

Alleviating the sign problem with contour deformations in heavy-dense QCD

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Outline

- ① Sign problem and reweighting
- ② Contour deformation in heavy-dense QCD
- ③ Manifold optimization
 - Local Fourier ansatz
- ④ Holomorphic flow
 - Partial flow

The Sign Problem

The path-integral weights are not generally real and positive, so they cannot be used directly as a Monte Carlo probability distribution.

$$Z_w = \int_{\mathcal{M}} \mathcal{D}\phi w[\phi], \qquad w[\phi] = e^{-S[\phi]}.$$

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The complex-action problem limits first-principles studies of ^{1 2}

- ▶ finite-density QCD,
- ▶ strongly correlated electrons away from half filling,
- ▶ dense nuclear matter,
- ▶ theories with topological terms,
- ▶ real-time quantum dynamics.

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Reweighting and average phase

For any positive reference measure $r[\phi]$,

$$\langle O \rangle_w = \frac{\int_{\mathcal{M}} \mathcal{D}\phi O[\phi] w[\phi]}{\int_{\mathcal{M}} \mathcal{D}\phi w[\phi]} = \frac{\int_{\mathcal{M}} \mathcal{D}\phi O[\phi] \frac{w[\phi]}{r[\phi]} r[\phi]}{\int_{\mathcal{M}} \mathcal{D}\phi \frac{w[\phi]}{r[\phi]} r[\phi]} = \frac{\langle O w/r \rangle_r}{\langle w/r \rangle_r}.$$

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The **average phase** σ measures the severity of the sign problem:

$\sigma \simeq 1 \implies$ mild phase cancellations,

$\sigma \simeq 0 \implies$ severe sign problem.

Contour deformation

We complexify the original variables and deform the integration manifold,

$$\mathcal{M} \longrightarrow \mathcal{M}', \quad \phi \in \mathcal{M}, \quad \phi' = \phi'(\phi) \in \mathcal{M}', \quad \mathcal{I}_{ij}[\phi] = \frac{\partial \phi'_i(\phi)}{\partial \phi_j}.$$

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Cauchy's theorem gives the same target partition function on any admissible homologous contour³:

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Phase-quenched partition function and phase reweighting on the deformed manifold

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$$\sigma_{\text{def}} = \left\langle \frac{\det \mathcal{J}}{|\det \mathcal{J}|} e^{-i \text{Im } S[\phi']} \right\rangle_r^{\text{def}} = \frac{Z_w}{Z_r^{\text{def}}}$$

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Z_w is contour invariant, whereas Z_r^{def} depends on the contour.

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Heavy-dense QCD in Polyakov gauge

- The Wilson gauge action is

$$S_g = -\frac{\beta}{6} \sum_x \sum_{\mu < \nu} \left[\text{Tr } U_{\mu\nu}(x) + \text{Tr } U_{\mu\nu}(x)^{-1} \right], \quad U_{\mu\nu}^{-1} = U_{\mu\nu}^\dagger \quad \text{only for } SU(3).$$

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$$S_f = -2N_f \sum_{\vec{x}} \log \left[\det \left(\mathbf{1} + h e^{\hat{\mu}} P(\vec{x}) \right) \det \left(\mathbf{1} + h e^{-\hat{\mu}} [P(\vec{x})]^{-1} \right) \right], \quad h = (2\kappa)^{N_t}, \quad \hat{\mu} = \mu a N_t = \frac{\mu}{T}.$$

In Polyakov gauge, before and after deformation

$$P(\vec{x}) = \text{diag} \left(e^{i\theta_1(\vec{x})}, e^{i\theta_2(\vec{x})}, e^{-i[\theta_1(\vec{x}) + \theta_2(\vec{x})]} \right) \in SU(3) \quad \longrightarrow \quad P(\vec{x}) \in SL(3, \mathbb{C}), \quad \theta_i(\vec{x}) \in \mathbb{C}.$$

***Only the Polyakov angles are deformed.**

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- ▶ Haar/Vandermonde contribution

$$S_V = - \sum_{\vec{x}} \log \left[\sin^2 \left(\frac{\theta_1(\vec{x}) - \theta_2(\vec{x})}{2} \right) \sin^2 \left(\frac{\theta_1(\vec{x}) + 2\theta_2(\vec{x})}{2} \right) \sin^2 \left(\frac{2\theta_1(\vec{x}) + \theta_2(\vec{x})}{2} \right) \right].$$

