Search for an Effective Change of Variable in QCD simulations

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work in collaboration with P. Boyle, T. Izubuchi, L. Jin, C. Jung, C. Lehner, and A. Tomiya

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(work in progress)

Background and Short summary (1/2)

Difficulties in taking the continuum limit

- Critical slowing down
- Topological freezing

cf. Talks by A. Tomiya, C. Jung, S. Foreman for related ideas for accelerating the simulation.

Our goal

Arrange a change of variable which makes the Monte Carlo calculation more efficient.

- In particular, we consider the trivializing maps. Nicolai '80, Lüscher '09 Lüscher constructed a flow that maps YM theory at finite β to the strong coupling limit.
- Several investigations have been made in this context. E.g.,
 - CP^{N-1} model calculation with the gradient flow. Engel, Schaefer '11 cf. Talks by M. Lüscher, R. Harlander, A. Hasenfratz for uses of the gradient flow
 - Machine learning studies (2D) scalar ϕ^4 theory Albergo et al. '19 2D U(1) gauge theory Kanwar et al. '20, Foreman, Izubuchi, L. Jin, X. Y. Jin, Osborn, Tomiya '21
 - Increase of the topological tunneling rate in Wilson-flowed HMC L. Jin LATTICE 2021 (4D YM theory)

He also shared us the result of adding a staple of the form: -- .

We have extended L. Jin's code to cover a wide range of smearing kernels, including all the shapes with footprint 2.

[2/19]

Background and Short summary (2/2)

However, adding higher order terms is costly because they induce larger number of terms for their complicated shapes.

- ∴ It is desirable to
 - have a measure of the effectiveness of adding a particular kernel
 - control the effect of the map on the resulting theory.

e.g., trivialize the UV part of the theory

In this talk,

 We discuss a way to measure effective action of flowed gluon field with the <u>Schwinger-Dyson equation</u>.

cf. Gonzalez-Arroyo, Okawa '87, de Forcrand et al. '00

In particular, we introduce a norm in the space of actions with their forces, by which the truncation error can be explicitly evaluated.

We explore a way to construct approximated trivializing maps using the Schwinger-Dyson equation step by step.

We show preliminary results of test calculations with several smearing kernels.

Though the results are for the 4D pure YM theory, the method may be generalized for a system with fermions (which is another field of study we are going to investigate).



• We consider a gauge system:

$$\langle \mathcal{O} \rangle_S \equiv \frac{\int (dU) e^{-S(U)} \mathcal{O}(U)}{\int (dU) e^{-S(U)}}$$

and parametrize the field $U=(U_{x,\mu})$ locally by the coordinates $(\theta^A)\equiv(\theta^a_{x,\mu})$:

$$e^{\theta_{x,\mu}^a T^a} U_{x,\mu}$$

$$\begin{bmatrix} T^a : su(3) \text{ generators, } tr(T^a T^b) = -\frac{1}{2} \delta^{ab} \\ \text{Haar measure } (dU) \text{ is then } (dU) \propto \prod_A d\theta^A \end{bmatrix}$$

• Lüscher proposed to look for a one-parameter family of maps $U = \mathcal{F}_t(V)$ s.t. the V-space effective action reaches the strong couping limit at t = 1 ("trivializing map"):

$$\begin{split} S_{\mathrm{eff},\,t}(V) &\equiv S\big(\mathcal{F}_t(V)\big) - \ln\,\det\mathcal{F}_{t*}(V) \\ S_{\mathrm{eff},\,t=1}(V) &= \mathrm{const.} \end{split} \qquad \begin{pmatrix} \mathcal{F}_{t*}(V) &= (\mathcal{F}_{t*}^{AB}(V)) \colon \mathrm{Jacobian\ matrix} \\ d\theta_{(U)}^A &= \mathcal{F}_{t*}^{AB}(V)\ d\theta_{(V)}^B \end{pmatrix} \end{split}$$

Since $S_{\text{eff},t}(V)$ approaches the strong coupling limit as we increase t, one can use this to generate more decorrelated configurations:

(i) generate configurations
$$\{V_i\}_{i=1,...,N_{\mathrm{conf}}}$$
 with $S_{\mathrm{eff},t}(V)$ $\left(N_{\mathrm{conf}}: \mathrm{sample\ size}\right)$

(ii) transform the field configurations: $U_i = \mathcal{F}_t(V_i)$

(iii) estimate
$$\langle \mathcal{O} \rangle_S$$
 by $\langle \mathcal{O} \rangle_S \approx \frac{1}{N_{\text{conf}}} \sum_i \mathcal{O}(U_i)$.

