

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:

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

If $w[U]$ not real *and* positive $\leftrightarrow S_{\text{eff}} \notin \mathbb{R}$: 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 $\frac{w}{r}$ → large cancellations → large uncertainties (exp. in V, μ);
- ▶ severity of the sign problem:

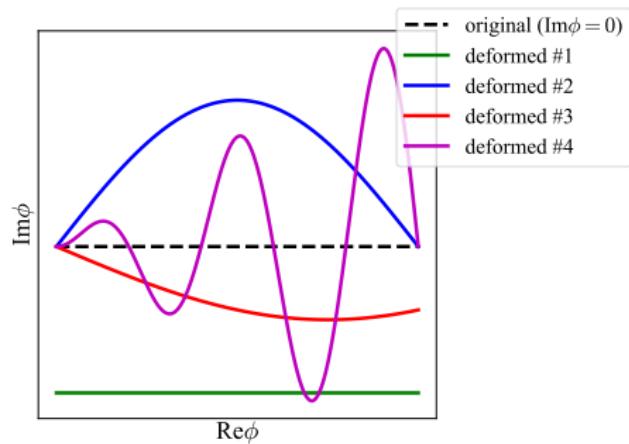
$$\left\langle \frac{w}{r} \right\rangle_r = \frac{\mathcal{Z}_w}{\mathcal{Z}_r} \quad \Rightarrow \quad \begin{cases} 1 & \sim \text{perfect!} \\ \approx 0 & \sim \text{not so much...} \end{cases}$$

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

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

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

Phase quenched partition function:

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

Severity of the sign problem:

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

Integration manifold optimisation \sim machine learning

The sign problem is milder if

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

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

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

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

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

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

Holomorphic flow

A. Alexandru et. al.: [[arXiv:hep-lat/1512.08764](https://arxiv.org/abs/hep-lat/1512.08764)]

- ▶ Specific way of doing contour deformations:

$$\int_{\mathcal{M}_0} \mathcal{D}\phi e^{-S_{\text{eff}}[\phi]} \xrightarrow{\text{deformation}} \int_{\mathcal{M}_{\text{def}}(t_f)} \mathcal{D}\phi_f e^{-S_{\text{eff}}[\phi_f]}$$

- ▶ Defined by the flow equation

$$\frac{d\phi_f}{dt_f} = \left(\frac{\partial S_{\text{eff}}}{\partial \phi_f} \right)^* \quad \text{with initial condition} \quad \phi_f(t_f = 0) = \phi .$$

- ▶ Along the flow

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

$$\frac{d}{dt_f} \text{Im} S_{\text{eff}} = \frac{1}{2i} \left[\frac{dS_{\text{eff}}}{dt_f} - \left(\frac{dS_{\text{eff}}}{dt_f} \right)^* \right] = \frac{1}{2i} \left[\left| \frac{dS_{\text{eff}}}{d\phi_f} \right|^2 - \left| \frac{dS_{\text{eff}}}{d\phi_f} \right|^2 \right] = 0 \sim \text{constant} .$$

- ▶ $\text{Re} S_{\text{eff}}$ increases monotonically $\implies \mathcal{Z}_{PQ}$ becomes smaller!
- ▶ Jacobian: $d\mathcal{J}/dt_f = (H\mathcal{J})^*$ with Hessian H and $\det \mathcal{J}(t_f = 0) = 1$
 \sim very expensive...

