Fighting the sign problem in a chiral random matrix model with contour deformations

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[arXiv:hep-lat/2301.12947]

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Outline

Structure of the talk:

1. introduction (the sign problem, the chRMT model and its sign problem);
2. methods (complexification, integration manifold optimisation, holomorphic flow);
3. results (with different *ansätze*, comparisons with holomorphic flow);
4. discussion and outlook.

What is the sign problem?

Grand canonical partition function of QCD:

$$\begin{aligned}\mathcal{Z} &= \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar{\psi}\; e^{-S[U,\psi,\bar{\psi}]} = \int \mathcal{D}U\; \det M[U] e^{-S_{\mathrm{g}}[U]} \\ &= \int \mathcal{D}U\; e^{-S_{\mathrm{eff}}[U]} = \int \mathcal{D}U\; w[U]\;.\end{aligned}$$

If $w[U]$ not real *and* positive $\leftrightarrow$ $S_{\mathrm{eff}} \notin \mathbb{R}$: MC with importance sampling not possible

$\sim$ **complex action problem**.

E.g.

- finite density/bariochemical potential QCD(-like models);
- Hubbard model of condensed matter physics (away from half filling);
- real time dynamics $\sim \langle f|e^{-iH}|i\rangle = \int \mathcal{D}x\; e^{iS[x]}$.

What is the sign problem?

Q: How to overcome the complex action problem?

A: Simulate what you can *and* reweight to the original theory!

Expectation value through reweighting ($r[\phi]$ real and positive):

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

Complex action problem reduces to the **sign problem**:

- large fluctuations in $\frac{w}{r}$ $\longrightarrow$ large cancellations $\longrightarrow$ large uncertainties (exp. in V, μ);
- severity of the sign problem:

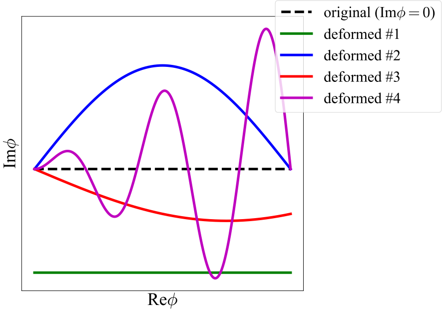
$$\left\langle \frac{w}{r} \right\rangle_r = \frac{\mathcal{Z}_w}{\mathcal{Z}_r} \qquad \Longrightarrow \qquad \begin{cases} 1 & \sim \text{perfect!} \\ \approx 0 & \sim \text{not so much\dots} \end{cases}$$

E.g. *phase quenched* theory $r = |w| \implies \det M \to |\det M|$.

Fighting the sign problem?

Why?:

- QCD;
- condensed matter physics (Hubbard model);
- neutron stars;
- hydrodynamic simulations at finite density;
- etc.



How?:
N-dim. integral over real fields to

- $2N$-dim. stochastic dynamics in the real and imaginary parts of complexified fields (e.g. *complex Langevin*);
- N-dim. integral with deformed integration contour/manifold into the complexified field space.

Complex contour deformations

Aim:

- searching for theories "closer" to the original theory;
- with real and positive weights;
- hence acquiring better signal-to-noise ratios in observables.

Set of integration manifolds $\mathcal{M}_{\rm def}(\{p\})$ parameterised with some finite set of real parameters $\{p\}$:

$$\mathcal{Z} = \int_{\mathcal{M}} \mathcal{D}\phi\, w[\phi] = \int_{\mathcal{M}_{\rm def}} \mathcal{D}\phi_{\rm def}\; w[\phi_{\rm def}] = \int_{\mathcal{M}_{\rm def}} \mathcal{D}X\;\; \det \mathcal{J}(X) w[\phi_{\rm def}(X)]\ .$$

Phase quenched partition function:

$$\mathcal{Z}^{\rm def}_{\rm PQ}(\{p\}) = \int_{\mathcal{M}_{\rm def}} \mathcal{D}X\; \Big| \det \mathcal{J}(X) w[\phi_{\rm def}(X)] \Big|\ .$$

Severity of the sign problem:

$$\left\langle \frac{w}{r} \right\rangle_r = \frac{\mathcal{Z}}{\mathcal{Z}^{\rm def}_{\rm PQ}(\{p\})} = \left\langle \frac{\det \mathcal{J} w[\phi_{\rm def}]}{|\det \mathcal{J} w[\phi_{\rm def}]|} \right\rangle^{\rm def}_{\rm PQ} := \langle e^{i\theta} \rangle\ .$$

