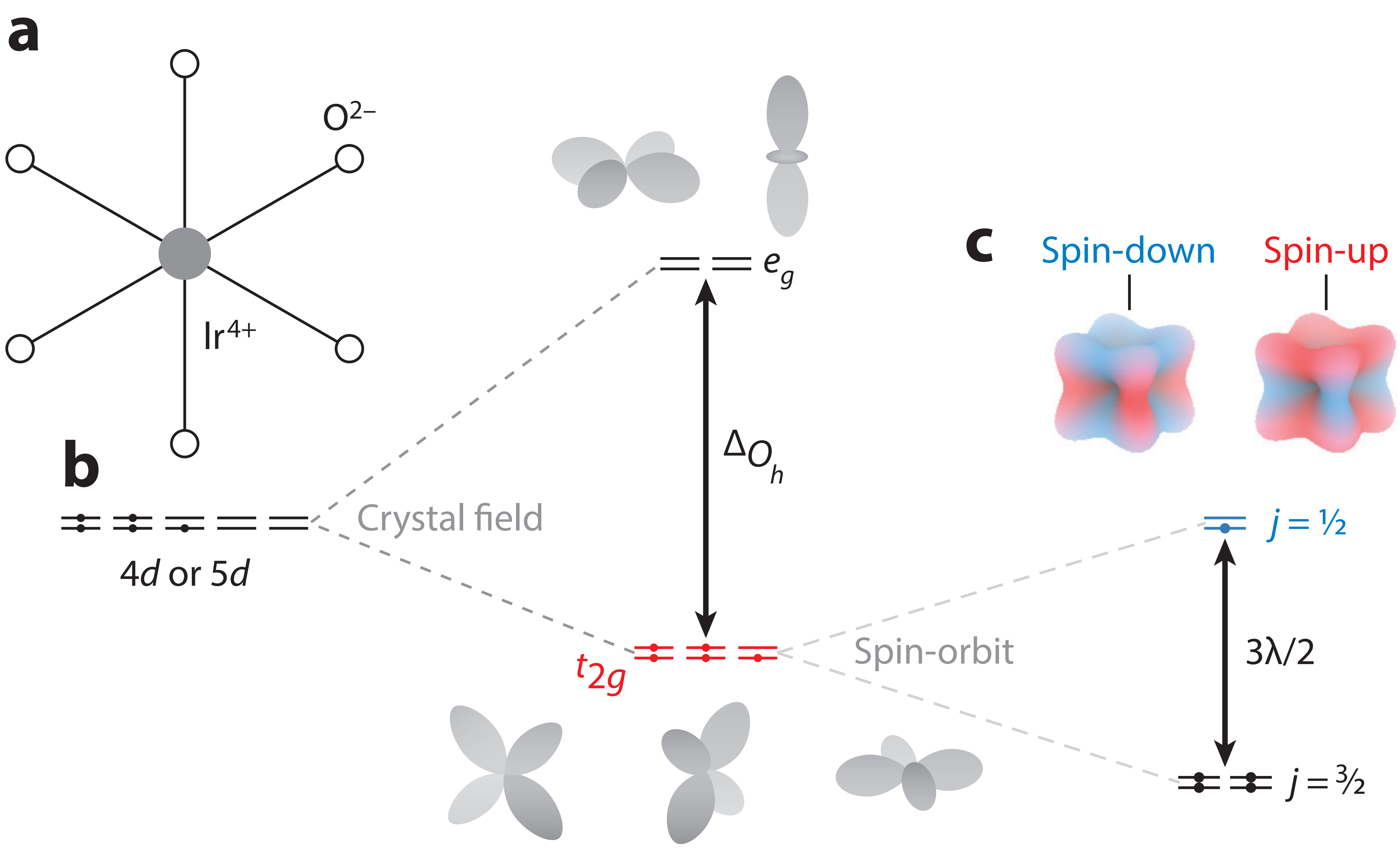
From the Hamiltonian to the state

- We discussed how entanglement is important. We also suggest tensor representation is a good language to describe the entangled wave function. However, how to get the ground state wave function? Especially for exponentially large Hilbert space.
- Usually we need to model a physical system first, then ask: what is the ground state wave function?

Physical systems $\leftrightarrow$ effective models

The model we just discussed seems very artificial ···

- We will focus on how to apply tensor network methods on the effective model.
- How to construct the effective model for a physical system is important but not discussed in the school due to the limit of time.