Holomorphic flow and Lefschetz thimbles

- ▶ Holomorphic flow tends towards the so-called **Lefschetz thimbles** as $t_f \rightarrow \infty$.
AuroraScience: [[arXiv:hep-lat/1205.3996](https://arxiv.org/abs/hep-lat/1205.3996)]
- ▶ Lefschetz thimbles: a given contour on which $\text{Im}S_{\text{eff}} = \text{constant}$.
- ▶ The thimble is the set of initial conditions for the equation

$$\frac{d\phi_f}{dt_f} = - \left(\frac{\partial S_{\text{eff}}}{\partial \phi_f} \right)^* \quad \text{for which } \phi_f(t_f \rightarrow \infty) = \phi^c ,$$

where

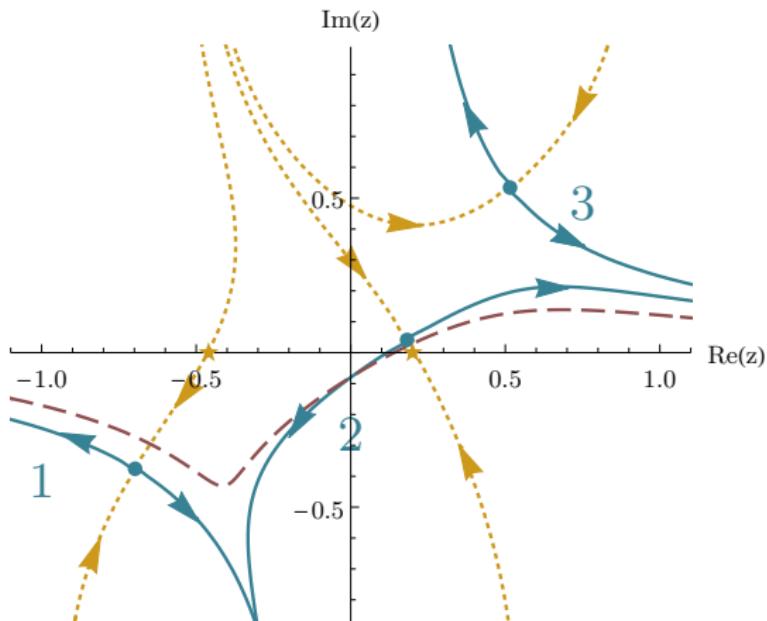
$$\left. \frac{\partial S_{\text{eff}}}{\partial \phi_f} \right|_{\phi_f = \phi^c} = 0 .$$

- ▶ Thimble structure of fermionic theories are usually quite complicated.
- ▶ Not smooth at zeroes of the fermion determinant.
- ▶ Cancellations between competing thimbles could become essential.
- ▶ Not necessarily the “best” contour either.
- ▶ If $\det \mathcal{J} \neq 1$: residual sign problem.

Lefschetz thimble: example

- ▶ Example with action [arXiv:hep-lat/2007.05436]

$$S(z) = \frac{1}{G} z^2 - \log[(p^2 + i\mu)^2 + (z + m)^2]$$



The Stephanov model

~ chiral random matrix model (Stephanov: [[arXiv:hep-lat/9604003](#)]):

$$\mathcal{Z} = \int \mathcal{D}U \det M[U] e^{-S_g[U]}$$

vs.

$$\mathcal{Z} = e^{N\mu^2} \int dW dW^\dagger \det^{N_f} (D + m) e^{-N \text{Tr}(WW^\dagger)},$$

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

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

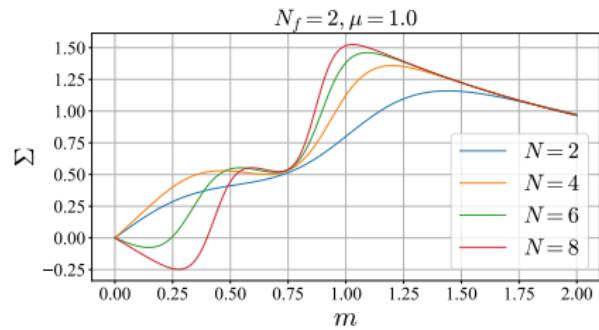
[[arXiv:hep-ph/0003017](#)]

The Stephanov model

Phase transitions:

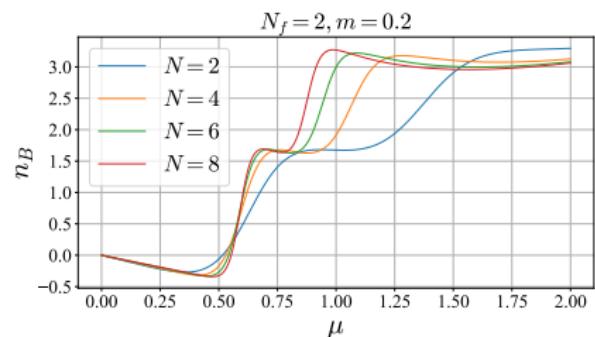
- chiral condensate

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



- baryon number density

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



The Stephanov model: the phase quenched theory

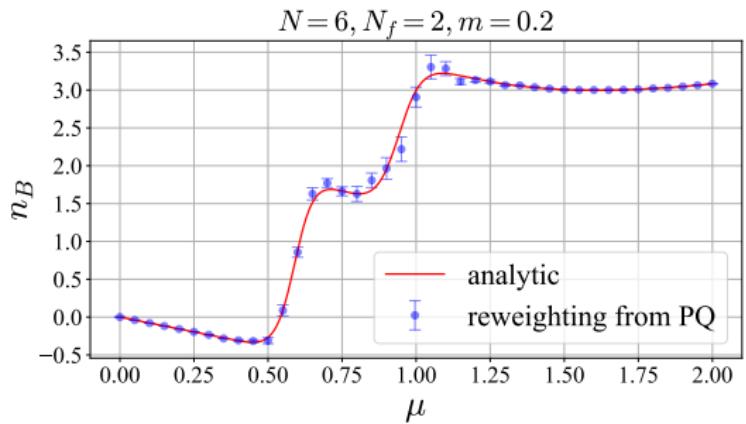
Phase quenched partition function:

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

E.g. baryon number density:

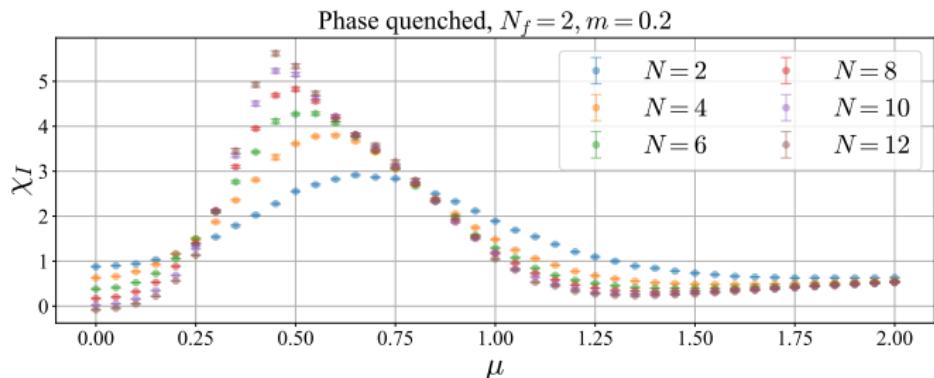
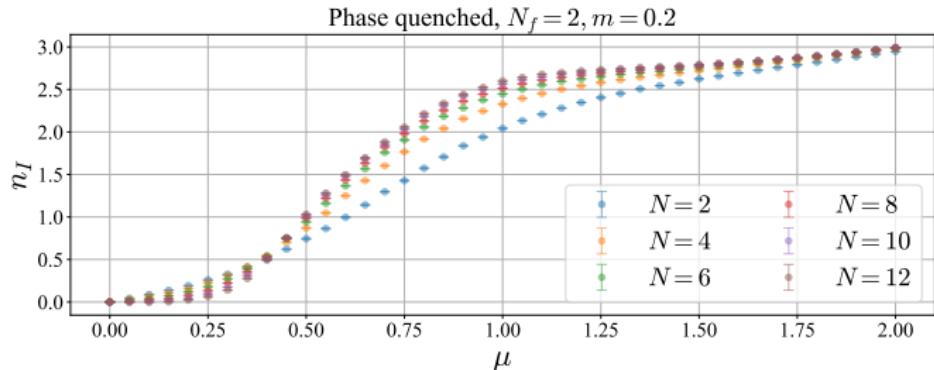
**Expectation values via
reweighting**

