Reducing the severity of the sign problem in 2+1D XY model

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in collaboration with

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Sign problem

Simulating euclidean quantum field theories on the lattice:

- at $\mu = 0$: action is real, path integral weights $\rightarrow$ Boltzmann weights
- at $\mu \neq 0$: action becomes complex, path integral weights are complex

Problem: at non-zero chemical potential path integral weights do not have a probabilistic interpretation

Can be overcome by simulating with $|e^{-S}|$ (PQ) or (for real partition functions) $|\mathrm{Re}\, e^{-S}|$ (SQ)

Sign problem

Expectation values of original theory reconstructed via reweighting

$$\langle O \rangle = \frac{\langle O e^{\imath\theta} \rangle_{PQ}}{\langle e^{\imath\theta} \rangle_{PQ}} = \frac{\left\langle O \frac{\cos\theta}{|\cos\theta|} \right\rangle_{SQ}}{\left\langle \frac{\cos\theta}{|\cos\theta|} \right\rangle_{SQ}}$$

where $e^{-S} = |e^{-S}| e^{\imath\theta}$

Large fluctuations in $e^{\imath\theta} \implies$ large cancellations $\implies$ large uncertainties

Sign problem

Reweighting is severely constrained by the sign problem

Uncertainties increase exponentially with chemical potential and volume

Two main approaches to alleviate the problem:

- complex Langevin: N-dim. integral over real fields enlarged to $2N$-dim. integral over real and imaginary parts of complex fields
- contour deformations: N-dim. integration manifold deformed

We pursue the second approach

The model

Action of the 2+1D XY model with non-zero chemical potential

$$S = -\beta \sum_{x} \sum_{n=0}^{2} \cos(\varphi_x - \varphi_{x+\hat{n}} + \imath\mu\delta_{n0})$$

Periodic boundary conditions in all three directions

The partition function is an integral over $\mathcal{M}_0 = [-\pi, \pi]^{N_0 N_1 N_2}$

$$Z(\mu) = \int \mathrm{d}\varphi_{000} \cdots \int \mathrm{d}\varphi_{N_0 N_1 N_2}\ e^{-S} \equiv \int_{\mathcal{M}_0} \mathcal{D}\varphi\ e^{-S}$$

The model has a second-order phase transition

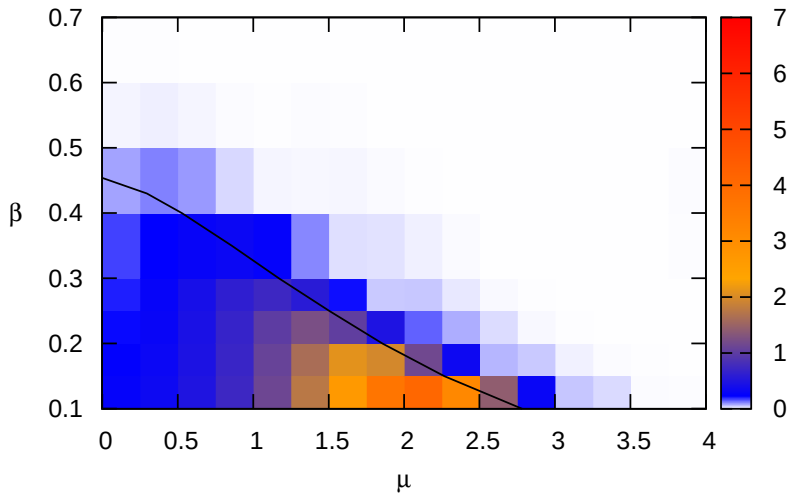
Complex Langevin

Sign problem for $\mu^2 > 0$ in original formulation

Worldline formulation: sign problem for $\mu^2 < 0$ but not for $\mu \in \mathbb{R}$

[Banerjee, Chandrasekharan, PRD (2010)]

Complex Langevin fails in disordered phase [Aarts, James, JHEP (2010)]



Difference between complex Langevin and worldline results for average action density

SQ reweighting

$Z(\mu)$ is real-valued and $Z(\mu) = Z(-\mu)$

Can be written in a manifestly real form

$$Z(\mu) = \int_{\mathcal{M}_0} \mathcal{D}\varphi \, \cos S^I \, e^{-S^R}$$

Integrand can still have negative values $\Longrightarrow$ not a probability weight

SQ reweighting

Simulate using $|\cos S^I \, e^{-S^R}|$ as probability weight (SQ)

Need to reweight to the theory described by $Z(\mu)$ to compute physical quantities

E.g. the action density

$$\frac{\langle S \rangle}{\Omega} = -\frac{\beta}{\Omega}\frac{\partial}{\partial\beta}\ln Z = \frac{\langle \mathrm{sgn}(\cos S^I)(S^R + S^I \tan S^I)\rangle_{SQ}}{\Omega\langle \mathrm{sgn}(\cos S^I)\rangle_{SQ}}$$

Problem: large errors when the average sign of $\cos S^I$ approaches 0

Improving the sign problem

Treat partition function as a multivariate contour integral

Deforming integration manifold away from the real submanifold

$$Z(\mu) = \int_{\mathcal{M}} \mathcal{D}\varphi \; e^{-S} = \int \mathcal{D}t \; e^{-S_{\text{eff}}}$$

t_x - real parameters of $\mathcal{M}$
$S_{\text{eff}} = S - \ln \det J$ - effective action including the log of the Jacobian

