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

Euclidean QFTs with non-zero chemical potential: complex action $\Longrightarrow$ complex path integral weights

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

Expectation values of original theory reconstructed via reweighting

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

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

Uncertainties increase exponentially with chemical potential and volume $\Longrightarrow$ improvement required

The model

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

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

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

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

Deforming integration manifold away from the real submanifold

$$Z(\mu) = \int_{\mathcal{M}} \mathcal{D}\varphi\ e^{-S} = \int \mathcal{D}t\ e^{-S_{\mathrm{eff}}}, \qquad S_{\mathrm{eff}} = S - \ln\det J$$

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

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 (SQ)

Severity of the sign problem measured by

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

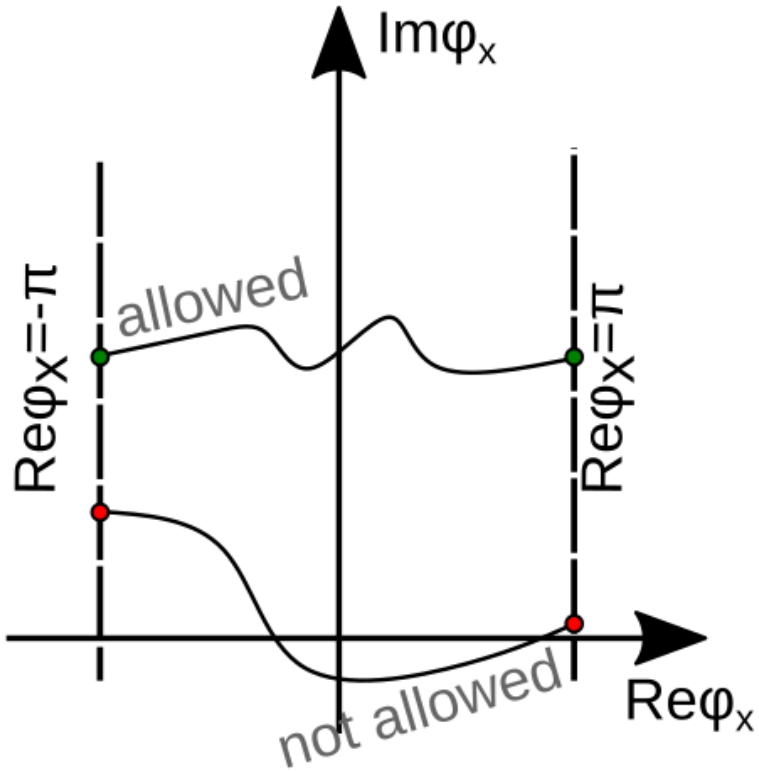
Deforming integration manifold changes the denominator $\Longrightarrow$ maximize $\langle \varepsilon \rangle_{SQ,\mu}$ with contour deformations

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

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

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

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 over x_0 ($\mu^2 = 0.15$):