Integration manifold optimisation $\sim$ machine learning

The sign problem is milder if

$$\frac{\mathcal{Z}}{\mathcal{Z}^{\mathrm{def}}_{\mathrm{PQ}}(\{p\})} \text{ is maximal!}$$

Y. Mori et. al. [arXiv:hep-lat/1705.05605]

Introducing a **cost function** and minimise it by varying $\{p\}$:

$$\mathcal{F}(\{p\}) = -\log\langle e^{i\theta}\rangle = -\log\mathcal{Z} + \log\mathcal{Z}^{\mathrm{def}}_{\mathrm{PQ}}(\{p\}) \ .$$

One can utilise machine learning algorithms (e.g. gradient descent) and compute gradients:

$$\nabla_p\mathcal{F}(\{p\}) = \nabla_p \log\mathcal{Z}_{\mathrm{PQ}}(\{p\}) = -\big\langle \nabla_p S_{\mathrm{eff}} - \nabla_p \log|\det\mathcal{J}|\big\rangle^{\mathrm{def}}_{\mathrm{PQ}} \ .$$

Holomorphic flow

A. Alexandru et. al.: `[arXiv:hep-lat/1512.08764]`

- Specific way of doing contour deformations:

$$\int_{\mathcal{M}_0} \mathcal{D}\phi \; e^{-S_{\text{eff}}[\phi]} \quad \xrightarrow{\text{deformation}} \quad \int_{\mathcal{M}_{\text{def}}(t_{\text{f}})} \mathcal{D}\phi_{\text{f}} \; e^{-S_{\text{eff}}[\phi_{\text{f}}]}$$

- Defined by the flow equation

$$\frac{\mathrm{d}\phi_{\text{f}}}{\mathrm{d}t_{\text{f}}} = \left(\frac{\partial S_{\text{eff}}}{\partial \phi_{\text{f}}}\right)^* \qquad \text{with initial condition} \qquad \phi_{\text{f}}(t_{\text{f}} = 0) = \phi \; .$$

- Along the flow

$$\frac{\mathrm{d}}{\mathrm{d}t_{\text{f}}} \mathrm{Re} S_{\text{eff}} = \frac{1}{2}\left[\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}t_{\text{f}}} + \left(\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}t_{\text{f}}}\right)^*\right] = \left|\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}\phi_{\text{f}}}\right|^2 \geq 0 \;\sim \text{monotonically increasing;}$$

$$\frac{\mathrm{d}}{\mathrm{d}t_{\text{f}}} \mathrm{Im} S_{\text{eff}} = \frac{1}{2i}\left[\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}t_{\text{f}}} - \left(\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}t_{\text{f}}}\right)^*\right] = \frac{1}{2i}\left[\left|\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}\phi_{\text{f}}}\right|^2 - \left|\frac{\mathrm{d}S_{\text{eff}}}{\mathrm{d}\phi_{\text{f}}}\right|^2\right] = 0 \;\sim \text{constant} \; .$$

- $\mathrm{Re} S_{\text{eff}}$ increases monotonically $\Longrightarrow$ $\mathcal{Z}_{\text{PQ}}$ becomes smaller!

- Jacobian: $\mathrm{d}\mathcal{J}/\mathrm{d}t_{\text{f}} = (H\mathcal{J})^*$ with Hessian H and $\det \mathcal{J}(t_{\text{f}} = 0) = 1$
$\sim$ very expensive. . .

The Stephanov model

$\sim$ **chiral random matrix model** (Stephanov: `[arXiv:hep-lat/9604003]`):

$$\boxed{\mathcal{Z} = \int \mathcal{D}U \, \det M[U] e^{-S_{\mathrm{g}}[U]}} \quad \text{vs.} \quad \boxed{\mathcal{Z} = e^{N\mu^2} \int \mathrm{d}W \mathrm{d}W^\dagger \, \det{}^{N_f}(D+m)\, e^{-N\mathrm{Tr}(WW^\dagger)}},$$

where:

- $W, W^\dagger \in \mathbb{C}^{N\times N}$, general complex matrices $\rightarrow 2N^2$ DoF;
- N_f : flavour number;
- μ : chemical potential;
- m : quark mass;
- and massless Dirac operator

$$D = \begin{pmatrix} 0 & iW+\mu \\ iW^\dagger + \mu & 0 \end{pmatrix} \in \mathbb{C}^{2N\times 2N}$$

