

# 経路最適化法を用いた $U(1)$ ゲージ理論における 符号問題への取り組み

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# Content

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1. Sign problem
2. Path Optimization
3. low dimensional QCD
4.  $U(1)$  one plaquette action
5. Summary

# Sign problem

- When  $S \in \mathbb{C}$ , serious cancellation occurs in integration at large volume. And, integrals cannot be obtained precisely.

$$\mathcal{Z} = \int \mathcal{D}x e^{-\text{Re}S - i\text{Im}S} \ll \int \mathcal{D}x e^{-\text{Re}S}$$

- Seriousness of the sign problem  
... average phase factor (APF)

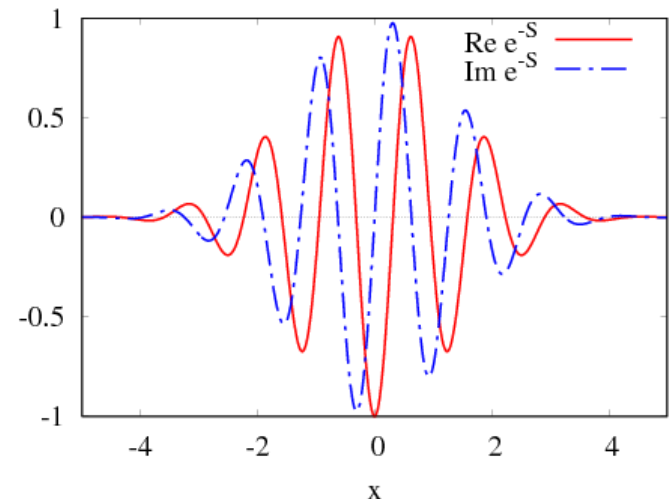
$$\begin{aligned} \text{APF} &= \frac{\int \mathcal{D}x e^{-\text{Re}S} e^{-i\text{Im}S}}{\int \mathcal{D}x e^{-\text{Re}S}} \\ &\sim e^{-\beta V \Delta f} \sim 0 \end{aligned}$$

- e.g. finite density QCD

$$\det(D(\mu))^* = \det(D(-\mu^*)) \in \mathbb{C}$$

ex.)  $e^{-S(x)} = (x + 10i)^{50} e^{-x^2/2}$

J. Nishimura and S. Shimasaki,  
PRD 92 (2015) 011501



# Path Optimization

**Y.M.**, K. Kashiwa, A. Ohnishi,  
Phys. Rev. D96 (2017) no.11, 111501

Optimize the integral path in the complexified variable space to weaken the sign problem.  
(Integral of holomorphic(analytic) function is independent of integral path.)

We can regard the sign problem as an optimization problem.

(ex.) One variable case

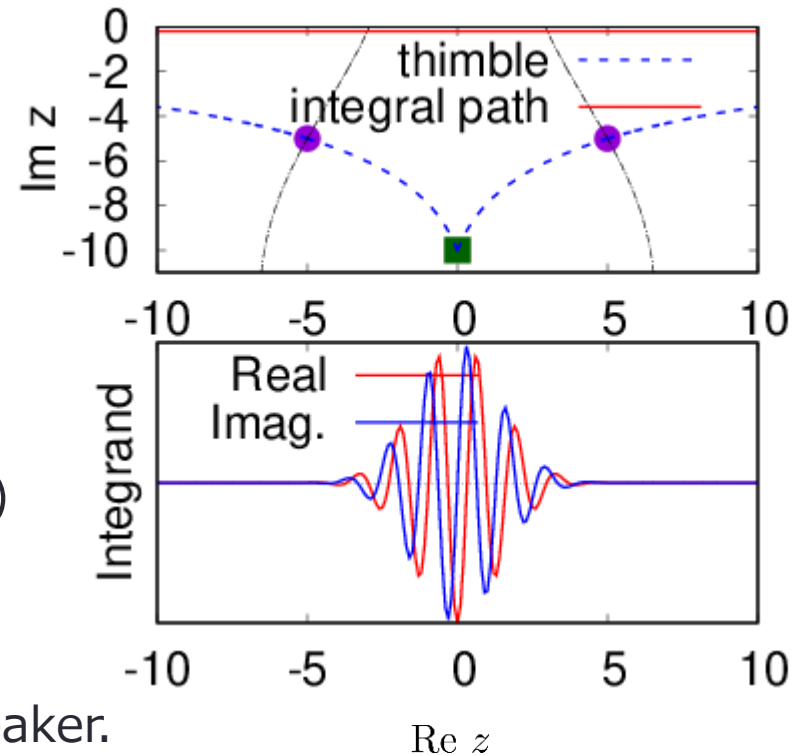
- Trial function (integral path)