- 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

Parametrizaitons with triangular Jacobian matrix

Including more neighbors in parametrization complicates the Jacobian

Introduce constraint to make Jacobian matrix triangular

1. With spatial neighbors

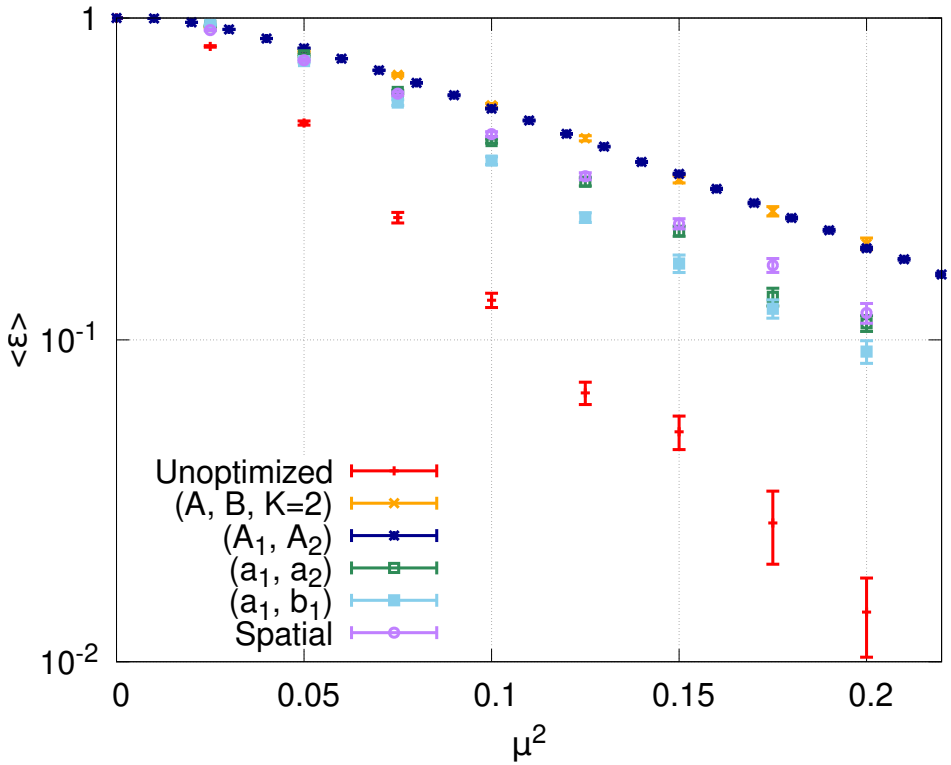
$$\varphi_x = t_x + \imath \sum_{k=1}^{K} \sum_{n=0}^{2} \theta_n^{(1)} \left[\bar{A}_{k,n} \cos(k(t_x - t_{x+\hat{n}})) + \bar{B}_{k,n} \sin(k(t_x - t_{x+\hat{n}})) \right]$$

2. With next-to-nearest temporal neighbor

$$\varphi_x = t_x + \imath \sum_{k=1}^{K} \left[\theta_0^{(1)} a_k \cos(k(t_x - t_{x+\hat{0}})) + \theta_0^{(2)} b_k \cos(k(t_x - t_{x+2\hat{0}})) \right]$$

