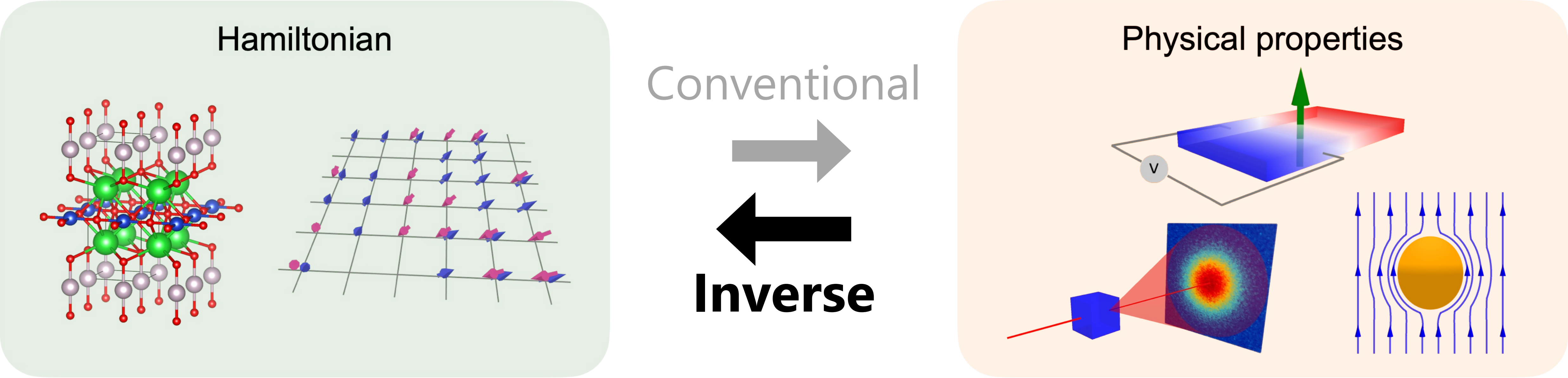


自動微分を用いた欲しい性質をもつハミルトニアンの逆設計:
バンドトポロジーと量子エンタングルメントへの応用

Koji Inui, The University of Tokyo

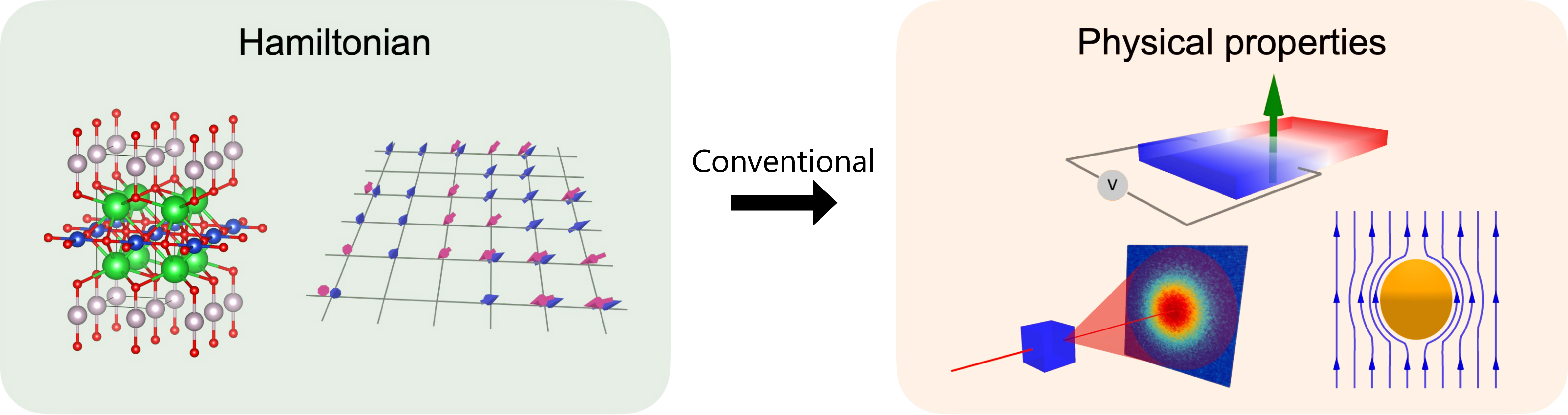
K. Inui, and Y. Motome, Commun. Phys. **6**, 37 (2023).
https://github.com/koji-inui/automatic-hamiltonian-design

2023/12/14 DLAP@上智大学

Table of contents

Inverse problem in materials science

Conventional theoretical approach

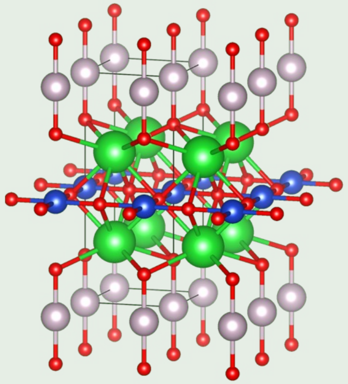


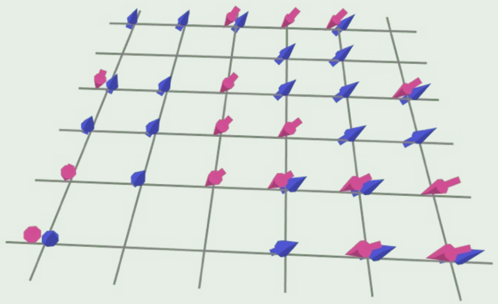
1. Construct the Hamiltonian based on phenomenology or first principles
2. Tune the parameters in the Hamiltonian by calculating physical properties of interest

Inverse problem in materials science

Conventional theoretical approach

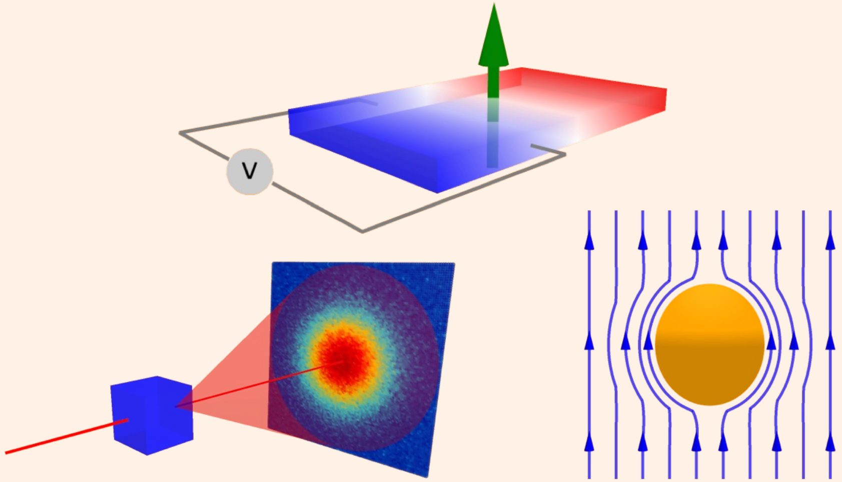
Hamiltonian





Conventional →

Physical properties



Parameter space

Hopping terms t_1, t_2, t_3 ...
Interaction terms U, V_1, V_2 ...
Temperature T
Magnetic field $H(\omega)$
Spin-orbit coupling λ
Lattice constant, a
Filling N
...

$\otimes$

Anisotropy
Site dependence
Layer dependence
Orbital dependence

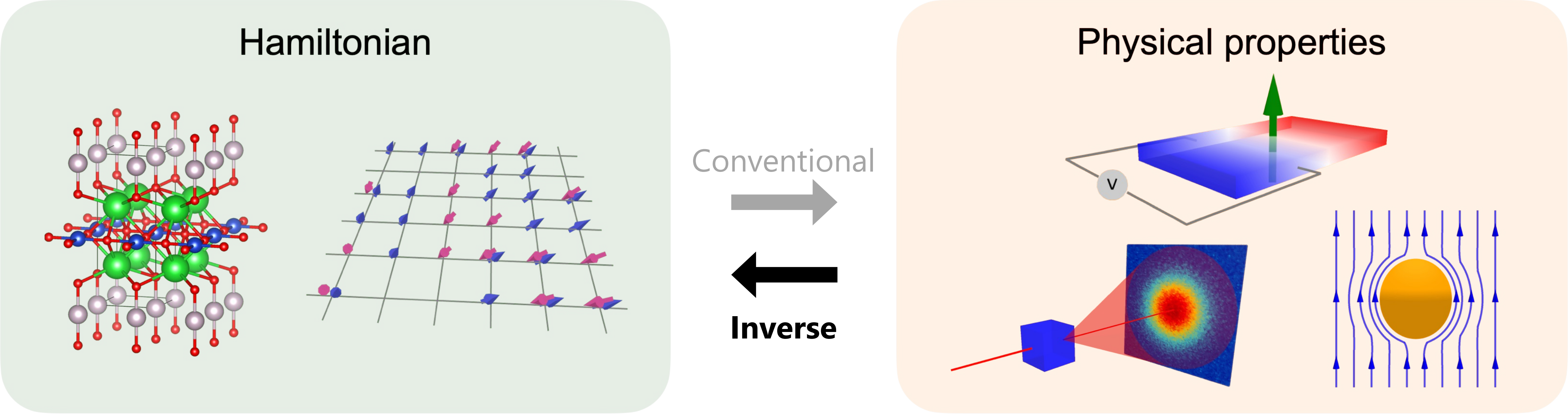
Construct a simple model
based on intuition and feedback

Calculate the physical properties of interest

Laborious to explore !

Inverse problem in materials science

Inverse approach



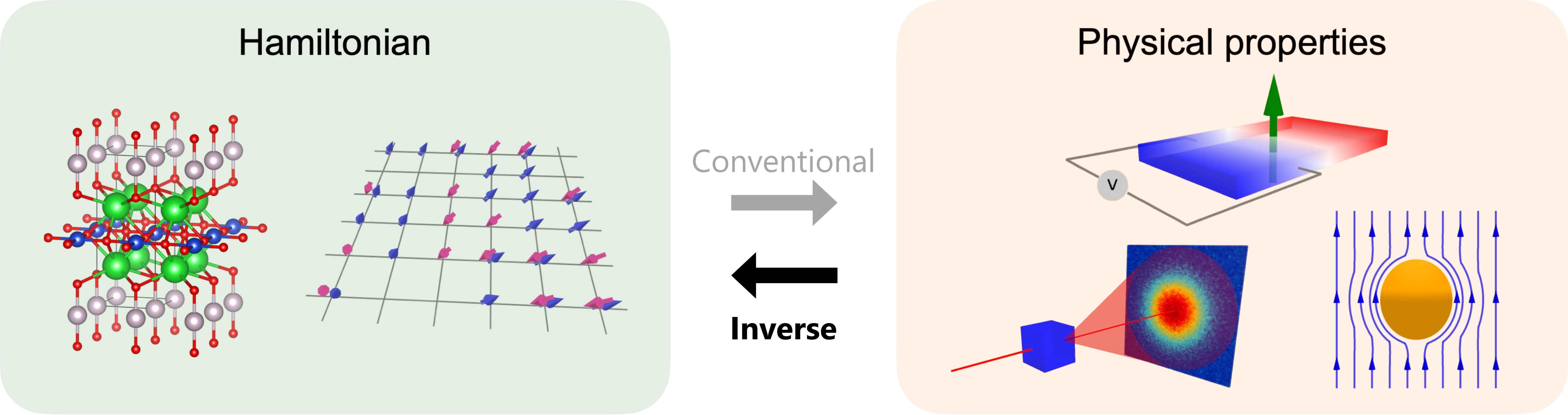
1. Prepare the desired physical properties
2. Construct a Hamiltonian to realize them directly