$$z(\cdot) : \mathbb{R} \rightarrow \mathbb{C}$$

- Cost function (function to minimize)

$$\mathcal{F}[z(t)] = |\mathcal{Z}| \{ |\text{APF}|^{-1} - 1 \}$$

oscillation of the integrand becomes weaker.



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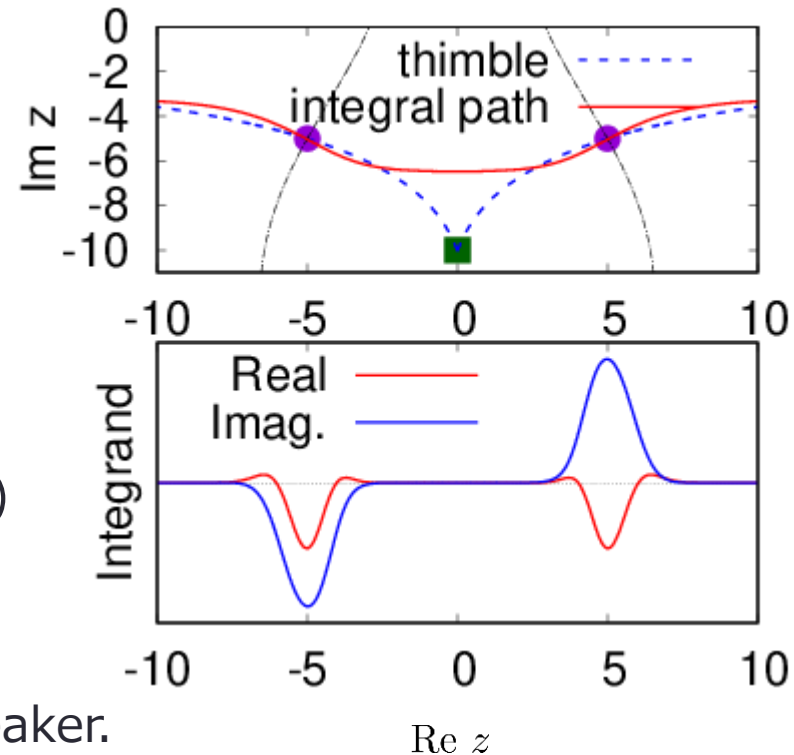
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# Neural Network for field theories

Neural Network(NN) is powerful to represent any functions of many inputs.

- Combination of linear and non-linear transformation

$$a_i = g(W_{ij}^{(1)} t_j + b_i^{(1)})$$

$$f_i = g(W_{ij}^{(2)} a_j + b_i^{(2)})$$

$$z_i(t) = t_i + i(\alpha_i f_i(t) + \beta_i)$$

$g(x)$  : Activation fn. (ex. tanh)