Lüscher constructed a trivializing flow for the Wilson action $S(U) = S_W(U)$, which can be expanded in powers of t:

• The flow is divided into infinitesimal steps, $t = m\epsilon$:

$$\mathcal{F}_{t=m\epsilon} = \mathcal{F}_{(m-1)\epsilon,\epsilon} \circ \mathcal{F}_{(m-1)\epsilon,\epsilon} \circ \cdots \circ \mathcal{F}_{\epsilon,\epsilon} \circ \mathcal{F}_{0,\epsilon}$$

• Each flow kernel is assumed to be the gradient of a scalar function $\tilde{S}_{t=m\epsilon}$:

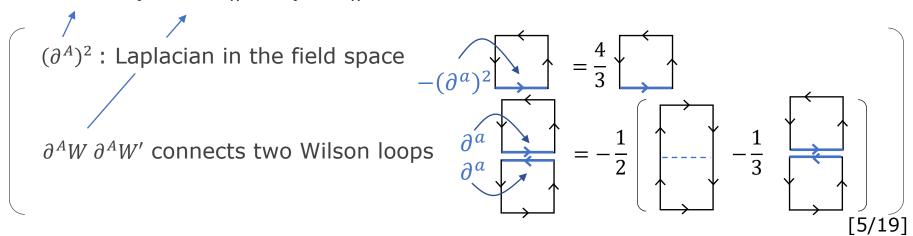
$$\mathcal{F}_{t,\epsilon}(U)_{x,\mu} = e^{-\epsilon T^a \partial_{x,\mu}^a \tilde{S}_t(U)} U_{x,\mu}. \qquad \left(\partial_{\theta_{x,\mu}^a} \equiv \partial_{x,\mu}^a \equiv \partial^A \right)$$

• Require that \mathcal{F}_t makes the effective action to be

$$S_{\text{eff},t}(V) = (1-t) S_W(\mathcal{F}_t(V))$$

 \Rightarrow the equation for \tilde{S}_t :

$$-(\partial^A)^2 \tilde{S}_t + t \ \partial^A S_W \ \partial^A \tilde{S}_t = S_W$$
 (up to an irrelevant constant; similarly below)



Equation for \tilde{S}_t :

$$[-(\partial^A)^2 + \underline{t \, \partial^A S_W \, \partial^A}] \, \tilde{S}_t = S_W$$

The derivative operator in the second term acts as adding a plaquette to \tilde{S}_t in all the possible ways (with a multiplication of t).

 \therefore The solution can be expressed by the *t*-expansion as:

$$\begin{split} \tilde{S}_t &= -\frac{\beta}{32} W_0 + \\ &+ t \frac{\beta^2}{192} (-\frac{4}{33} W_1 + \frac{12}{119} W_2 + \frac{1}{33} W_3 - \frac{5}{119} W_4 + \frac{3}{10} W_5 - \frac{1}{5} W_6 + \frac{1}{9} W_7) \\ &+ O(t^2) \end{split}$$
 NLO terms: footprint 2 shapes

 $W_0, ..., W_7$: Wilson loops

$$W_0 = \Sigma$$
 $+ c.c.$ $W_1 = \Sigma$ $+ c.c.$ $W_2 = \Sigma$ $+ c.c.$ $+ c.c.$ $+ c.c.$ $+ c.c.$ $+ c.c.$

$$W_5 = \sum \left(\begin{array}{c} \\ \\ \\ \end{array} \right) + c.c. \qquad W_6 = \sum \left(\begin{array}{c} \\ \\ \\ \end{array} \right) + c.c. \qquad W_7 = \sum \left(\begin{array}{c} \\ \\ \\ \end{array} \right)$$

HMC algorithm with the trivializing map (1/1)

Lüscher's proposal Lüscher '09

Perform the <u>Hybrid Monte Carlo (HMC)</u> updates in the *V*-space Duane et al. '87

using the effective action $S_{\text{eff.}\,t}(V)$ as the potential:

$$H(\pi, V) \equiv \frac{1}{2} (\pi^A)^2 + S_{\text{eff}, t}(V).$$

The exact formula for the gradient $\partial^A S_{\mathrm{eff},\,t}(V)$ was also derived for finite ϵ in terms of \tilde{S}_t . We also use this formula to calculate $\partial^A S_{\mathrm{eff},\,t}(V)$ for a given map \mathcal{F}_t .