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

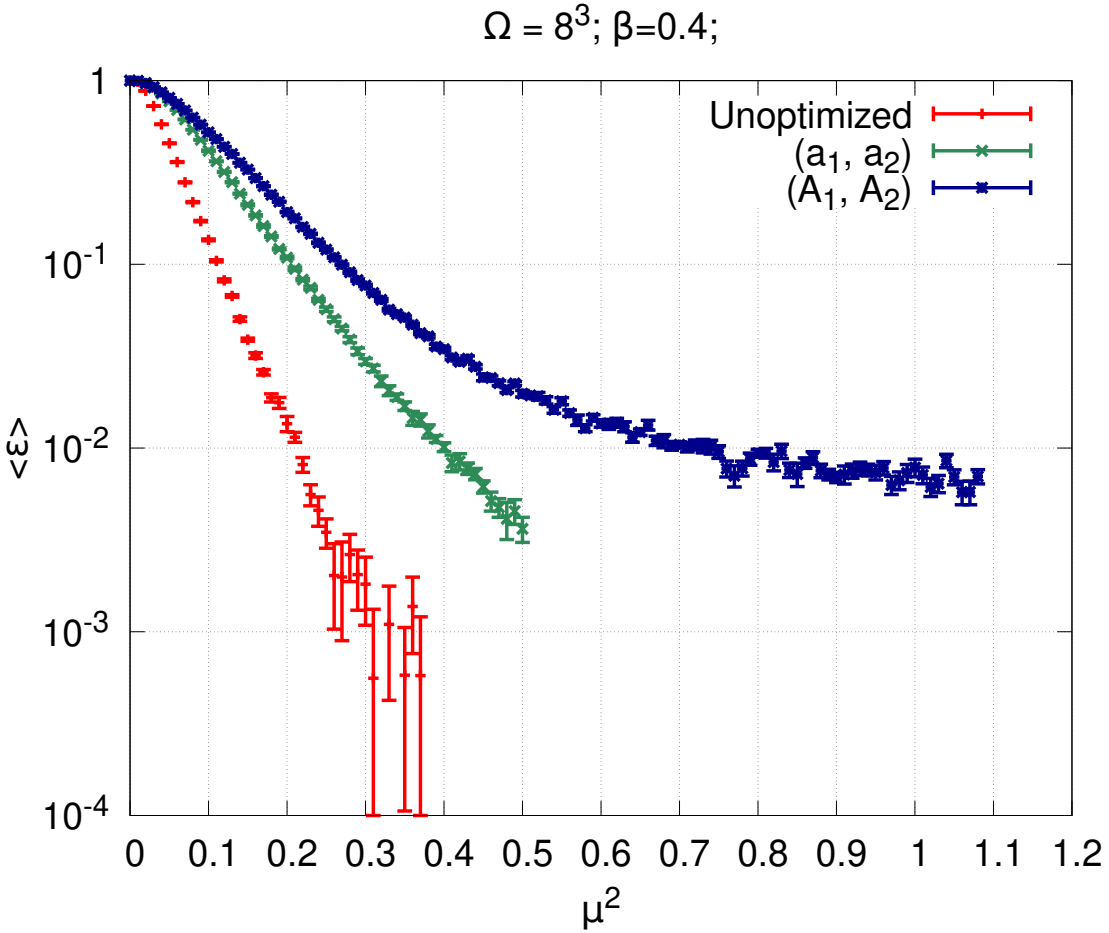
Comparing parametrizations



- Spatial neighbors: no effect
- Next-to-nearest neighbors at 1^{st} order worse than nearest neighbors at 2^{nd} order
- Triangular Jacobian matrix: less improvement but reduced cost

Best choice: only nearest temporal neighbors, 2^{nd} order, translational invariance

