The sign problem in low dimensional QCD studied by using the path optimization

Yuto Mori (Kyoto Univ.)

Kouji Kashiwa (Fukuoka Inst. Tech.)
Akira Ohnishi (YITP)

2019/6/26 XQCD2019 @ Tokyo

Content

1. Sign problem, Path Optimization
2. 0+1 dimensional QCD
   1. w/ diagonal gauge fixing
   2. w/o diagonal gauge fixing (one link variable)
3. 1+1 dimensional QCD(preliminary)
4. Summary

Sign problem

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

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

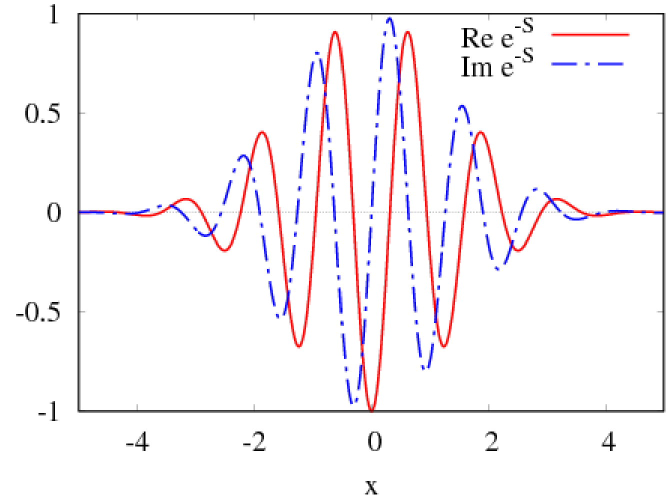
- Seriousness of the sign problem
  $\cdots$ average phase factor (APF)

$$\mathrm{APF} = \frac{\int \mathcal{D}x e^{-\mathrm{Re}S} e^{-i\mathrm{Im}S}}{\int \mathcal{D}x e^{-\mathrm{Re}S}}$$

$$\sim e^{-\beta V \Delta f} \sim 0$$

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.

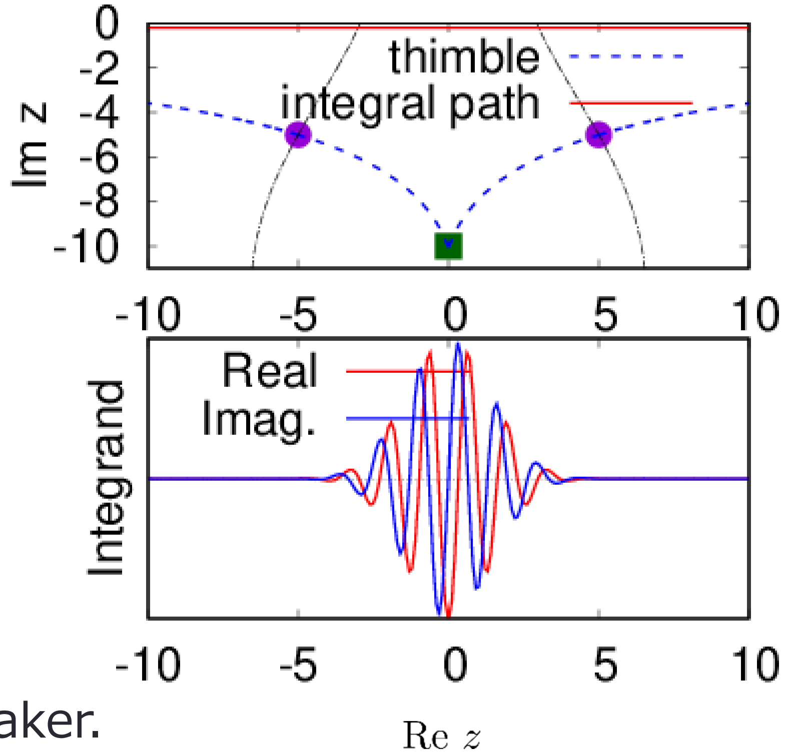
(ex.) One variable case

- Trial function (integral path)

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

- Cost function (function to minimize)

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



oscillation of the integrand becomes weaker.