• Note that the previous *t*-expansion is obtained from the requirement:

$$S_{\text{eff},t}(V) = (1-t)S(\mathcal{F}_t(V)).$$

It is this $S_{\text{eff},t}(V)$ that we directly work with in the HMC.

∴ We can alternatively impose

$$S_{\text{eff},t}(V) = (1-t)S(V),$$

aiming to use the map at finite t.

If the map can be constructed accurately, we can use the guided (Hybrid) Monte Carlo algorithm to reduce the costs from the Jacobian.

Horowitz '91; use different action in the Molecular Dynamics process not the one that appears in the Boltzmann weight.

Such a map can be constructed step by step:

Let us assume that the effective action at t is constructed such that

$$S_{\text{eff}, t}(V) = (1 - t) S(V).$$

• We transform the field infinitesimally as $V \mapsto \mathcal{F}_{t,\epsilon}(V)$ and require the effective action at $t + \epsilon$ to be

$$S_{\mathrm{eff},\,t+\epsilon}(V) = S_{\mathrm{eff},\,t}\big(\mathcal{F}_{t,\epsilon}(V)\big) - \ln\det\mathcal{F}_{t,\epsilon,*}(V), \qquad --- \text{(A)}$$

$$\stackrel{*}{=} (1-t-\epsilon)\,S(V).$$
requirement; the infinitesimal map $\mathcal{F}_{t,\epsilon}(V)$ is specificed by this equation.

• The composition ordering will be reversed from the ordinary flow:

$$\mathcal{F}_{t=m\epsilon} = \mathcal{F}_{0,\epsilon} \circ \mathcal{F}_{\epsilon,\epsilon} \circ \mathcal{F}_{(m-1)\epsilon,\epsilon} \circ \mathcal{F}_{(m-1)\epsilon,\epsilon}.$$

$$\begin{array}{l} \text{\mathcal{C} eff, $t=m\epsilon(V)$} \\ &= S_{\mathrm{eff, }(m-1)\epsilon} \big(\mathcal{F}_{(m-1)\epsilon,\epsilon}(V) \big) - \ln \det \mathcal{F}_{(m-1)\epsilon,\epsilon,*}(V) \\ &= S_{\mathrm{eff, }(m-2)\epsilon} \big(\mathcal{F}_{(m-2)\epsilon,\epsilon}(\mathcal{F}_{(m-1)\epsilon,\epsilon}(V)) \big) - \ln \det \mathcal{F}_{(m-2)\epsilon,\epsilon,*} \big(\mathcal{F}_{(m-1)\epsilon,\epsilon}(V) \big) - \ln \det \mathcal{F}_{(m-1)\epsilon,\epsilon,*}(V) \\ &= \cdots \\ &= S_{\mathrm{eff, }t=0} \big(\mathcal{F}_{0,\epsilon} \circ \cdots \circ \mathcal{F}_{(m-1)\epsilon,\epsilon}(V) \big) - \sum_{\ell} \ln \det \mathcal{F}_{\ell\epsilon,\epsilon,*} \big(\mathcal{F}_{(\ell+1)\epsilon,\epsilon} \circ \cdots \circ \mathcal{F}_{(m-1)\epsilon,\epsilon}(V) \big) \\ &= S(\mathcal{F}_{m\epsilon}) - \ln \det \mathcal{F}_{m\epsilon,*} \end{aligned}$$

The trivializing map with the requirement

$$S_{\text{eff.}\,t}(V) = (1-t)\,S(V)$$

can be formally related to Lüscher's trivializing map $\mathcal{F}_t^{(L)}$:

superscript (L) in this page refers to Lüscher's map

• We assume the same gradient form for the kernels:

$$\mathcal{F}_{t,\epsilon}(U)_{x,\mu} = e^{-\epsilon T^a \partial_{x,\mu}^a \tilde{S}_t(U)} U_{x,\mu}.$$