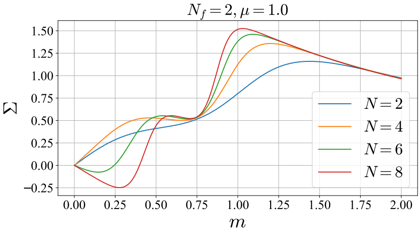
`[arXiv:hep-ph/0003017]`

The Stephanov model

Phase transitions:

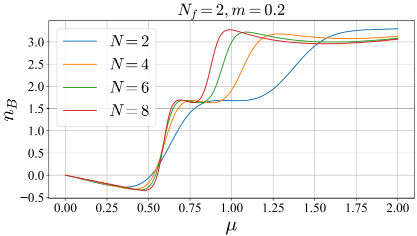
- chiral condensate

$$\Sigma(m, \mu) = \frac{1}{2N} \frac{\partial \log \mathcal{Z}}{\partial m}$$



- baryon number density

$$n_B(m, \mu) = \frac{1}{2N} \frac{\partial \log \mathcal{Z}}{\partial \mu}$$



The Stephanov model: the phase quenched theory

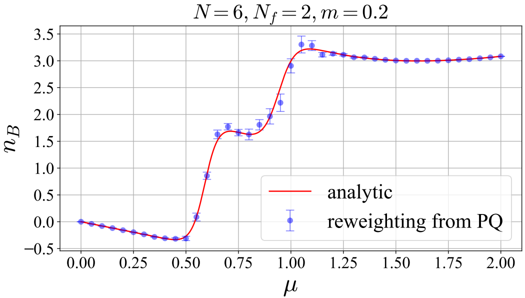
Phase quenched partition function:

$$\mathcal{Z}_{\mathrm{PQ}} = e^{N\mu^2} \int \mathrm{d}W\mathrm{d}W^\dagger \, |\det{}^{N_f}(D+m)| \, e^{-N\mathrm{Tr}(WW^\dagger)} \, .$$

E.g. baryon number density:

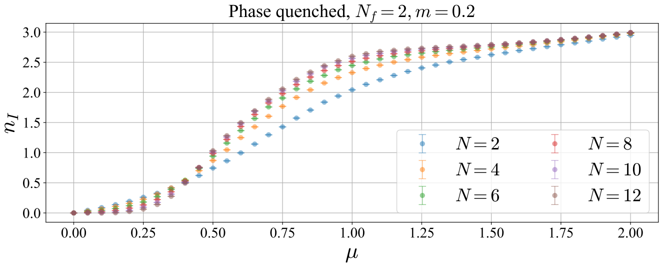
Expectation values via reweighting

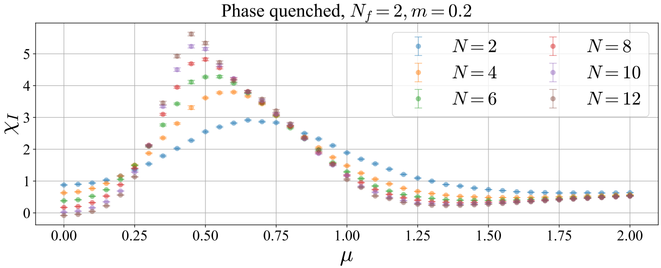
$$\langle \mathcal{O} \rangle = \frac{\left\langle \mathcal{O} \frac{\det^{N_f}(D+m)}{|\det^{N_f}(D+m)|} \right\rangle_{\mathrm{PQ}}}{\left\langle \frac{\det^{N_f}(D+m)}{|\det^{N_f}(D+m)|} \right\rangle_{\mathrm{PQ}}} \, .$$



The Stephanov model: pion condensation in the PQ theory

Transition to pion condensed phase:

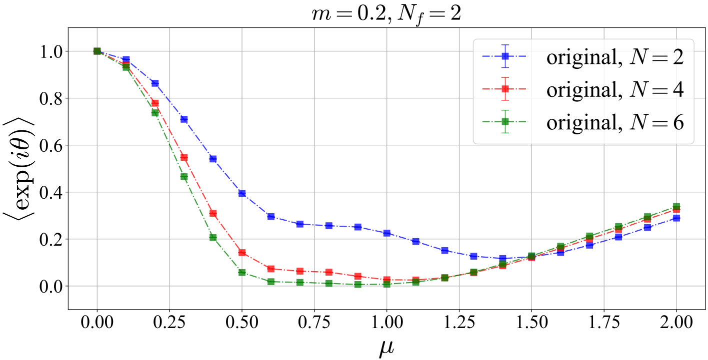




The Stephanov model and its sign problem at finite μ

Severity of the sign problem (average phase):

$$\langle e^{i\theta} \rangle = \frac{\mathcal{Z}}{\mathcal{Z}_{\mathrm{PQ}}} = \left\langle \frac{\det^{N_f}(D+m)}{|\det^{N_f}(D+m)|} \right\rangle_{\mathrm{PQ}} .$$



The Stephanov model: integration contour deformations

Complexification:

$$\begin{aligned} W &= A + iB & \rightarrow \qquad X &= \alpha + i\beta \\ W^\dagger &= A^\mathrm{T} - iB^\mathrm{T} & \rightarrow \qquad Y &= \alpha^\mathrm{T} - i\beta^\mathrm{T} \end{aligned}$$

where $A, B \in \mathbb{R}^{N\times N}$ and $\alpha, \beta \in \mathbb{C}^{N\times N}$.

$\longrightarrow$ α, β can be parameterized by A, B and some set of parameters $\{p\}$.

Partition functions:

- deformations are chosen such that $\mathcal{Z}$ remains invariant,
- while $\mathcal{Z}_{\mathrm{PQ}} \equiv \mathcal{Z}_{\mathrm{PQ}}(\{p\})$ does not!

The Stephanov model: Jacobian of contour deformations

We parameterize the deformed integration manifold with the undeformed variables:

$$\mathcal{Z} = \int\limits_{\mathcal{M}_{\mathrm{def}}} \mathrm{d}\alpha \mathrm{d}\beta \, e^{-S_{\mathrm{eff}}[\alpha,\beta]} = \int\limits_{\mathcal{M}_{\mathrm{def}}} \mathrm{d}A \mathrm{d}B \, \det \mathcal{J} e^{-S_{\mathrm{eff}}[\alpha(A,B),\beta(A,B)]} \, ,$$

where $S_{\mathrm{eff}} = N \mathrm{Tr}(XY) - N_f \log\det(D+m)$ and $\mathcal{J} = \frac{\partial(\alpha,\beta)}{\partial(A,B)} \in \mathbb{C}^{2N^2 \times 2N^2}$.

"New" average phase after deformation:

$$\langle e^{i\theta} \rangle = \left\langle \frac{\det^{N_f}(D+m) \det\mathcal{J}}{|\det^{N_f}(D+m) \det\mathcal{J}|} e^{-iN\mathrm{Im}\mathrm{Tr}(XY)} \right\rangle_{\mathrm{PQ}}^{\mathrm{def}}$$

Results: *ansatz* #1

Motivation:

μ can be transformed out of the Dirac operator via a constant imaginary shift in A:

$$D = \begin{pmatrix} 0 & iW + \mu \\ iW^\dagger + \mu & 0 \end{pmatrix} = \begin{pmatrix} 0 & (iA - B) + \mu \\ (iA^{\mathrm{T}} + B^{\mathrm{T}}) + \mu & 0 \end{pmatrix}$$

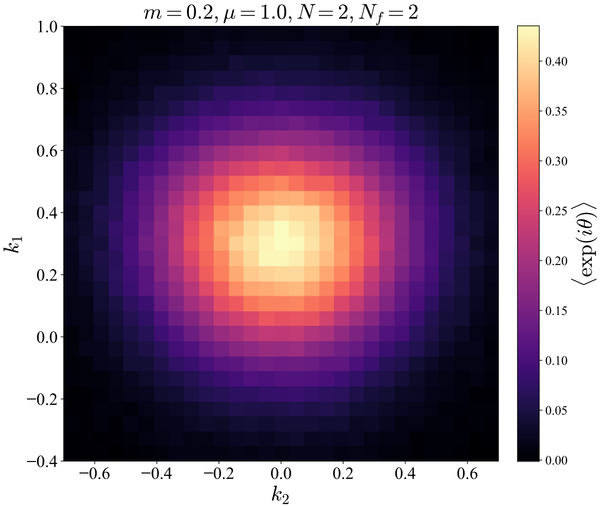
The *ansatz*:

$$\alpha = A + ik_1 \mathrm{id}$$
$$\beta = B + ik_2 \mathrm{id}$$

with $k_1, k_2 \in \mathbb{R}$ and $\det \mathcal{J} = 1$.