Multi-dim. Cauchy's theorem: $Z(\mu)$ invariant $\implies$ same physical predictions

Improving the sign problem

Exploit the reality of the partition function

$$Z(\mu) = \int \mathcal{D}t \ \cos(S^I_{\text{eff}})\, e^{-S^R_{\text{eff}}}$$

Use $|\cos S^I_{\text{eff}}|\, e^{-S^R_{\text{eff}}}$ as weight in importance sampling

Severity of the sign problem measured by

$$\langle \varepsilon \rangle_{sQ,\mu} \equiv \langle \text{sgn}(\cos S^I_{\text{eff}}) \rangle_{sQ} = \frac{\int \mathcal{D}t \ \cos S^I_{\text{eff}}\, e^{-S^R_{\text{eff}}}}{\int \mathcal{D}t \ |\cos S^I_{\text{eff}}|\, e^{-S^R_{\text{eff}}}} = \frac{Z}{Z_{sQ}}$$

Deforming integration manifold changes the denominator $\Longrightarrow$ affects the sign problem

Improving the sign problem

Cost function: ratio of configurations with negative and positive $\cos S^I_{\text{eff}}$

$$\frac{N_-}{N_+} = \frac{\int \mathcal{D}t\ \Theta(-\cos S^I_{\text{eff}})\,|\cos S^I_{\text{eff}}|e^{-S^R_{\text{eff}}}}{\int \mathcal{D}t\ \Theta(\cos S^I_{\text{eff}})\,|\cos S^I_{\text{eff}}|e^{-S^R_{\text{eff}}}}$$

Task: minimize N_-/N_+ with respect to p_i coefficients that parametrize the integration contours

Use gradient descent

Improving the sign problem

Derivative with respect to Fourier coefficient p_i

$$\mathcal{F}_i \equiv \frac{\partial}{\partial p_i}\left(\frac{N_-}{N_+}\right) = \frac{N_-}{N_+}\Big(\langle F_i\rangle_- - \langle F_i\rangle_+\Big)$$

$$F_i = -\frac{\partial S^R_{\text{eff}}}{\partial p_i} - \tan S^I_{\text{eff}} \frac{\partial S^I_{\text{eff}}}{\partial p_i}$$

In jth optimization step

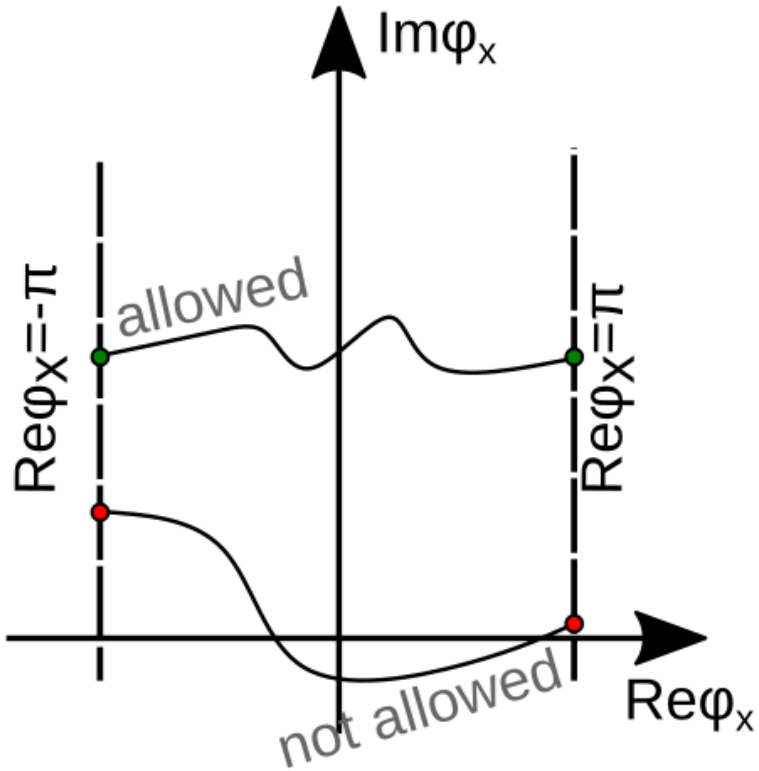
$$\boldsymbol{p}^{(j+1)} = \boldsymbol{p}^{(j)} - \alpha_j \boldsymbol{\mathcal{F}}^{(j)}, \qquad \alpha_j = \frac{\left|\left(\boldsymbol{p}^{(j)} - \boldsymbol{p}^{(j-1)}\right)^T \cdot \left(\boldsymbol{\mathcal{F}}^{(j)} - \boldsymbol{\mathcal{F}}^{(j-1)}\right)\right|}{||\boldsymbol{\mathcal{F}}^{(j)} - \boldsymbol{\mathcal{F}}^{(j-1)}||^2}$$

Assumptions for contour deformation

Integration endpoints in φ_x: $-\pi$ and π

Periodicity in $\mathrm{Re}\varphi_x \implies$
endpoints can be shifted in
imaginary direction

Choose $t_x = \mathrm{Re}\varphi_x$



$\mathrm{Im}\varphi_x$ Fourier-series in variables t_x

Assumptions for contour deformation

Deforming contours independently does not lead to improvement
$\Longrightarrow$ φ_x should not depend only on t_x