 \Rightarrow equation for \tilde{S}_t :

$$[-(\partial^A)^2 + (1-t)\partial^A S \partial^A] \tilde{S}_t = S$$

Comparing this expression with the counterpart in Lüscher's map:

$$[-(\partial^A)^2 + \underline{t} \partial^A S \partial^A] \tilde{S}_t^{(L)} = S,$$

we notice that t is replaced by 1 - t.

 \therefore Writing $t = m\epsilon$ ($0 \le t \le 1$) and $1 \equiv n\epsilon$,

$$\mathcal{F}_{t=m\epsilon} = \mathcal{F}_{0,\epsilon} \circ \cdots \circ \mathcal{F}_{(m-1)\epsilon,\epsilon}$$
$$= \mathcal{F}_{(n-1)\epsilon,\epsilon}^{(L)} \circ \cdots \circ \mathcal{F}_{(n-m)\epsilon,\epsilon}^{(L)}.$$

At t = 1, $\mathcal{F}_{t=1} = \mathcal{F}_{t=1}^{(L)}$, and thus it does not contradict with the <u>uniqueness argument</u>. Lüscher '09

This also suggests that complicated shapes can easily appear even at t = 0. [9/19]

Schwinger-Dyson equation

Schwinger-Dyson equation (1/3)

Truncation error seems unvoidable in the construction.

. We would like to measure the goodness of a trivializing map for a given kernel.



Schwinger-Dyson equation to estimate the effective couplings ("tomography"):

Gonzalez-Arroyo, Okawa '87 Application to gauge systems: de Forcrand et al. '00

• Let us expand $S_{\text{eff}}(V)$ in terms of Wilson loops and their products:

$$S_{\rm eff}(V) = \sum_j \beta_j W_j$$
 -- (1) We omit the *t*-dependence momentarily. j runs over an infinite dimensional space.

• We then consider an infinitesimal variation using W_i as the kernel:

$$\delta V = -\epsilon T^A \partial^A W_i$$
.

The path integral is invariant under this variation (Schwinger-Dyson equation):

$$0 = \delta \int (dV) \ e^{-S_{\text{eff}}(V)} = \int (dV) \ e^{-S_{\text{eff}}(V)} \epsilon \left[-(\partial^A)^2 \ W_i + \partial^A S_{\text{eff}} \ \partial^A W_i \right].$$
 -- (2)

Combining (1) and (2),

$$\beta_j \langle \partial^A W_j \partial^A W_i \rangle_{S_{\text{eff}}} = \langle (\partial^A)^2 W_i \rangle_{S_{\text{eff}}}.$$

 $\beta_j \left<\partial^A W_j \right. \partial^A W_i \right>_{S_{\rm eff}} = \left<(\partial^A)^2 W_i\right>_{S_{\rm eff}}.$ From the expectation values, we can estimate β_j .

Schwinger-Dyson equation:

cf. Gonzalez-Arroyo, Okawa '87, de Forcrand et al. '00

$$\sum_{j} \beta_{j} \left\langle \partial^{A} W_{j} \partial^{A} W_{i} \right\rangle_{S_{\text{eff}}} = \left\langle (\partial^{A})^{2} W_{i} \right\rangle_{S_{\text{eff}}}. \qquad -- (3)$$

- In practice, it is difficult to track all the infinite number of couplings.
 - We mimic the exact effective action $S_{\rm eff}(V) = \sum_j \beta_j W_j$ by a truncated action:

$$S'_{\rm eff}(V) = \sum_j' \beta_j' W_j$$
. Prime symbols indicate truncation. j runs a finite range.