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

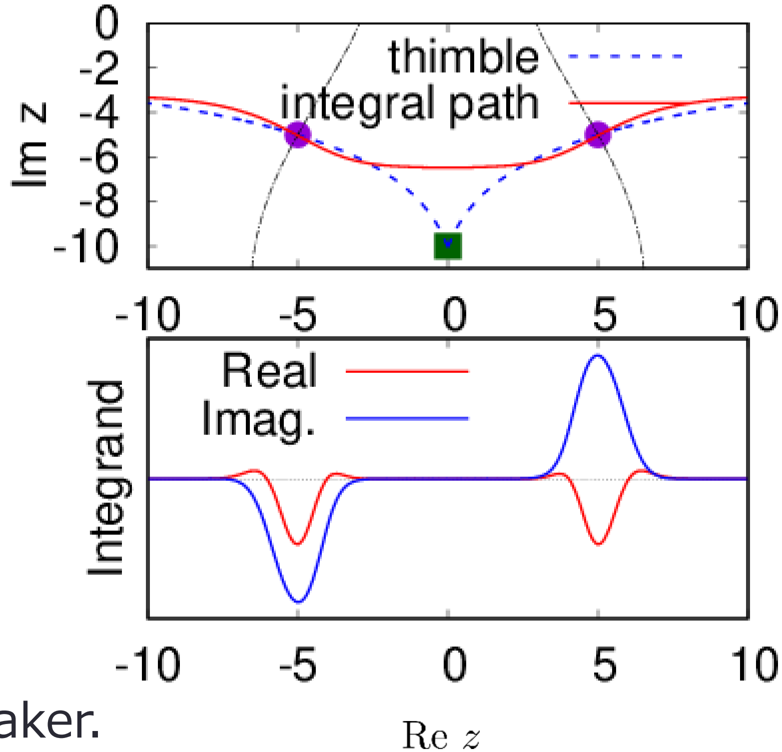
- Trial function (integral path)

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

- Cost function (function to minimize)

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

oscillation of the integrand becomes weaker.



ex.) One-site Hubbard Model

- Hamiltonian

$$\hat{H} = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow)$$

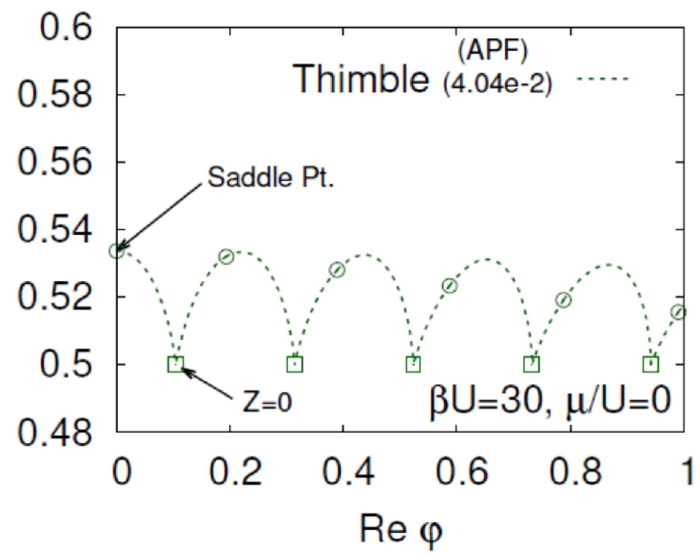
- Path integral representation

$$\mathcal{Z} = \sqrt{\frac{\beta U}{2\pi}} \int d\varphi [1 + \exp(\beta U(i\varphi + \mu/U + 1/2))]^2 \exp[-\beta U \varphi^2/2]$$