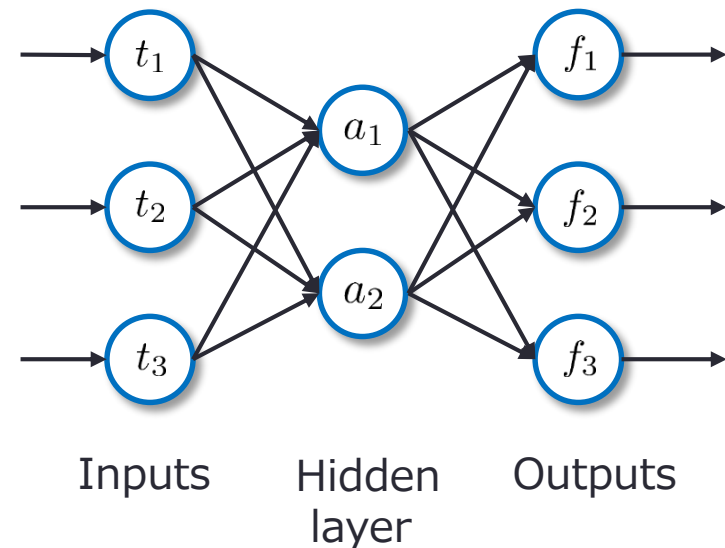
※  $W, b, \alpha, \beta$  : parameters

- Any fn. can be reproduced  
at (# of units of hidden layer)  $\rightarrow \infty$   
(Universal approximation theorem)

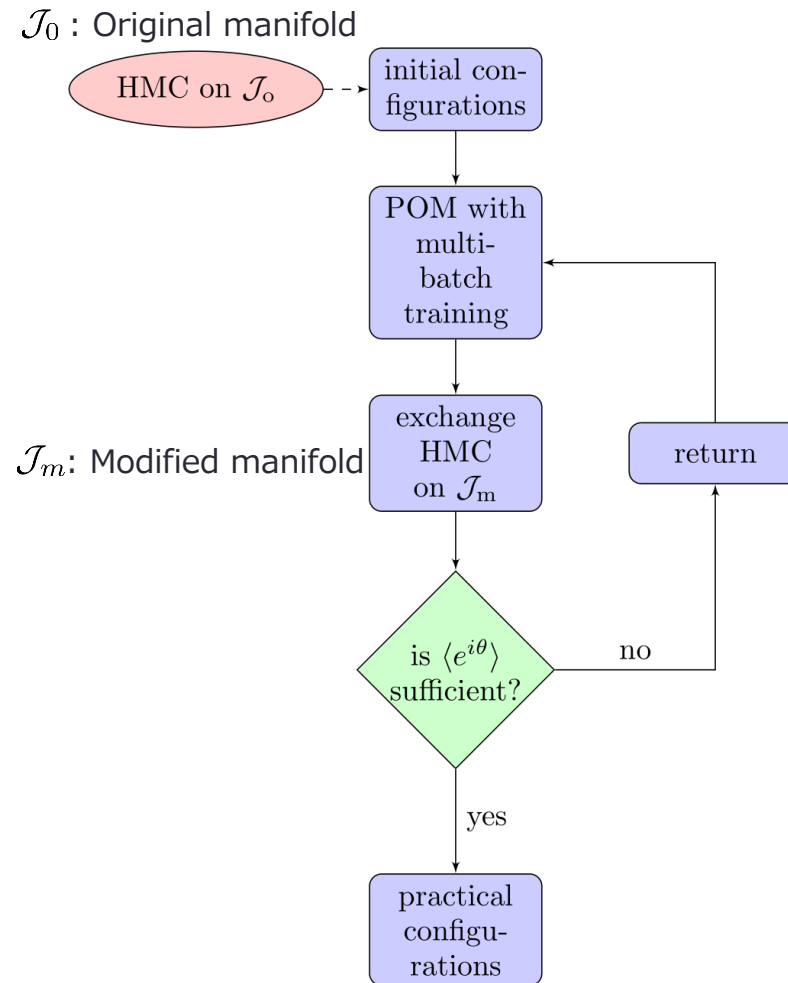
G. Cybenko, MCSS 2, 303 (1989)

K. Hornik, Neural networks 4, 251 (1991)

- We input the real part of variables,  
and obtain the imaginary part from outputs.