Benefits

- It can bypass the laborious exploration

Inverse problem in materials science

Inverse approach

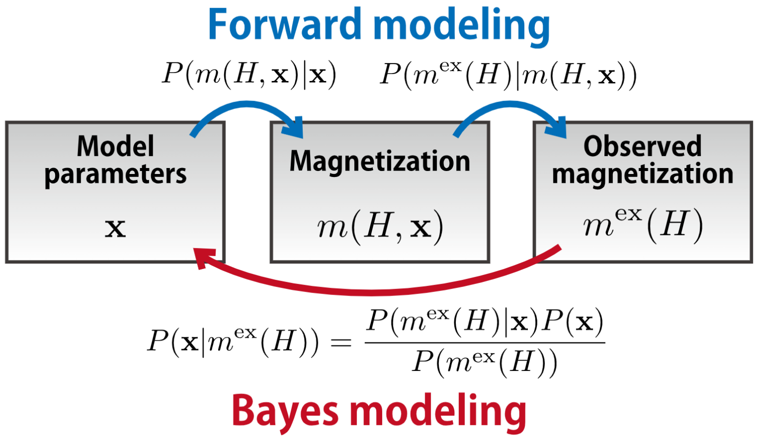


1. Prepare the desired physical properties
2. Construct a Hamiltonian to realize them directly

Benefits
- It can bypass the laborious exploration
- It can reach the qualitatively new principles and materials

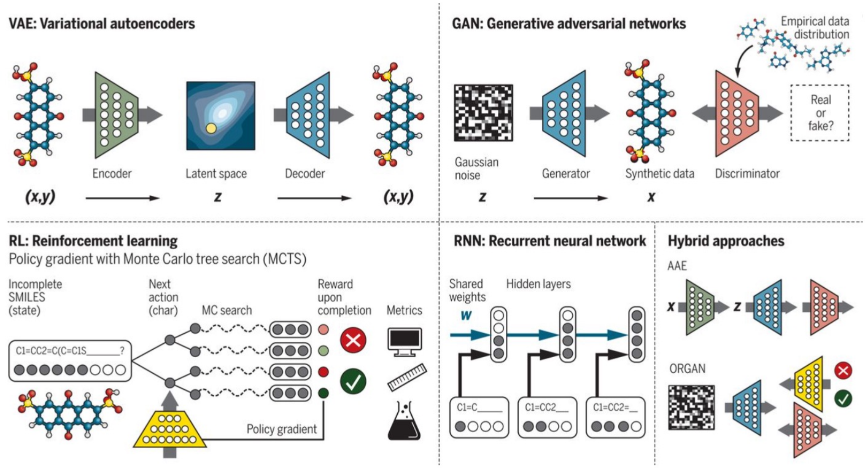
Previous studies to estimate Hamiltonians

Bayesian optimization



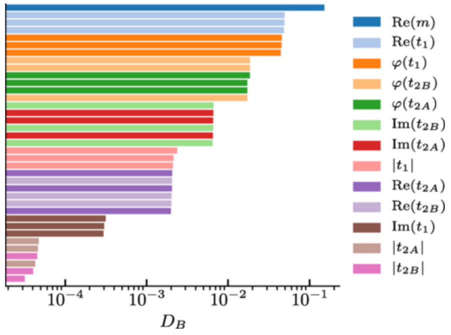
R. Tamura and K. Hukushima, Phys. Rev. B **95** (2017) 164407.
K. Obinata, S. Katakami, Y. Yue, and M. Okada, J. Phys. Soc. Jpn. **88** (2019) 064802.

Generative models



B. Sanchez-Lengeling and A. Aspuru-Guzik, Science **361** (2018) 360.

Machine learning



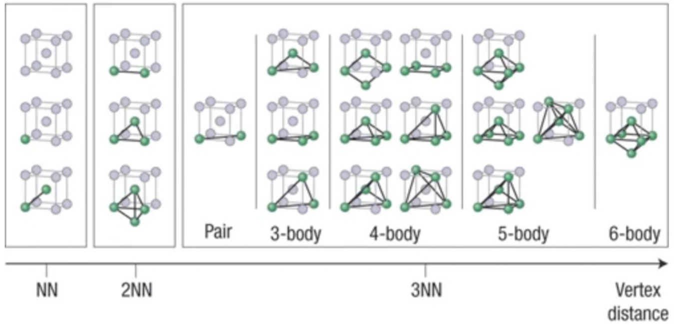
T. Mertz and R. Valenti, Phys. Rev. Research **3** (2021) 013132.

Perturbation theory

$$c_j \to \quad c_j - \alpha \frac{\partial \mathrm{Cost}(\{c_j\})}{\partial c_j}$$

H. Fujita, Y. O. Nakagawa, S. Sugiura, and M. Oshikawa, Phys. Rev. B **95** (2017) 164407.

Genetic algorithm



G. L. W. Hart *et al.*, Nat. Mater. **4** (2005) 391.
A. Ajoy and P. Cappelaro, Phys. Rev. Lett. **110** (2013) 220503.

- Difficulty in learning because of the cost of collecting data and computation
- The validity of the results is not guaranteed
- Limitations on the models and physical quantities that can be applied

Research Purpose

Develop a versatile framework to
discover Hamiltonians with the desired properties

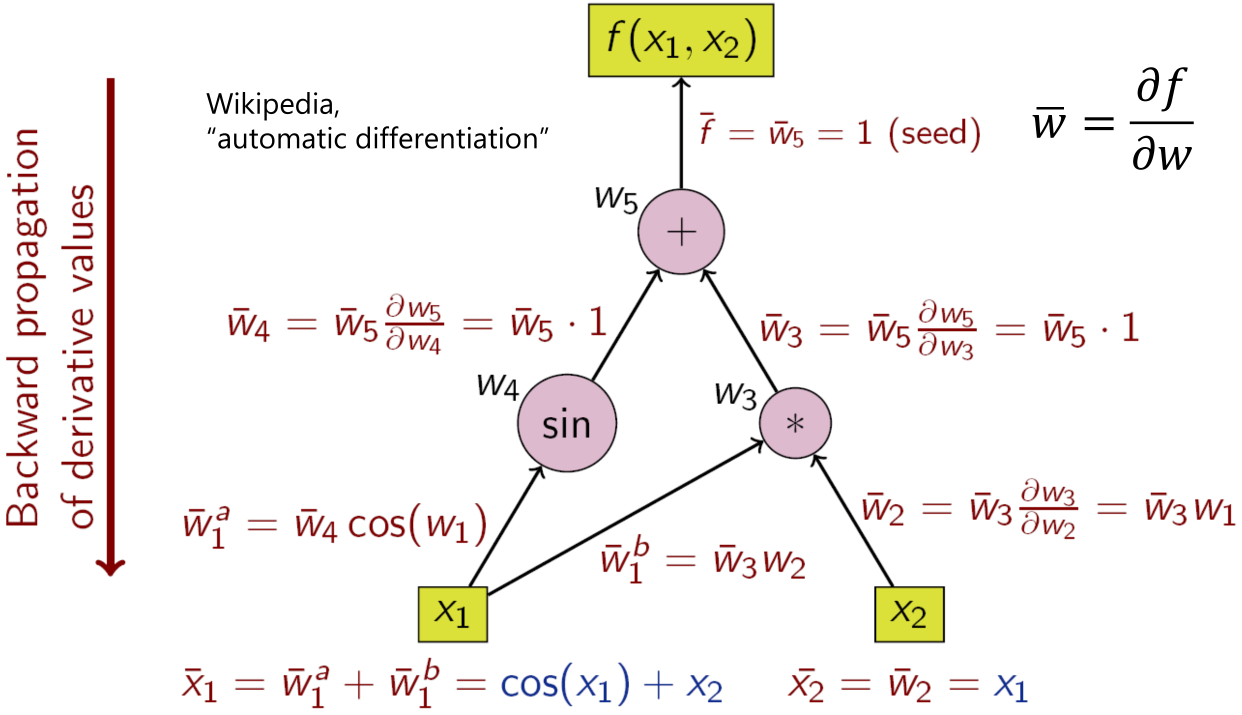
↓

Proof of concept of the framework through application to
anomalous Hall effect and quantum entanglement.

Framework

Automatic differentiation (Backpropagation)

Analytical derivatives of (almost) any function can be computed by applying the chain rule



Software libraries

PyTorch

jax.numpy.linalg.eigh

```
jax.numpy.linalg.eigh(a, UPLO=None, symmetrize_input=True)
```

Return the eigenvalues and eigenvectors of a complex Hermitian

While it is used as backpropagation in deep learning, it can be applied to versatile applications.

Some studies use over a trillion parameters

W. Fedus *et al.*, J. mach. Learn. Res. **23** (2022) 120.

(This framework does NOT use neural networks)

Framework

Prepare a Hamiltonian $\mathscr{H}(\boldsymbol{\theta})$ with parameters $\boldsymbol{\theta}$

↓

Calculate an objective function $L(\boldsymbol{\theta})$ representing desired physical properties

↓

Calculate the derivatives $\partial L(\boldsymbol{\theta})/\partial\boldsymbol{\theta}$ by using automatic differentiation

↓

Update $\boldsymbol{\theta}$ to minimize $L(\boldsymbol{\theta})$ by using $\partial L(\boldsymbol{\theta})/\partial\boldsymbol{\theta}$

↓

Obtain the Hamiltonian $\mathscr{H}(\boldsymbol{\theta}_{\mathrm{opt}})$ satisfying the desired physical properties

Repeat until convergence

Numerical method

Diagonalization · Hartree-Fock · Band calculation

Kohn-Sham eq. · DMFT · …

Example) $L(\boldsymbol{\theta}) = -\langle P(\boldsymbol{\theta})\rangle$

$$L(\boldsymbol{\theta}) = \sum_{\boldsymbol{k}} \left(S_{\mathrm{target}}(\boldsymbol{k}) - S(\boldsymbol{k},\boldsymbol{\theta})\right)^2$$

Many parameters can be optimized simultaneously

⬇

Possibility to discover unprecedented Hamiltonians beyond human intuition

Framework

Neural networks

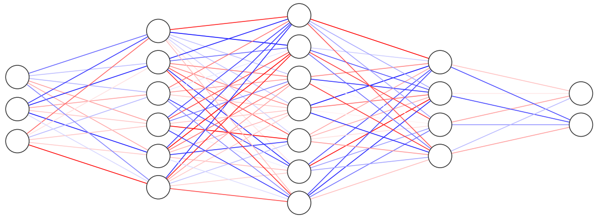
Fixed

Data

Parametrized

Parameters $\boldsymbol{\theta}$

Neural network model

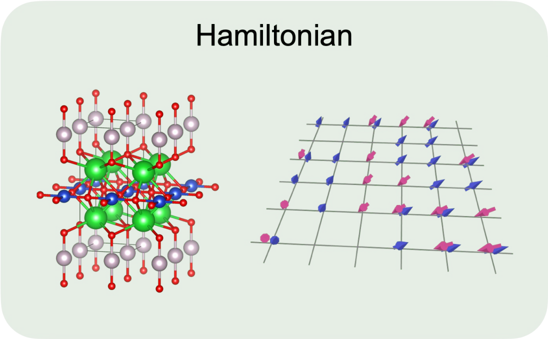


Objective function

Example)

$$L(\boldsymbol{\theta}) = \frac{1}{N}\sum_x \left(y^x_{\mathrm{pred}}(\boldsymbol{\theta}) - y^x_{\mathrm{ans}}\right)^2$$

Our framework



Parametrized

Hamiltonian

$\mathcal{H}(\boldsymbol{\theta})$ ← Parameters $\boldsymbol{\theta}$

Diagonalization	Hartree Fock
Band calculation	DMFT
Perturbation	…

Fixed

Numerical method

Example)

$$L(\boldsymbol{\theta}) = -\langle P(\boldsymbol{\theta}) \rangle$$

Objective physical properties

Result 1
Rediscovery of the Haldane model

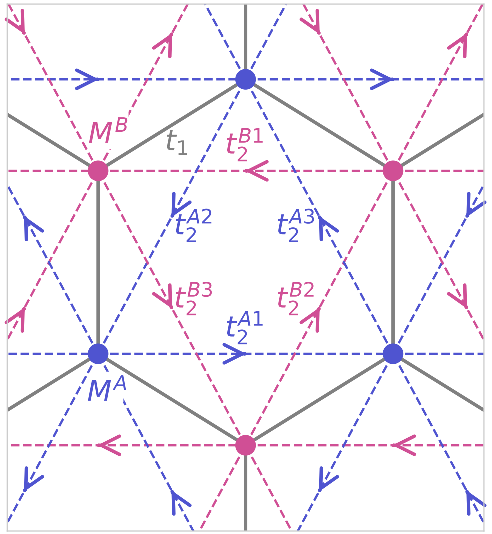
Tight binding model on honeycomb lattice