• To determine β'_i , we use the truncated counterpart of (3):

$$\sum_{j}' \beta_{j}' \left\langle \partial^{A} W_{j} \ \partial^{A} W_{i} \right\rangle_{S_{\text{eff}}} = \left\langle (\partial^{A})^{2} W_{i} \right\rangle_{S_{\text{eff}}}. \quad -- \quad (4)$$
(*i* is also restricted to the finite range)

• Such β'_j give the best approximation of $S_{\text{eff}}(V)$ in the sence that it minimizes the norm

$$\|S_{\rm eff}-S_{\rm eff}'\|$$
, where $\|\mathcal{O}\|^2\equiv\langle(\partial^A\mathcal{O})^2\rangle_{S_{\rm eff}}$. (short proof in the next page)

The truncation error is calculable because it is merely the difference of the forces squared.

Schwinger-Dyson equation (3/3)

cf. Gonzalez-Arroyo, Okawa '87

$$\sum_{j} \beta_{j} \left\langle \partial^{A} W_{j} \partial^{A} W_{i} \right\rangle_{S_{\text{eff}}} = \left\langle (\partial^{A})^{2} W_{i} \right\rangle_{S_{\text{eff}}}. \qquad -- (3)$$

$$\sum_{j}' \beta_{j}' \left\langle \partial^{A} W_{j} \partial^{A} W_{i} \right\rangle_{S_{\text{eff}}} = \left\langle (\partial^{A})^{2} W_{i} \right\rangle_{S_{\text{eff}}}. \qquad -- (4)$$

Proof $[\beta'_j]$ determined by (4) minimizes $||S_{eff} - S'_{eff}||$

• We subtract (4) from (3) to obtain

$$\sum_{j}' (\beta_{j} - \beta_{j}') \langle \partial^{A} W_{j} \partial^{A} W_{i} \rangle_{S_{\text{eff}}} = 0$$
.

This is nothing but the stationary point condition:

$$\begin{split} \frac{\partial}{\partial \beta_i'} \|S_{\text{eff}} - S_{\text{eff}}'\|^2 &= \frac{\partial}{\partial \beta_i'} \langle [\partial^A (S_{\text{eff}} - S_{\text{eff}}')]^2 \rangle_{S_{\text{eff}}} \\ &= -2 \sum_j' \left(\beta_j - \beta_j' \right) \left\langle \partial^A W_j \, \partial^A W_i \right\rangle_{S_{\text{eff}}} = 0 \end{split}$$

• Since the norm $\|\mathcal{O}\|^2 = \langle (\partial^A \mathcal{O})^2 \rangle_{S_{\mathrm{eff}}}$ is non-negative for real-valued functions \mathcal{O} , the stationary point corresponds to the minimum of $\|S_{\mathrm{eff}} - S'_{\mathrm{eff}}\|$.

Comment - Mandelstam relation (1/1)

 Some of the basis functions are not linearly independent because of the group theoretic relations ("Mandelstam constraints").

Mandelstam '79

Relevant example

$$+2 + 2W_0$$

$$\text{``} \quad (\operatorname{tr} U)^2 = \operatorname{tr}(U^2) + 2\operatorname{tr} U^\dagger \quad \left[U \in SU(3) \right]$$

$$\begin{array}{l} \text{``} \quad \operatorname{Diagonalizing} \quad U \sim \operatorname{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}), \\ \\ \operatorname{lhs} = \left(e^{i\theta_1} + e^{i\theta_2} + e^{i\theta_3} \right)^2 \\ \\ = e^{2i\theta_1} + e^{2i\theta_2} + e^{2i\theta_3} \\ \\ + 2(e^{-i\theta_1} + e^{-i\theta_2} + e^{-i\theta_3}) \quad = \operatorname{rhs} \end{array}$$

Expressions involving higher powers of U can be further derived, e.g., by the Cayley-Hamilton theorem:

$$U^3 = (\operatorname{tr} U)U^2 - \frac{1}{2}[(\operatorname{tr} U)^2 - \operatorname{tr}(U)^2]U + \mathbb{I}.$$

• To perform the tomography, we need to be careful that the effective action is expanded by linearly independent functions.

Otherwise, we have zero modes and the linear equation cannot be inverted.

Design the flow with the Schwinger-Dyson equation (1/1)

Equation for determining $\beta'_{i,t}$:

Boyle, Izubuchi, L. Jin, Jung, NM, Tomiya, work in progress

$$\left\langle -(\partial^A)^2 W_i + \sum_j' \beta_{j,t}' \partial^A W_j \partial^A W_i \right\rangle_{S_{\text{eff}},t} = 0 \quad -- (4')$$

We further use (4') to design approximated trivializing maps:

• We parametrize \tilde{S}_t in the same truncated space:

$$\tilde{S}_t(V) = \sum_{k}' \gamma_{k,t} W_k$$
.