# Flowchart of POM



# 0+1 dim. QCD

YM, Kashiwa, Ohnishi,  
arXiv:1904.11140

Application to gauge theories

## ● 1-species of Staggered fermion

cf. CLM: Aarts, et al.(2010)

LTM: Schmidt, et al.(2016),  
Di Renzo, et al.(2017)

$$S = \frac{1}{2} \sum_{\tau} (\bar{\chi}_{\tau} e^{\mu} U_{\tau} \chi_{\tau+\hat{0}} - \bar{\chi}_{\tau+\hat{0}} e^{-\mu} U_{\tau}^{-1} \chi_{\tau}) + m \sum_{\tau} \bar{\chi}_{\tau} \chi_{\tau}$$

$$\mathcal{Z} = \int \mathcal{D}U \det D[U] = \int dU \det[X_N + (-1)^N e^{\mu/T} U + e^{-\mu/T} U^{-1}]$$

$$X_N = 2 \cosh(E/T), \quad E = \operatorname{arcsinh} m, \quad T = 1/N$$

One link variable, No plaquette



# 1 dim. QCD one link

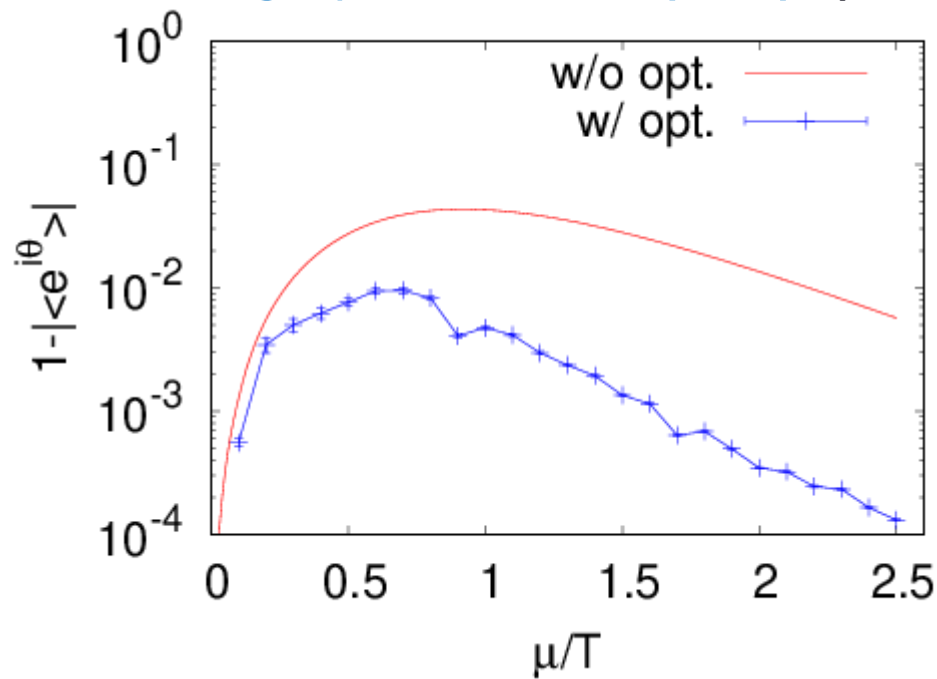
YM, Kashiwa, Ohnishi,  
arXiv:1904.11140

- **Complexification the link variable**

$$\mathcal{U}(U) = U \prod_a e^{y_a \lambda_a / 2} \quad y_a(U) : \text{trial function}$$

We generate the configurations by HMC and optimize NN parameters by stochastic gradient descent(SGD, Adadelata).

- **1 – average phase factor(APF)** ( $m = 0.05$ ,  $T = 0.5$ )



After some steps of optimization,  
1-APF becomes  
3~100 times  
smaller than before.

# 1+1D QCD

YM, Kashiwa, Ohnishi,  
in progress

- Action with staggered fermion (strong coupling)

$$S = \bar{\chi}_x D_{xy} \chi_y$$

$$D_{xy} = m\delta_{x,y} + \frac{1}{2}(-1)^{x_0} \{ \delta_{x+\hat{1},y} U_{1,x} - \delta_{x,y+\hat{1}} U_{1,y}^{-1} \} \\ + \frac{1}{2} \{ \delta_{x+\hat{0},y} e^{\mu} U_{0,x} - \delta_{x,y+\hat{0}} e^{-\mu} U_{0,y}^{-1} \}$$