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

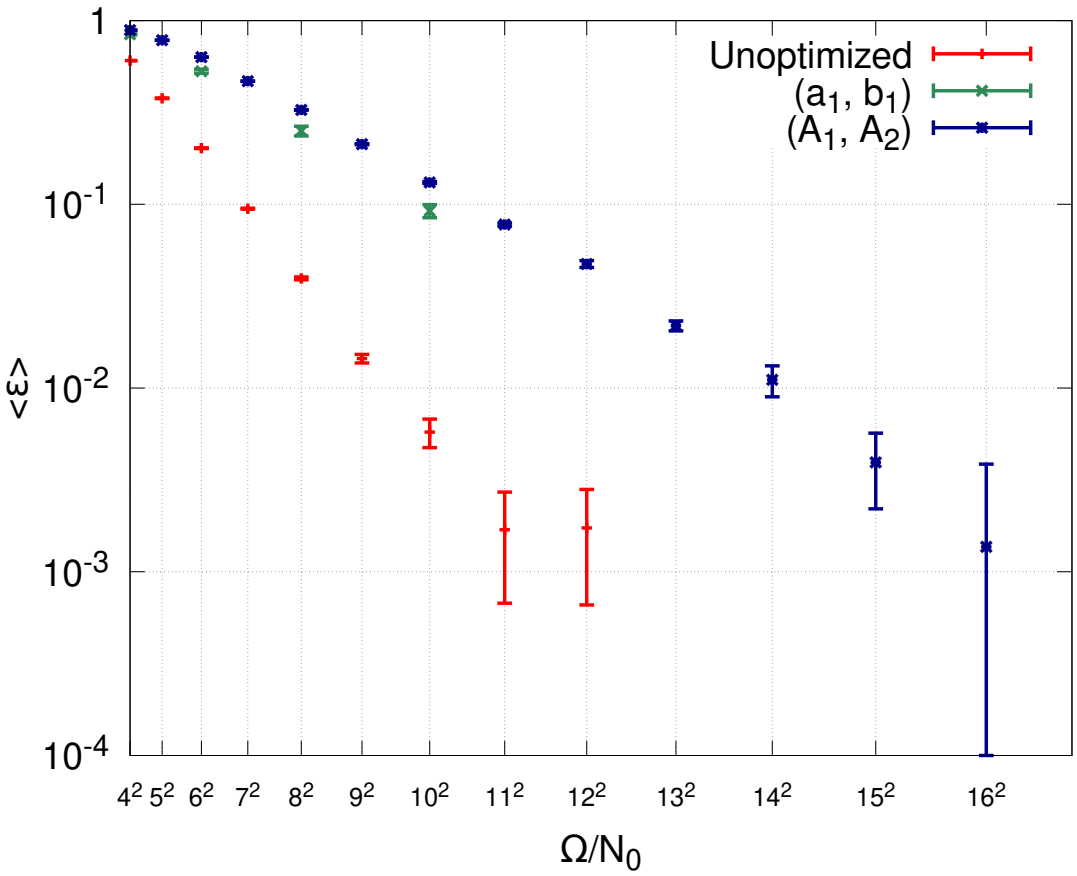


Fit

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

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

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

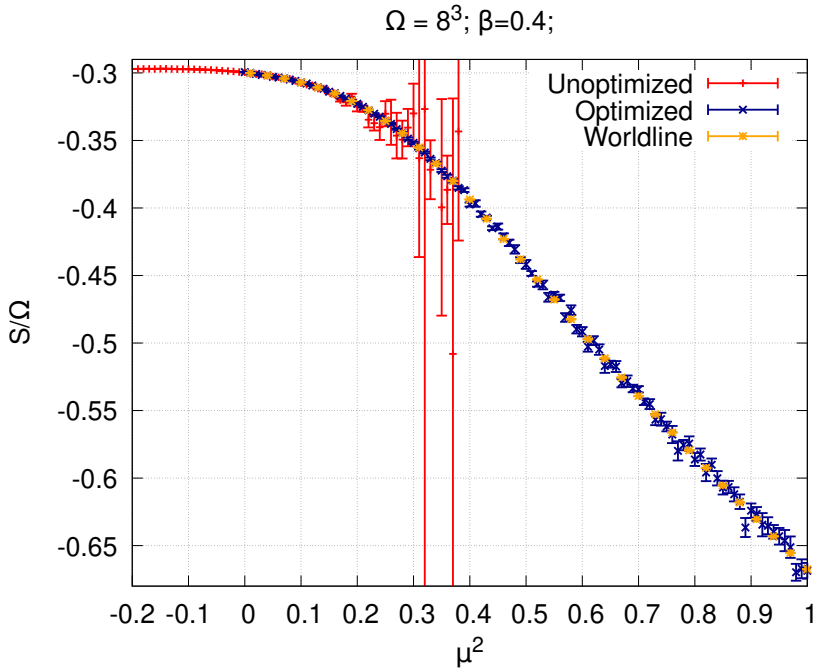


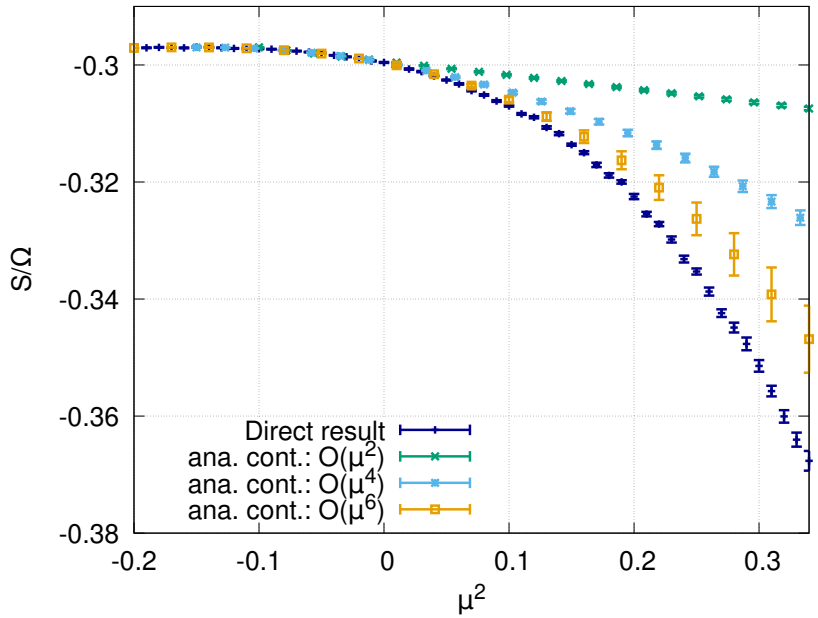
Fit

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

- 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





Compare to worldline results [Banerjee, Chandrasekharan, PRD (2010)] and analytic continuation from imaginary chemical potential

