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MLPhYs 学術変革領域研究(A) 学習物理学の創成
Foundation of "Machine Learning Physics"

Self-learning Monte Carlo with an equivariant transformer

Information Technology Center /
Department of Advanced Materials Science (AMS),
Graduate School of Frontier Sciences
The University of Tokyo

UTokyo 東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

GRADUATE SCHOOL OF FRONTIER SCIENCES
THE UNIVERSITY OF TOKYO

Yuki Nagai

Yuki Nagai and Akio Tomiya, "Self-Learning Monte Carlo with Equivariant Transformer", J. Phys. Soc. Jpn. 93, 114007 (2024)

Outline

- Introduction: Self-learning Monte Carlo
- Transformer and Attention mechanism
- Equivariant Transformer
- Summary

Self-learning Monte Carlo

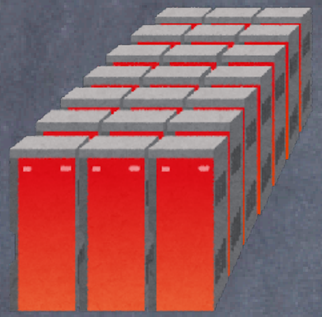
Spins **Electrons** **Atoms/molecules** **Lattice QCD**

Condensed matters, quantum chemistry, high-energy physics

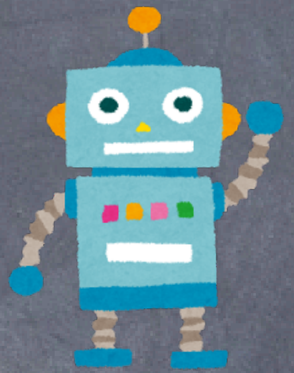
Introduction: Self-learning Monte Carlo

Speedup with Machine learning

Scientific simulations

A →  → B

quantum mechanics etc

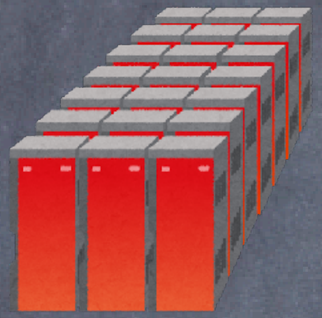
A →  → B

AI: effective model

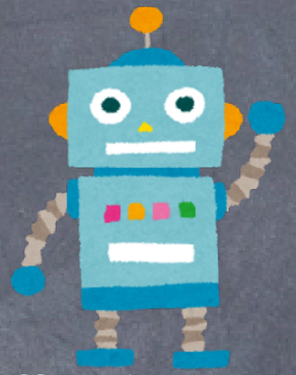
We can speedup simulations!

Speedup with Machine learning

Scientific simulations

A →  → B

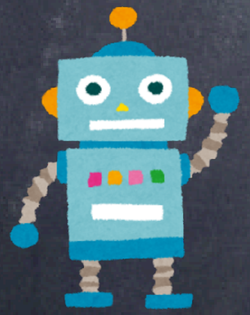
quantum mechanics etc

A →  → B

AI: effective model

We can speedup simulations!

However,



$B_1, B_2, B_3, \ldots$

$B_1, B_2, B_3 \neq B$!

We know this. -> **Hallucinations**

seen in ChatGPT, Gemini

Can we do the accurate simulations even if we use "not so accurate" machine learning model? -> Self-learning MC!

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Self-learning Monte Carlo

We focus on **Markov-chain Monte Carlo method**

We usually calculate physical observables with a partition function $Z=\int \exp(-S)$ or $\sum \exp(-\beta H)$

Configurations → **Heavy tasks** → Boltzmann weight

Configurations → **effective model** → Boltzmann weight

Spins **Electrons** **Atoms, molecules** **Lattice QCD**

In MCMC, there are two parts

1. proposing new configuration
2. evaluating Boltzmann weight

To propose a new configuration, we use the effective model

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Self-learning Monte Carlo

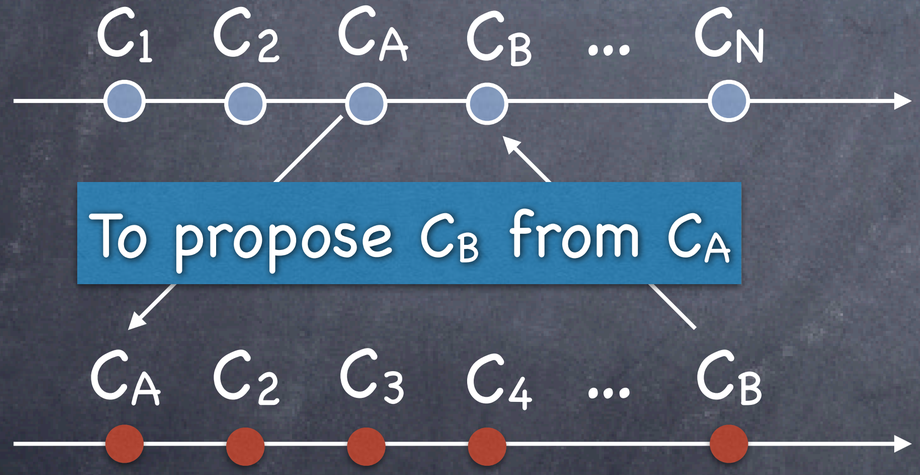
Self-learning Monte Carlo method (SLMC)

Self-learning Hybrid Monte Carlo method (SLHMC)

To speed up the Markov Chain Monte Carlo (MCMC) simulations

SLMC

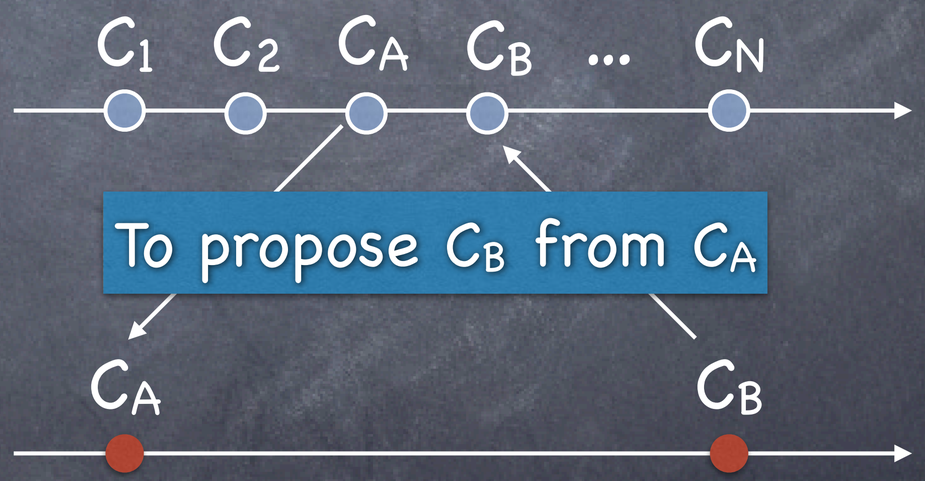
Markov chain with the probability W(C)



Another Markov chain with the probability W'(C)

SLHMC

Markov chain with the probability W(C)



Machine learning molecular dynamics

Machine learning techniques are used for proposing new configuration!

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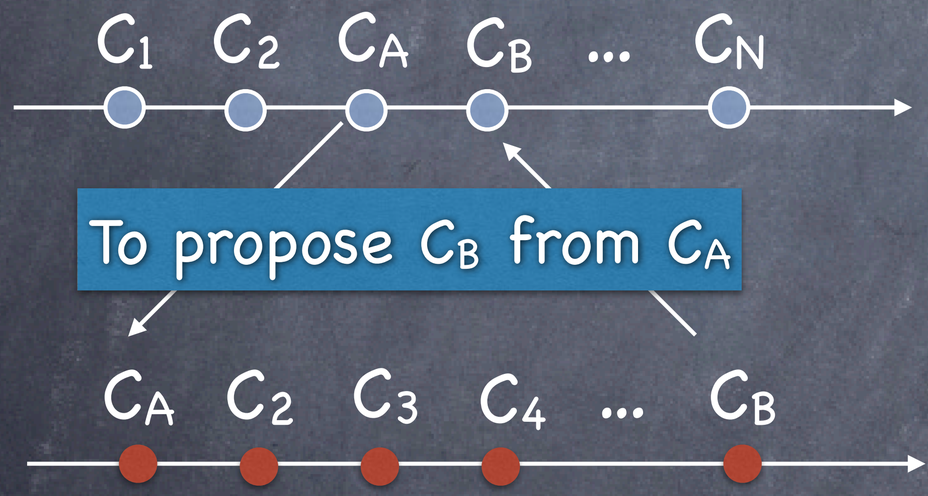
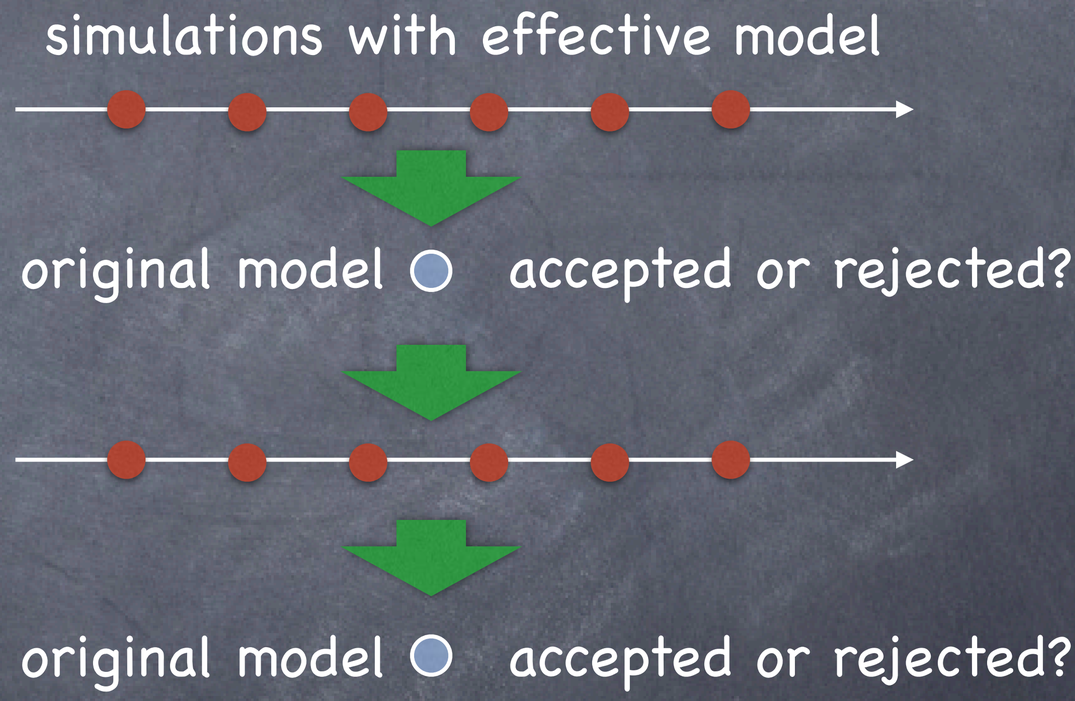
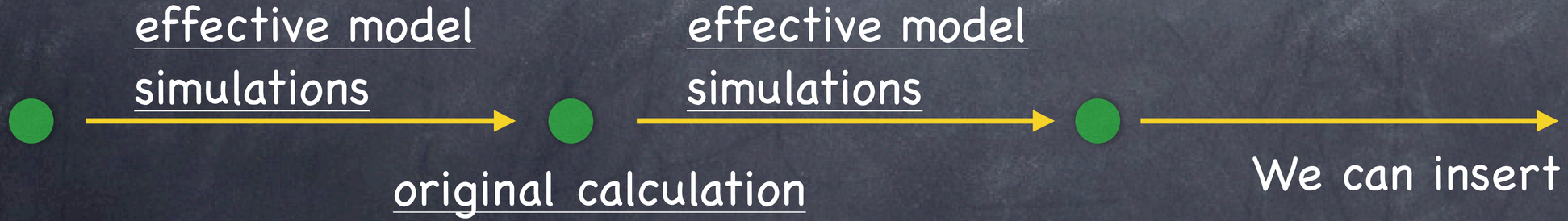
How to avoid scientific hallucinations?