Results: *ansatz* #1

$\alpha = A + ik_1\mathrm{id}$
$\beta = B + ik_2\mathrm{id}$



Results: *ansatz* #2

Motivation:

When μ is transformed out of the Dirac operator via $A \to A + ik\mathrm{id}$:

$$\mathrm{Tr}(XY) = \mathrm{Tr}(AA^{\mathrm{T}} + BB^{\mathrm{T}}) - Nk^2 + 2ik\mathrm{Tr}A$$

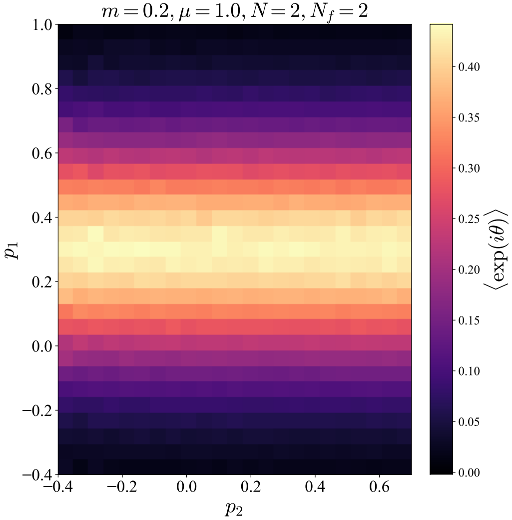
The *ansatz*:

$$\begin{aligned}\alpha &= A + ip_1\mathrm{id} + p_2\mathrm{Tr}A\mathrm{id}\\ \beta &= B\end{aligned}$$

with $p_1, p_2 \in \mathbb{R}$ and $\det\mathcal{J} = 1 + Np_2$.

Results: *ansatz* #2

$$\alpha = A + ip_1\mathrm{id} + p_2\mathrm{Tr}A\mathrm{id}$$
$$\beta = B$$



Results: many-parameter *ansätze*

20-parameter linear *ansatz*:

$$\alpha = (a + b\mathrm{Tr}A + c\mathrm{Tr}B)\mathrm{id} + (1+d)A + eB$$
$$\beta = (f + g\mathrm{Tr}A + h\mathrm{Tr}B)\mathrm{id} + jA + (1+k)B$$

with $a, b, \ldots, k \in \mathbb{C}$ *and* all are zero before contour deformation;

$$\det\mathcal{J} = \big((1+d)(1+k) - ej\big)^{N^2-1}\big[\big((1+d)+Nb\big)\big((1+k)+Nh\big) - (e+Nc)(j+Ng)\big] \,.$$

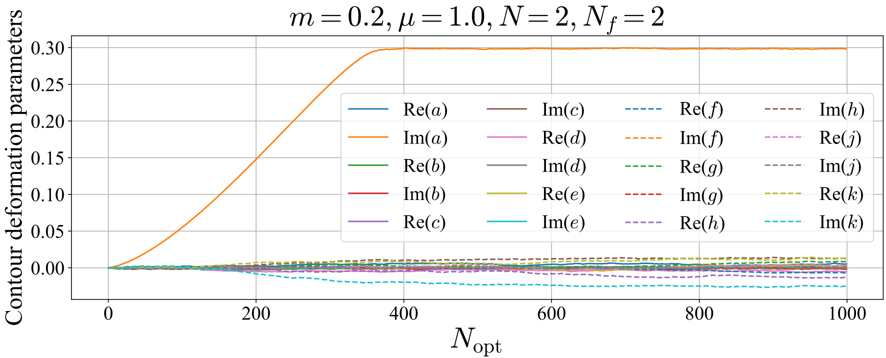
Proper scan is not feasible: too many parameters:

- too costly to scan,
- impossible to visualize,

but can be handled with the *integration manifold optimisation* approach.