By differentiating (4') with respect to t,

• We require $\dot{\beta}'_{j,t}=-rac{eta'_{j,t}}{1-t}$ so that $eta'_{j,t}=(1-t)eta'_{j,t=0}=(1-t)eta_{j,t=0}'$.

The linear equation for $\gamma_{k,t}$:

$$\begin{split} \sum_{k}' \gamma_{k,t} \left\langle \left[-(\partial^{B}) W_{k} + \partial^{B} S_{\text{eff},\,t} \; \partial^{B} W_{k} \right] \left[-(\partial^{A}) W_{i} + \partial^{A} S_{\text{eff},\,t}' \; \partial^{A} W_{i} \right] \right\rangle_{S_{\text{eff},\,t}} \\ &= -\frac{1}{1-t} \left\langle \partial^{A} S_{\text{eff},\,t}' \partial^{A} W_{i} \right\rangle_{S_{\text{eff},\,t}}. \end{split}$$

By the minimization theorem, this determination corresponds to minimizing the norm $\|S'_{\text{eff},t} - (1-t)S\|$.



- Physical field space U: Wilson action ($\beta = 2.0$) $4^3 \times 8$ lattice
- We perform the tomography in the *V*-space with the following three maps:
 - Lüscher's with leading order terms (Wilson flow)
 Lüscher's up to NLO order (Wilson flow + O(t) term)

 Deviation from $(1-t)S_W(V)$ can also happen because of the difference between V and $U = \mathcal{F}_t(V)$ (composition ordering not reversed)
 - Coefficients $\gamma_{i,t}$ determined by the Schwinger-Dyson (SD) equation \leftarrow still ongoing

$$\epsilon = 0.1$$
 in all cases.

See Kagimura-Tomiya-Yamamura '15 for the tomography after the Wilson flow in the subspace W_0 , W_{1r} with a <u>demon algorithm</u>.

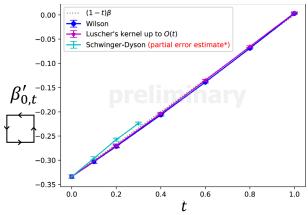
Creutz '83, Hasenbusch et al. '94

• We prepare the truncated space to be 11-dimensional space spanned by

$$W_0, W_{1r}, W_{1c}, \dots, W_{4r}, W_{4c}, W_5, W_7.$$
 operators with the footprint up to 2 rectangle and chair separated W_6 omitted because it is linearly dependent

- Configs are generated by the ordinary HMC. The map \mathcal{F}_t is then applied to the same configs (sample size $N_{\rm conf}=200$).
- Computations are carried out on facilities of the USQCD Collaboration,
 which are funded by the Office of Science of the U.S. Department of Energy.

• The coefficient of plaquettes almost follows the optimal trajectory for $\beta = 2.0$:

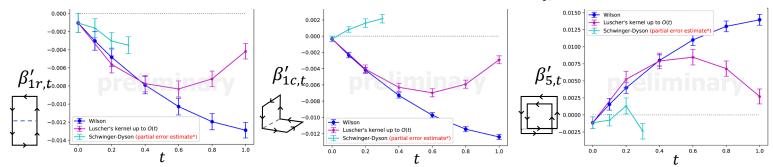


Statistical errors are estimated with the Jackknife method.

* Statistical errors for SD are estimated for a given mean value of $\gamma_{j,t}$; statistical errors propagated from preceding $\gamma_{j,t}$ are not taken into account.

• In the SD map, $\beta'_{j,t}$ should be 0 for $j \neq 0$ by construction, once error of $\gamma_{j,t}$ are taken properly. We will include it and improve statistics/methods further.