SLMC

Markov chain with the probability W(C)







We can insert a teacher in MCMC!

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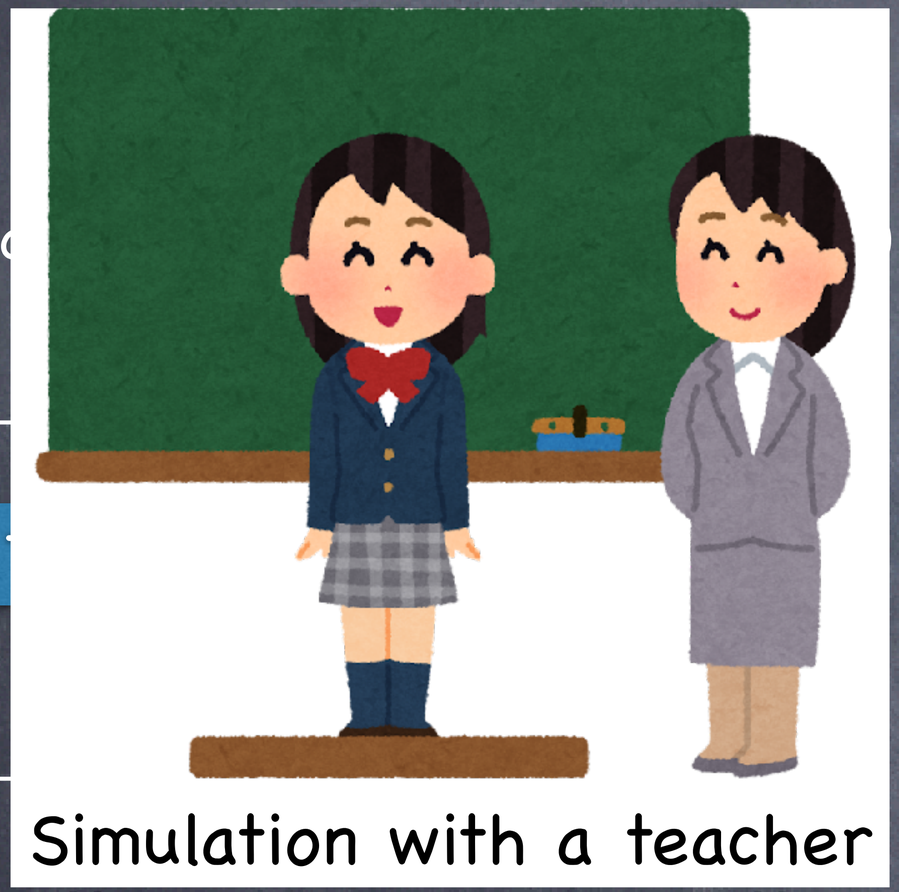
How to avoid scientific hallucinations?



Simulation with a teacher

In conventional machine learning simulations

Bad model -> bad data -> hallucination

In SLMC

Bad model -> bad acceptance ratio
-> longer simulation time
-> no hallucination

model accuracy → time

one possible verifier for scientific simulations

effective model simulations → original calculation → effective model simulations → We can insert a teacher in MCMC!

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Self-learning Monte Carlo

Spin systems

J. Liu, Y. Qi, Z. Y. Meng, and L. Fu, Phys. Rev. B 95, 041101(R) (2017)

H. Kohshiro and YN,,
"Effective Ruderman–Kittel–Kasuya–Yosida-like Interaction in Diluted Double-exchange Model: Self-learning Monte Carlo Approach",
J. Phys. Soc. Jpn. 90, 034711 (2021)

YN and A. Tomiya, "Self-learning Monte Carlo with equivariant Transformer", J. Phys. Soc. Jpn. 93, 114007 (2024)

Fermion+classical spins

Electrons

YN, H. Shen, Y. Qi, J. Liu, and L. Fu
"Self-learning Monte Carlo method: Continuous-time algorithm",
Physical Review B 96, 161102(R) (2017) ***Editors' Suggestion***

YN, M. Okumura, A. Tanaka
"Self-learning Monte Carlo method with Behler-Parrinello neural networks",
Phys. Rev. B **101**, 115111 (2020)

Continuous time Quantum Monte Carlo

Atoms/molecules

Machine-learning MD

YN, M. Okumura, K. Kobayashi, and M. Shiga,
"Self-learning Hybrid Monte Carlo: A First-principles Approach",
Phys. Rev. B **102**, 041124(R) (2020)

K. Kobayashi, YN, M. Itakura, and M. Shiga,
"Self-learning hybrid Monte Carlo method for isothermal–isobaric ensemble: Application to liquid silica",
J. Chem. Phys. **155**, 034106 (2021)

YN, Yutaka Iwasaki, Koichi Kitahara, Yoshiki Takagiwa, Kaoru Kimura, Motoyuki Shiga, "High-Temperature Atomic Diffusion and Specific Heat in Quasicrystals", Phys. Rev. Lett. 132, 196301 (2024)

Bo Thomsen, YN, Keita kobayashi, Ikutaro Hamada, and Motoyuki Shiga, "Self-learning path integral hybrid Monte Carlo with mixed ab initio and machine learning potentials for modeling nuclear quantum effects in water", J. Chem. Phys. 161, 204109 (2024)

Lattice QCD

SU(N) Gauge theory on the lattice

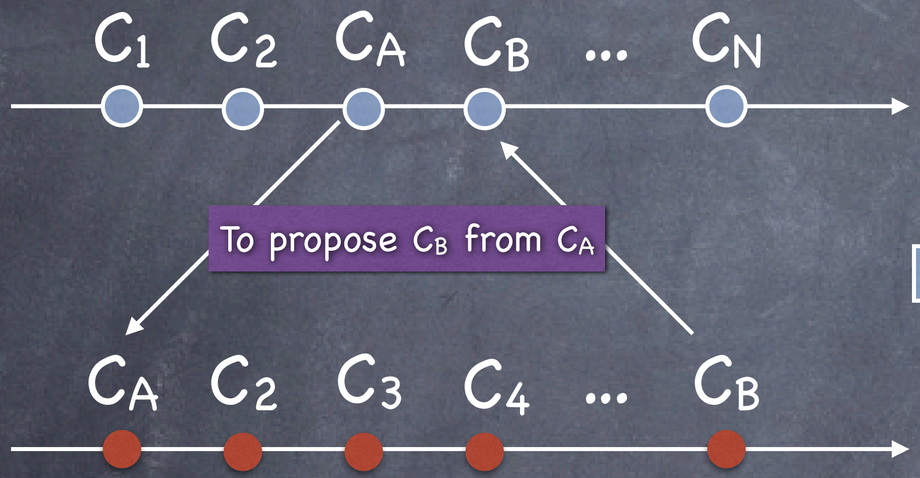
YN, Akinori Tanaka, Akio Tomiya,
"Self-learning Monte-Carlo for non-abelian gauge theory with dynamical fermions",
Phys. Rev. D 107, 054501 (2023)

YN and Akio Tomiya,
"Gauge covariant neural network for 4 dimensional non-abelian gauge theory",
Phys. Rev. D 111, 07450 (2025)

J. Liu, Y. Qi, Z. Y. Meng, and L. Fu, Phys. Rev. B 95, 041101(R) (2017)

Concept of SLMC

Markov chain with the probability W(C)



Another Markov chain with the probability W'(C)

Acceptance ratio for the Metropolis-Hastings algorithm

$$A(C_B, C_A) = \min\left(1, \frac{W(C_B)}{W(C_A)}\frac{g(C_A|C_B)}{g(C_B|C_A)}\right)$$

$g(C_B|C_A)$:Proposal probability

$$A(C_B, C_A) = \min\left(1, \frac{W(C_B)}{W(C_A)}\frac{W'(C_A)}{W'(C_B)}\right)$$

If W'(C)=W(C),
the acceptance ratio is **one**!