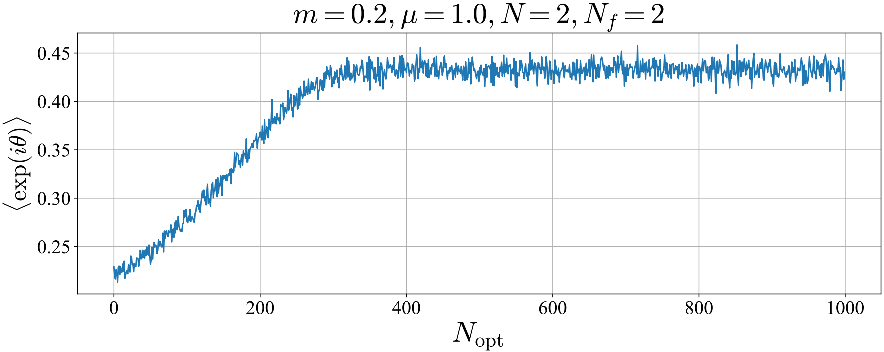
Results: many-parameter *ansätze*

Interestingly only a **single important parameter** emerges $\Longrightarrow$ $\boxed{\mathrm{Im}(a) = k_1 = p_1}$

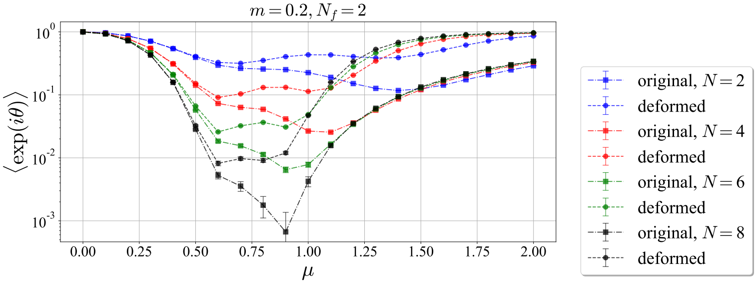


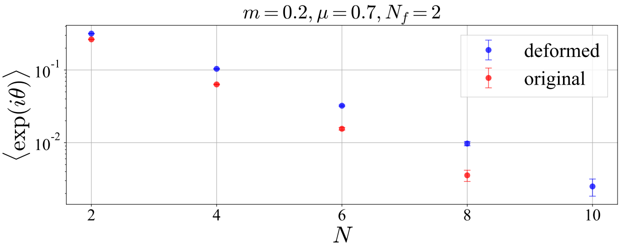
Results: many-parameter *ansätze*

Visible improvement in the sign problem:



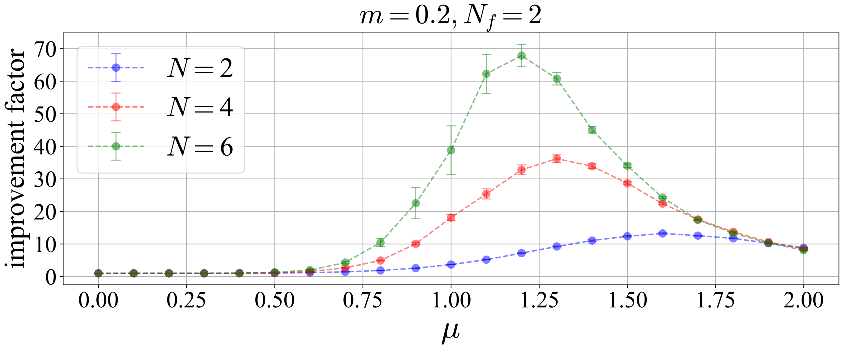
Results: μ- and N-dependence at $N_f = 2$ ($\mathrm{Im}(a) = k_1 = p_1$)





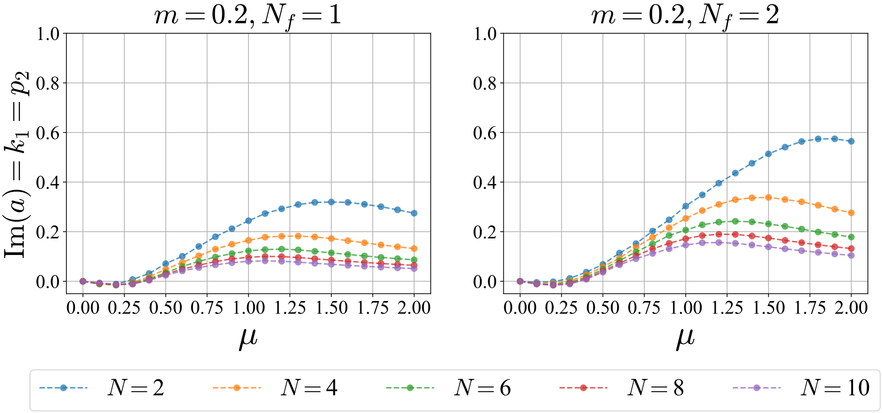
Results: improvement on the sign problem ($\mathrm{Im}(a) = k_1 = p_1$)