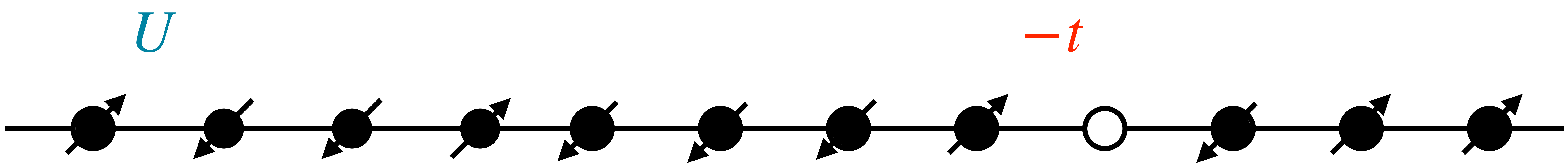


Jeffrey G. Rau, Eric Kin-Ho Lee, and Hae-Young Kee, Ann. Rev. Cond. Vol. 7:195-221 (2016)

Hubbard model

- Minimum model with correlation effects

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

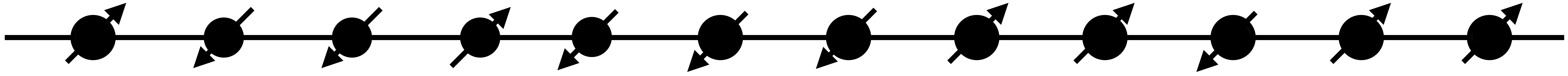


Pauli exclusion principle

Quantum Heisenberg model

- At half-filling, large U limit. The charge degrees of freedom is frozen. We have an effective model with spin degrees of freedom only. (Through degenerate perturbation theory)

$$H = -J \sum_{\langle i,j \rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j$$



Spin model

- Classical spin models and quantum spin models
  - The spin configuration is describe by number or states.
  - Classical model
    $$\{\sigma_i\} = \{\uparrow, \downarrow, \cdots, \uparrow\}$$
  - Quantum spin model
    $$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow, \uparrow, \cdots, \uparrow\rangle + |\downarrow, \downarrow, \cdots, \downarrow\rangle)$$

Transverse field Ising model

- $H = -J \sum_i \sigma_i^z \sigma_{i+1}^z - h \sum_i \sigma_i^x$
- $\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \cdots \otimes \mathscr{H}_N$
- $\sigma_i^z \sigma_{i+1}^z = \mathbf{1}_1 \otimes \cdots \otimes \sigma_i^z \otimes \sigma_{i+1}^z \otimes \cdots \otimes \mathbf{1}_N$

Exact diagonalization for quantum models and its limitation

- $\hat{H}$ is a $2^N \times 2^N$ complex matrix.
- To find ground state, we need to diagonalize $\hat{H}$
- To study the wave function evolution, we need to study operator like $e^{-i\hat{H}t}$.
- Scale exponentially with system size!
  - How much memory do we need to store a a $2^N \times 2^N$ complex matrix for N=10, 20, 30?

Advantages for tensor network methods

- Variational wave function encapsulate information of entanglement efficiently.
- Can use density matrix renormalization group (DMRG) to get the ground state efficiently.
- DMRG has no sign problem! Can be used to study frustrated systems, spin-orbit coupled systems, etc.

- (Day 1) tensor network for ground states: MPS, MPO and DMRG. Prof. Chia-Min Chung's talk and tutorial!

Time-evolution of correlated many-body systems

- Exact diagonalization gives the full information. We can have $|\psi(t)\rangle$ for arbitrary t.
- However, we usually cannot study a system beyond ~20 spins.
  - tensor network method
    - TEBD : approximate the time-evolution operator, $e^{-i\hat{H}dt}$, using quantum gates.
    - TDVP : constrain the time evolution to a specific manifold of matrix-product states.

Advantages for tensor network methods

- When the wave function evolve as a function of time, how entanglement is build via unitary evolution?
- How the understanding of entanglement pattern helps us developing physical picture for correlated quantum many-body dynamics?

- (Day 3) tensor network for dynamics: TEBD, TDVP.
  Mr. Kai-Hsin Wu, Prof. Ying-Jer Kao, Prof. Ian McCulloch's talk and tutorial.

Tensor networks for classical statistical mechanics

Statistical mechanics

- The microscopic theory behind thermodynamics (macroscopic theory).
- Renormalization group: relate coupling constants at different scales!
- The RG equation and fixe points.

Renormalization group equation

- renormalization group (RG) prescription in tensor space.
- tensor RG equation
- fix-point tensor

- (Day 2) tensor network and statistical mechanics.
- A textbook implementation of the real-space renormalization group, Prof. Naoki Kawashima
- Renormalization of the Tensor Network for Classical Models, Prof. Pochung Chen

2022 summer school for
physics and tensor-network methods in correlated systems

- Date: 29-31, August, 2022
- Venue: R620, Physics Building, NTHU

- Day 1&2: MPS and MPO (Finding ground states, SPTs, SETs)
- Day 2: Tensor renormalization group (Connection with statistical mechanics)
- Day 3: Dynamics and tensor network (Finding how a state evolve as a function of time)