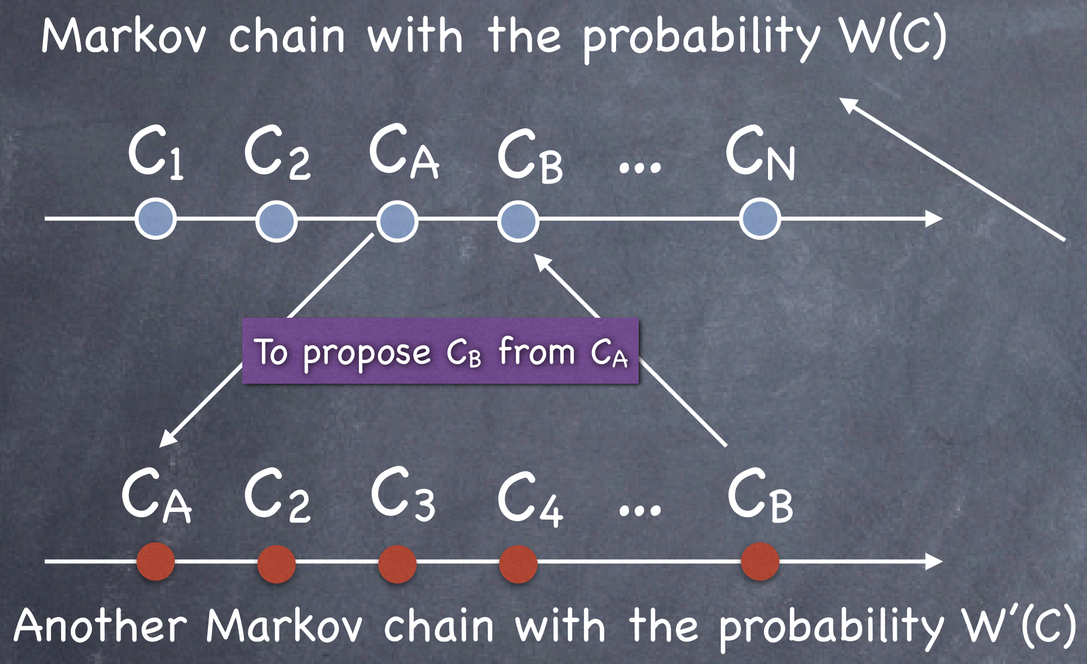
If the computational cost of the proposal Markov chain is small, we can speed up the simulation

How to construct the Markov chain with W'(C)? ->Machine learning technique!

$W(C) = \exp(-\beta H(C))$ -> $W'(C) = \exp(-\beta H_{eff}(C))$ We construct the effective Hamiltonian

Self-learning Monte Carlo

for lattice QCD



YN, Akinori Tanaka, Akio Tomiya,
"Self-learning Monte-Carlo for non-abelian gauge theory with dynamical fermions",
Phys. Rev. D 107, 054501 (2023)

$$S[U] = S_g[U] + S_f[U],$$

$$S_f[U] = -\log \det M^\dagger M,$$

integrated fermion action

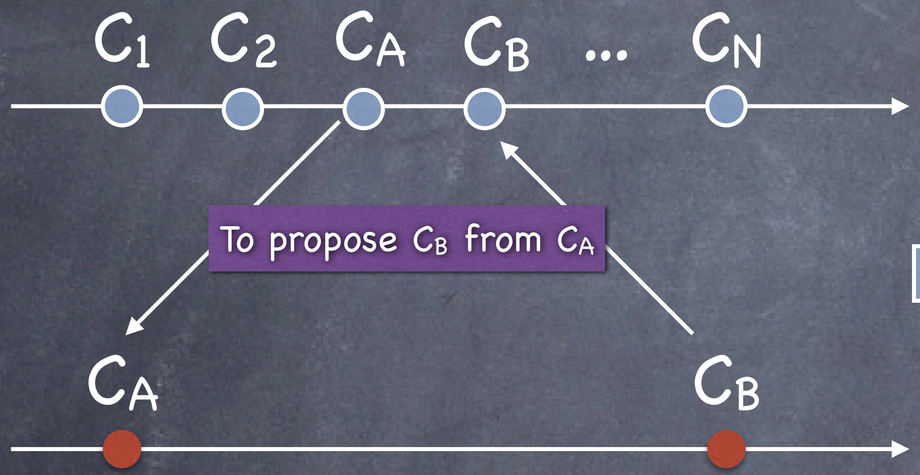
effective model without fermion actions

$$S^\theta_{\rm eff}[U] = \sum_n \left[\beta_{\rm plaq} \sum_{\mu=1}^{4} \sum_{\nu>\mu} \left(1 - \frac{1}{2} {\rm tr} U_{\mu\nu}(n) \right) + \beta_{\rm rect} \sum_{\mu=1}^{4} \sum_{\nu\neq\mu} \left(1 - \frac{1}{2} {\rm tr} R_{\mu\nu}(n) \right) \right]$$
$$+ \beta^{\mu=1}_{\rm Pol} \sum_{n_2,n_3,n_4} {\rm tr} \left[\prod_{n_1=0}^{N_1-1} U_1(\vec{n}, n_4) \right] + \beta^{\mu=2}_{\rm Pol} \sum_{n_1,n_3,n_4} {\rm tr} \left[\prod_{n_2=0}^{N_2-1} U_2(\vec{n}, n_4) \right]$$
$$+ \beta^{\mu=3}_{\rm Pol} \sum_{n_1,n_2,n_4} {\rm tr} \left[\prod_{n_3=0}^{N_3-1} U_3(\vec{n}, n_4) \right] + \beta^{\mu=4}_{\rm Pol} \sum_{n_1,n_2,n_3} {\rm tr} \left[\prod_{n_4=0}^{N_4-1} U_4(\vec{n}, n_4) \right] + \beta_{\rm const},$$

YN, M. Okumura, K. Kobayashi, and M. Shiga, Phys. Rev. B 102, 041124(R) (2020)

Concept of SLHMC

Markov chain with the probability W(C)



Machine learning molecular dynamics (MLMD)

Acceptance ratio for the Metropolis-Hastings algorithm in Hybrid Monte Carlo

$$A(C_B, C_A) = \min\left(1, \frac{W(C_B)}{W(C_A)}\right)$$

if the MD is time-reversal symmetric

MLMD conserves the energy of the effective model

MLMD DOES NOT conserve the energy of the original model

If the MD conserves the energy of the original model the acceptance ratio is **one**!

If the computational cost of the MLMD is small, we can speed up the simulation

In the field of atom and molecular systems, machine learning molecular dynamics was proposed in 2007

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K. Kobayashi, YN, M. Itakura, and M. Shiga, J. Chem. Phys. **155**, 034106 (2021)

Self-learning Hybrid Monte Carlo

for materials

We developed the SLHMC for NPT ensemble

MLMD simulation sometimes becomes unstable with NPT

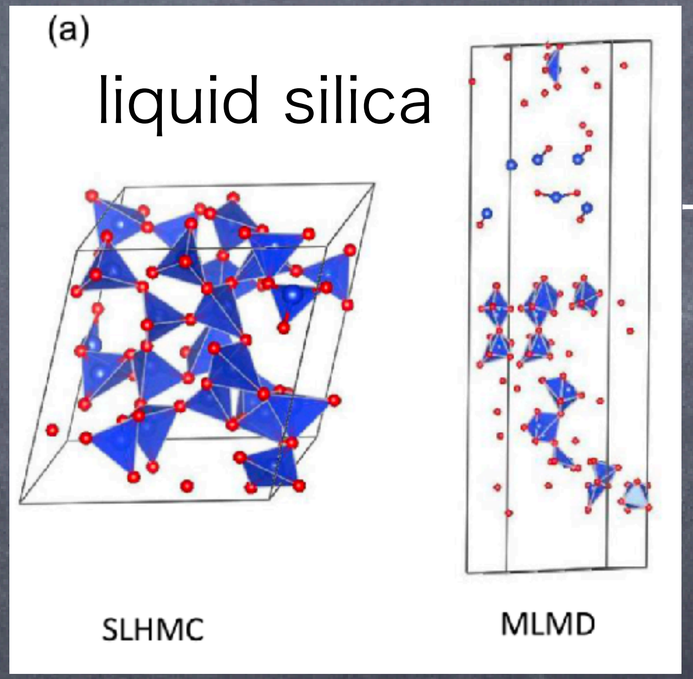
TABLE I. Acceptance ratio P_{ac} and mean MCMC interval dt_m of SLHMC for liquid silica with 72 and 216 atoms. N means the number of atoms. t_{eff} is the product of P_{ac}, dt_m, and the number of MCMC steps (20 000).

N	Temperature (K)	P_{ac} (%)	dt_m (fs)	t_{eff} (ps)
	2500	34.1	242	1646
72	3000	31.0	217	1343
	3500	33.8	235	1590
	2373	27.2	210	1142
216	3000	23.8	188	893
	3500	17.4	111	388

DFT calculation every 200 fs

1ns long time simulation with DFT accuracy

after 50 ps at 4000K (72 atoms)



MLMD

Trained with 8600

->structure is broken

SLHMC

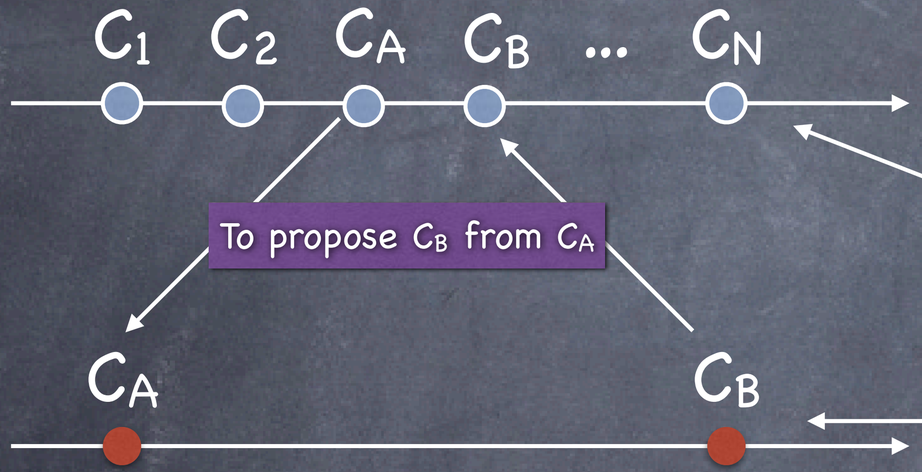
stable because bad structures are rejected

->Stable simulation!