Two sublattices

Maximize anomalous Hall conductivity σ_{xy}

$$\mathcal{H} = \sum_i M^a c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_1 c_i^\dagger c_j + \sum_{\langle\langle i,j \rangle\rangle} t_2^d c_i^\dagger c_j,$$

$(d \in \{A1, A2, A3, B1, B2, B3\})$



$\boldsymbol{k} = 100\times100$

t_1 is fixed to 1. M^a $(a \in \{A, B\})$

$t_2^d = \sigma(r^d)\exp(i\phi^d) \quad 0 < |t_2^d| < 1$

➡ $\boldsymbol{\theta} = \{M^A, M^B, \{r^a\}, \{\phi^a\}\}$: 14 parameters

Objective function : $L(\boldsymbol{\theta}) = -\sigma_{xy}(\boldsymbol{\theta})$

$$\sigma_{xy} = -\frac{\Omega}{N_{\boldsymbol{k}}} \sum_{m,n,\boldsymbol{k}} \left(f(E_{\boldsymbol{k}n}, \beta) - f(E_{\boldsymbol{k}m}, \beta)\right) \mathrm{Im}\left(\frac{\langle \boldsymbol{k}n | (\frac{\partial \mathcal{H}}{\partial k_y}) | \boldsymbol{k}m \rangle \langle \boldsymbol{k}m | (\frac{\partial \mathcal{H}}{\partial k_x}) | \boldsymbol{k}n \rangle}{(E_{\boldsymbol{k}n} - E_{\boldsymbol{k}m})^2 + i\delta} \right),$$

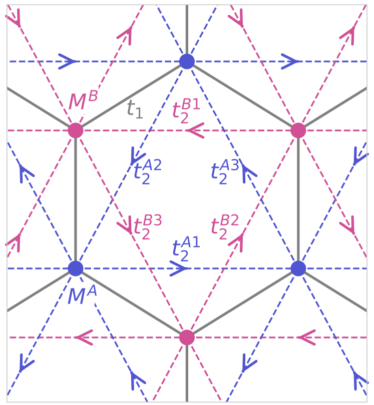
Set finite temperature to avoid $\frac{\partial \sigma_{xy}}{\partial \boldsymbol{\theta}}$ becomes 0

Tight binding model on honeycomb lattice

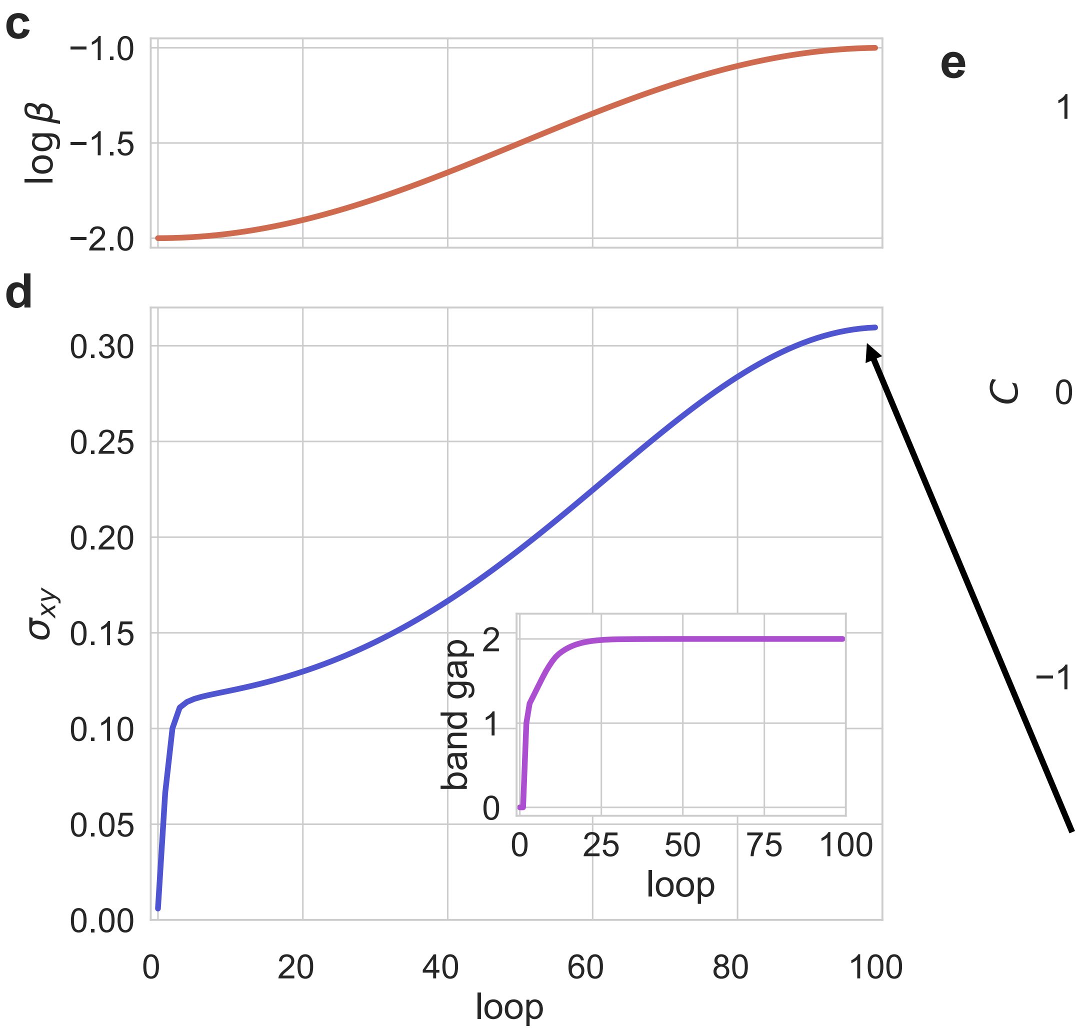
Two sublattices

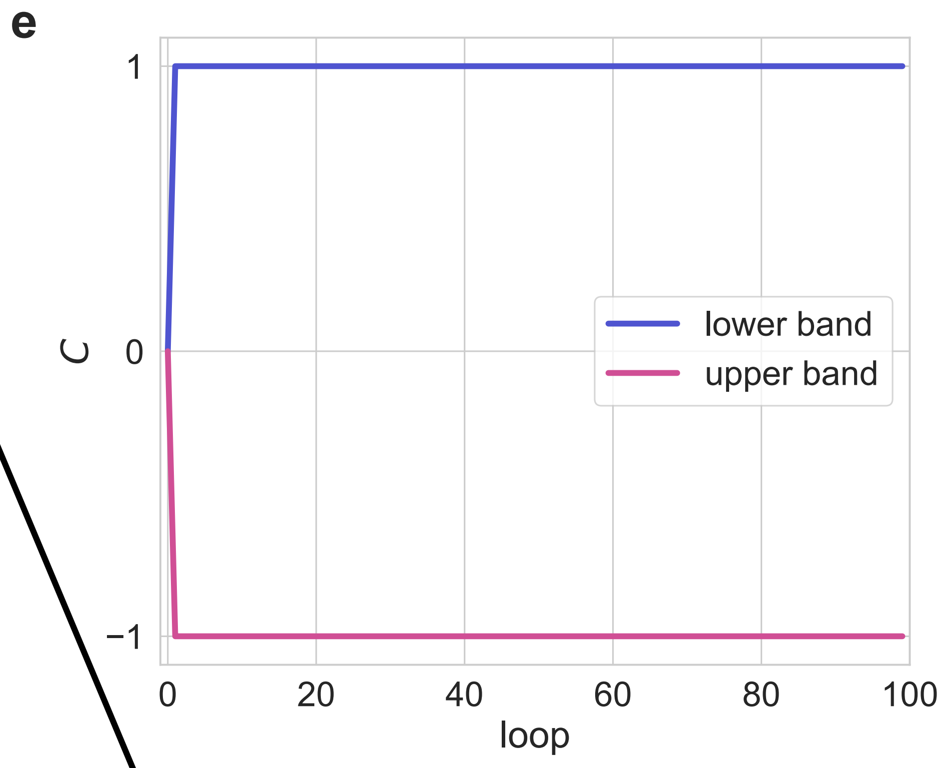
Increasing σ_{xy} automatically changes the Chern numbers to +1 and -1

$$\mathcal{H} = \sum_i M^a c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_1 c_i^\dagger c_j + \sum_{\langle\langle i,j \rangle\rangle} t_2^d c_i^\dagger c_j,$$



$$\boldsymbol{\theta} = \{M^A, M^B, \{r^a\}, \{\phi^a\}\}$$





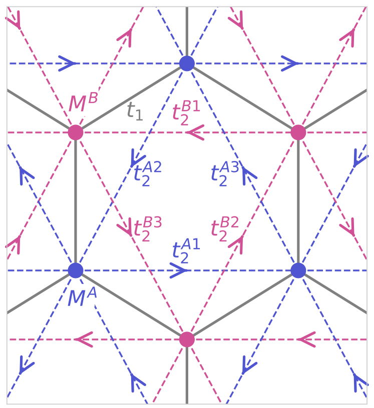
※ $\sigma_{xy} < 1$ due to finite temperature

Tight binding model on honeycomb lattice

Two sublattices

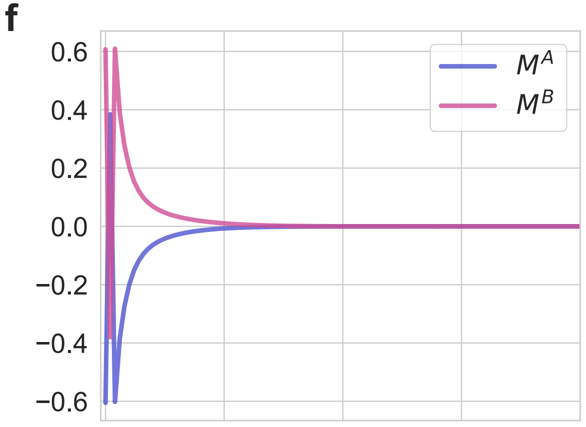
Optimized parameters correspond to the center of the $C = 1$ phase in the Haldane model

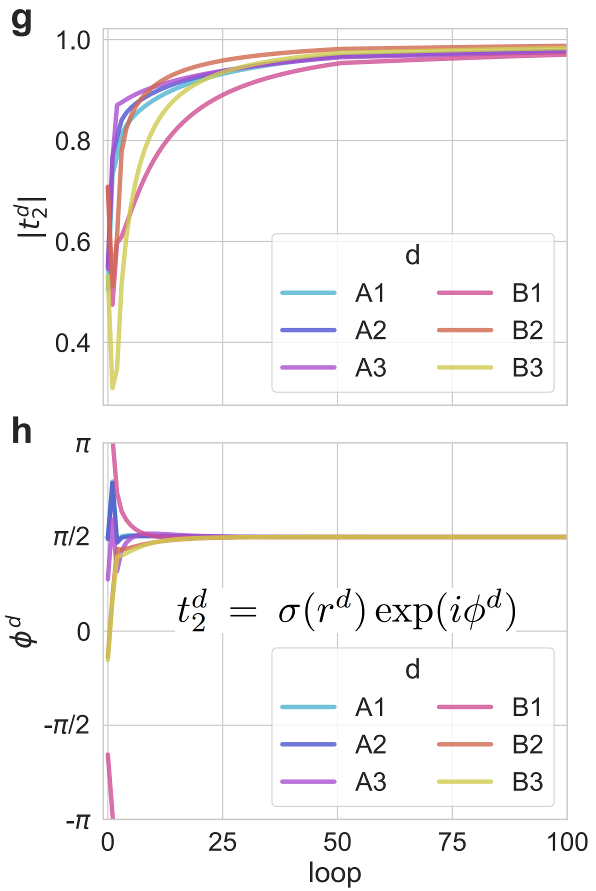
$$\mathcal{H} = \sum_i M^a c_i^\dagger c_i + \sum_{\langle i,j \rangle} t_1 c_i^\dagger c_j + \sum_{\langle\langle i,j \rangle\rangle} t_2^d c_i^\dagger c_j,$$