- Polyakov gauge (without diagonal gauge fixing)

$$U_{0,x} \begin{cases} = \mathbb{1} & (x_0 \neq N_\tau) \\ \in \text{SU}(3, \mathbb{C}) & (x_0 = N_\tau) \end{cases}$$

※There still remains the gauge degree of freedom depending on only x

- Complexification

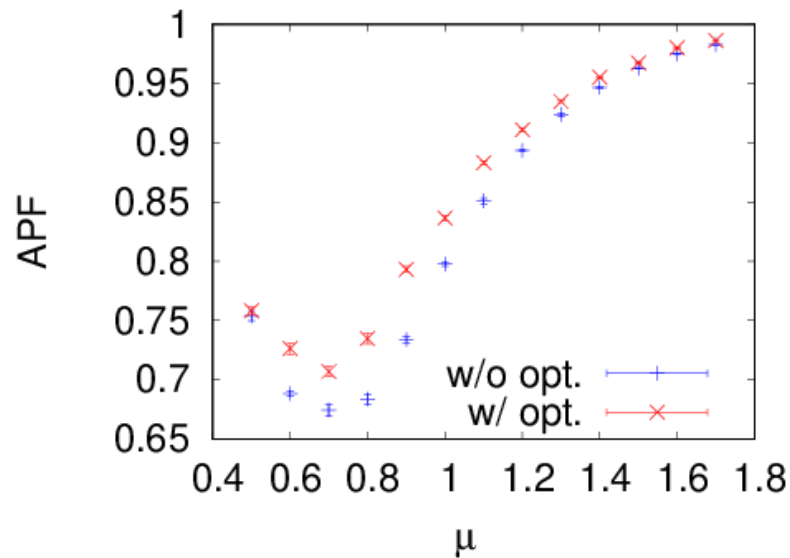
$$U_{\nu,x} \in \text{SU}(3) \rightarrow \mathcal{U}_{\nu,x}(U) \in \text{SL}(3, \mathbb{C})$$

# 1+1D QCD

YM, Kashiwa, Ohnishi,  
in progress

$2 \times 2$  Lattice,  $N_f = 2, m = 0.1$

Average phase factor



Average phase factor can be slightly enhanced by the deformation of manifold.

...Is there upper bound of APF?  
Is the optimization failed?  
(and Why?)

→We study the U(1) gauge theory to investigate this reason

# U(1) one plaquette action

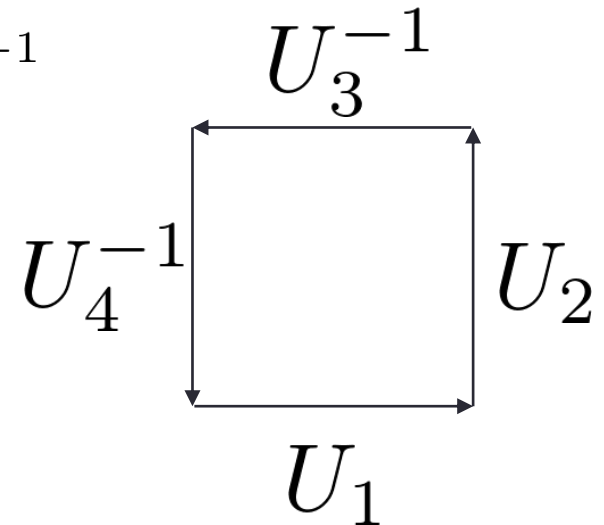
Kashiwa and YM,  
arXiv:2007.04167.

## ●Action

$$S = \frac{\beta}{2}(P + P^{-1}), \quad P = U_1 U_2 U_3^{-1} U_4^{-1}$$

## ●Partition function

$$Z = \int \prod_i dU_i e^{-S} = \underbrace{I_0(\beta)}_{\text{Modified Bessel fn.}}$$