- Analysis by Lefschetz thimble

  Tanizaki, Hidaka, Hayata, 2016

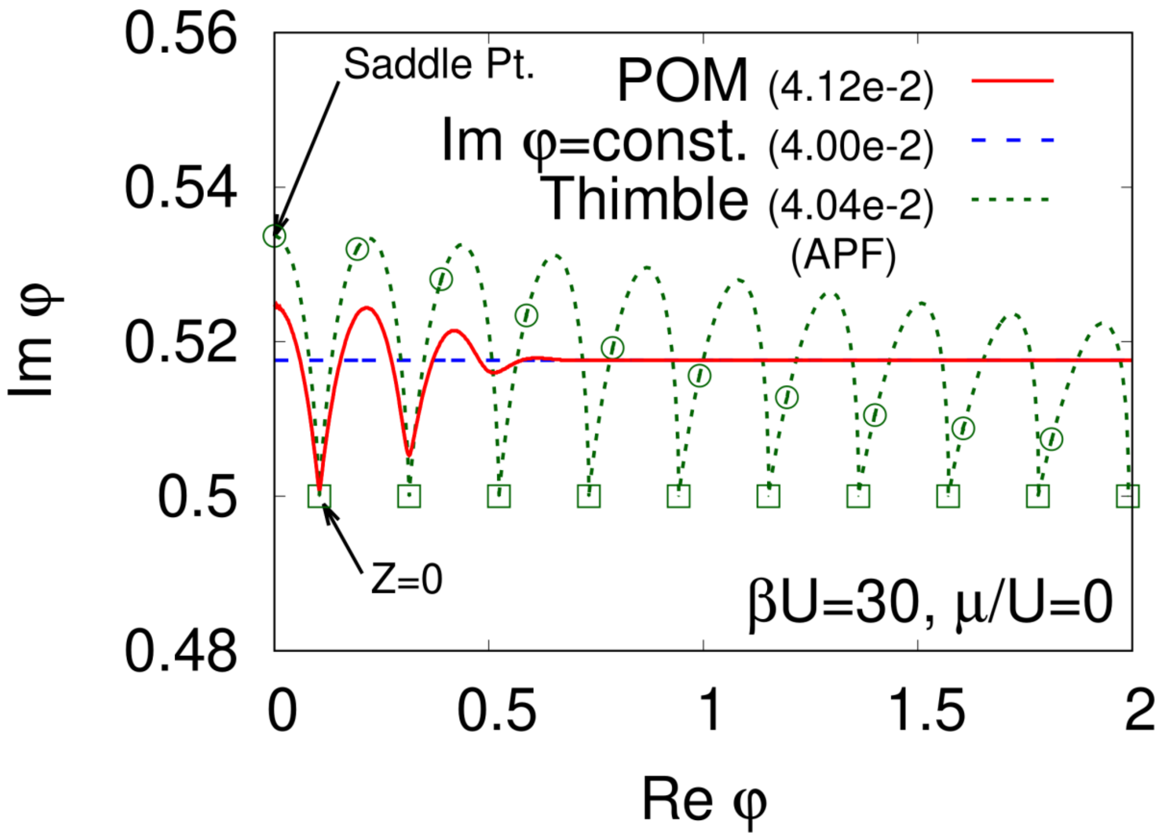
  - Number of relevant thimbles increases with $\beta = 1/T$



ex.) One-site Hubbard Model

Ohnishi, YM, Kashiwa, in progress

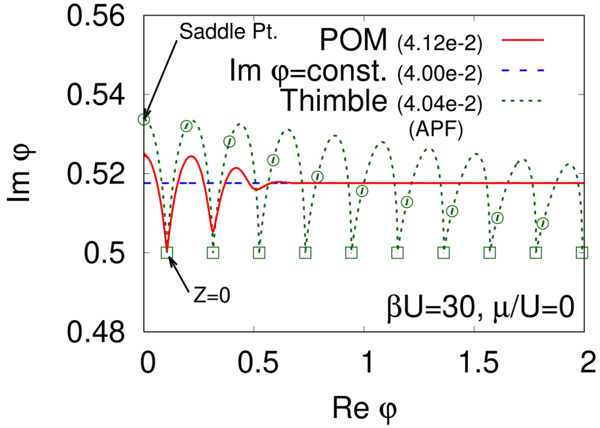
•Integral Path



- There is a gap between the POM and thimble even around the saddle pt.
- The average phase factors are almost same.