Chemical potential alters interaction between temporal neighbors
$\Longrightarrow$ include dependence on nearest temporal neighbor

Jacobian can become complicated $\Longrightarrow$ use only one temporal neighbor

Assumptions for contour deformation

Parametrization

$$\varphi_x = t_x + \imath\left\{A_{0,x_0} + \sum_{k=1}^{K}\left[A_{k,x_0}\cos(k(t_x - t_{x+\hat{0}})) + B_{k,x_0}\sin(k(t_x - t_{x+\hat{0}}))\right]\right\}$$

φ_x and φ_y on the same time slice have the same coefficients

Effective action

$$S_{\text{eff}} = S - \sum_x \ln\frac{\partial\varphi_x}{\partial t_x} - \sum_{x_1,x_2}\ln\left(1 - (-1)^{N_0}\prod_{x_0}\frac{1-\partial\varphi_x/\partial t_x}{\partial\varphi_x/\partial t_x}\right)$$

Not enforcing temporal translational invariance

Optimization at $\beta = 0.4$ on $\Omega = N_0 N_1 N_2 = 8 \times 4^2, 8 \times 6^2, 8^3, 8 \times 10^2$ lattices with $K = 2$

For every simulated μ, coefficients were initialized using the optimization results from the previous μ run

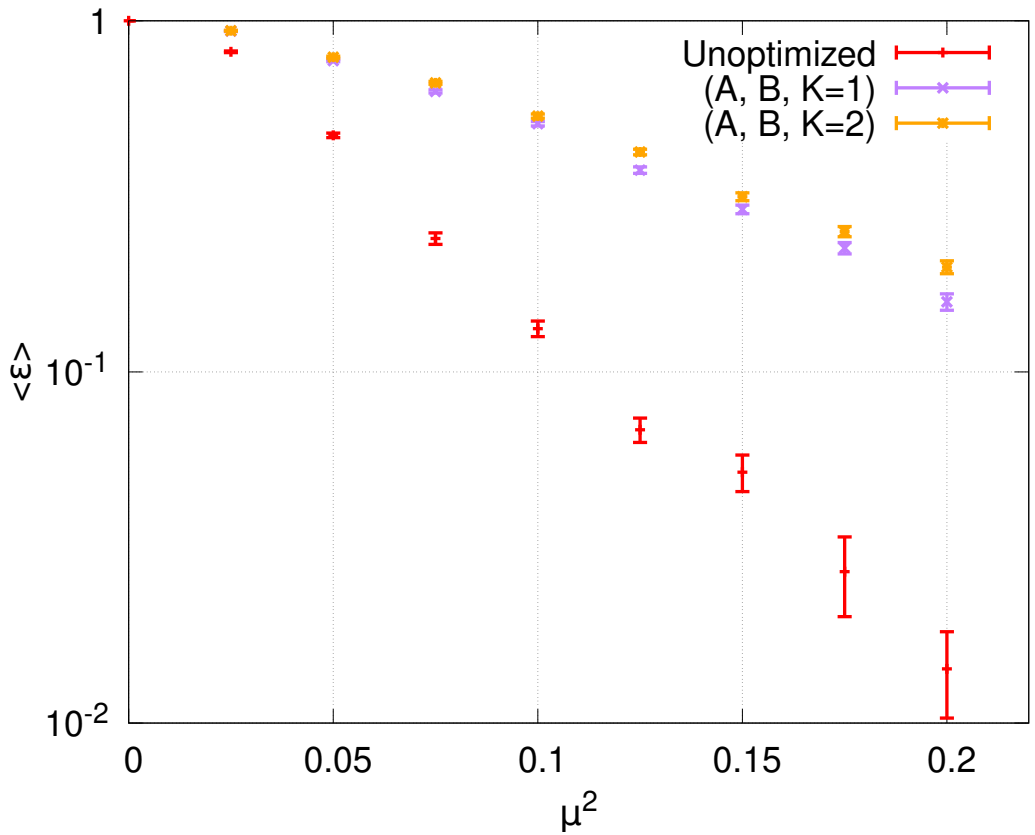
Averaging coefficients over x_0:

- A_0: 0.000855 ± 0.004658
- A_1: -0.121 ± 0.002
- B_1: 0.000249 ± 0.001684
- A_2: 0.0145 ± 0.0018
- B_2: 0.000436 ± 0.001164

Obtained coefficients are:

- independent of lattice site
- non-zero for the cosine terms only
- independent of spatial volume