Self-learning Hybrid Monte Carlo

for lattice QCD

Markov chain with the probability W(C)



Machine learning molecular dynamics (MLMD)

target action

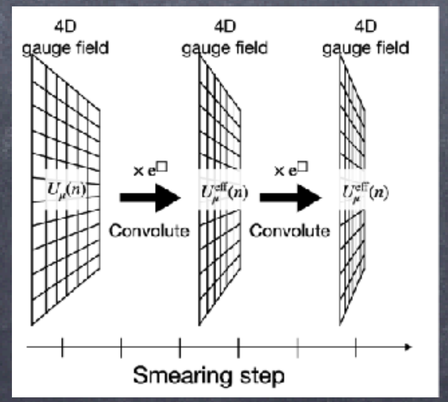
$$S[U] = S_{\rm g}[U] + S_{\rm f}[\phi, U; m_{\rm l}],$$

effective action

$$S_\theta[U] = S_{\rm g}[U] + S_{\rm f}[\phi, U_\theta^{\rm NN}[U]; m_{\rm h}],$$

if ml < mh, the computational cost reduces

$U^{\rm NN}$: trainable stout smearing



YN and Akio Tomiya,
“Gauge covariant neural network for 4 dimensional non-abelian gauge theory”,
Phys. Rev. D 111, 07450 (2025)

Problems of SLMC

Configurations → **Heavy tasks** → Boltzmann weight

Configurations → **effective model** → Boltzmann weight

How to construct effective models?

Quality of the effective model is very important

In previous studies,

for example, a linear regression is used to construct the effective model inspired by the physical insight

Use Transformer!!

Transformer and Attention mechanism

Generative AIs

https://arxiv.org/abs/1706.03762

OpenAI ChatGPT

Gemini

DeepL

deepseek

These AI have same architecture called Transformer

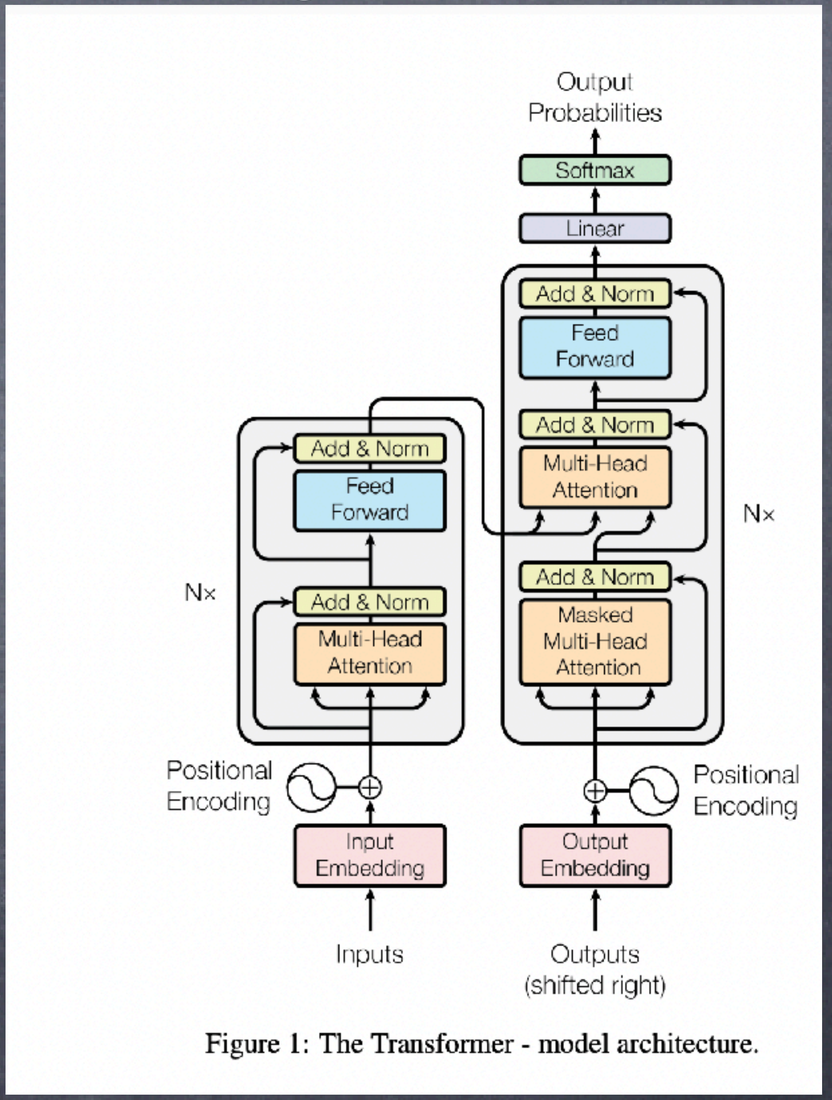


Figure 1: The Transformer - model architecture.

Transformer

AI Chat, Visualization, language translation

protein foldings etc.

Scaling laws of Transformer

https://arxiv.org/abs/2001.08361

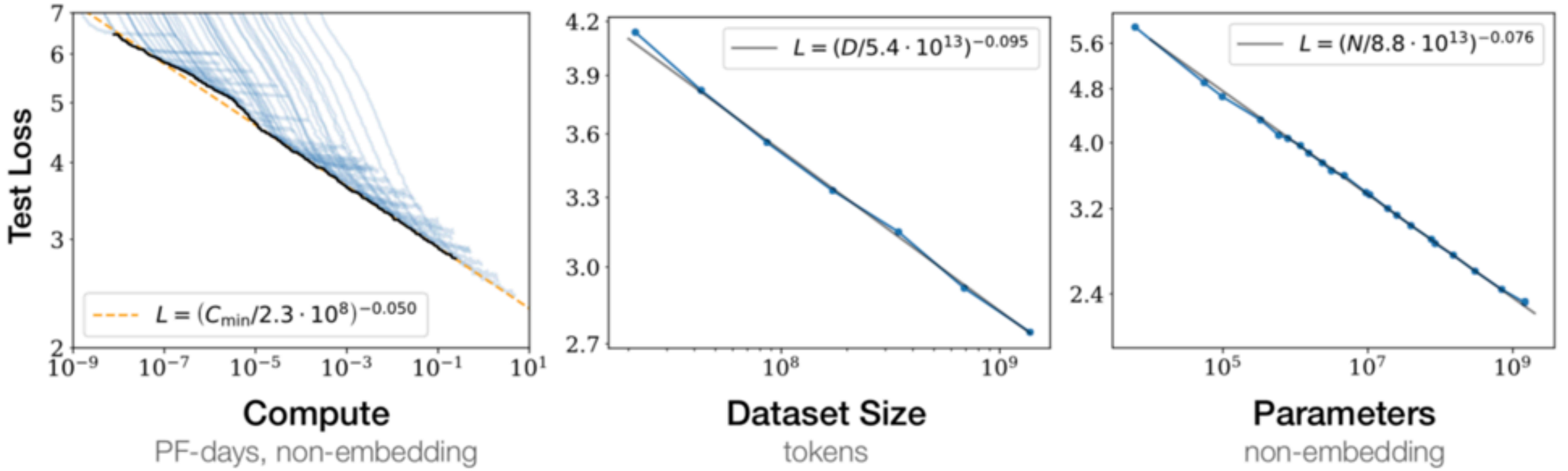


Figure 1 Language modeling performance improves smoothly as we increase the model size, datasetset size, and amount of compute[2] used for training. For optimal performance all three factors must be scaled up in tandem. Empirical performance has a power-law relationship with each individual factor when not bottlenecked by the other two.

It requires huge data (e.g. GPT uses all electric books in the world)
= weak inductive bias, large data makes prediction better

Attention learns Non-local correlations

"Attention is all you need" (arXiv:1706.03762)

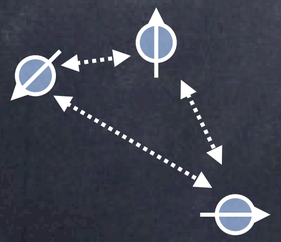
Attention is an important building block in the transformer

Language model (chat, translation etc..)

"Attention" layer can capture non-local relations between words

Physics

Can we use Attention layer to learn **non local correlation**?



If so, we can design a new model in physics

What is the attention mechanism?

There are many websites to explain the transformer and attention mechanism, in terms of language processing...

I try to explain the attention in terms of simple mathematics

This came from discussions with Dr. Tomiya

1. We consider a vector/matrix/tensor **A** Ai or Aij or Aijk
2. We make three variables **K,Q,V** from **A**

   $K = W^K A$, $Q = W^Q A$, $V = W^V A$ **W^k, W^Q, W^V: trainable parameters**
3. We generate new vector/matrix/tensor **B**

$$B_l = A_l + \sum_i P_i^l V_i \qquad P = \sigma(QK^T)$$

correlation between Q and K

l=i or ij or ijk

What is the attention mechanism?

K = W^KA, Q = W^QA, V = W^VA **W^k,W^Q,W^V:trainable parameters**

3. We generate new vector/matrix/tensor **B**

$$B_l = A_l + \sum_i P_i^l V_i$$

weighted sum

$$P = \sigma(QK^T)$$

σ :nonlinear funciton

correlation between Q and K

self-attention mechanism

This is most simplest architecture

In generative AIs, they use the multi-head attention

Simple mechanism but very effective!

How can we use this in physics?

Equivariant transformer

Difference between AI and Physics

Generative AIs: huge number of the parameters (Billions, Trillions)

We have to gather huge amount of data
We need large computational resources and money

We do not want to gather and train data by ourselves

But, we want to use transformers because of good properties

Physics: small number of parameters

When there are too many parameters in a machine learning model,
I feel like I don't really understand what's going on.

If the computation is too heavy, it's impossible to speed up the simulation

We want to reduce the number of parameters in transformers

Incorporating natural laws can simplify the model -> Symmetries!