ex.) One-site Hubbard Model

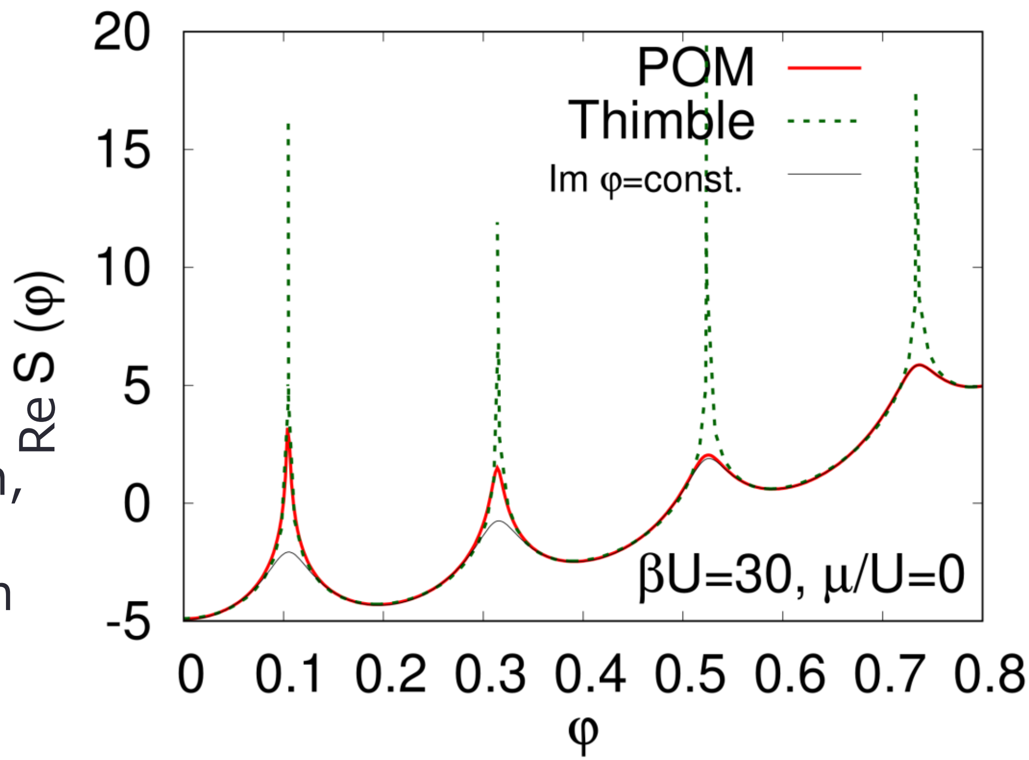
Ohnishi, YM, Kashiwa,
in progress



- Potential barrier is mild above on the blue line.

→To use MCMC calculation, we should choose moderately optimized path or use the annealing or tempering algorithm.

- Integrand



Neural Network for field theories

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

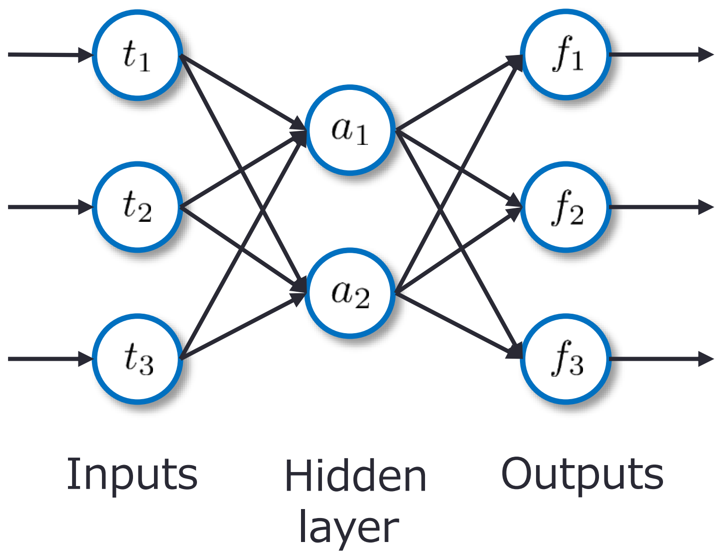
- Combination of linear and non-linear transformation

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

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

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

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



- Any fn. can be reproduced at (# of units of hidden layer) $\to \infty$ (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.

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

0+1D QCD

YM, Kashiwa, Ohnishi, arXiv:1904.11140

Application to gauge theories

- 1-spiecies of Staggered fermion

cf. CLM: Aarts, et al.(2010)
LTM: Schmidt, et al.(2016), Di Renzo, et al.(2017)

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

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

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

One link variable, No plaquette

0+1D QCD

YM, Kashiwa, Ohnishi, arXiv:1904.11140

There are two ways of complexifying link variables.