***Regularize the logarithmic singularities of S_V inside the argument w of $\sin(w)$ via $w \rightarrow w + \epsilon$, with $\epsilon \rightarrow 0$.**

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***Regularize the logarithmic singularities of S_V inside the argument w of $\sin(w)$ via $w \rightarrow w + \epsilon$, with $\epsilon \rightarrow 0$.**

- ▶ The effective action is ⁴⁵

$$S_{\text{eff}} = S_g + S_V + S_f + S_{\mathcal{J}},$$

⁴_{hep-lat/2007.05436}

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Manifold optimization

The sign problem is weaker when $\sigma_{\text{def}} = Z_w/Z_r^{\text{def}}$ is larger. Since Z_w does not depend on the manifold parameters, maximizing σ_{def} is equivalent to minimizing the deformed phase-quenched partition function.

Parameterize a family of manifolds by a finite set $\{p\}$,

$$\mathcal{M} \longrightarrow \mathcal{M}'(\{p\}),$$

and optimize $\{p\}$ using the cost function ^{6 7}

$$\mathcal{F}(\{p\}) = -\log \sigma(\{p\}) = -\log Z_w + \log Z_r^{\text{def}}(\{p\}).$$

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Only the phase-quenched partition function changes, so

$$\nabla_p \mathcal{F}(\{p\}) = \nabla_p \log Z_r^{\text{def}}(\{p\}) = - \left\langle \nabla_p \text{Re } S_r^{\text{eff}}(\{p\}) \right\rangle_r^{\text{def}}.$$

Consequently,

$$\min_{\{p\}} \mathcal{F}(\{p\}) \iff \max_{\{p\}} \sigma(\{p\}).$$

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Manifold optimization

Local Fourier ansatz¹²

$$\tilde{\theta}_k(\vec{x}) = \theta_k(\vec{x}) + i \sum_{m,n=0}^N \lambda_{mn}^{(k)} \cos[m\theta_1(\vec{x}) + n\theta_2(\vec{x})]$$

$k = 1, 2$. There are $2(N+1)^2$ real parameters. The same coefficients $\lambda_{mn}^{(k)}$ are used at every spatial site.

PQ sample on $\mathcal{M}(\lambda_r) \longrightarrow \nabla_\lambda \mathcal{F} = - \left\langle \nabla_\lambda S_r^{\text{eff}} \right\rangle_r \longrightarrow \lambda_{r+1}$

N_{opt} : number of successive parameter updates.

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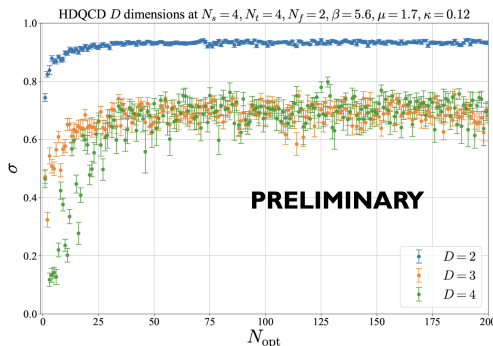
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Rapid increase followed by a plateau after roughly 30–50 updates: $D = 2 \simeq 0.93$, while $D = 3, 4 \simeq 0.70$.



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Holomorphic Flow Equations

- ❶ The fields evolve according to,

$$\frac{d\phi'_i}{dt} = \left(\frac{\partial S[\phi']}{\partial \phi'_i} \right)^*, \quad \phi'_i(t=0) = \phi_i.$$

- ❷ The Jacobian obeys

$$\frac{d\mathcal{J}}{dt} = (\mathcal{H}\mathcal{J})^*, \quad \mathcal{H}_{ij} = \frac{\partial^2 S}{\partial \phi'_i \partial \phi'_j},$$

with $\phi' = \phi$, $\mathcal{J} = 1$, and $\det \mathcal{J} = 1$ at $t = 0$.¹

The flow defines a family of deformed integration manifolds parameterized by the fictitious flow time t , with