Fermion and spin model

We want to focus on a simple lattice model

fermions and classical spins

$$H = -t \sum_{\alpha,\langle i,j\rangle} (\hat{c}^{\dagger}_{i\alpha}\hat{c}_{j\alpha} + \mathrm{h.c.}) + \frac{J}{2}\sum_{i} \mathbf{S}_i \cdot \hat{\sigma}_i - \mu \sum_{\alpha,i} \hat{c}^{\dagger}_{i\alpha}\hat{c}_{i\alpha},$$

called double exchange model
in condensed matter physics

Partition function:

$$Z = \sum_{\{\mathbf{S}\}} \prod_{n} (1 + e^{-\beta(\mu - E_n(\{\mathbf{S}\}))})$$

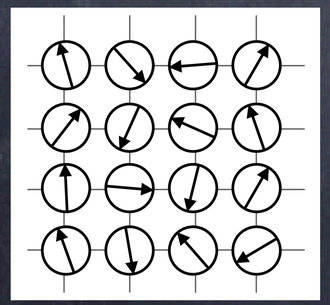
Input: spin configurations {S}

diagonalization

Output: Boltzmann weight

Configurations: classical spins $\{S_i\}$

S_i: i-th three dimensional vector in spin space



We want to replace the diagonalization

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Fermion and spin model

We want to focus on a simple lattice model

fermions and classical spins

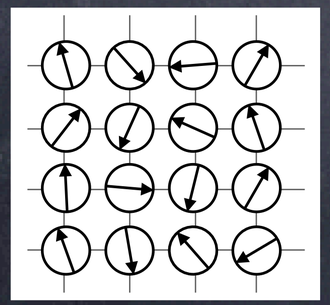
$$H = -t \sum_{\alpha,\langle i,j\rangle} (\hat{c}^{\dagger}_{i\alpha}\hat{c}_{j\alpha} + \mathrm{h.c.}) + \frac{J}{2}\sum_{i} \mathbf{S}_i \cdot \hat{\sigma}_i - \mu \sum_{\alpha,i} \hat{c}^{\dagger}_{i\alpha}\hat{c}_{i\alpha},$$

called double exchange model
in condensed matter physics

If J is small, we can use the perturbation theory

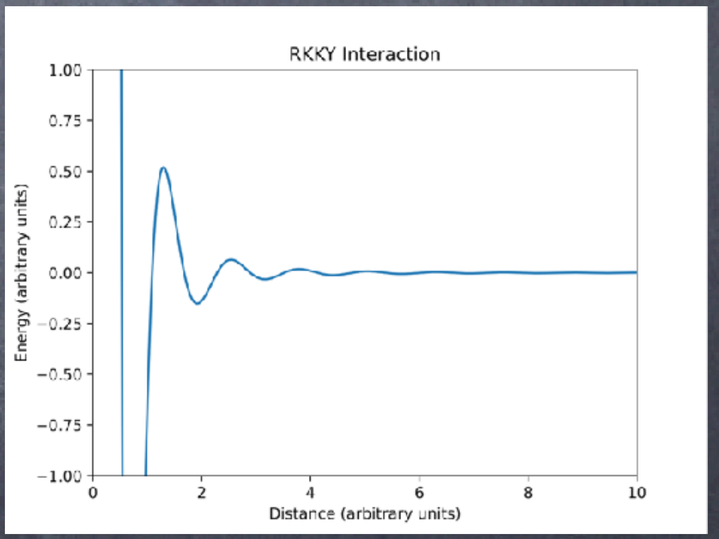
the **Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction** models

$$H_{\mathrm{RKKY}} = -\sum_{\langle i,j\rangle_n} J_n \mathbf{S}_i \cdot \mathbf{S}_j$$



We can integrate out fermion degrees of freedom

fermion + spin -> spin



Fermion and spin model

We want to focus on a simple lattice model

fermions and classical spins

$$H = -t \sum_{\alpha,\langle i,j\rangle} (\hat{c}^{\dagger}_{i\alpha}\hat{c}_{j\alpha} + \mathrm{h.c.}) + \frac{J}{2}\sum_{i} \mathbf{S}_i \cdot \hat{\sigma}_i - \mu \sum_{\alpha,i} \hat{c}^{\dagger}_{i\alpha}\hat{c}_{i\alpha},$$

called double exchange model
in condensed matter physics

We want to consider large J region

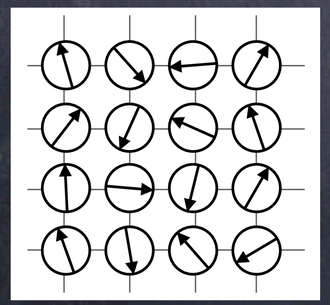
Simple effective model

J. Liu, H. Shen, Y. Qi, Z. Y. Meng, and L. Fu, Phys. Rev. B 95, 241104(R)(2017)

J_n^{eff}: n-th nearest neighbor interaction

$$H_{\mathrm{eff}}^{\mathrm{Linear}} = -\sum_{\langle i,j\rangle_n} J_n^{\mathrm{eff}} \mathbf{S}_i \cdot \mathbf{S}_j + E_0$$

This is a linear model
by integrating out fermion degrees of freedom



similar to RKKY model
derived by physicist

There are only few parameters J_n^{eff}

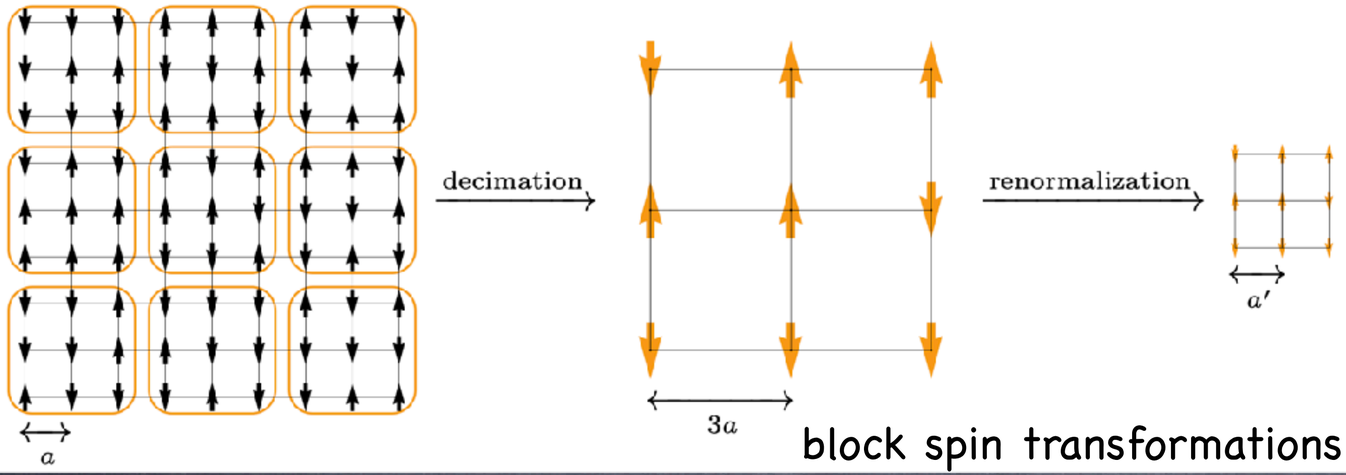
Num. of parameters is too small! How to improve this model?

東京大学情報基盤センター
INFORMATION TECHNOLOGY CENTER, THE UNIVERSITY OF TOKYO

Fermion and spin model

How to construct model?

In physics, we know the renormalization group analysis



block spin transformations

Charlie Duclut., "Nonequilibrium critical phenomena :exact Langevin equations, erosion of tilted landscapes" Université Pierre et Marie Curie - Paris VI, 2017.

Spins are renormalized

Renormalized spin should have same symmetries

Spins become "effective" spins

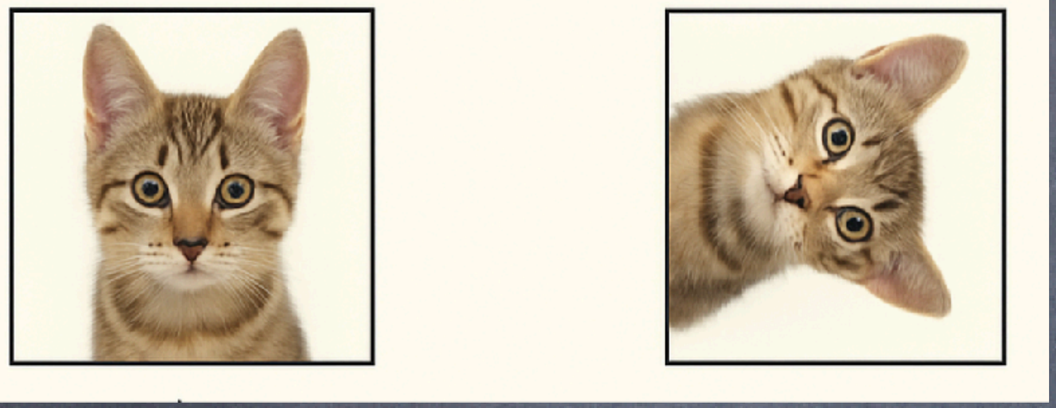
$$H_{\mathrm{eff}} = -\sum_{\langle i,j\rangle_n} J_n^{\mathrm{eff}} \mathbf{S}_i^{\mathrm{NN}} \cdot \mathbf{S}_j^{\mathrm{NN}} + E_0$$

Heisenberg model for effective spins

If we can construct effective spins, we can construct effective model!

We need an equivariant model

What is equivariance?



A. Cat or Not?

Rotate input image

→ Still recognized as a cat

Output unchanged → **Invariant**

B. Where are the cat's ears?

Rotate input image

→ Output (ear position) also rotates

Output changes accordingly

→ **Equivariant**

Equivariance =
Output transforms with input

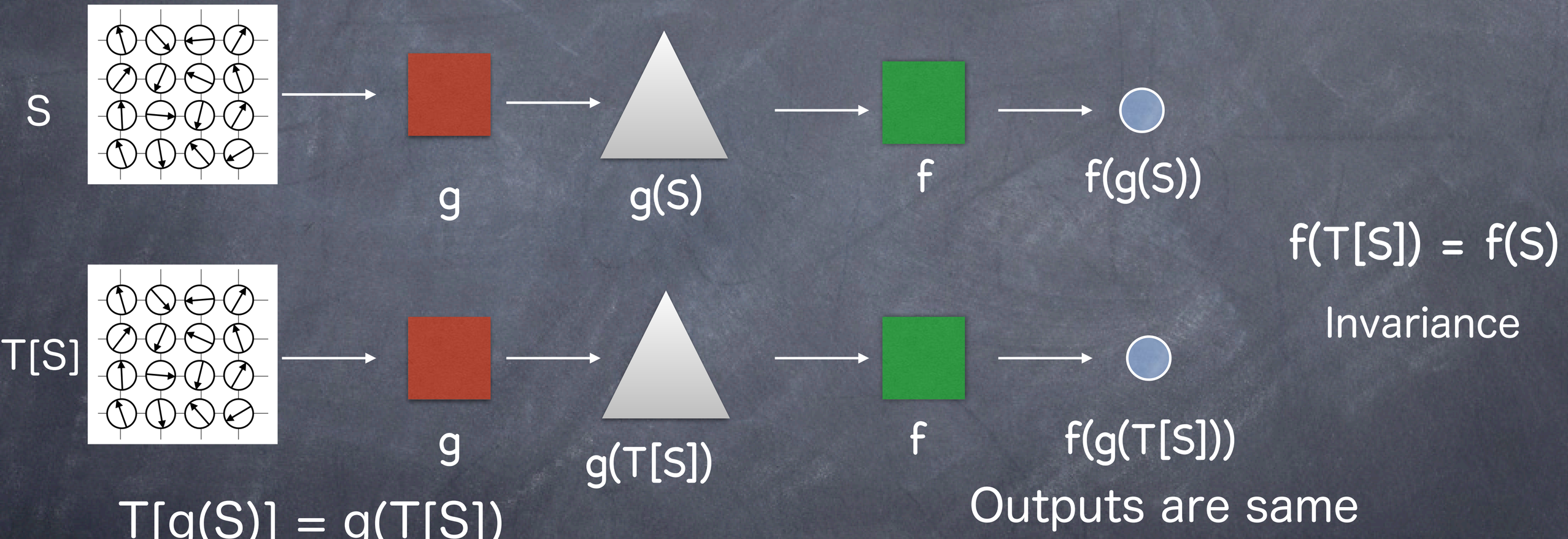
Hamiltonian: Rotational **invariant**

Effective spin:

must be rotational **equivariant**

Invariance and equivariance

We make equivariant networks and make the output invariant



T[g(S)] = g(T[S])