① Complexification after diagonal gauge fixing

$$U = \mathrm{diag}(e^{ix_1}, e^{ix_2}, e^{ix_3}), \ (x_3 = -(x_1 + x_2))$$

$$\mathcal{Z} = \int dx_1 dx_2 \underline{H(x)} \exp(-S(x))$$

Haar measure

$$H(x) = \frac{8}{3\pi^2} \prod_{a<b} \sin^2\left(\frac{x_a - x_b}{2}\right)$$

$$e^{-S(x)} = \prod_a (X_N + 2\cos(x_a - i\mu))$$

$x_a \in \mathbb{R} \to z_a \in \mathbb{C}$ $z_a(x) = x_a + i y_a(x), \ y_a(x)$: trial function

② Complexification without diagonal gauge fixing

$$U \in \mathrm{SU}(3) \to \mathcal{U} \in \mathrm{SL}(3, \mathbb{C})$$

- ex. $\mathcal{U}(U) = U \prod_a \exp(y_a \lambda_a)$ $y_a(U)$: trial function

0+1D QCD diagonal gauge

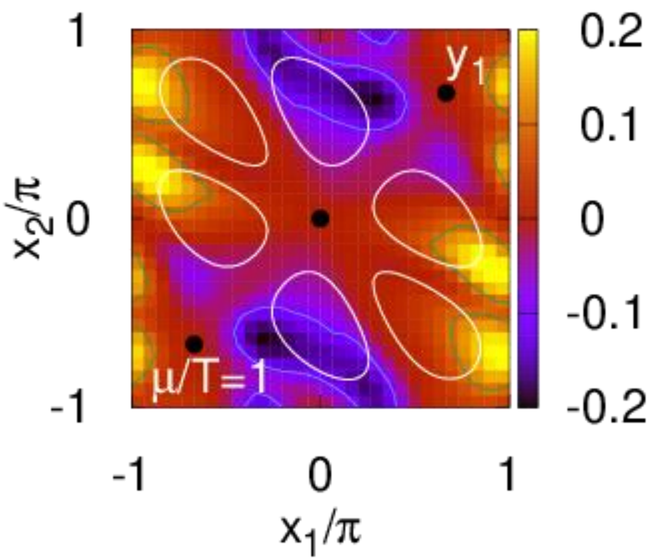
YM, Kashiwa, Ohnishi, arXiv:1904.11140

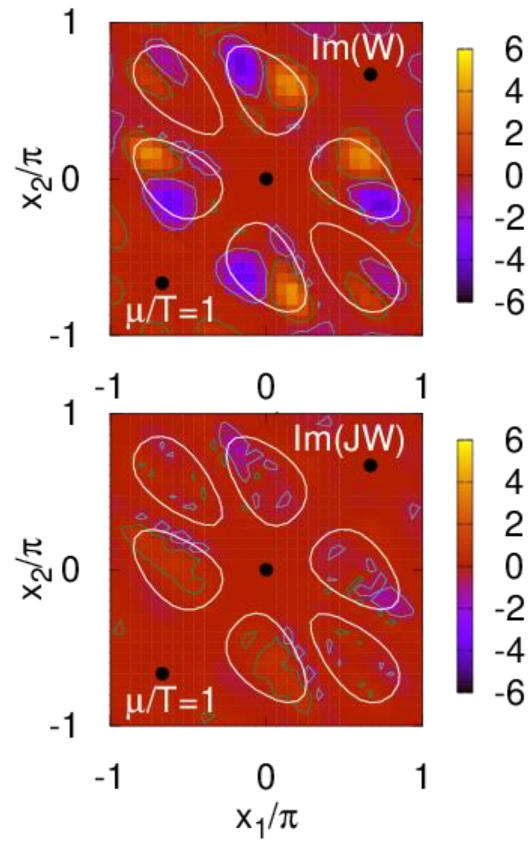
① Complexification after diagonal gauge fixing

$$\mathcal{Z} = \int dz_1 dz_2 H(z) e^{-S(z)} = \int dx_1 dx_2 J H(z(x)) e^{-S(z(x))}$$