## ●Gauge fixing

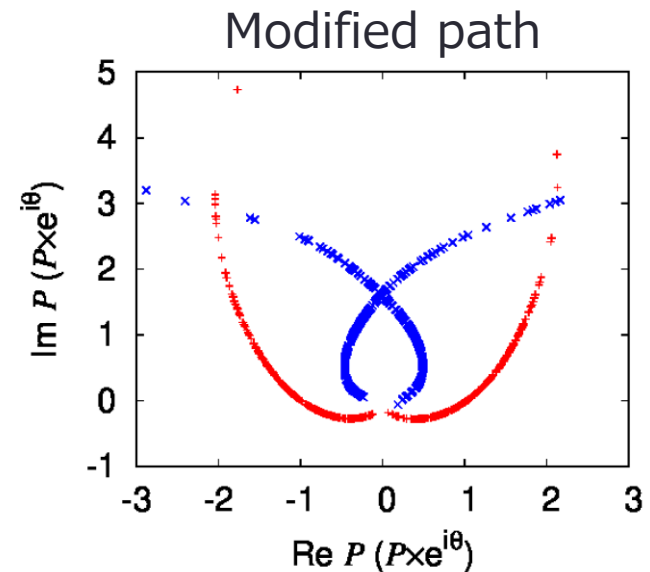
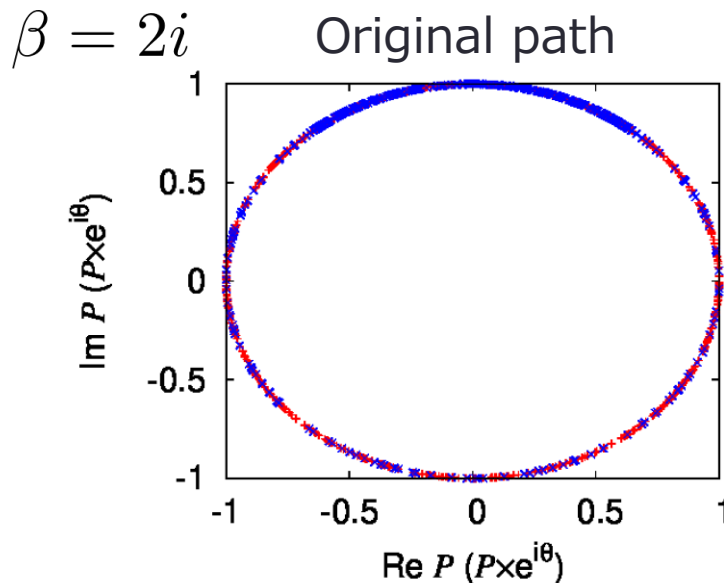
1~3 link variables among 4 can be fixed as a unit element

$$U_n = \begin{cases} \mathbb{I} & n : \text{fixed variable} \\ U_n & \text{otherwise} \end{cases}$$

# U(1) | integral path

Kashiwa and YM,  
arXiv:2007.04167.

- In the following,  $\beta$  is pure imaginary and we use the gauge fixing:  $U_n = \begin{cases} \mathbb{I} & n \neq 1 \\ P & n = 1 \end{cases}$
- We complexify the variable  $\mathcal{P} = P \times e^{y(P)}$ ,  $y(P) \in \mathbb{R}$  and optimize  $y(P)$
- Scatter plot of  $\mathcal{P}$  and  $\mathcal{P} \times e^{i\theta}$  ( $\theta$ : phase of  $J e^{-S}$ , probability:  $|J e^{-S}|$ )



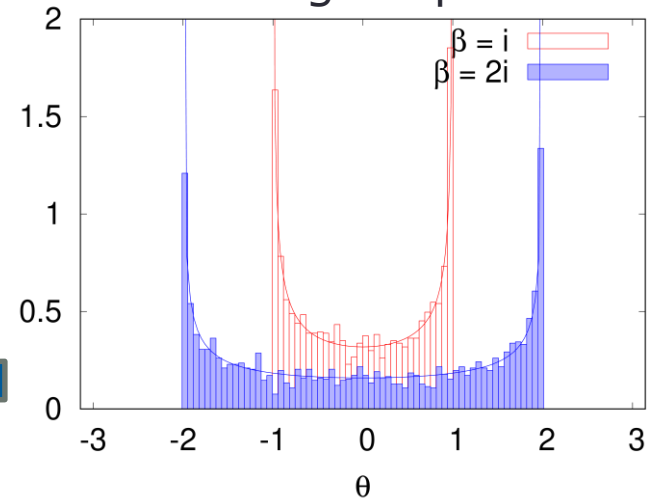
# U(1) | phase histogram

Kashiwa and YM,  
arXiv:2007.04167.