Not enforcing temporal translational invariance



Significant improvement in the sign problem even at first order

Second-order terms bring marginal improvement

Parametrizaitons with triangular Jacobian matrix

Including more neighbors in parametrization complicates the Jacobian

Introduce constraint to make Jacobian matrix triangular

1. With spatial neighbors

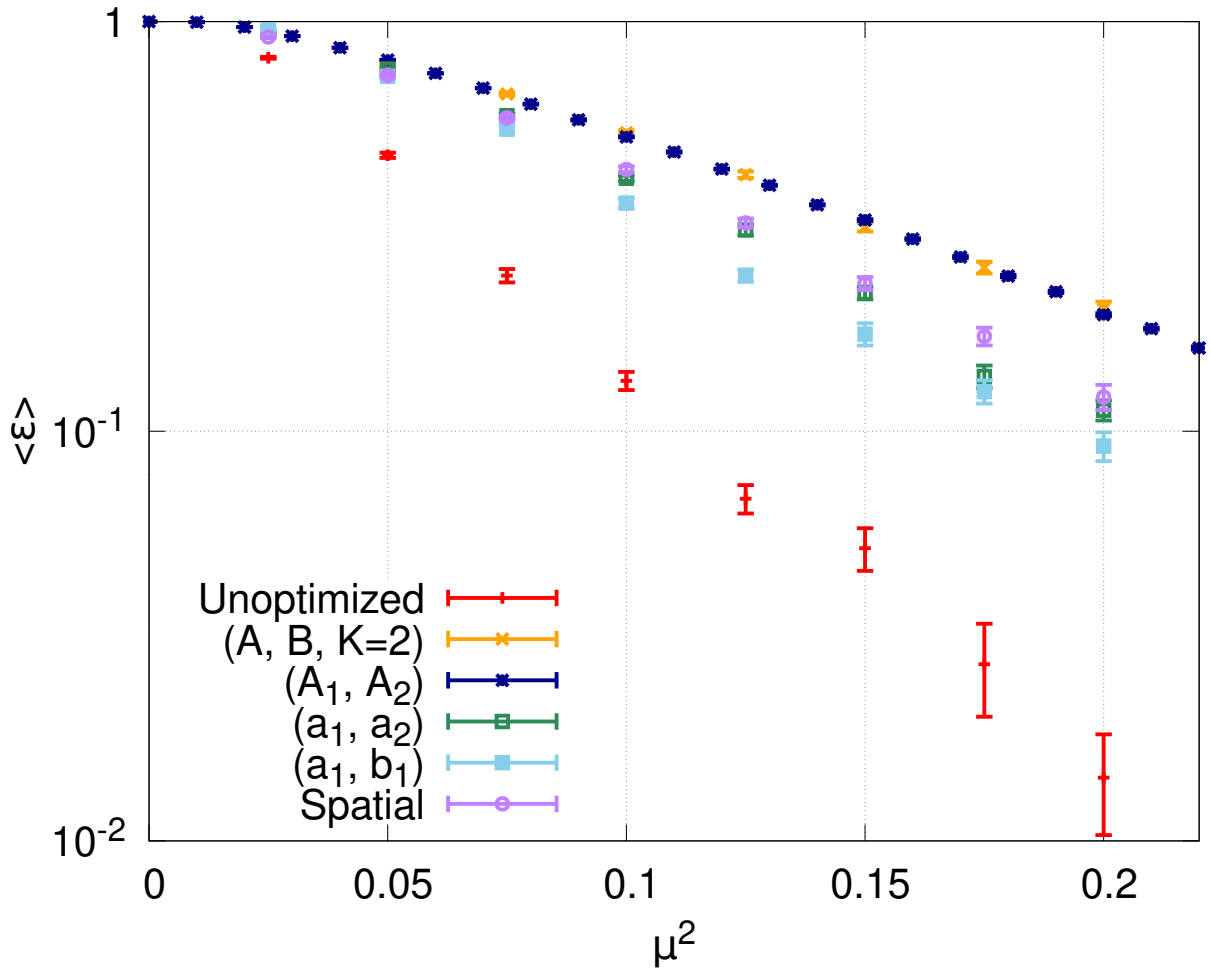
$$\varphi_x = t_x + \imath \sum_{k=1}^{K} \sum_{n=0}^{2} \theta_{n,x}^{(1)} \left[\bar{A}_{k,n} \cos(k(t_x - t_{x+\hat{n}})) + \bar{B}_{k,n} \sin(k(t_x - t_{x+\hat{n}})) \right]$$

2. With next-to-nearest temporal neighbor

$$\varphi_x = t_x + \imath \sum_{k=1}^{K} \left[\theta_{0,x}^{(1)} a_k \cos(k(t_x - t_{x+\hat{0}})) + \theta_{0,x}^{(2)} b_k \cos(k(t_x - t_{x+2\hat{0}})) \right]$$

$$\theta_{i,x}^{(j)} = \begin{cases} 1 & \text{if } x_i < N_i - j, \\ 0 & \text{otherwise.} \end{cases}$$