Optimization of z by gradient descent method

$m = 0.05,\ T = 0.5,\ \mu/T = 1.0$





$W = He^{-S}$

Phase of J cancels that of W

0+1D QCD diagonal gauge

YM, Kashiwa, Ohnishi, arXiv:1904.11140

① Complexification after diagonal gauge fixing

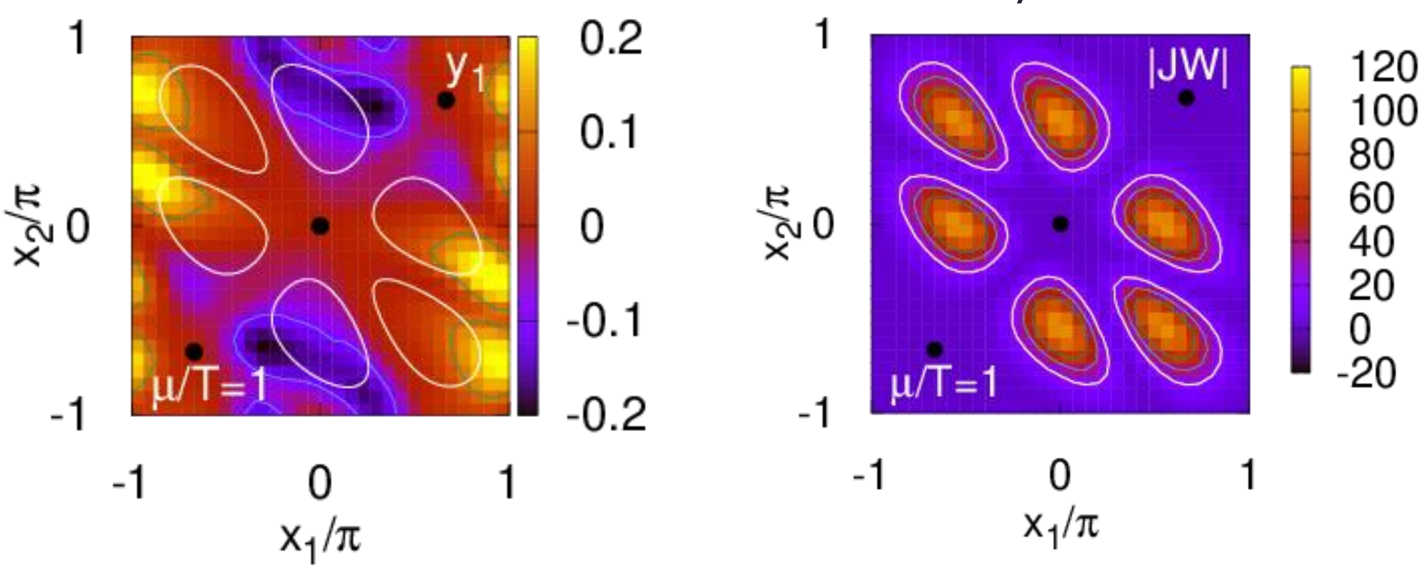
$$\mathcal{Z} = \int dz_1 dz_2 H(z) e^{-S(z)} = \int dx_1 dx_2 J H(z(x)) e^{-S(z(x))}$$

Optimization of z by gradient descent method

$$m = 0.05,\ T = 0.5,\ \mu/T = 1.0$$

$$H(x) = \frac{8}{3\pi^2} \prod_{a<b} \sin^2\left(\frac{x_a - x_b}{2}\right)$$

→Separation of probability distribution. Difficulty in HMC.