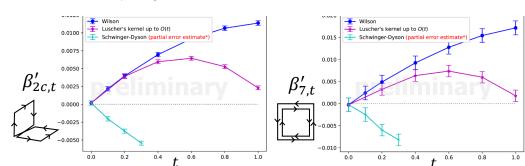
Some couplings seem to get closer to the optimal trajectory $\beta'_{j,t} = 0$:



However, some couplings deviate more:

Luscher's kernel up to O(t)

 $\beta'_{2r,t}$ °

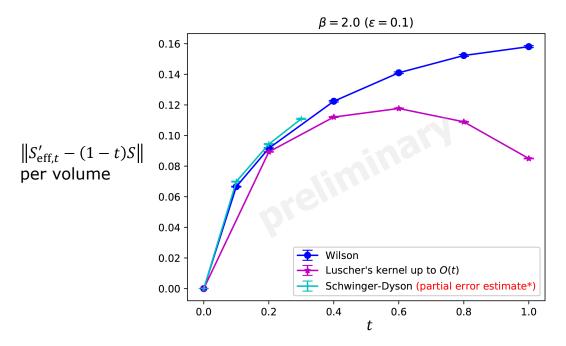


 $\gamma_{i,t}$ may be poorly estimated with $N_{\rm conf}=200$.

[16/19]

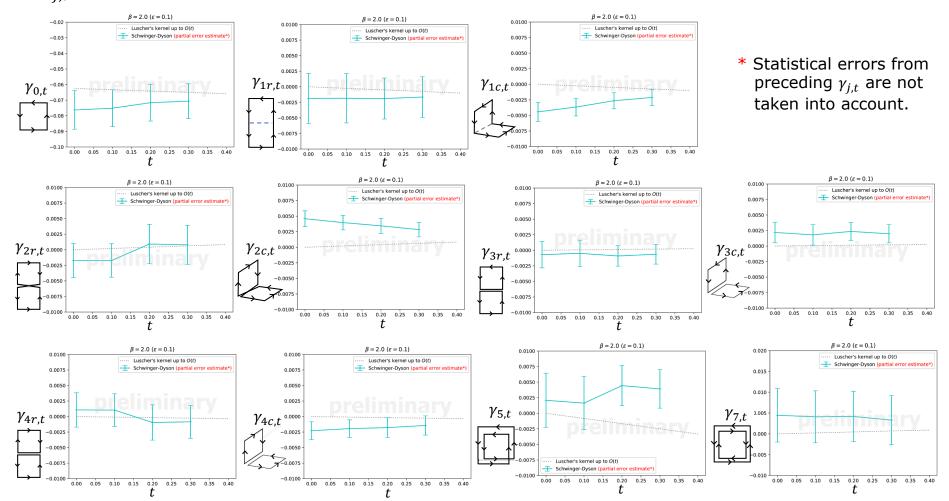
• Because of the minimization theorem, SD method should give $S'_{eff,t}$ that minimizes $||S'_{eff,t} - (1-t)S||$.

In this preliminary study, however, the deviation of $\beta'_{j,t}$ from the optimal trajectory is reflected as larger values of $\|S'_{\text{eff},t} - (1-t)S\|$:



* Statistical errors for SD are estimated for a given mean value of $\gamma_{j,t}$; statistical errors propagated from preceding $\gamma_{i,t}$ are not taken into account.

- In our setup with $\beta = 2.0$, Lüscher's map turns out to work quite well.
- (Though the coefficients $\gamma_{j,t}$ are poorly estimated,) $\gamma_{j,t}$ actully take similar values to those of Lüscher's [up to O(t)] kernel in this case:



We would like to observe whether the difference becomes significant at larger β . (future work)

We are also developing an alternative way of estimating γ_{it} more accurately.

[18/19]

Summary and Outlook

Summary

 We discussed a way to measure effective action of flowed gluon field with the Schwinger-Dyson equation.

In particular, we introduced a norm in the space of actions with their forces, by which the truncation error can be explicitly evaluated.

We also explored a way to construct approximated trivializing maps using the Schwinger-Dyson equation step by step.

We showed preliminary results of test calculations with several kernels.

Outlook

- Reduce the statistical noise in the determination of $\gamma_{j,t}$.
- Investigate at larger β and volume.
 - difference between Lüscher's and SD maps
 - autocorrelation, topological tunneling rate
- Include fermion

Benefit of our method: analytical calculations not mandatory.

Investigate the uses of field transformations in other contexts.