Parametrizaitons with triangular Jacobian matrix



Parametrizaitons with triangular Jacobian matrix

Including spatial neighbors in the parametrization has no effect

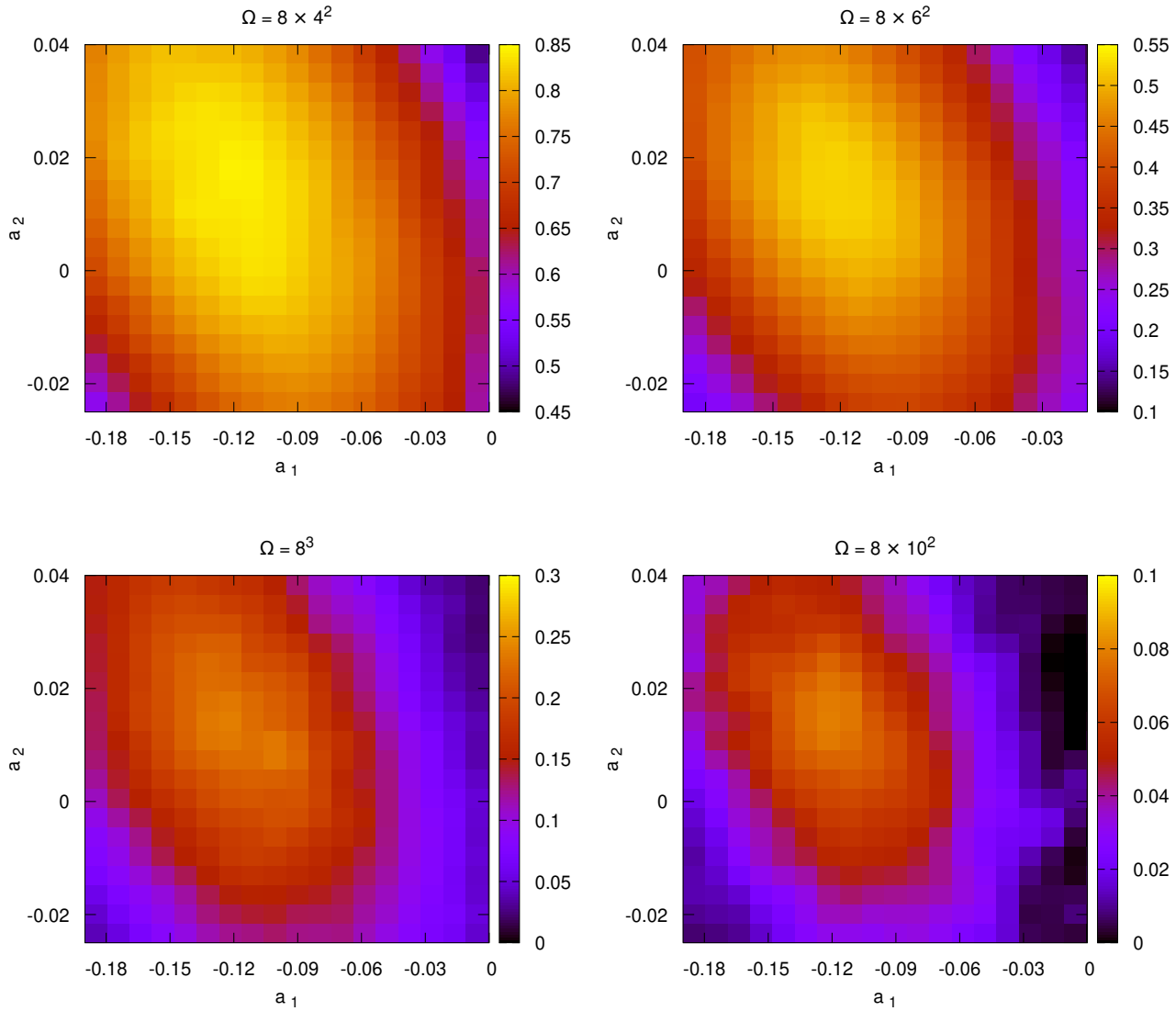
Including next-to-nearest neighbors at first order improves less than including second-order nearest-neighbor terms

Imposing constraints to make the Jacobian matrix triangular decreases amount of improvement but can reduce computational cost in complicated models

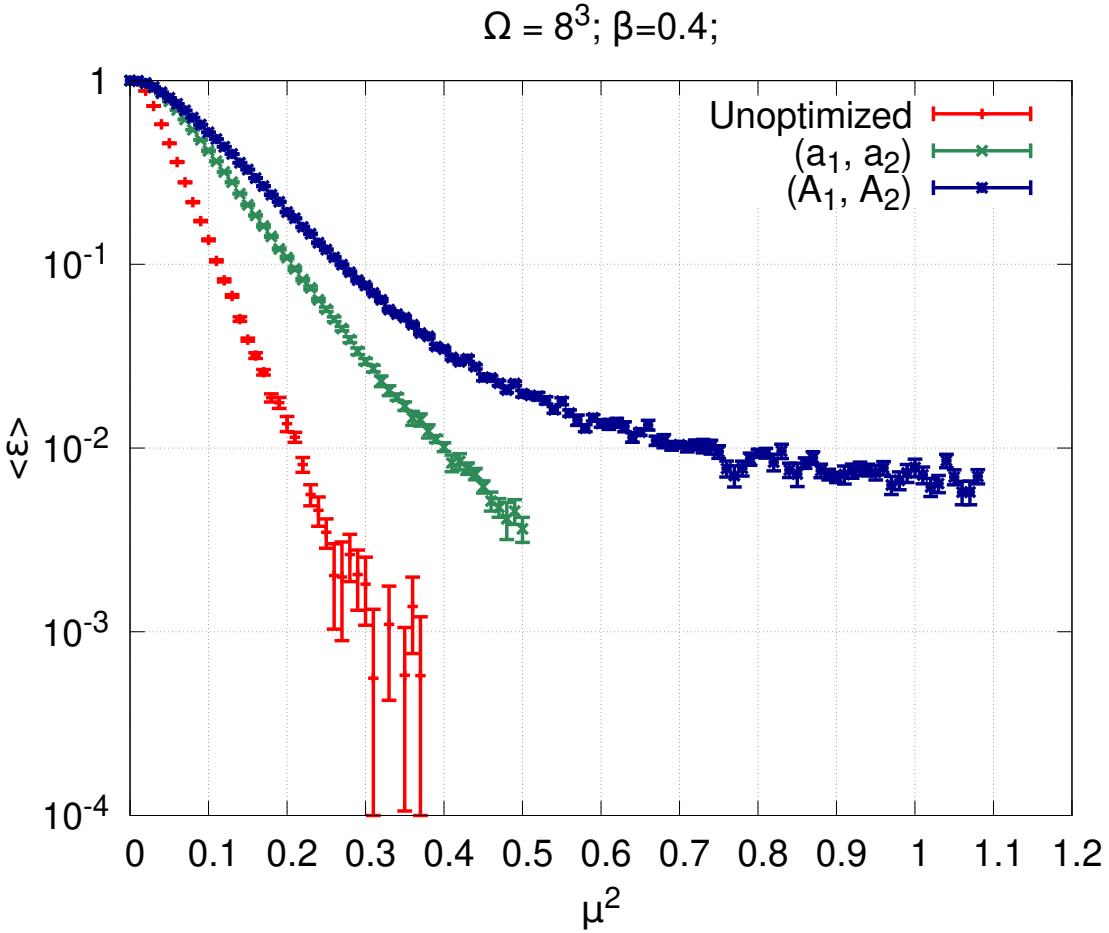
Best choice: explicitly translationally invariant parametrziation, only nearest temporal neighbors up to second order