Phase transition at $\mu_c^2 \approx 0.54$

Reducing cost of optimization

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

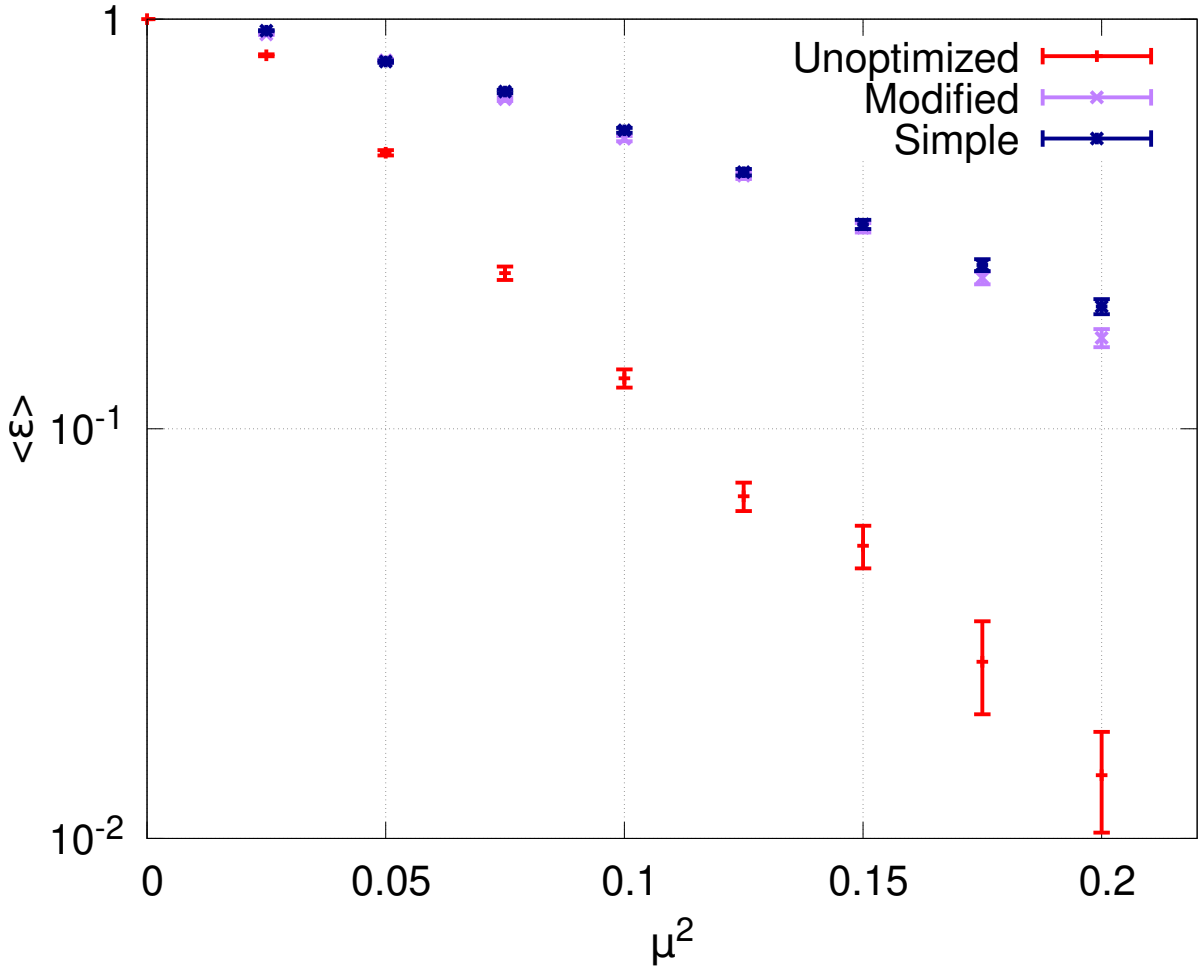
Evaluate gradient of cost function on this fixed set of configurations

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

Generate new configurations when overlap between w and r becomes too small

Reducing cost of optimization



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

Summary and outlook

- Applied path optimization on 2+1D XY model at non-zero chemical potential to reduce the sign problem
- Improvement is exponential in squared chemical potential and volume
- Possible to simulate past phase transition on optimized manifold
- Optimization time can be significantly reduced by generating configurations only at the start of the procedure
- Moving on to fermionic models and gauge theories with fermions