0+1D QCD one link

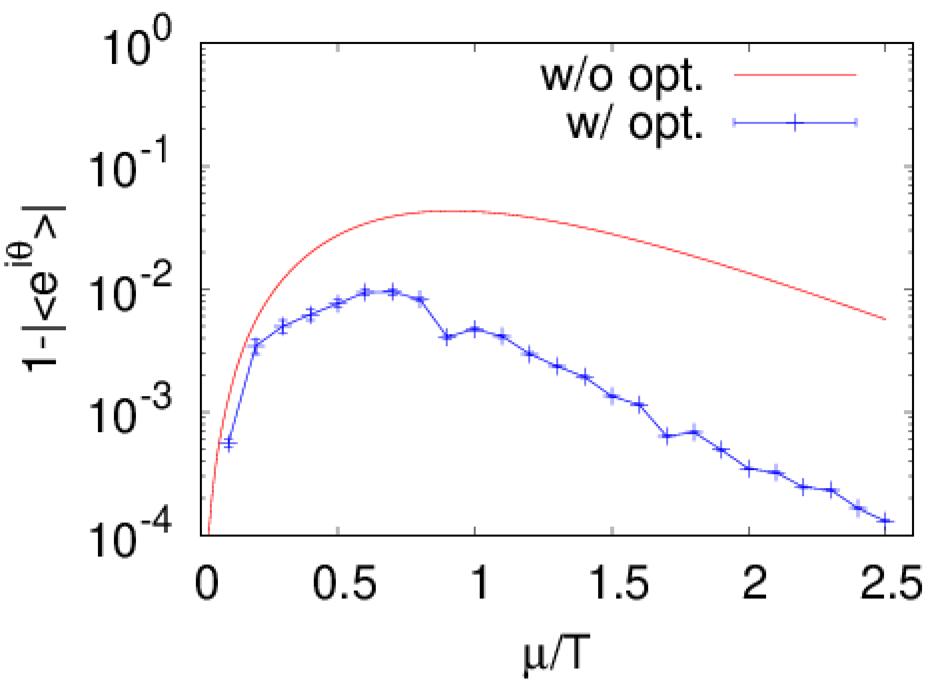
YM, Kashiwa, Ohnishi, arXiv:1904.11140

② Complexification without diagonal gauge fixing

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

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

- 1 – average phase factor(APF)



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

0+1D QCD one link

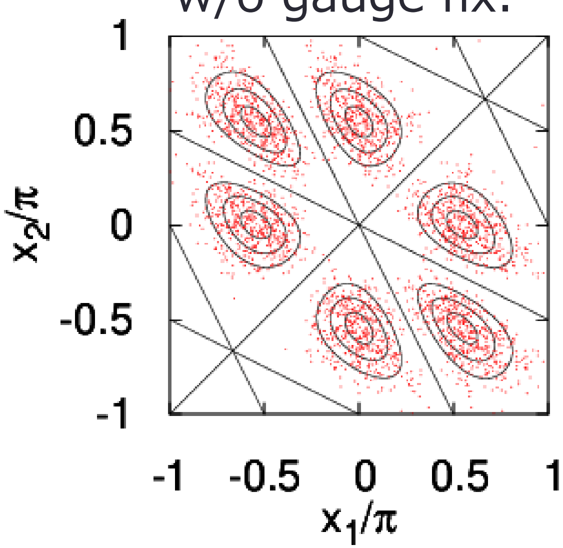
YM, Kashiwa, Ohnishi, arXiv:1904.11140

- Eigenvalue distribution

$$PUP^{-1} = \mathrm{diag}(e^{iz_1}, e^{iz_2}, e^{-i(z_1+z_2)})$$

Six separated region are produced by HMC

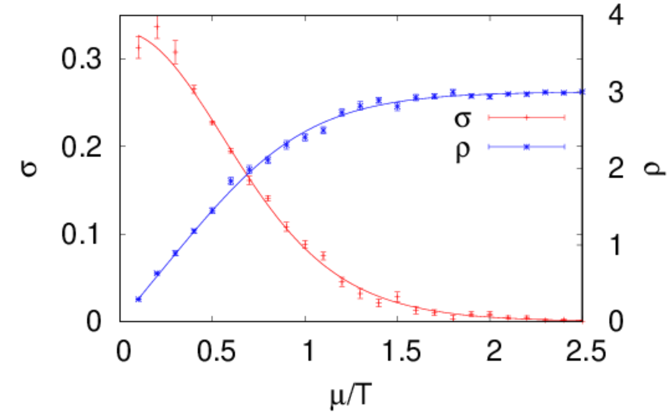
w/o gauge fix.

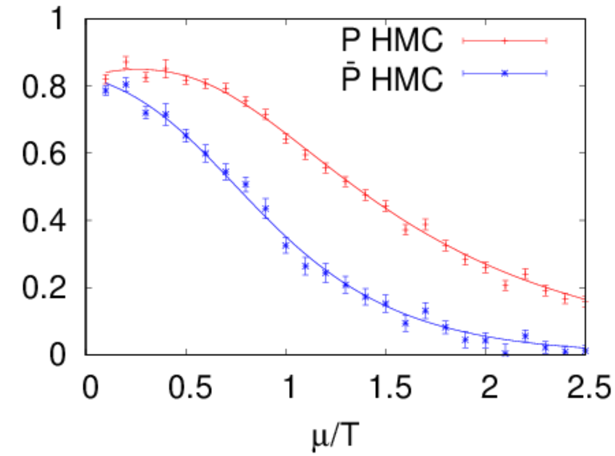


$m = 0.05,\ T = 0.5,\ \mu/T = 1.0$

- Expectation value

Consistent with exact solutions.