Scans in (a_1, a_2) coefficient space

Average sign at $\beta = 0.4, \mu^2 = 0.15$



μ dependence of $\langle\varepsilon\rangle_{SQ,\mu}$

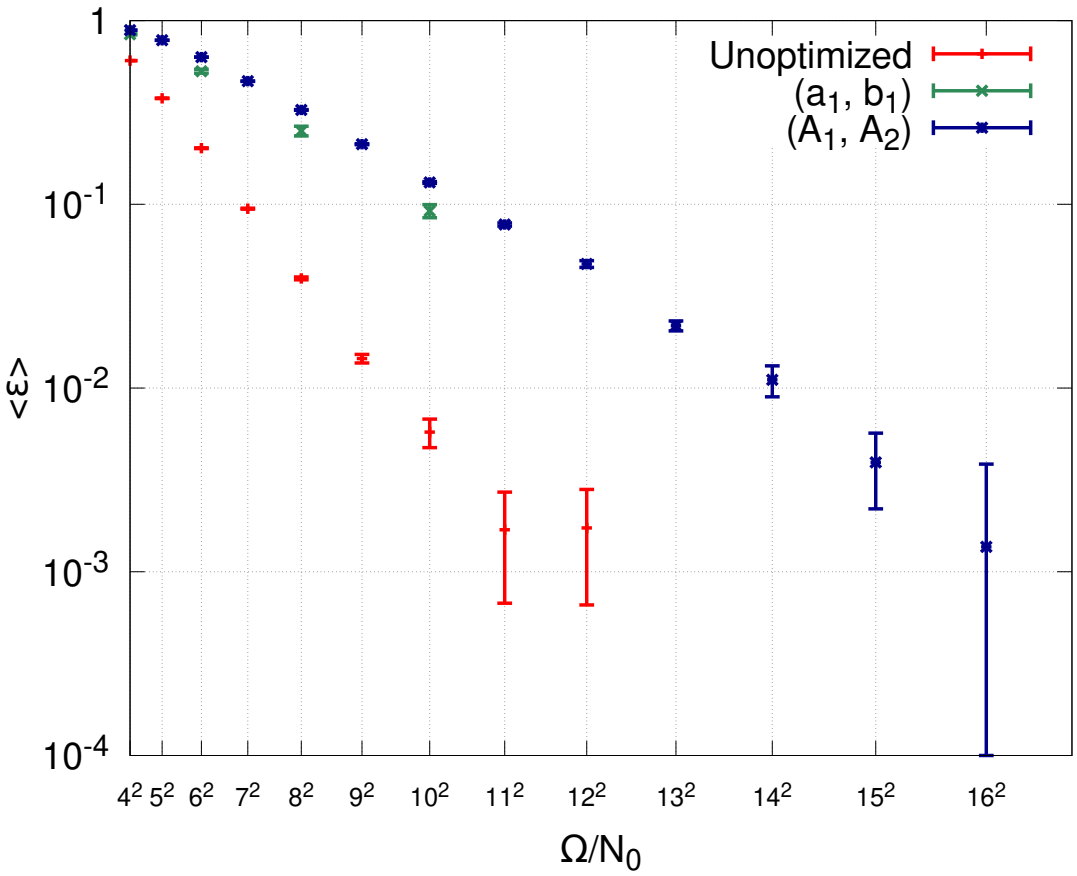


Fit

$\langle\varepsilon\rangle_{SQ,\mu} \sim e^{-C^{(\mu)}\mu^2}$

- unopt.
  $C^{(\mu)} \approx 24$
- (a_1, a_2)
  $C^{(\mu)} \approx 13$
- (A_1, A_2)
  $C^{(\mu)} \approx 10$

Volume dependence of $\langle \varepsilon \rangle_{sQ,\mu}$



Fit

$\langle \varepsilon \rangle_{sQ,\mu} \sim e^{-C^{(V)}V}$

- unopt.
  $C^{(V)} \approx 0.0073$
- (a_1, a_2)
  $C^{(V)} \approx 0.0032$
- (A_1, A_2)
  $C^{(V)} \approx 0.0031$

Action density

Simulating with $|\cos S^I_{\text{eff}}| e^{-S^R_{\text{eff}}}$ and reweighting to obtain predictions