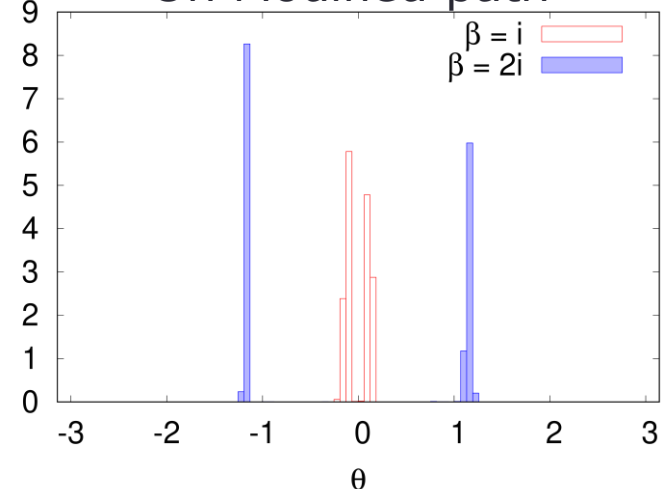
- Normalized histogram of phase  $\theta$  ( $\theta$ : phase of  $Je^{-S}$ )
- $\theta$  distribution becomes well localized by optimization.
- There remains global sign problem  
→ exchange Monte Carlo is needed.  
So we use exchange HMC in this work,



On original path



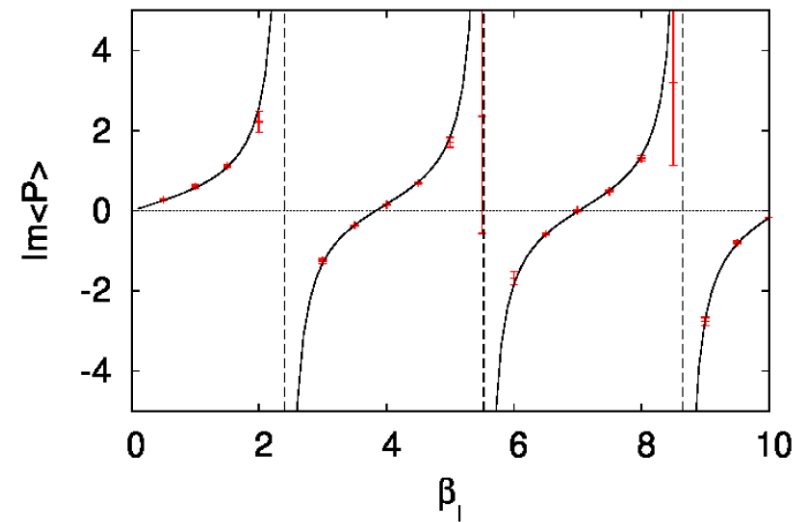
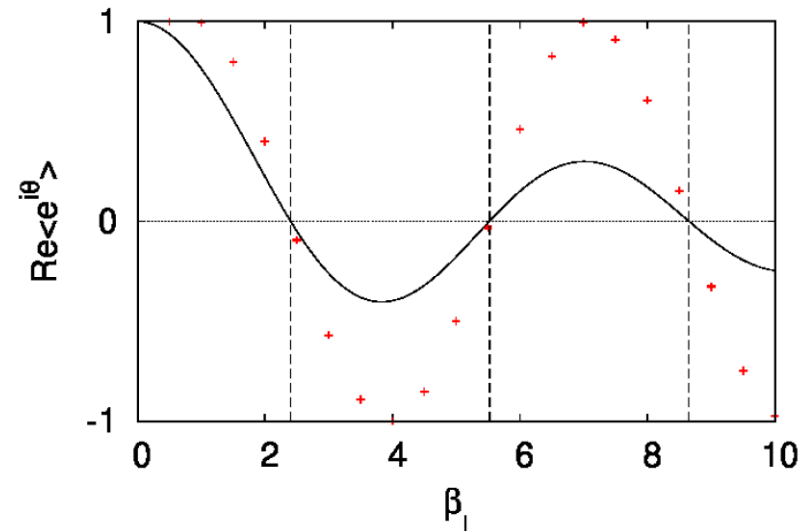
On Modified path



# U(1) | expectation value

Kashiwa and YM,  
arXiv:2007.04167.