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



The Stephanov model: pion condensation in the PQ theory

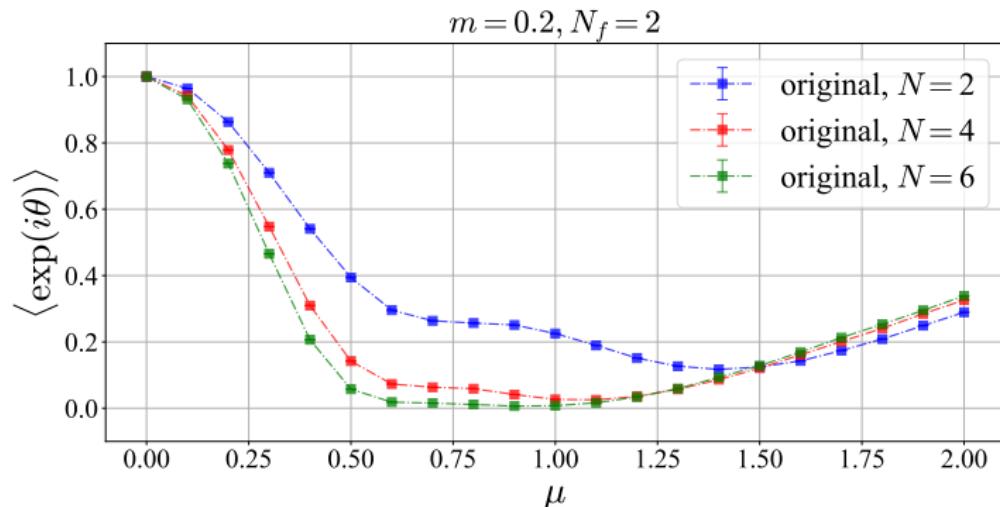
Transition to pion condensed phase:



The Stephanov model and its sign problem at finite μ

Severity of the sign problem (average phase):

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



Complex Langevin method does not work for this model:

J. Bloch et. al [[arXiv:hep-lat/1712.07514](https://arxiv.org/abs/hep-lat/1712.07514)].

The Stephanov model: integration contour deformations

Complexification:

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

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

→ 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 $\mathcal{Z}_{PQ} \equiv \mathcal{Z}_{PQ}(\{p\})$ does not!

The Stephanov model: Jacobian of contour deformations

We parameterize the deformed integration manifold with the undeformed variables:

$$\mathcal{Z} = \int_{\mathcal{M}_{\text{def}}} d\alpha d\beta e^{-S_{\text{eff}}[\alpha, \beta]} = \int_{\mathcal{M}_{\text{def}}} dA dB \det \mathcal{J} e^{-S_{\text{eff}}[\alpha(A, B), \beta(A, B)]},$$

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

“New” average phase after deformation:

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

Results: *ansatz* #1

Motivation:

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

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

The *ansatz*:

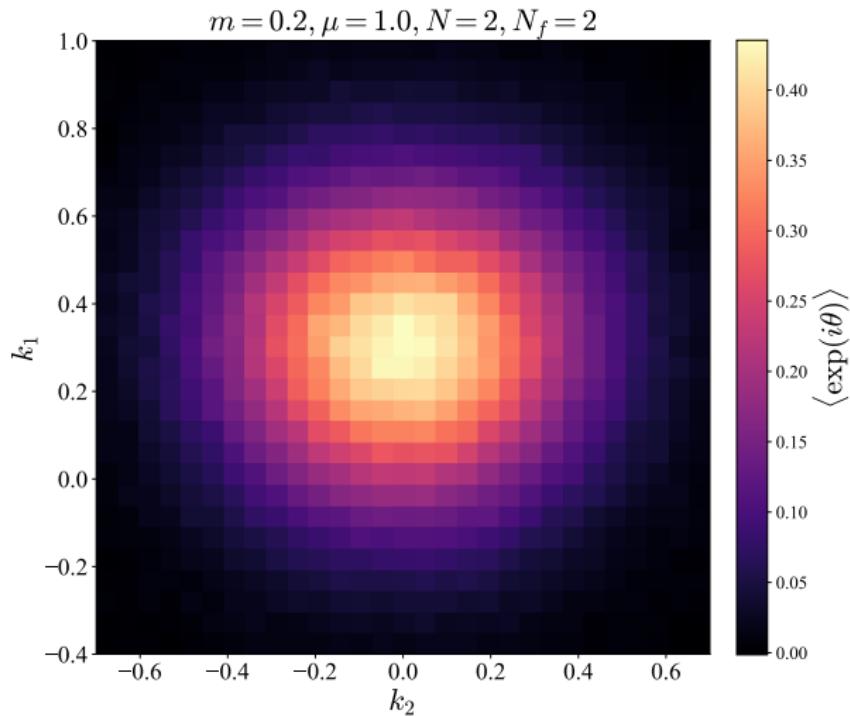
$$\alpha = A + ik_1 \text{id}$$

$$\beta = B + ik_2 \text{id}$$

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

Results: *ansatz* #1

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



Results: *ansatz* #2

Motivation:

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

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

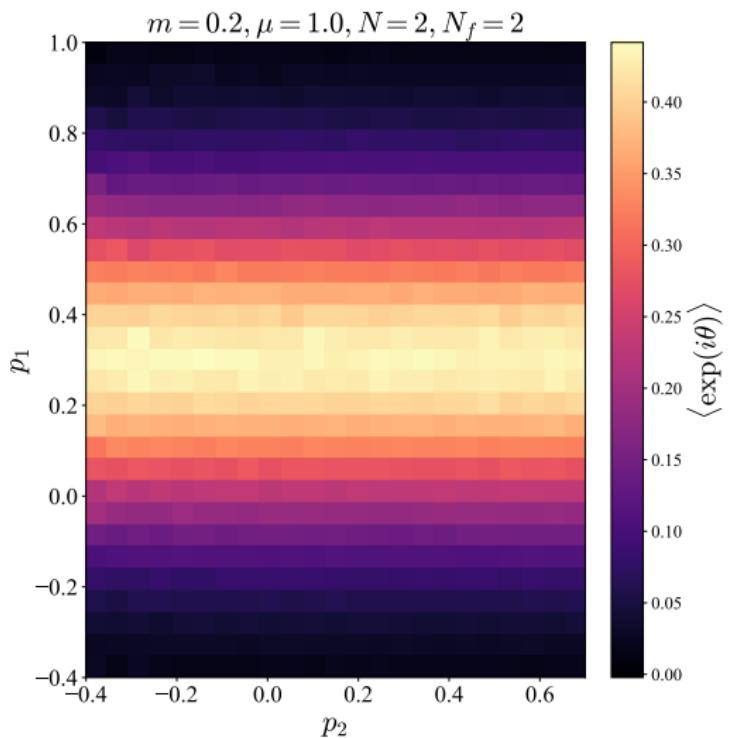
The *ansatz*:

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

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

Results: *ansatz* #2

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



Results: many-parameter *ansätze*

20-parameter linear *ansatz*:

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

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

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

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.