Equivariance

f(T[S]) = f(S)

Invariance

Outputs are same

CNN uses equivariance

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

How to construct the attention layer

1. We consider a vector/matrix/tensor **A** Ai or Aij or Aijk

⇨ We consider spin "matrix" $[\hat{S}]_{i\mu} = [\vec{S}_i]_\mu$

$\vec{S}_i$ is a classical spin on i-th site (vector)

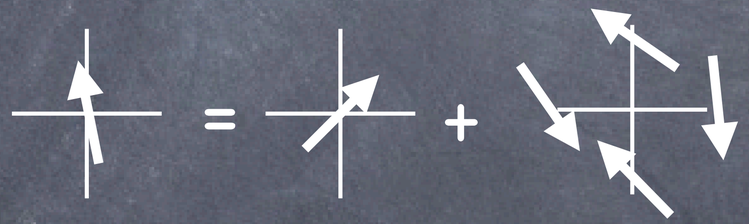
2. We make three variables **K,Q,V** from **A**

K = W^KA, Q = W^QA, V = W^VA

⇨ We introduce "operators" $\hat{S}^{\mathrm{Q}} = \bar{W}^{\mathrm{Q}}\hat{S}$ $\hat{S}^{\mathrm{K}} = \bar{W}^{\mathrm{K}}\hat{S}$ $\hat{S}^{\mathrm{V}} = \bar{W}^{\mathrm{V}}\hat{S}$

$$[\bar{W}^\alpha \hat{S}]_{i\mu} \equiv \sum_{\langle i,j\rangle_n} W^\alpha_n \hat{S}_{j\mu}$$

n-th nearest neighbors



W^k,W^Q,W^V:trainable parameters

W^k,W^Q,W^V do not depend on the site i (translational symmetry)

num. of parameters becomes a few

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

How to construct the attention layer

3. We generate new vector/matrix/tensor **B**

$$B_l = A_l + \sum_i P_i^l V_i$$

$$\Rightarrow \quad \hat{S}^{(l)} \equiv \mathcal{N}(\hat{S}^{(l-1)} + \check{M}\hat{S}^{\mathrm{V}}) \qquad [\mathcal{N}(\hat{S})]_{i\mu} = [\vec{S}_i]_\mu / ||\vec{S}_i||$$

$P = \sigma(QK^T)$ correlation between Q and K

$$\Rightarrow \quad [\check{M}]_{ij} = \mathrm{ReLU}\left(\frac{1}{\sqrt{3}} \sum_{\mu=1}^{3} \hat{S}^{\mathrm{Q}}_{i\mu} \hat{S}^{\mathrm{K}}_{j\mu}\right)$$

$\hat{S}^{(l)}$ has spin-rotational equivariance

R[g(S)] = g(R[S])

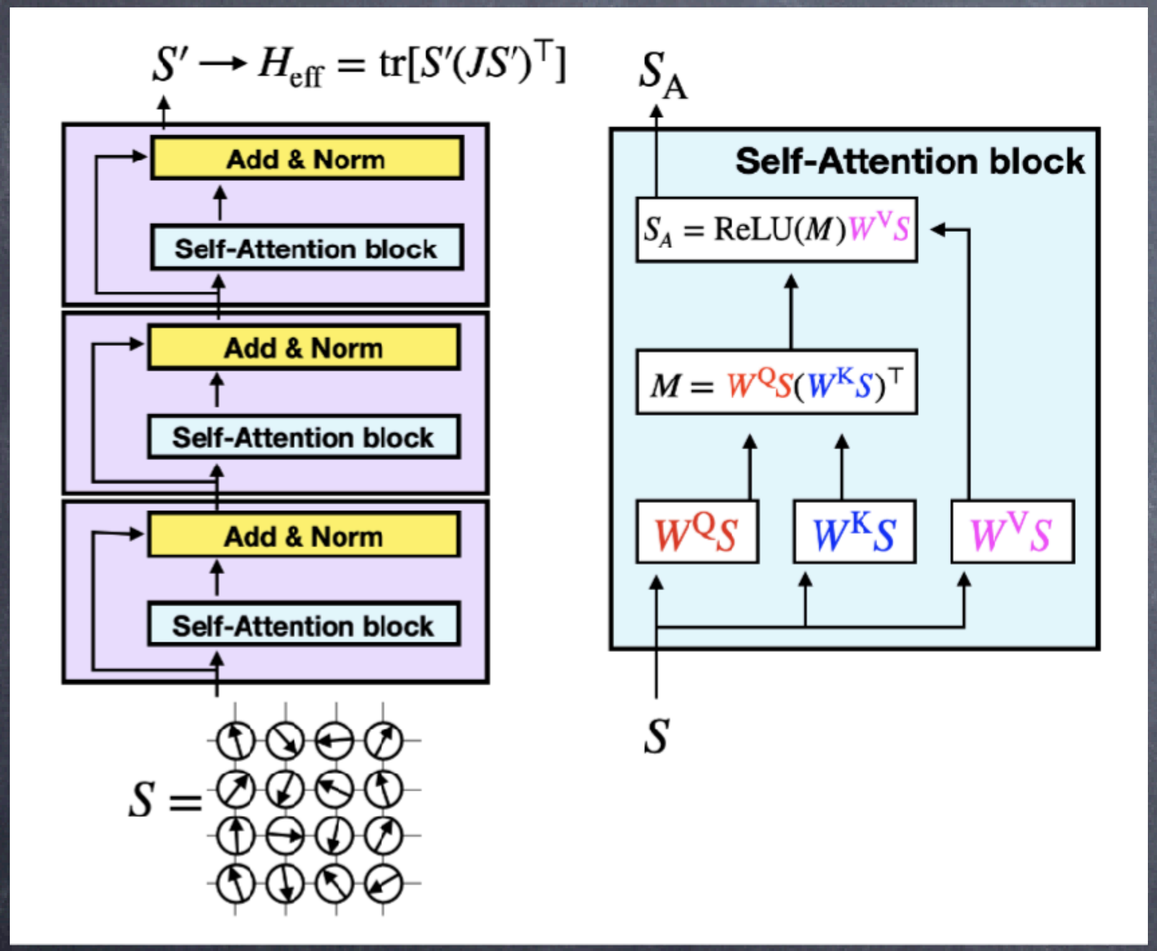
The "effective" spin $S^{(L)}$ can be regarded as a physical spin

-> renormalized spin

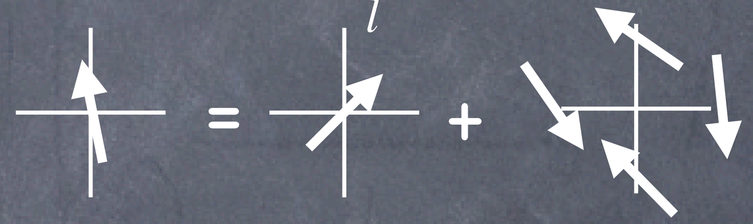
We can build a model!

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

Equivariant Transformer for spin systems



$$K_i = \sum_l W_l S_{i+l}$$



W only mixes neighbor spins
(short range interaction)