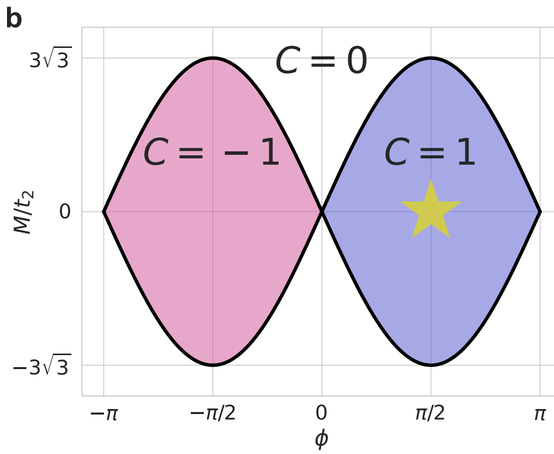
$$\boldsymbol{\theta} = \{M^A, M^B, \{r^a\}, \{\phi^a\}\}$$

$$L(\boldsymbol{\theta}) = -\sigma_{xy}(\boldsymbol{\theta})$$





The phase diagram of the Haldane model



Different initial conditions also converge to the same state
→ Our framework automatically rediscover the Haldane model

Result 2

Discovery of a new Hamiltonian on a triangular lattice

Tight binding model on triangular lattice

Four sublattices

Maximize anomalous Hall conductivity σ_{xy}

$\boldsymbol{k} = 100\times100$

$$\mathcal{H} = \sum_{\langle i,j\rangle} t_1^{ij} c_i^\dagger c_j + \sum_{\langle\langle i,j\rangle\rangle} t_2^{ij} c_i^\dagger c_j + \sum_{\langle\langle\langle i,j\rangle\rangle\rangle} t_3^{ij} c_i^\dagger c_j$$

$$t_1^{ij} = \exp(i\phi_1^{ij})$$

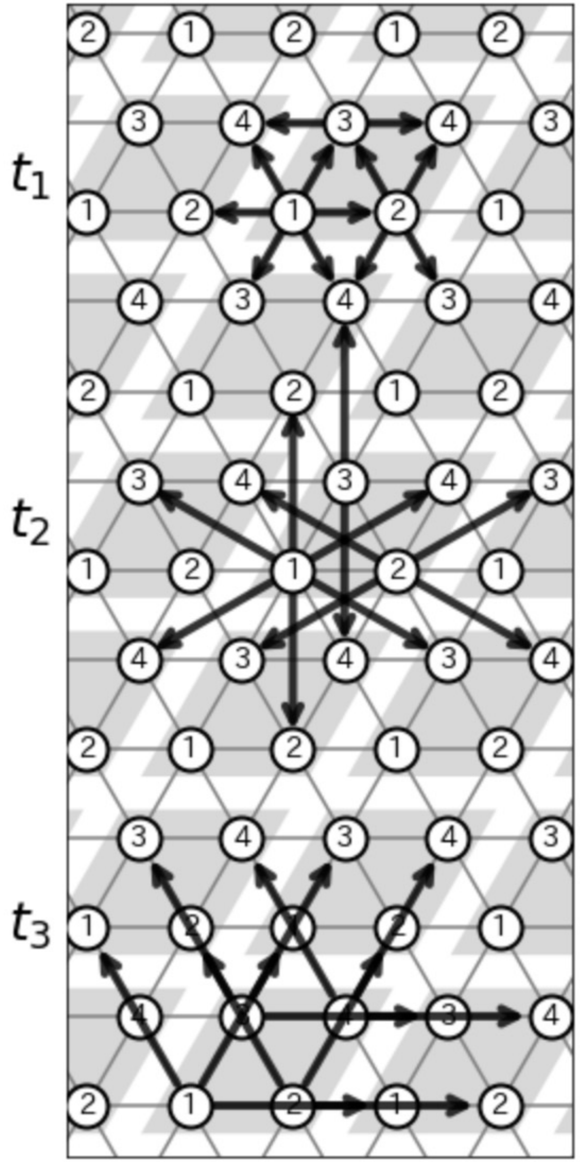
$$t_m^{ij} = \sigma(r_m)\exp(i\phi_m^{ij}) \text{ for } m \in \{2,3\}$$

$$\boldsymbol{\theta} = \{r_2, r_3, \{\phi_1^{ij}\}, \{\phi_2^{ij}\}, \{\phi_3^{ij}\}\}$$: 38 parameters

$$L(\boldsymbol{\theta}) = -\sigma_{xy}(\boldsymbol{\theta})$$

Fixed to half-filling

$$\sigma_{xy} = -\frac{\Omega}{N_{\boldsymbol{k}}} \sum_{m,n,\boldsymbol{k}} (f(E_{\boldsymbol{k}n},\beta) - f(E_{\boldsymbol{k}m},\beta))\,\mathrm{Im}\left(\frac{\langle \boldsymbol{k}n|(\frac{\partial\mathcal{H}}{\partial k_y})|\boldsymbol{k}m\rangle\langle \boldsymbol{k}m|(\frac{\partial\mathcal{H}}{\partial k_x})|\boldsymbol{k}n\rangle}{(E_{\boldsymbol{k}n} - E_{\boldsymbol{k}m})^2 + i\delta}\right),$$

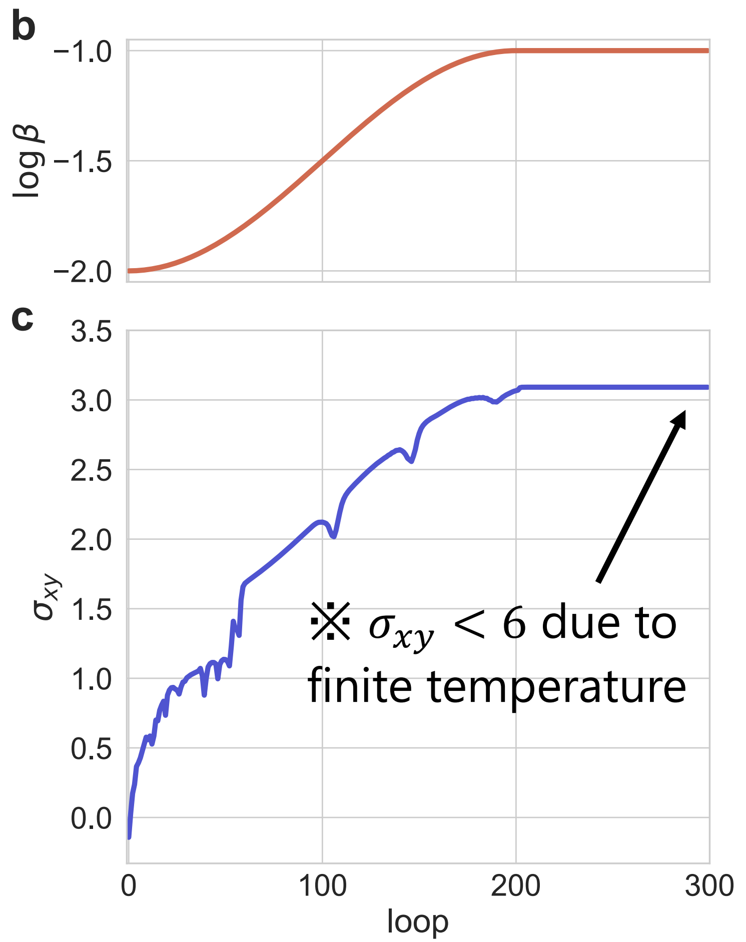


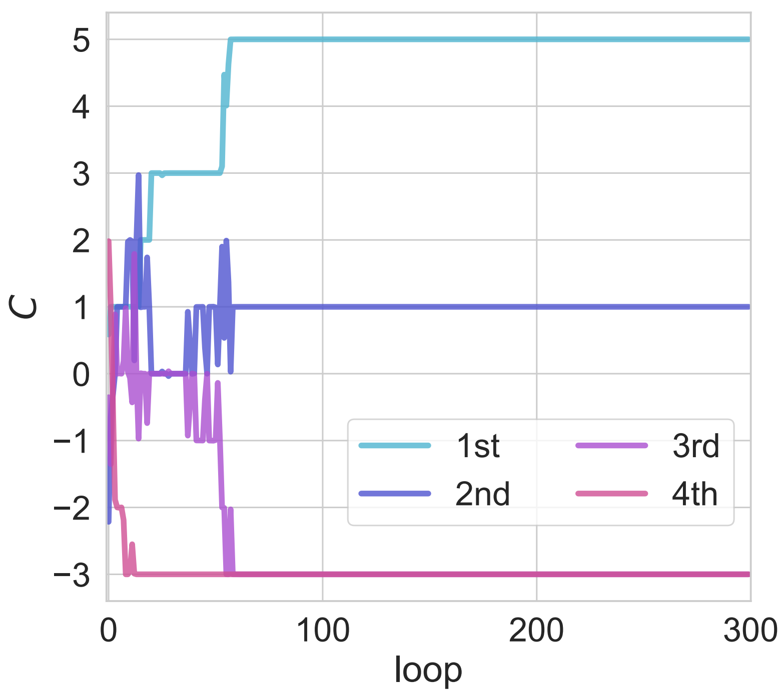
Tight binding model on triangular lattice

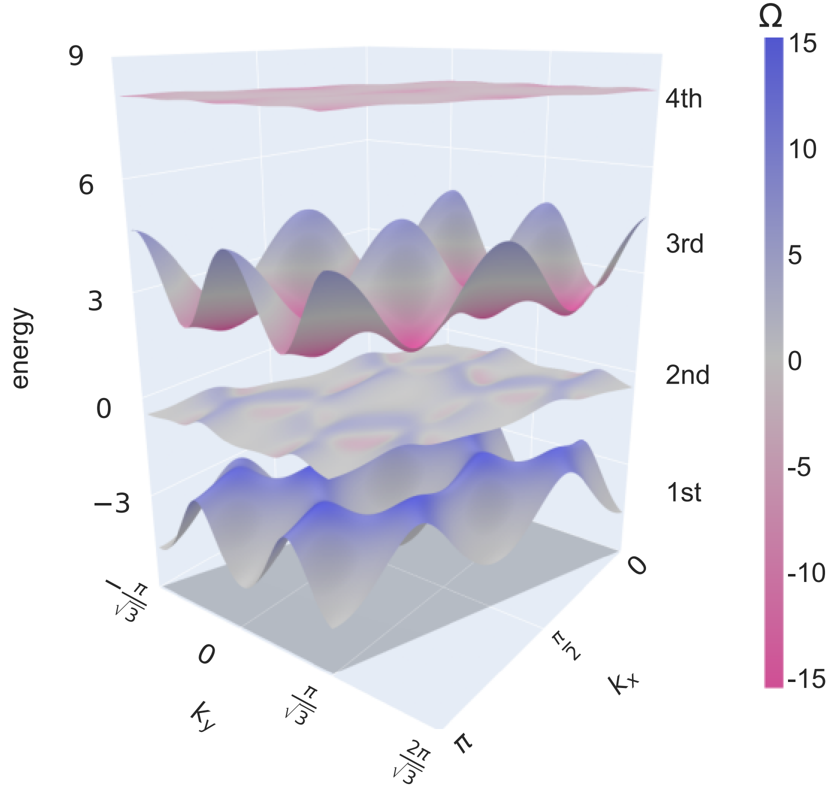
Four sublattices

Increasing σ_{xy} automatically changes the Chern numbers to [5,1,-3,-3]

$$\mathcal{H} = \sum_{\langle i,j \rangle} t_1^{ij} c_i^\dagger c_j + \sum_{\langle\langle i,j \rangle\rangle} t_2^{ij} c_i^\dagger c_j + \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} t_3^{ij} c_i^\dagger c_j \qquad L(\boldsymbol{\theta}) = -\sigma_{xy}(\boldsymbol{\theta})$$