1+1D QCD

YM, Kashiwa, Ohnishi, in progress

- Action with staggered fermion (strong coupling)

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

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

- Polyakov gauge (without diagonal gauge fixing)

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

- Complexification

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

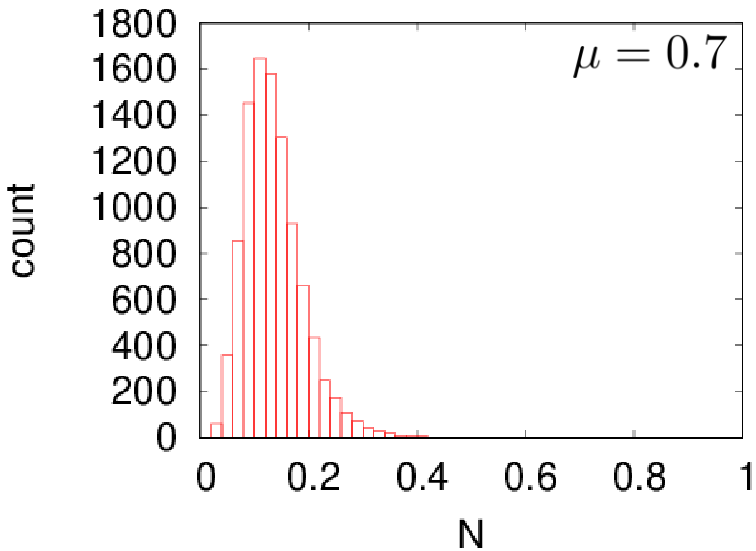
1+1D QCD

YM, Kashiwa, Ohnishi, in progress

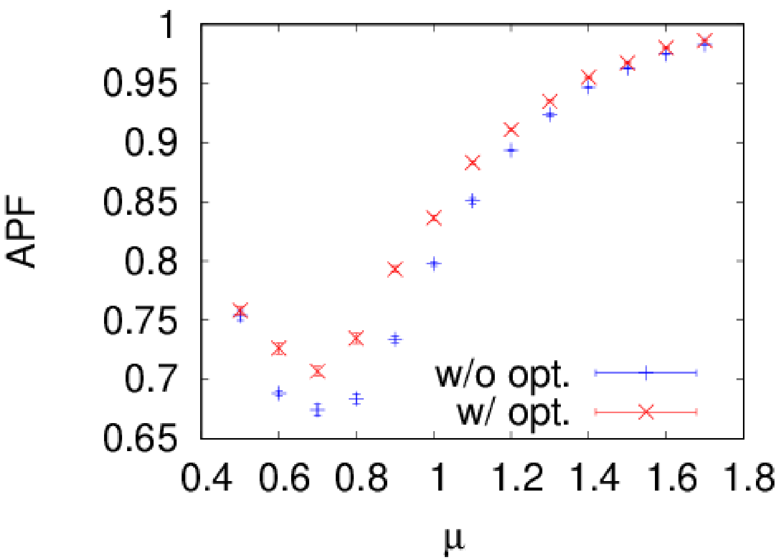
2×2 Lattice, $N_f = 2, m = 0.1$

Unitarity norm after opt.

$$N = \max_{x,\nu} \mathrm{tr}(\mathcal{U}^\dagger_{\nu,x}\mathcal{U}_{\nu,x} - \mathbb{1})^2$$



Average phase factor



Average phase factor can be slightly enhanced by the deformation of manifold.
···Is there upper bound of APF?

Summary

- 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 0+1 dim. QCD with and without diagonal gauge fixing.
  - Average phase factor becomes large and exact results are reproduced in observable calculations.
  - Without gauge fixing, eigenvalue distribution agrees with gauge fixed results, and HMC works well.
- In 1+1D QCD, works in progress.