Back-up: improving the sign problem

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

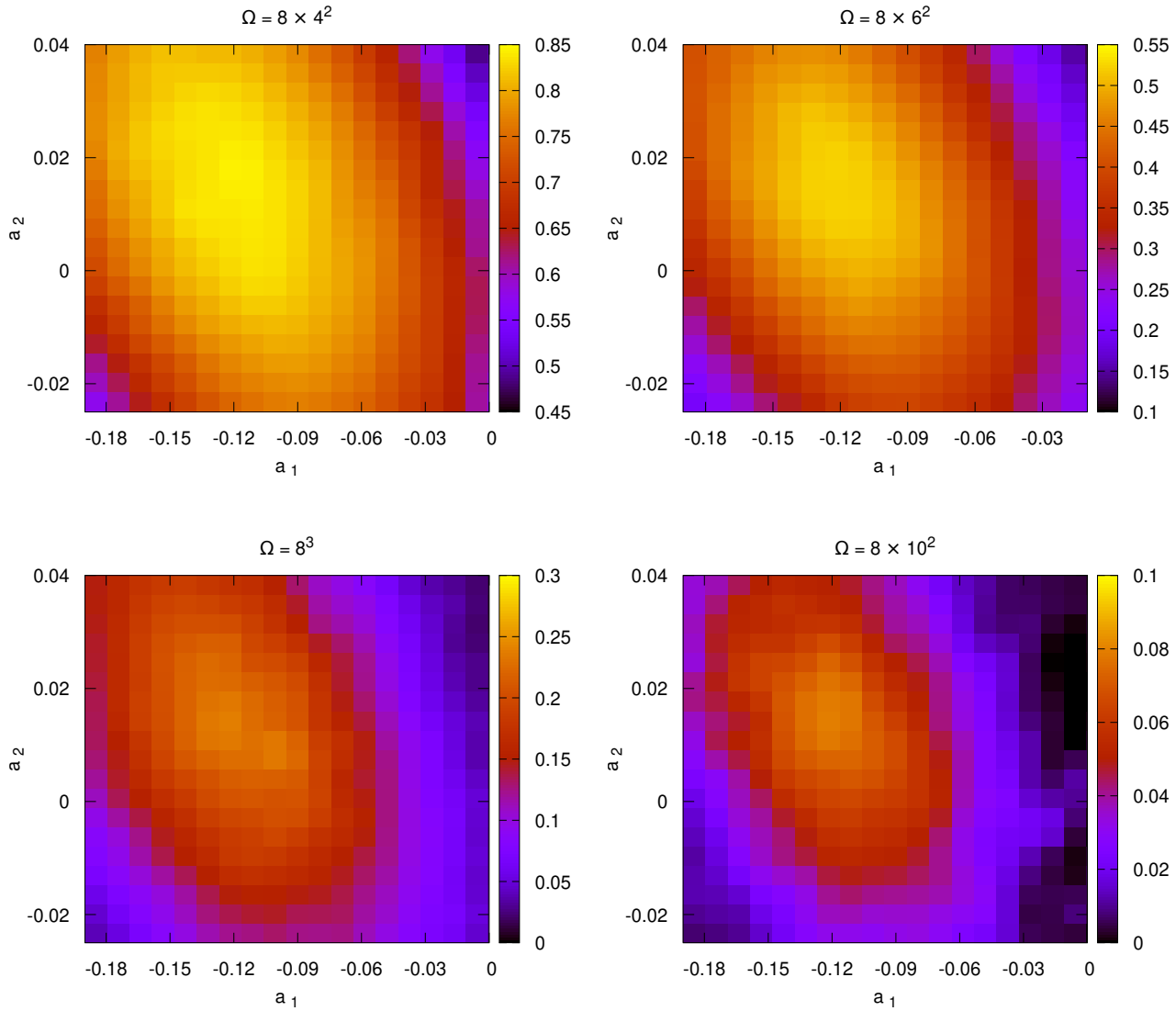
$$\frac{N_-}{N_+} = \frac{\int \mathcal{D}t\ \Theta(-\cos S^I_{\text{eff}})\,|\cos S^I_{\text{eff}}|e^{-S^R_{\text{eff}}}}{\int \mathcal{D}t\ \Theta(\cos S^I_{\text{eff}})\,|\cos S^I_{\text{eff}}|e^{-S^R_{\text{eff}}}}$$

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

Use gradient descent

Back-up: scans in (a_1, a_2) coefficient space

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



Back-up: reducing computational cost

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