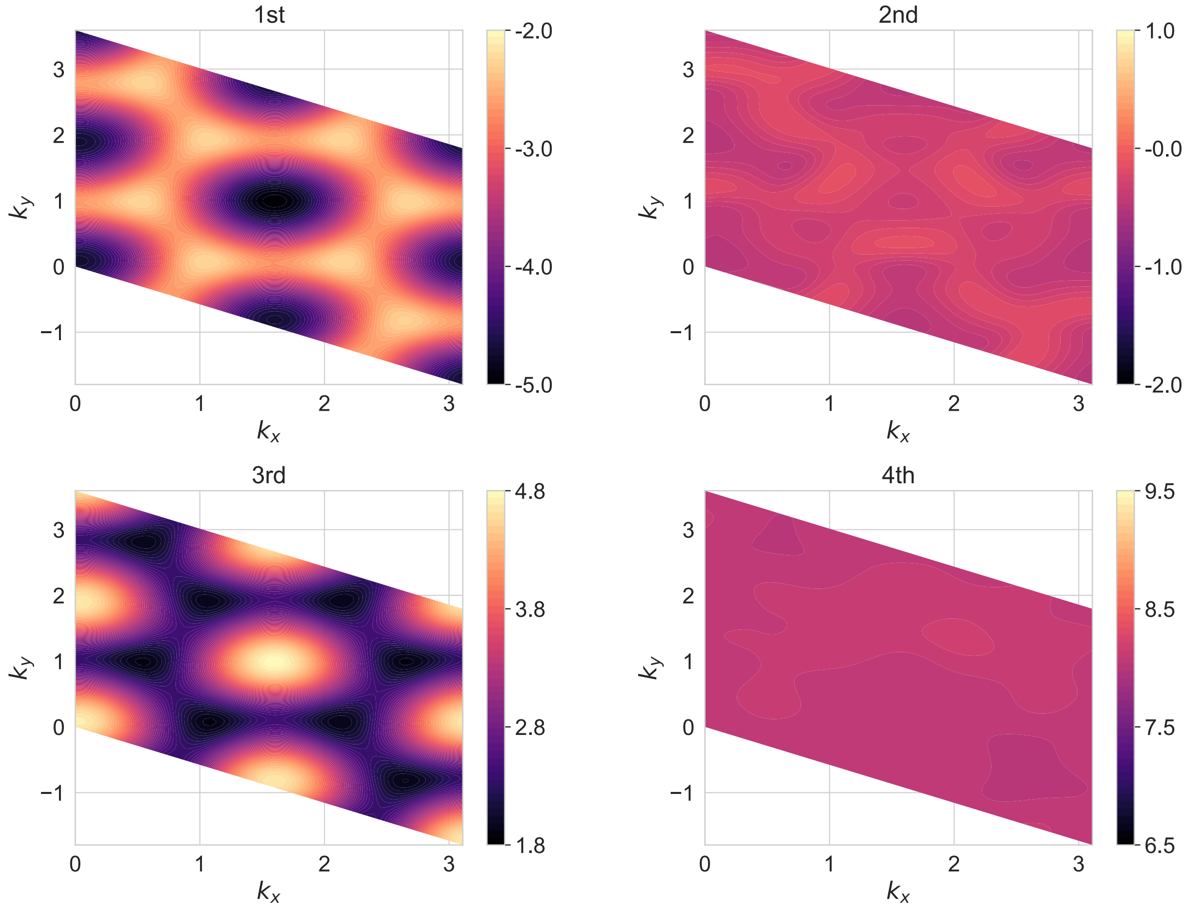
The total Chern number has a large value of 6

Tight binding model on triangular lattice

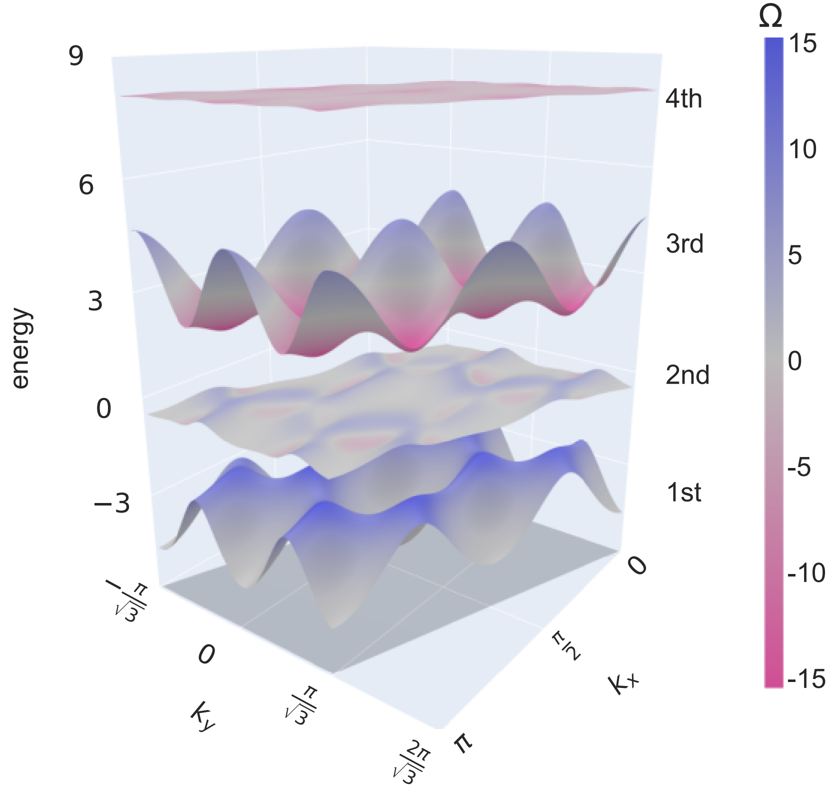
Four sublattices

(approximately) three-fold rotational symmetry appears automatically

$$\mathcal{H} = \sum_{\langle i,j \rangle} t_1^{ij} c_i^\dagger c_j + \sum_{\langle\langle i,j \rangle\rangle} t_2^{ij} c_i^\dagger c_j + \sum_{\langle\langle\langle i,j \rangle\rangle\rangle} t_3^{ij} c_i^\dagger c_j \qquad L(\boldsymbol{\theta}) = -\sigma_{xy}(\boldsymbol{\theta})$$



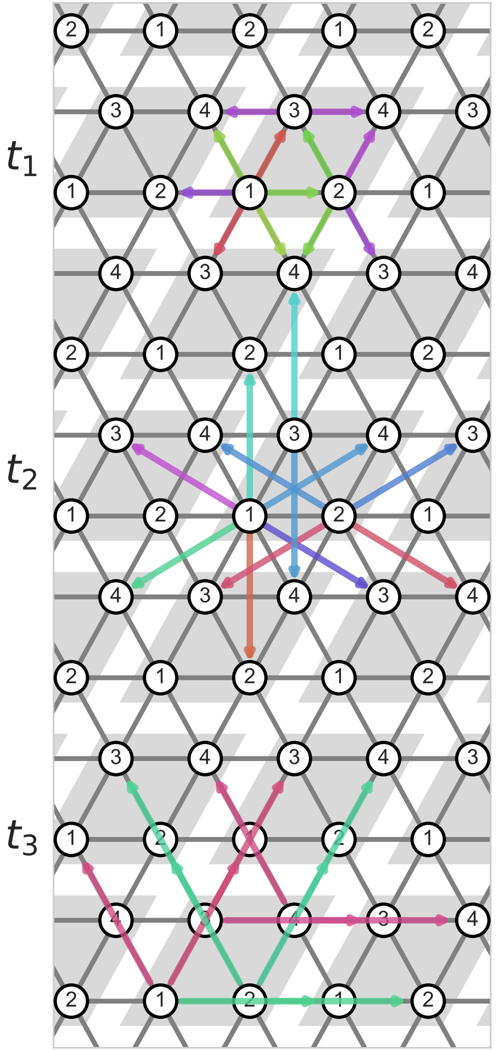
Top view



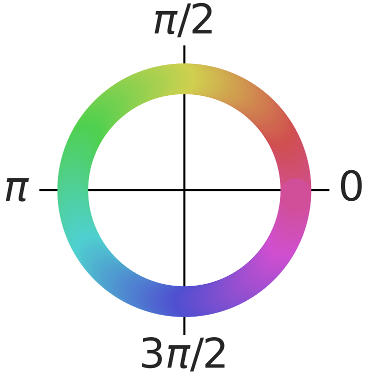
Tight binding model on triangular lattice