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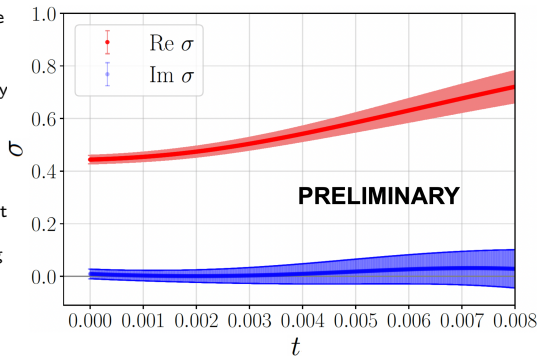
Holomorphic-flow identities:

$$\frac{d}{dt} \text{Re } S[\phi'(t)] = \sum_i \left| \frac{\partial S}{\partial \phi'_i} \right|^2 \geq 0, \quad \frac{d}{dt} \text{Im } S[\phi'(t)] = 0.$$

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Partial flow (Polyakov-loop eigenvalues)

- ▶ Only the Polyakov-loop eigenangles are flowed.
- ▶ The real part of the average phase increases with flow time. The imaginary part remains consistent with zero.
- ▶ At finite flow time, the phase cancellations are reduced and σ improves.
- ▶ For now, all configurations are gathered at zero flowtime and reweighted to finite flowtime (leading to the errors growing with flowtime).
- ▶ Eventually, we plan to use a cheap approximation of the finite flowtime Jacobian in the accept-reject step, and later reweight to the exact Jacobian.



$$D = 4, N_s = 4, N_t = 4, N_f = 2, \Delta t = 10^{-8}, \mu = 1.0, \kappa = 0.12, \epsilon = 10^{-2}, \tau = 150, \beta = 5.6.$$

* Local Fourier gives a plateau average phase around $\sigma \approx 0.6$ for this particular set of parameters.

Conclusions

Contour deformation changes the sampling problem without changing the target theory.

For the present application to a four-dimensional lattice gauge theory in the heavy-dense limit of QCD:

- ▶ The local Fourier manifold provides a computational improvement with a block-local Jacobian.
- ▶ The holomorphic field and Jacobian flows provide an independent, action-driven deformation.
- ▶ We found that at large-flow region the data becomes statistically noisy due to reweighting. To-do: Finite-flow simulations.
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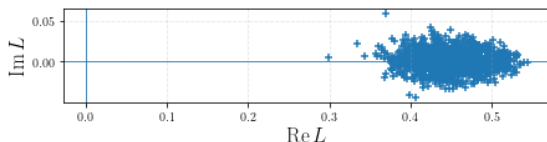
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Thanks!

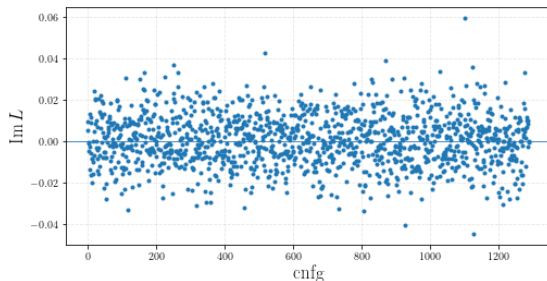
Backup

Polyakov-loop diagnostics



The volume-averaged traced Polyakov loop is

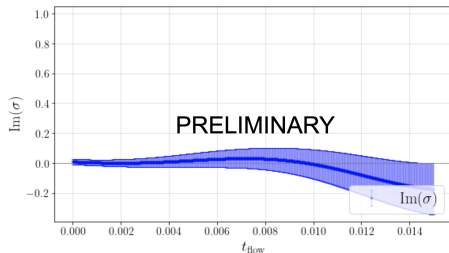
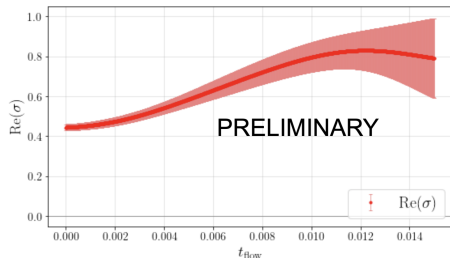
$$L = \frac{1}{3N_s^3} \sum_{\vec{x}} \text{Tr } P_{\vec{x}}.$$



The complex-plane distribution and Monte Carlo history provide compact diagnostics of phase fluctuations and balance configurations.

- Currently 2000 configurations.

Partial flow at large t_{flow}



Parameters: $D = 4$, $N_s = 4$, $N_t = 4$, $N_f = 2$, $\Delta t = 10^{-8}$, $\mu = 1.0$, $\kappa = 0.12$, $\epsilon = 10^{-2}$, $\tau = 150$, $\beta = 5.6$;