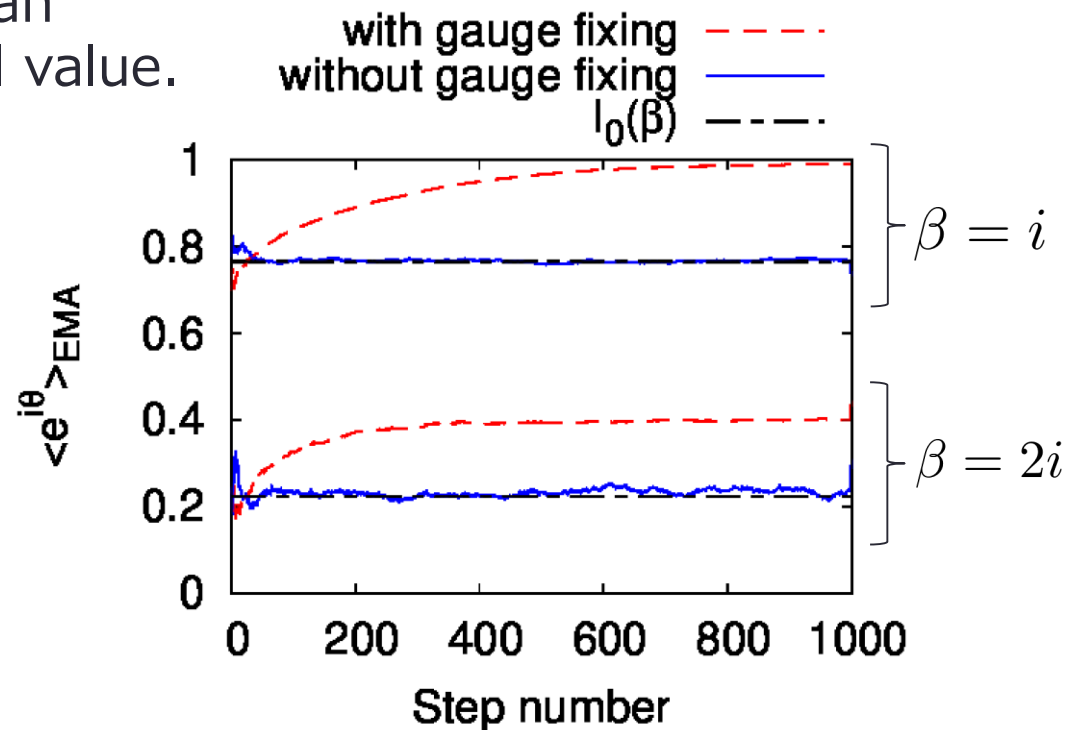
- Average phase factor
  - APF can be enhanced.  
(solid line :APF on original path)
  - The upper bound is caused by global sign problem
- Expectation value of Plaquette
  - Analytic results (solid line) are reproduced except the region near zero point of  $\mathcal{Z}$ .  
...exchange HMC works well.



# U(1) | effect of gauge fixing

Kashiwa and YM,  
arXiv:2007.04167.

- Average phase factor as a function of optimization step with/without gauge fixing
- With gauge fixing, APF can approach to the maximal value.
- Without gauge fixing, optimization fails.
- The symmetry may be difficult to learn





# Summary

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- In the path optimization method, we can regard the sign problem as an optimization problem.
  - Neural Network and optimization methods (SGD) developed in machine learning are helpful.
- We apply this method to  $U(1)$  gauge theory with one plaquette action
  - With gauge fixing, average phase factor becomes large and exact results are reproduced in observable calculations.
  - Without gauge fixing, the optimization fails.
- We will study this reason.