Four sublattices

Fictitious flux takes regular values

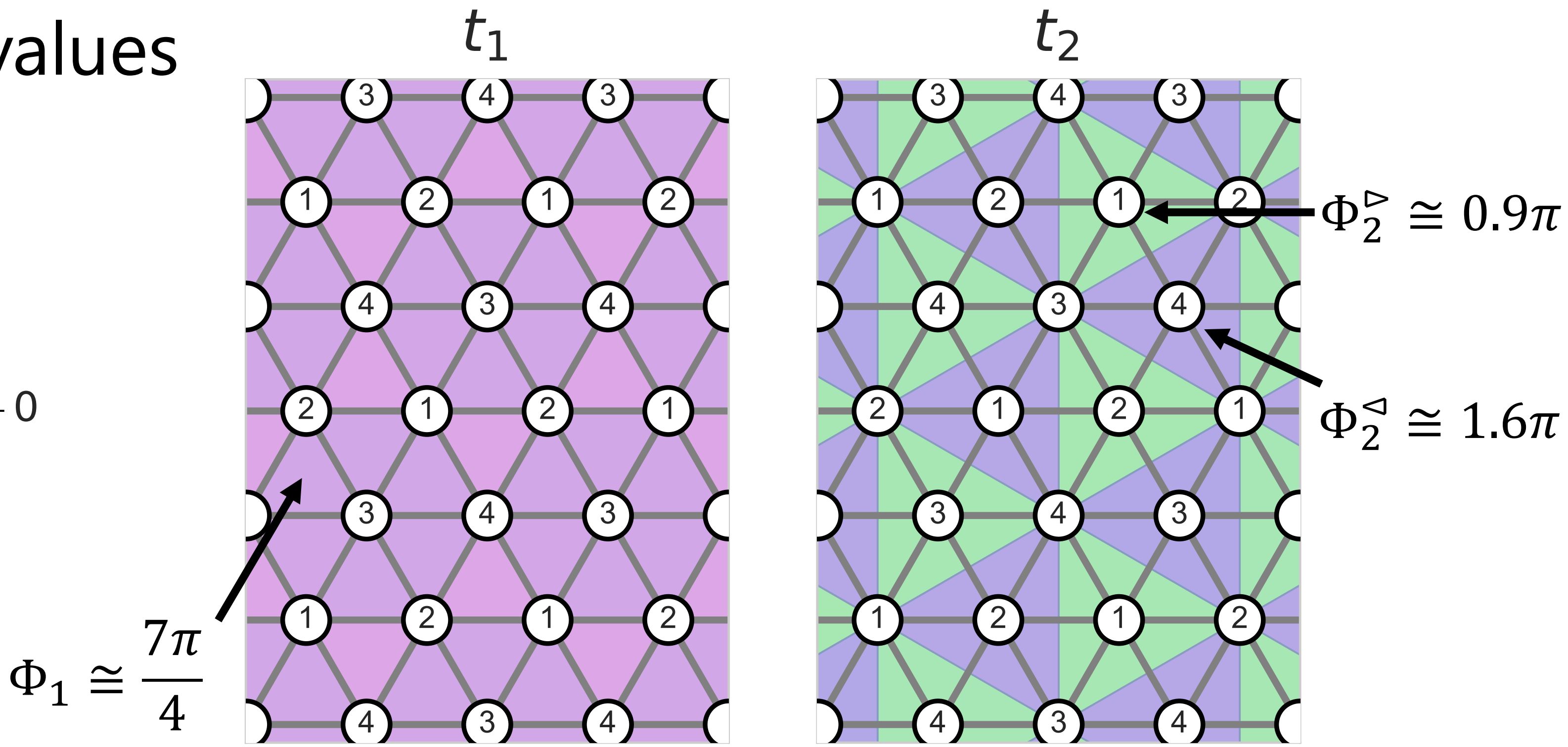


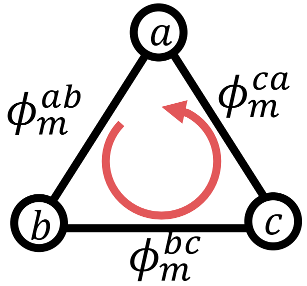
ϕ_m^{ij}, Φ_m



$|t_2|, |t_3| = 1$

$\phi_{ij}^3 \in (0, \pi)$





fictitious flux

$$\Phi_m = \sum \phi_m^{ij}$$

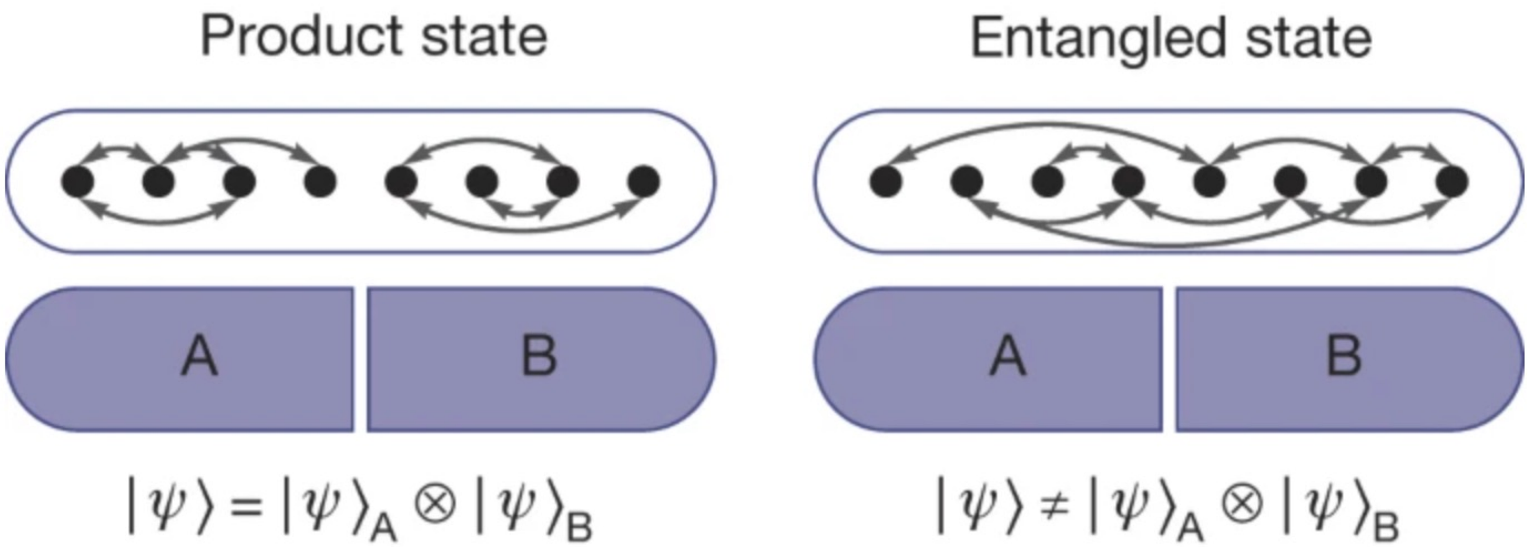
As far as we know, such a Hamiltonian has never been reported.
This proves that our framework can discover new Hamiltonians.

Result 3

Application to quantum entanglement in many-body systems

Entanglement entropy (EE)

The measure of quantum entanglement in quantum many-body systems.



R Islam *et.al.*, Nature **528**, 77 (2015)

$S_A = 0$ $\qquad$ $S_A > 0$

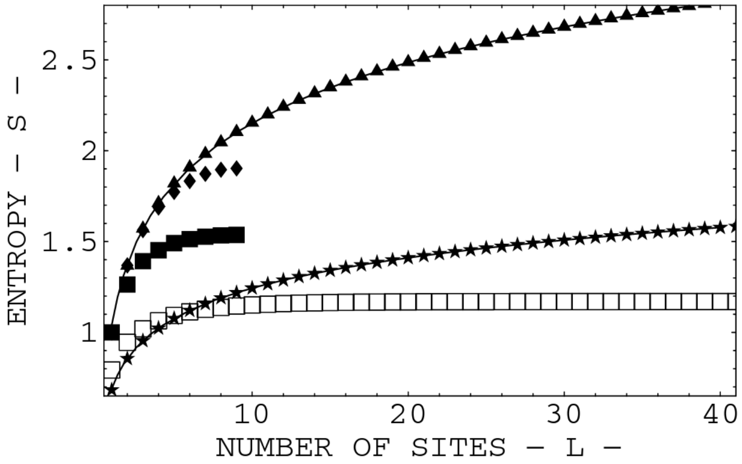
$$\rho = |\psi\rangle\langle\psi| \qquad \rho_A = \mathrm{Tr}_B \rho$$

Entanglement entropy $\quad S_A = -\mathrm{Tr}_A \rho_A \log \rho_A$

Entanglement entropy in various quantum phenomena

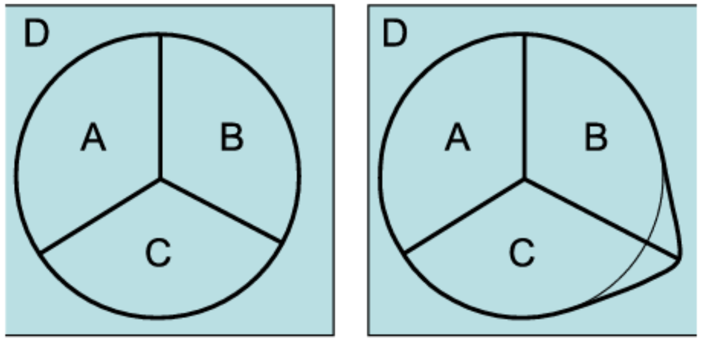
Quantum
Phase transition

G.Vidal, *et.al.*, PRL. **90**, 227902 (2003)



Topological
order

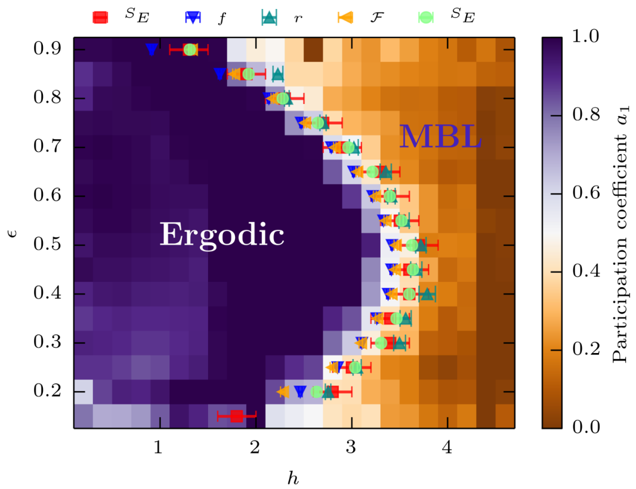
A. Kitaev and J. Preskill, PRL. **96**, 110404 (2006)



$$S_{\text{topo}} \equiv S_A + S_B + S_C - S_{AB} - S_{BC} - S_{AC} + S_{ABC}.$$

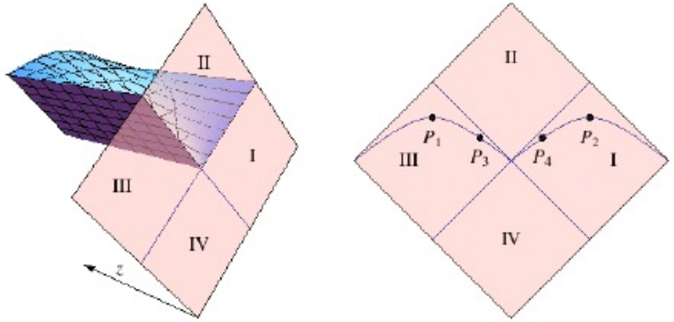
Many-body
localization

D. J. Luitz, *et.al.*, PRB. **91**, 081103(R) (2015)



Black holes

T. Hartman and J. Maldacena, JHEP. **91**, (R) (2006)



$$S_A = \frac{c}{6}\log\left(2\cosh\frac{2\pi t}{\beta}\right) + S_{\text{div}}\ .$$

Quantum entanglement appears in various field such as condensed matter physics, high-energy physics, and quantum information.

Designing quantum entanglement

Conventional research has focused on investigating quantum entanglement properties of specific quantum systems.

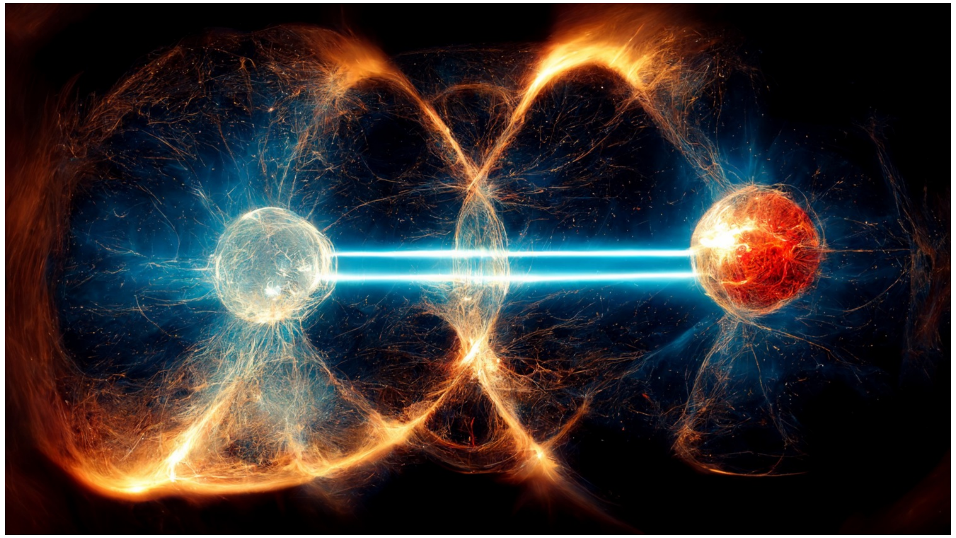
Hamiltonian

$$\mathcal{H}$$

Conventional →

← **Inverse**

Entanglement properties



Meanwhile, considering applications like quantum computation, we need methods to design a system with desired quantum entanglement properties by solving **inverse problems**.

Objective function

Objective:
Designing Hamiltonians with large entanglement in the ground state

Is it OK to increase EE of the ground state? → **No**.

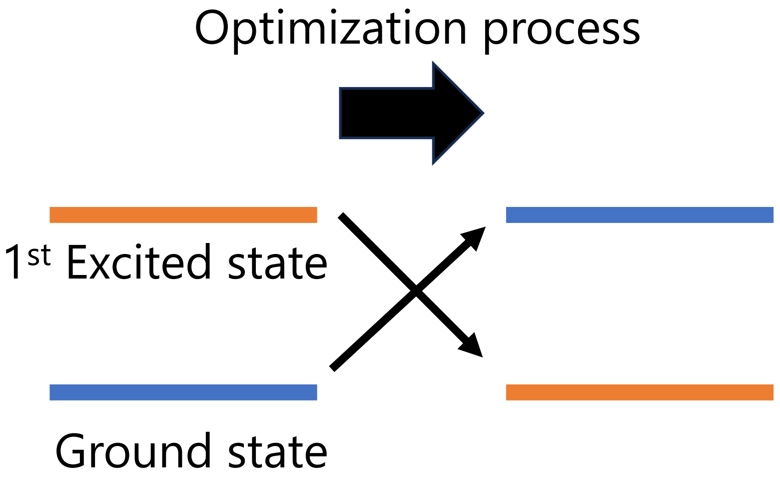
$$L = -S_A$$

Objective function

Objective:
Designing Hamiltonians with large entanglement in the ground state

Is it OK to increase EE of the ground state? → **No**.

😥 The optimization becomes unstable when switching the ground states



EE of the ground state
suddenly change

Objective function

Objective:
Designing Hamiltonians with large entanglement in the ground state

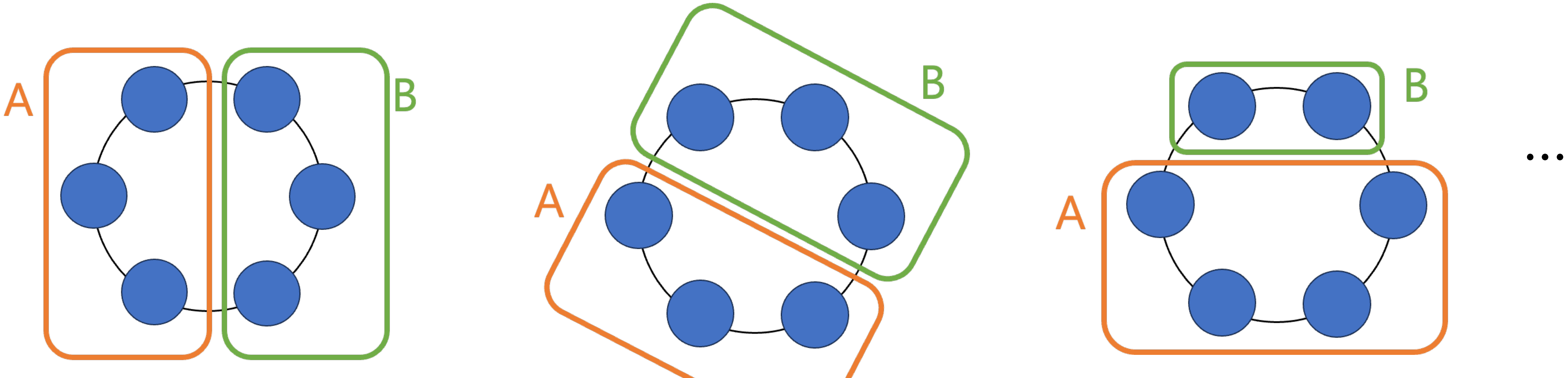
Is it OK to increase EE of the ground state? → **No**.