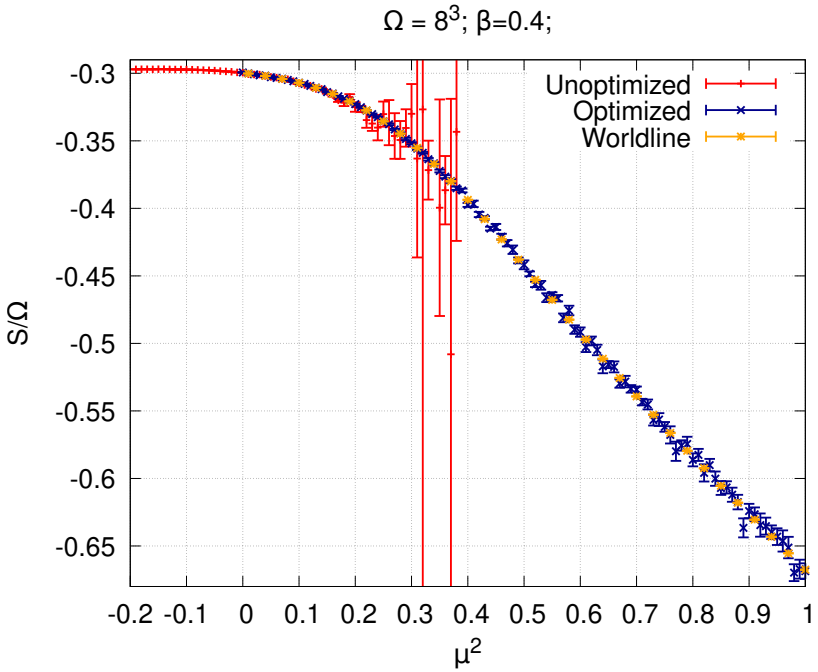
$$\frac{\langle S \rangle}{\Omega} = -\frac{\beta}{\Omega} \frac{\partial}{\partial \beta} \ln Z = \frac{\langle \varepsilon (S^R + S^I \tan S^I_{\text{eff}}) \rangle_{SQ}}{\Omega \langle \varepsilon \rangle_{SQ}}$$

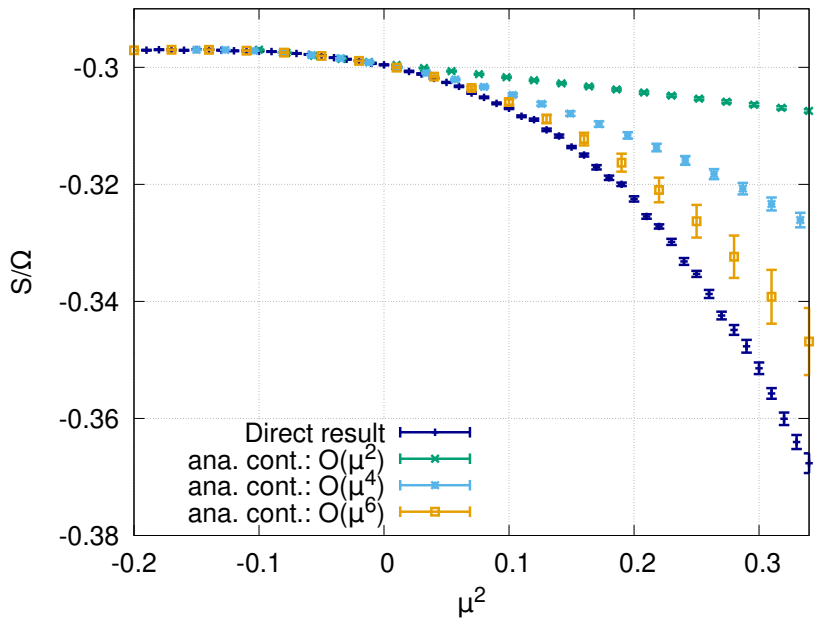
Compare to worldline results for verification

No sign problem for imaginary μ, can also use analytic continuation from $\mu^2 < 0$ to $\mu^2 > 0$

Simulations carried out at $\beta = 0.4$, second order phase transition at $\mu_c^2 \approx 0.54$

Action density





Compare to analytic continuation from imaginary chemical potential and worldline results

Optimization with additional reweighting

Reduce computational cost by generating configurations only at the start of optimization

Evaluate gradient on this fixed set of configurations

Configurations distributed according to original weight
$r = |\cos S^I_{\mathrm{eff},0}\, e^{-S^R_{\mathrm{eff},0}}|$

Reweight to distribution $w = |\cos S^I_{\mathrm{eff},1}\, e^{-S^R_{\mathrm{eff},1}}|$ evaluated on updated contours