like block spin transformations

S → K = W^{K}S
S → Q = W^{Q}S
S → V = W^{V}S

M = W^{Q}SS+W^{K}

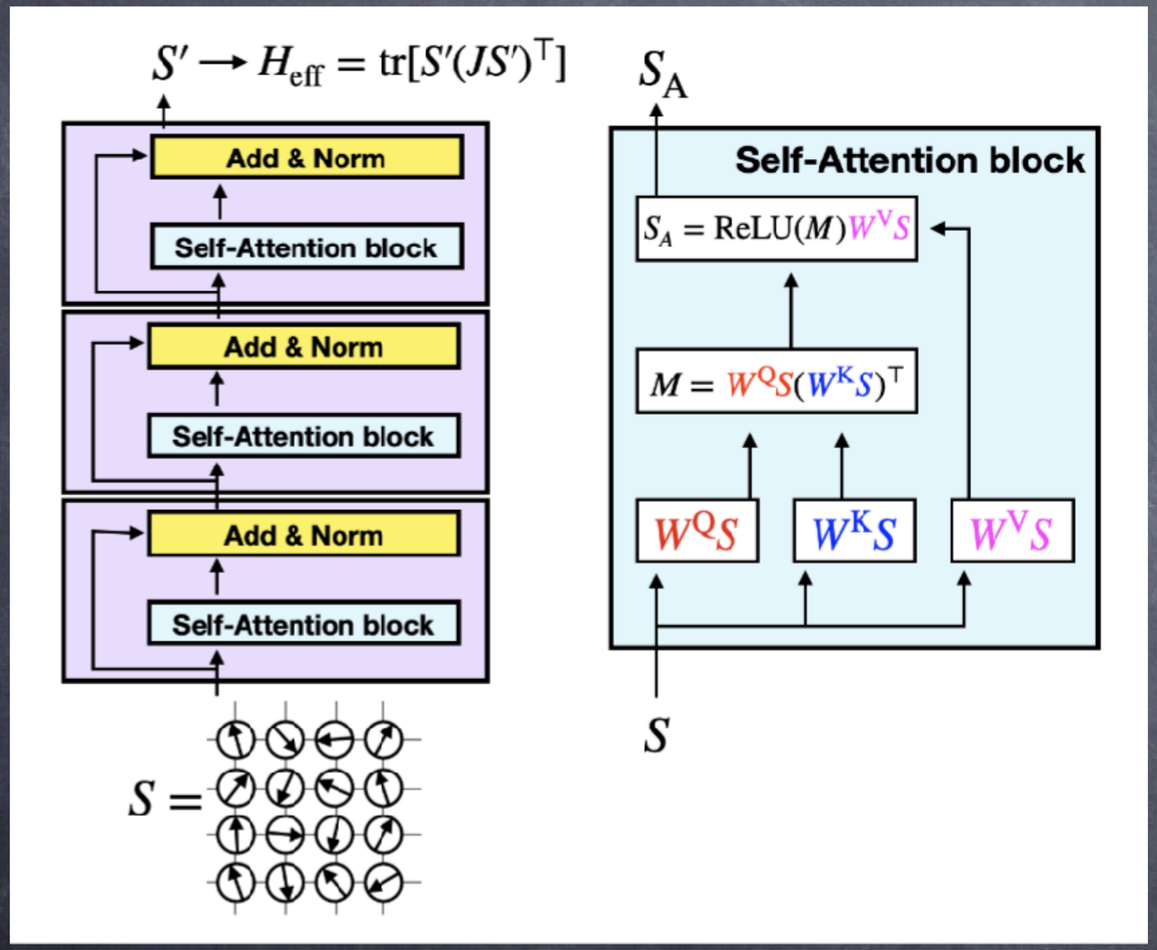
Rotational and translational invariant

S′ = S + ReLU(M) W^{V}S

Long range correlation is included

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

Equivariant Transformer for spin systems



$$\mathcal{N}(\mathbf{S}_i) = \mathbf{S}_i / \|\mathbf{S}_i\|$$

Layer 1

$$S_1 = \mathcal{N}(S + \mathrm{ReLU}(M^1(S))W^{V1}S)$$

Layer 2

$$S_2 = \mathcal{N}(S_1 + \mathrm{ReLU}(M^2(S_1))W^{V2}S_1)$$

Layer 3

$$S_3 = \mathcal{N}(S_2 + \mathrm{ReLU}(M^3(S_2))W^{V3}S_2)$$

Last Heisenberg model with effective spins

$$E = \sum_i \sum_l J_l \vec{S}_{3i} \cdot \vec{S}_{3i+l} + E_0$$

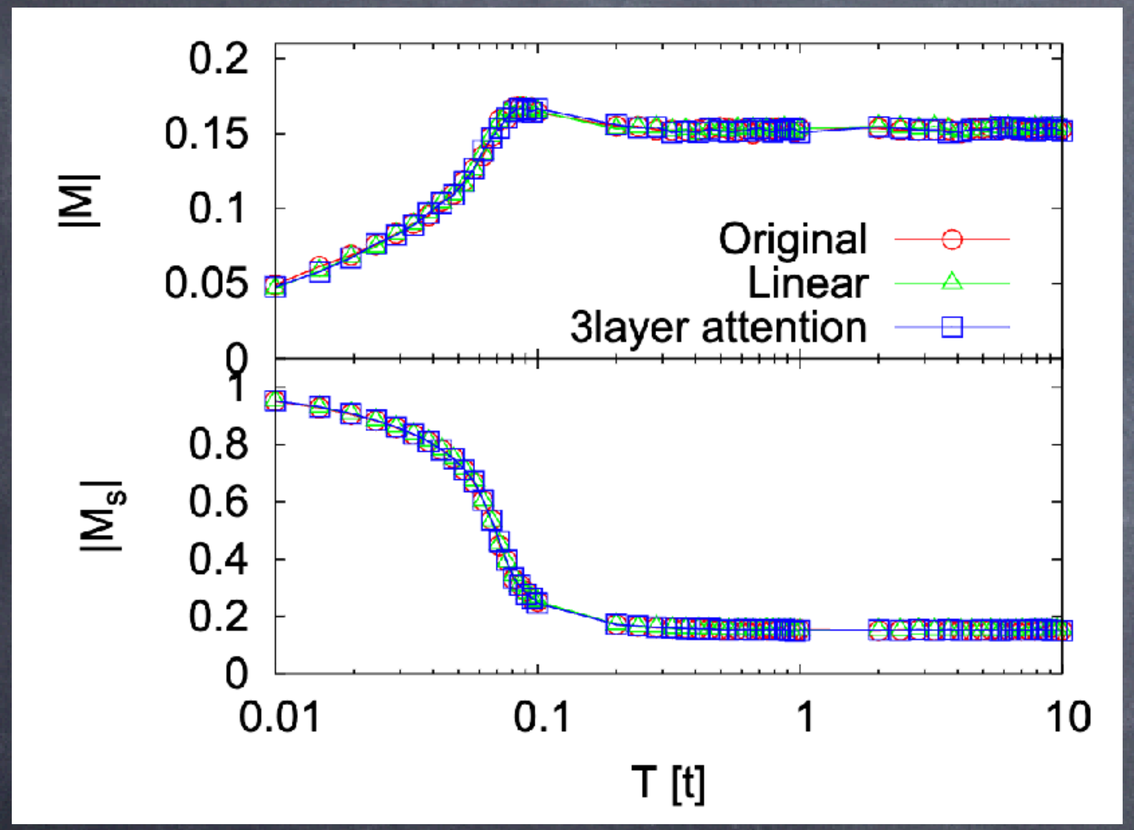
If the second term is zero

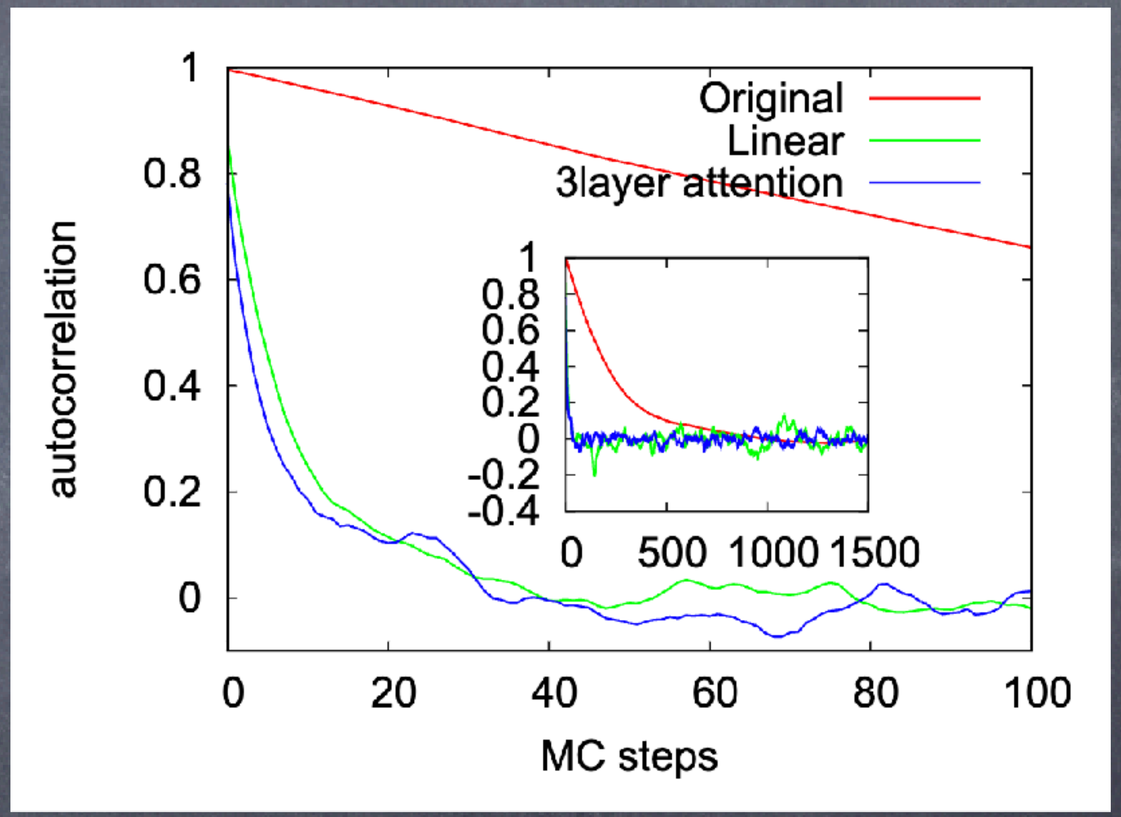
$$E = \sum_i \sum_l J_l \vec{S}_i \cdot \vec{S}_{i+l} + E_0$$ we get linearized model

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

Results

2D double exchange model(fermion + classical spin)