😥 There are several ways of partitioning into A and B

Group g=1,
Pattern $\xi = 1$

Group g=1,
Pattern $\xi = 2$

Group g=2,
Pattern $\xi = 1$



Objective function

Thermally ensemble EE (TEEE)

$$S^C_{g,\xi}(\boldsymbol{\theta}) = \frac{\sum_n \exp(-\beta E_n(\boldsymbol{\theta}) S_{n,g,\xi}(\boldsymbol{\theta})}{\sum_n \exp(-\beta E_n(\boldsymbol{\theta}))},$$

n: index of eigenstate
(g,ξ): partitioning pattern
E_n: Energy of state n
$S_{n,g,\xi}$: EE at state n, partitioning (g,ξ)
β: inverse temperature

Mean of TEEE for partitions

$$\bar{S}^C(\boldsymbol{\theta}) = \frac{1}{\sum_g N_g} \sum_{g\xi} S^C_{g,\xi}(\boldsymbol{\theta})$$

Std of TEEE for partitions

$$\Delta S^C(\boldsymbol{\theta}) = \sum_g \sqrt{\frac{1}{N_g} \sum_\xi (S^C_{g,\xi}(\boldsymbol{\theta}) - \bar{S}^C_g(\boldsymbol{\theta}))^2}$$

$$\bar{S}^C_g(\boldsymbol{\theta}) = \frac{1}{N_g} \sum_\xi S^C_{g,\xi}(\boldsymbol{\theta})$$

😁 L does not change when switching the ground states

$$L(\boldsymbol{\theta}) = \underline{-\bar{S}^C(\boldsymbol{\theta})} + \lambda \underline{\Delta S^C(\boldsymbol{\theta})} \qquad \lambda > 0$$

Maximize TEEE — Make TEEE uniform for partitions

Quantum spin systems on a honeycomb lattice

K. Inui, and Y. Motome, in preparation

$$\mathcal{H}(\boldsymbol{\theta}) = \sum_{ij\mu} J_{ij}^{\mu} \hat{\sigma}_i^{\mu} \hat{\sigma}_j^{\mu}$$

$$J_{ij}^{\mu} = \frac{\theta_{ij}^{\mu}}{\sqrt{\sum_{\mu} \theta_{ij}^{\mu\,2}}}.$$

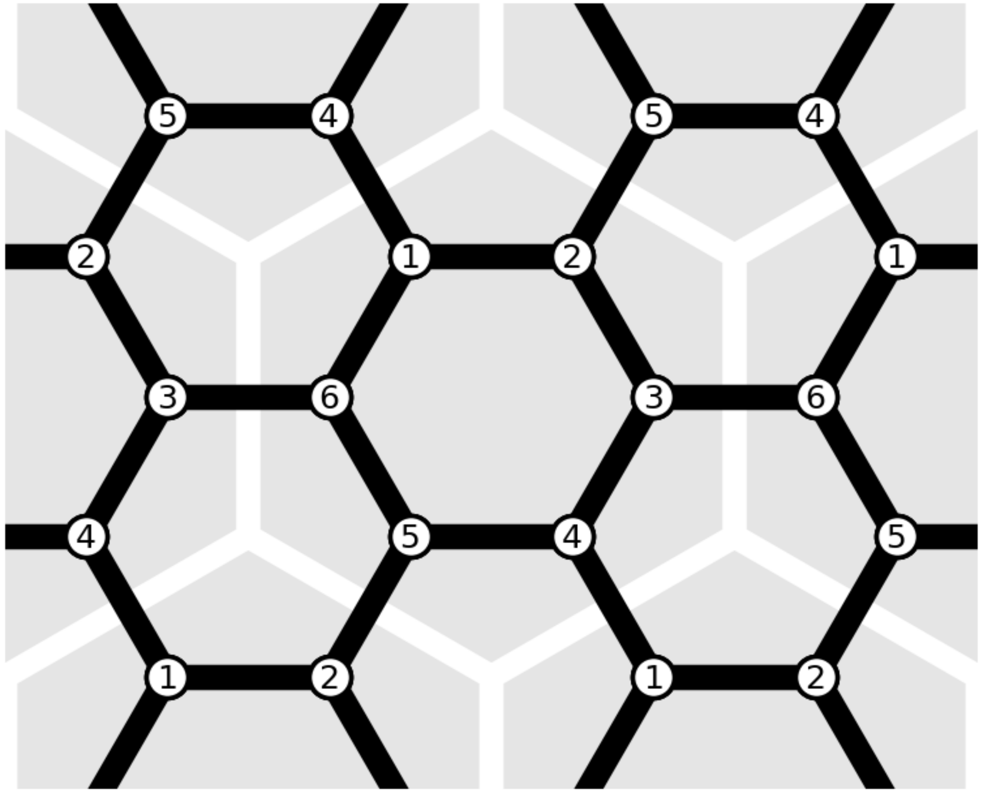
$\mu \in \{x, y, z\}$

18 parameters

$$\sum_{\mu} J_{ij}^{\mu\,2} = 1$$

Bipartition patterns

group g	index ξ	A	B
1	1	(1,2,3)	(4,5,6)
	2	(2,3,4)	(1,5,6)
	3	(3,4,5)	(1,2,6)
	4	(1,2,4)	(3,5,6)
	5	(1,3,4)	(2,5,6)
	6	(3,4,6)	(1,2,5)
	7	(2,3,5)	(1,4,6)
	8	(2,4,5)	(1,3,6)
	9	(1,4,5)	(2,3,6)



Quantum spin systems on a honeycomb lattice

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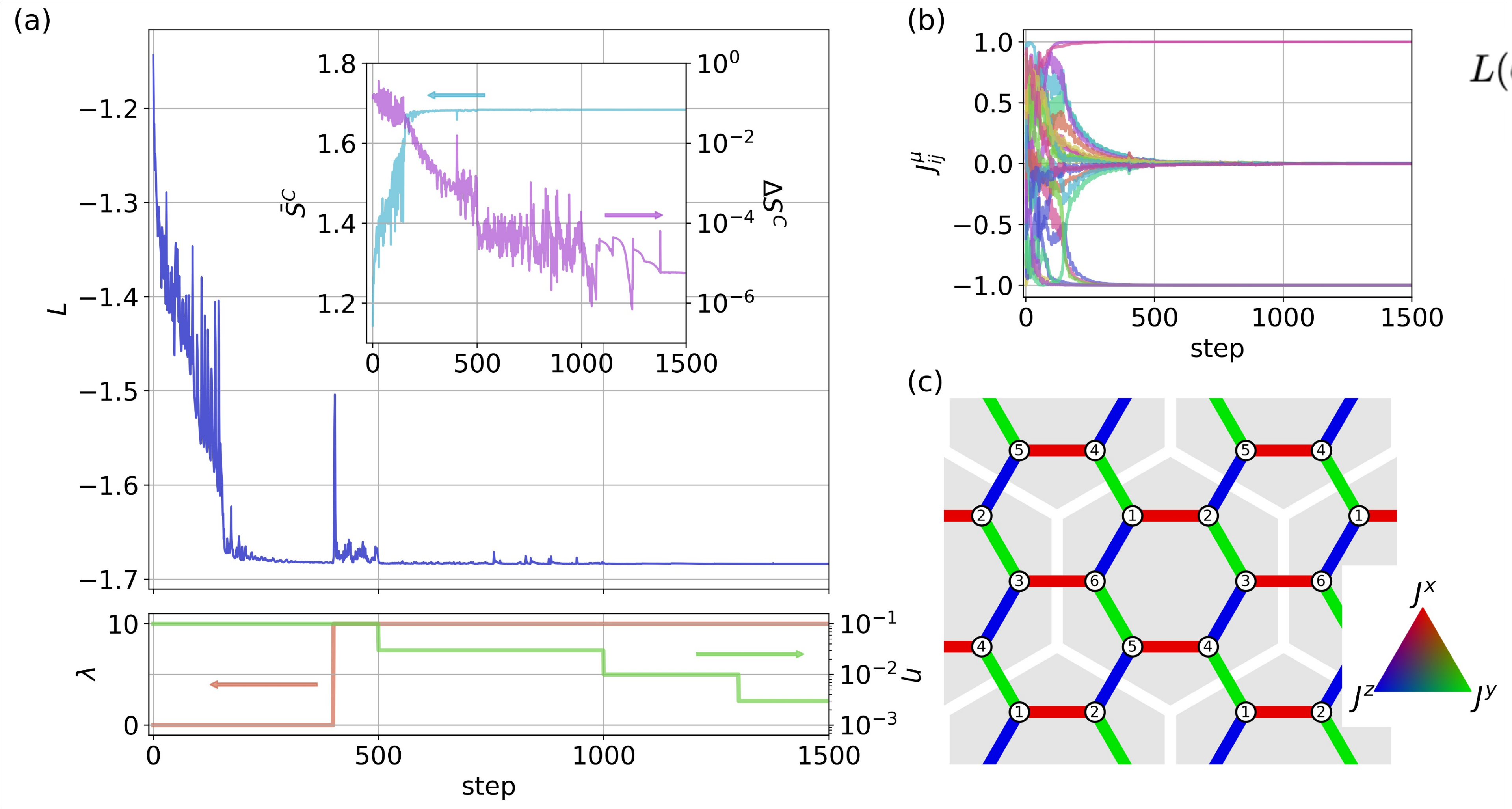


$$L(\boldsymbol{\theta}) = -\bar{S}^C(\boldsymbol{\theta}) + \lambda \Delta S^C(\boldsymbol{\theta})$$

$$\mathcal{H}(\boldsymbol{\theta}) = \sum_{ij\mu} J_{ij}^{\mu} \hat{\sigma}_i^{\mu} \hat{\sigma}_j^{\mu}$$

$$\sum_{\mu} J_{ij}^{\mu\,2} = 1$$

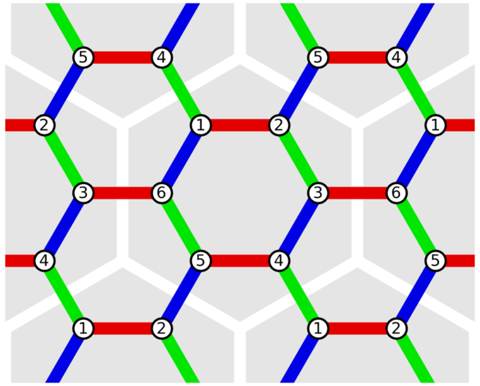
By increasing the quantum entanglement, the **Kitaev model** automatically appears