Optimization with additional reweighting

Cost function

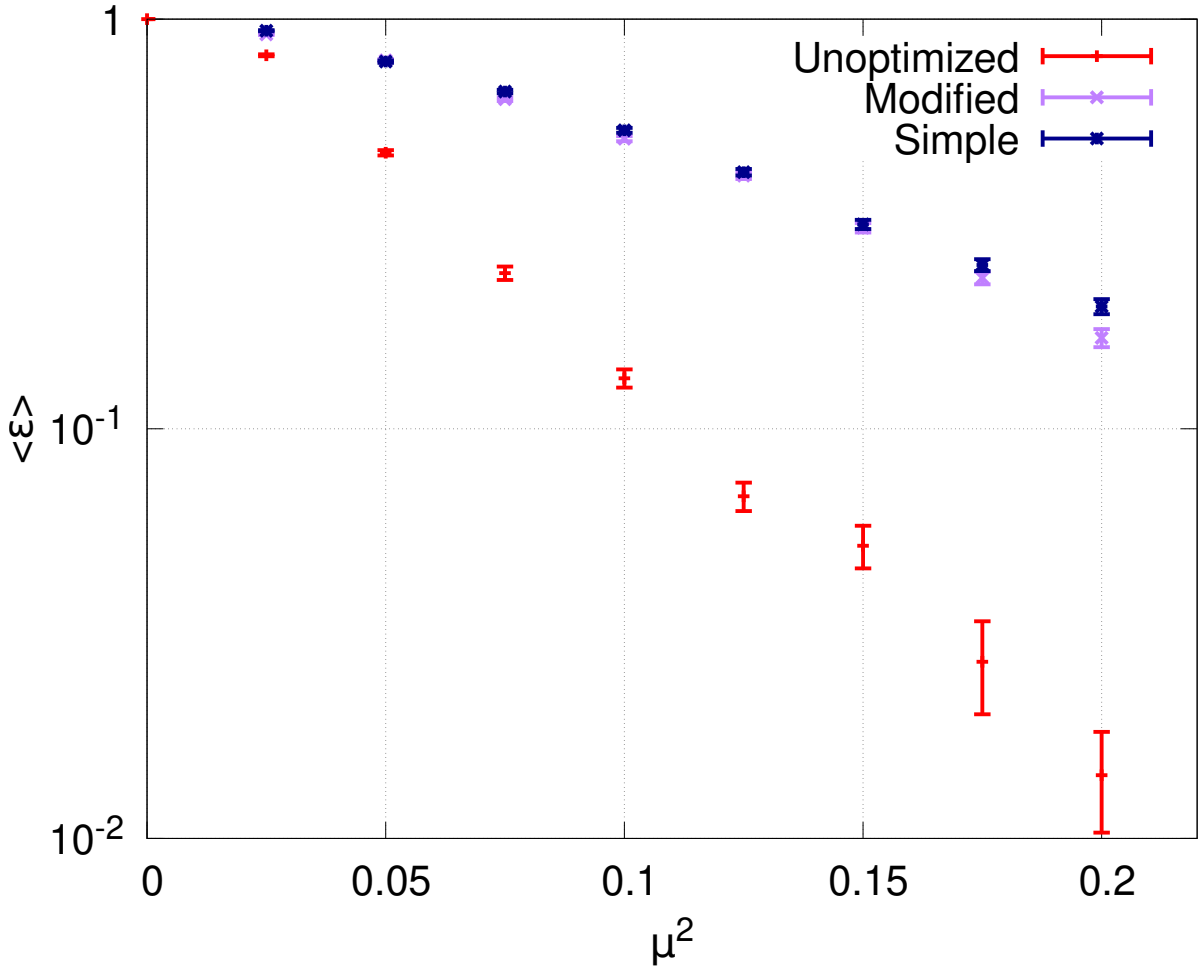
$$\frac{N_-}{N_+} = \frac{\langle \Theta(-\cos S^I_{\mathrm{eff},1}) \frac{w}{r} \rangle_r}{\langle \Theta(\cos S^I_{\mathrm{eff},1}) \frac{w}{r} \rangle_r}$$

Gradient

$$\frac{\partial}{\partial p_i} \left(\frac{N_-}{N_+} \right) = \frac{N_-}{N_+} \left[\frac{\langle \Theta(-\cos S^I_{\mathrm{eff},1}) F_i \frac{w}{r} \rangle_r}{\langle \Theta(-\cos S^I_{\mathrm{eff},1}) \frac{w}{r} \rangle_r} - \frac{\langle \Theta(\cos S^I_{\mathrm{eff},1}) F_i \frac{w}{r} \rangle_r}{\langle \Theta(\cos S^I_{\mathrm{eff},1}) \frac{w}{r} \rangle_r} \right]$$

Monitor overlap between w and r (denominators), generate new configurations when it becomes too small

Optimization with additional reweighting



Using $(A, B, K = 2)$ parametrization, same improvement

Summary

Applied path optimization on 2+1D XY model at non-zero chemical potential to reduce the sign problem

The optimized manifold has explicit translational invariance

The optimal choice of contour coefficients is independent of the spatial size of the system

The reduction of the sign problem is exponential in both the chemical potential and the volume

Possible to simulate past the phase transition on the optimized manifolds

Optimization time can be significantly reduced by generating configurations only at the start of the procedure

Outlook

Move on to gauge theories with fermions, e.g. high-density QCD:

$$Z = \int \mathcal{D}U \prod_x \det\left(1 + (2\kappa)^{N_T} e^{\mu/T} P(\boldsymbol{x})\right)^{2N_f} \det\left(1 + (2\kappa)^{N_T} e^{-\mu/T} P(\boldsymbol{x})^{-1}\right)^{2N_f} e^{-S_{plaq}[U]}$$

Plaquette action makes finding adequate parametrizations difficult

Can use algorithms to flow towards optimal manifold,
e.g. holomorphic flow, but they are expensive at large volumes

Learn main characteristics of optimized manifolds from holomorphic flow to make an ansatz for contour deformations