Statistical improvement $\sim$ $\left(\langle e^{i\theta}\rangle^{\text{def}}/\langle e^{i\theta}\rangle^{\text{original}}\right)^2$ $\propto$ 1/(length of the simulation)



Results: optimal contour parameters ($\mathrm{Im}(a) = k_1 = p_1$)

μ- and N-dependence:

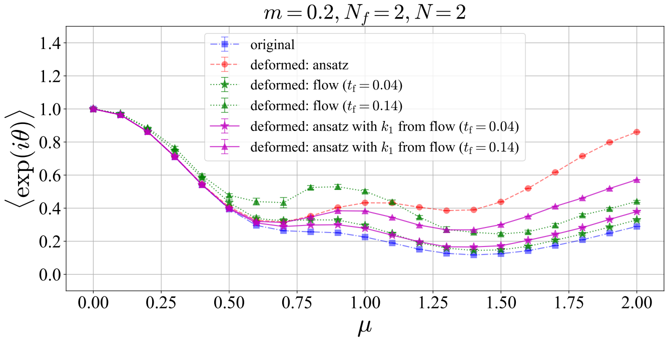


Results: holomorphic flow vs. *integration manifold optimisation*

Q: "Does the two methods find the same deformed contour?"

$$\langle \alpha_{\mathrm{f}}^{ij} - A^{ij} \rangle = \big\langle \mathrm{Tr}(\alpha_{\mathrm{f}} - A) \big\rangle (t_{\mathrm{f}}) \delta^{ij} \qquad \longleftrightarrow \qquad \langle \alpha^{ij} - A^{ij} \rangle = i k_1 N \delta^{ij}$$

hence: $\quad k_1 = \mathrm{Im} \big\langle \mathrm{Tr}(\alpha_{\mathrm{f}} - A) \big\rangle (t_{\mathrm{f}}) / N.$



- The majority of the improvement comes from the constant shift, but there seems to be more and more as t_{f} is increased.

Piecewise optimisation of the trace

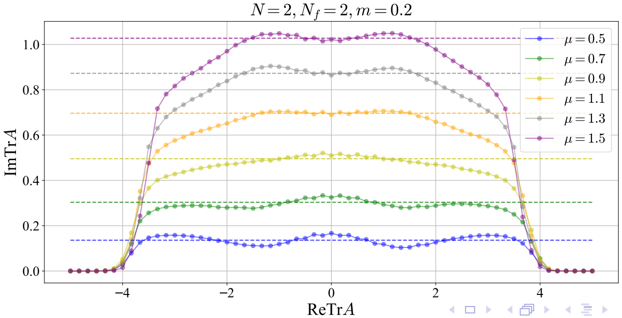
$\sim$ deforming only $t = \mathrm{Tr}A$.

Ansatz ($\beta = B$):

$$A = \frac{t}{N}\mathrm{id} + \left(A - \frac{t}{N}\mathrm{id}\right) = \frac{t}{N}\mathrm{id} + \tilde{A} \quad \rightarrow \quad \alpha = \frac{\tau}{N}\mathrm{id} + \tilde{A}\,,$$

$\mathrm{Tr}\tilde{A} = 0$ and $\tau = t + if(t; \{y_k\}, \{x_k\})$ where f is some (e.g. linear) interpolation function.

- $\{y_k\}$: parameters to optimise;
- $\{x_k\}$: nodes on the original contour.



Discussion and outlook

Findings:

- The sign problem in theories with a fermion determinant could be improved through complex contour deformations.
- Deformations that weaken the sign problem the most (i.e. some constant shift $\propto i \cdot \mathrm{id}$) has no direct counterpart in full-QCD.
- Still, numerically the improvement appears to be exponential in V and μ.
- The optimisation method (i.e. machine learning) is an applicable way to find the optima of the deformation parameters in different änsatze.
- Results with holomorphic flow demonstrate that there is still more than the constant shift.

To do:

- We shall use a more realistic toy model of QCD, or continue with chRMT but only with deformations allowed in full-QCD.
- Planned: applications in heavy dense QCD in 2 and/or 4 dimensions.

The End

Thank you for your attention.

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