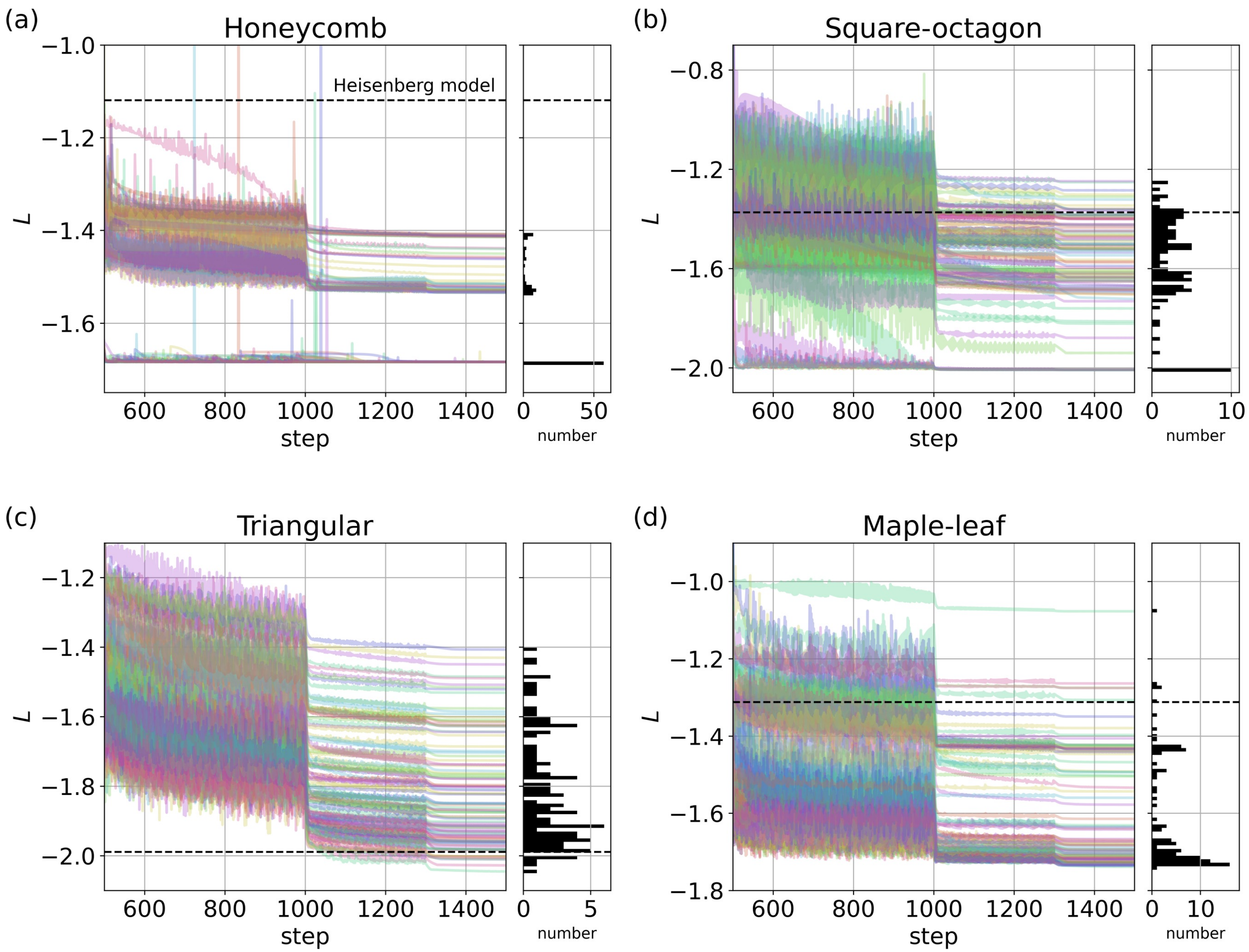
Various Lattices

K. Inui, and Y. Motome, in preparation

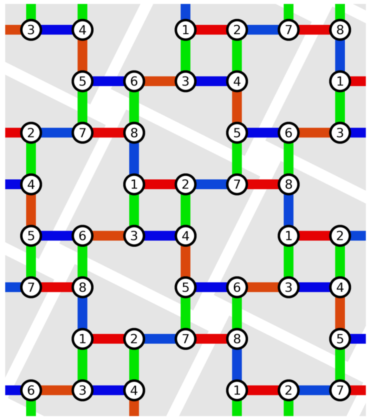
We run calculation with 100 different initial conditions.

Kitaev model

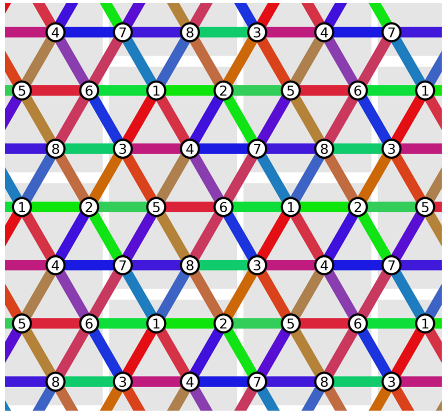




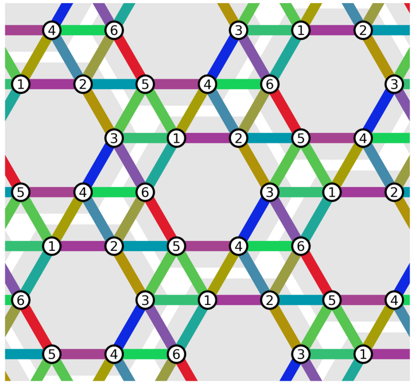
Kitaev model



Inhomogeneous

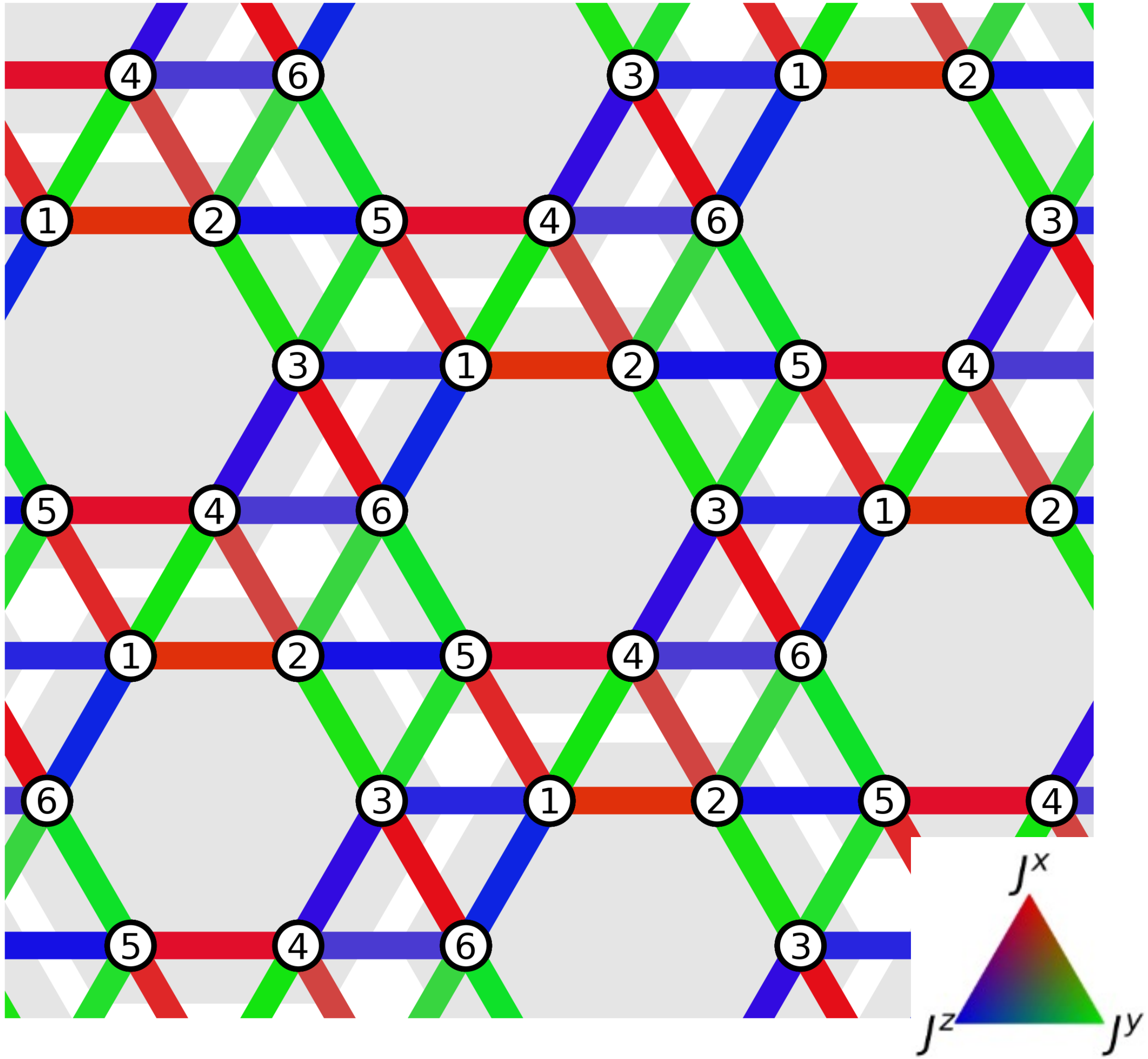


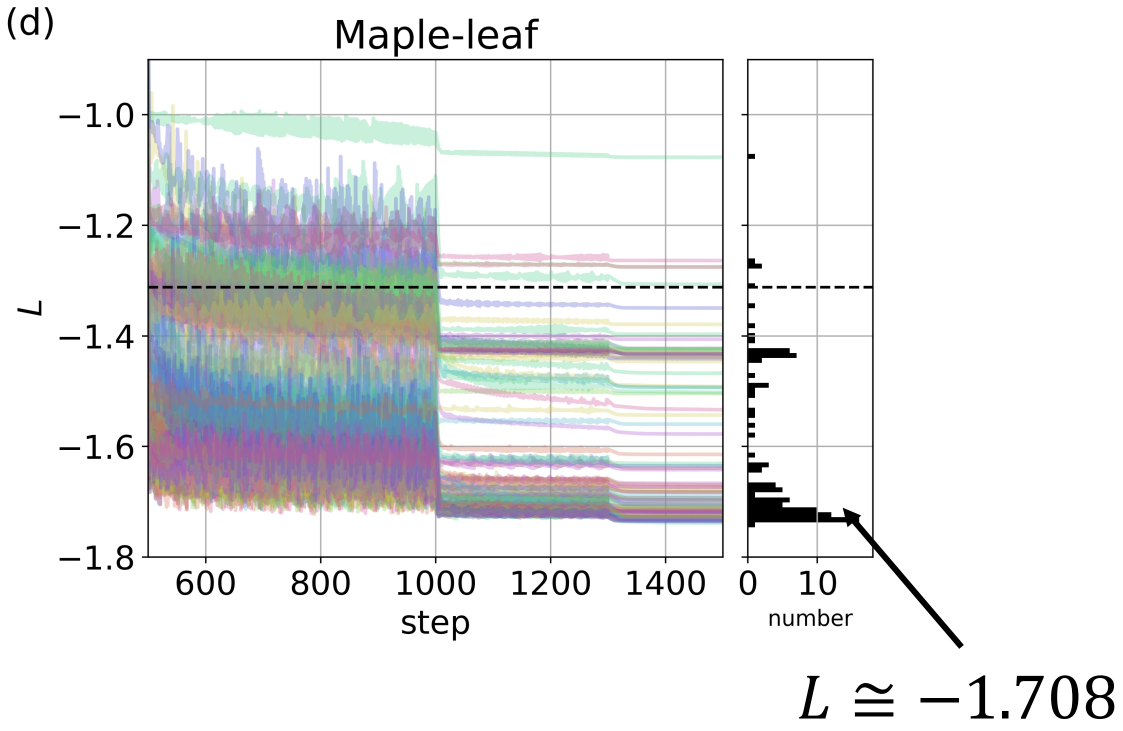
Inhomogeneous



Maple-leaf lattice

K. Inui, and Y. Motome, in preparation





We found a new Kitaev-like model with large quantum entanglement.

Summary and perspective

K. Inui, and Y. Motome, Commun. Phys. **6**, 37 (2023).
https://github.com/koji-inui/automatic-hamiltonian-design

We have developed and demonstrated a framework to automatically construct a Hamiltonian with the desired properties using automatic differentiation.

We apply this framework to maximizing the Hall conductivity
1. Rediscovering the Haldane model on honeycomb lattices
2. Discovery of a new Hamiltonian with large Hall coefficient and topologically nontrivial properties on a triangular lattice

We apply it to maximizing the entanglement entropy
1. The method is found to generate the Kitaev model on the honeycomb lattice.
2. It generate a new model with large enganglement on the maple-leaf lattice.

Perspective: the method has a wide range of applicability beyond entanglement

Numerical methods
- Tensor networks
- DMRG
- DFT

Physical properties
- Topological entanglement entropy
- Superconductivity
- Reproduction of experiments