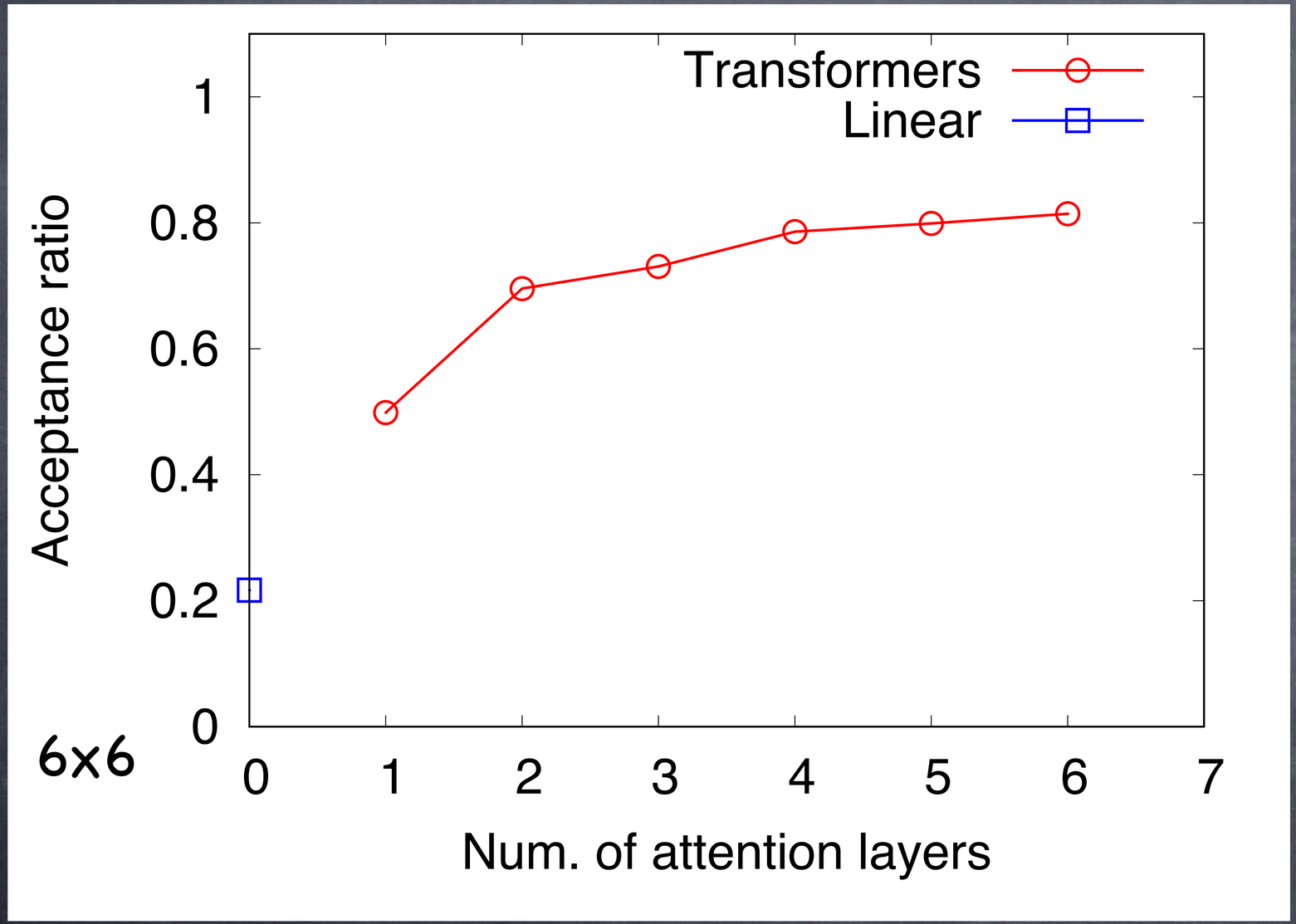
magnetization
and staggered magnetization

Autocorrelation time is reduced

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

Results

N=6



6-th nearest neighbors

$$K_i = \sum_l W_l S_{i+l}$$

Num. of parameters per layer

7+7+7 = 21

Last layer: nearest neighbors

$$E = \sum_i \sum_l J_l \vec{S}_{3i} \cdot \vec{S}_{3i+l}$$

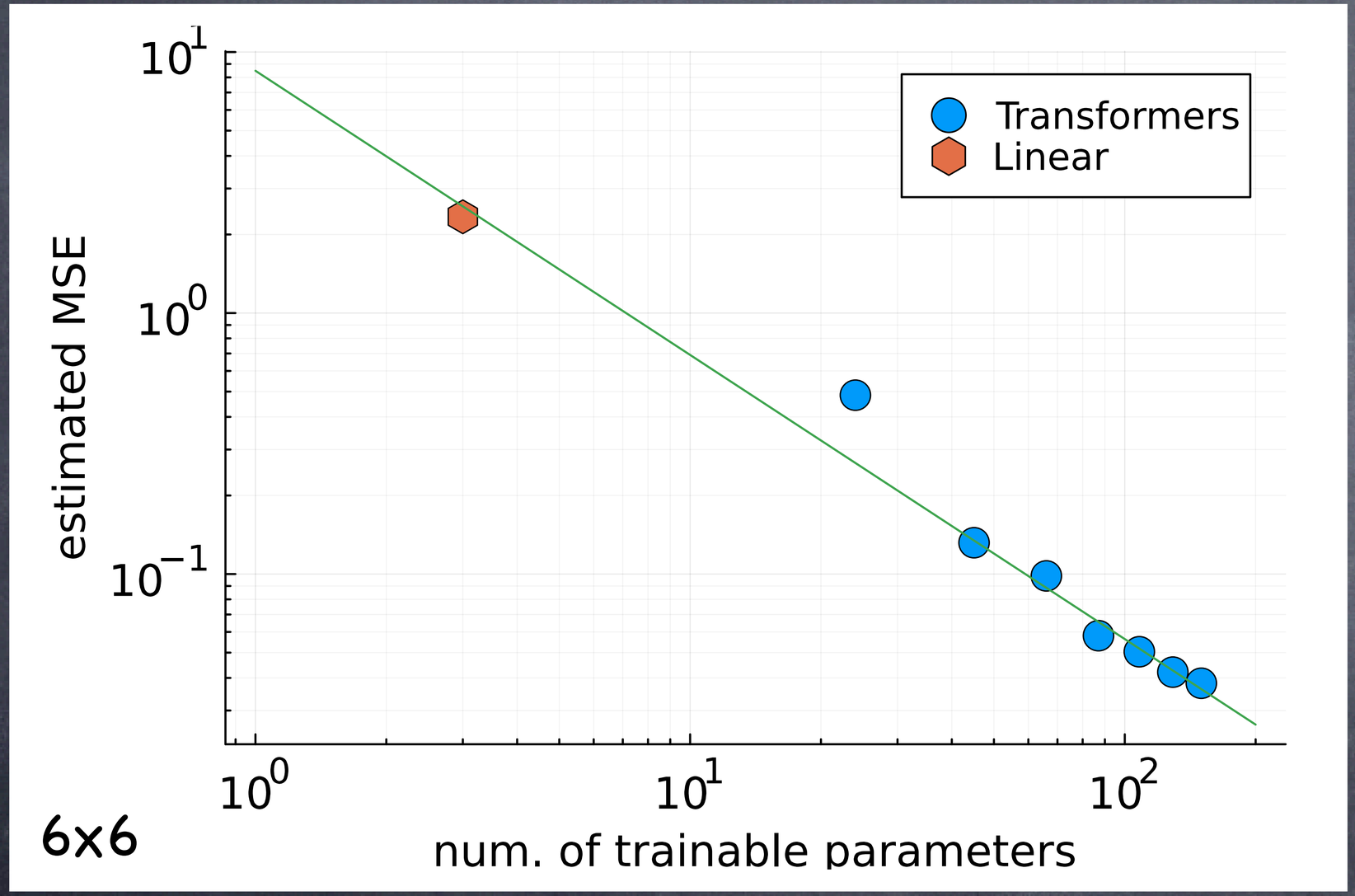
Num. of parameters is small

High acceptance ratio!

Yuki Nagai and Akio Tomiya, J. Phys. Soc. Jpn. 93, 114007 (2024)

Results

arXiv: 2306.11527



6-th nearest neighbors

$$K_i = \sum_l W_l S_{i+l}$$

Num. of parameters per layer

7+7+7 = 21

Scaling law?

This is like the scaling laws in Large Language Models

This is MC simulation

We generate data as we want

Application to LatticeQCD

2. We make three variables **K,Q,V** from **A**

K = W^KA, Q = W^QA, V = W^VA

We introduced "operators" $\hat{S}^{\mathrm{Q}} = \bar{W}^{\mathrm{Q}}\hat{S}$ ⇨ Effective gauge field U^Q is needed

3. We generate new vector/matrix/tensor **B**

$$B_l = A_l + \sum_i P_i^l V_i \qquad P = \sigma(QK^T)$$ correlation between Q and K

We introduced inner product of spins ⇨ What is "inner product" in gauge field?

We can use Wilson loop as an inner product

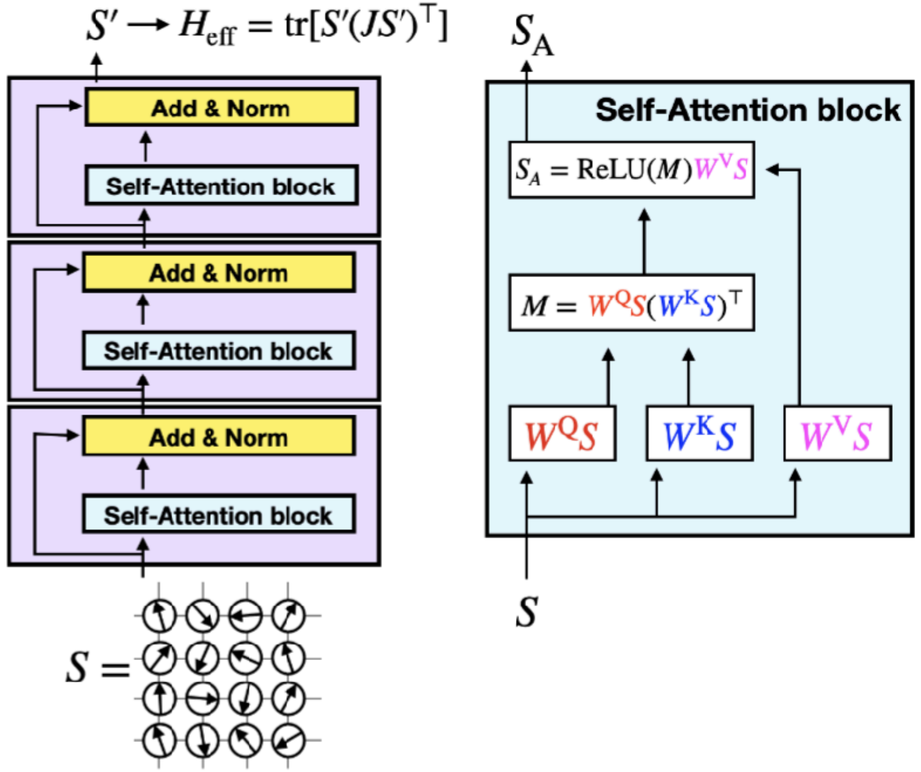
Yuki Nagai, Hiroshi Ohno, Akio Tomiya, "CASK: A Gauge Covariant Transformer for Lattice Gauge Theory", PoS, DOI:10.22323/1.466.0030, arXiv:2501.16955

Summary

Summary

Yuki Nagai and Akio Tomiya, “Self-Learning Monte Carlo with Equivariant Transformer”, J. Phys. Soc. Jpn. 93, 114007 (2024)

Equivariant Transformer in spin systems



Equivariant with respect to spin-rotational and translational symmetries

We found the scaling law!

We can improve models with increasing num. of layers

“Transformer and Attention” is very useful!