Interlude 1: AdaDelta optimisation

Parameter updates are computed with the AdaDelta algorithm [[arXiv:1212.5701](https://arxiv.org/abs/1212.5701)]:

→ i.e. change in parameter vector \mathbf{p} at optimisation step t :

$$\Delta \mathbf{p}_t = -\frac{\sqrt{\mathcal{E}(\Delta \mathbf{p}^2)_{t-1} + \varepsilon}}{\sqrt{\mathcal{E}(\mathbf{g}^2)_t + \varepsilon}} \mathbf{g}_t \quad \text{with gradient } \mathbf{g}_t = \nabla_p \mathcal{F}(\mathbf{p}_t)$$

and a decaying average defined as $\mathcal{E}(\pi)_t = \gamma \mathcal{E}(\pi)_{t-1} + (1 - \gamma) \pi_t$.

Interlude 2: parameter constraints and logarithmic barriers

Possible problems:

- ▶ many-parameter deformation *ansätze* do not guarantee the convergence of the integral,
- ▶ $|\det \mathcal{J}| > 0$, otherwise problematic $(A, B) \mapsto (\alpha, \beta)$ mapping.

Finiteness

from the action:

$$\text{Tr}(X(A, B)Y(A, B)) = \mathbf{v} \cdot \mathbf{M} \cdot \mathbf{v}^T + \dots$$

$$\mathbf{v} = (A_{11}, \dots, A_{NN}, B_{11}, \dots, B_{NN}) \in \mathbb{R}^{2N^2}$$

and \mathbf{M} has details of the quadratic form
($\mathbf{M} = \text{id}_{2N^2 \times 2N^2}$ for no deformation).

For the integral to be convergent: $\text{Re } \lambda_i > 0$
($i = 1, \dots, 2N^2$)

Constraint via logarithmic barriers:

Modifying the cost function to minimize:

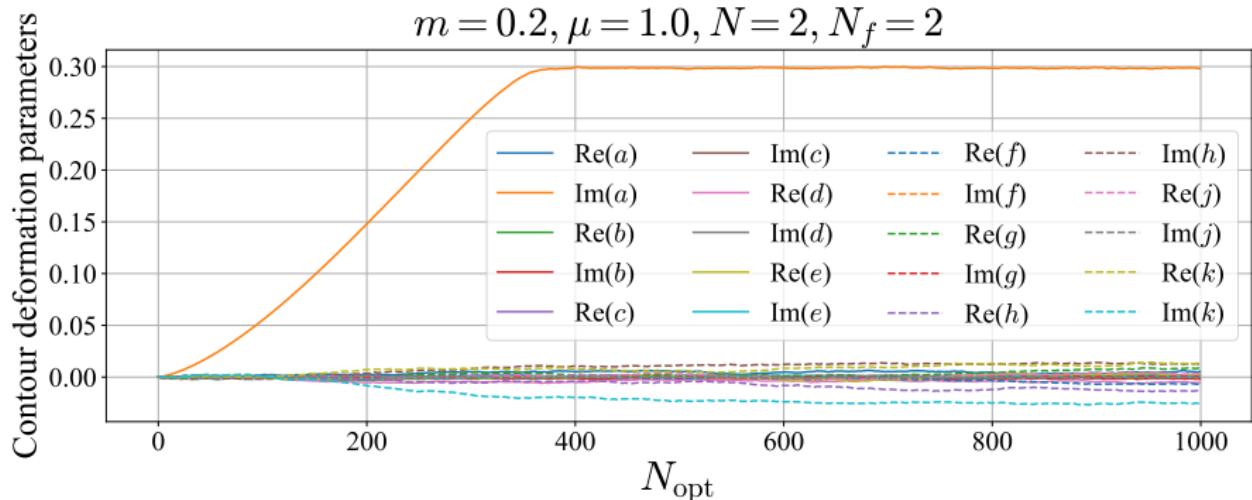
$$\begin{aligned} \mathcal{F}(\{p\}) \\ \downarrow \\ \mathcal{F}(\{p\}) - \frac{1}{t} \left[\log(|\det \mathcal{J}|) + \sum_i^{2N^2} \log(\text{Re } \lambda_i) \right] \end{aligned}$$

Results: many-parameter *ansätze*

Interestingly only a **single important parameter** emerges

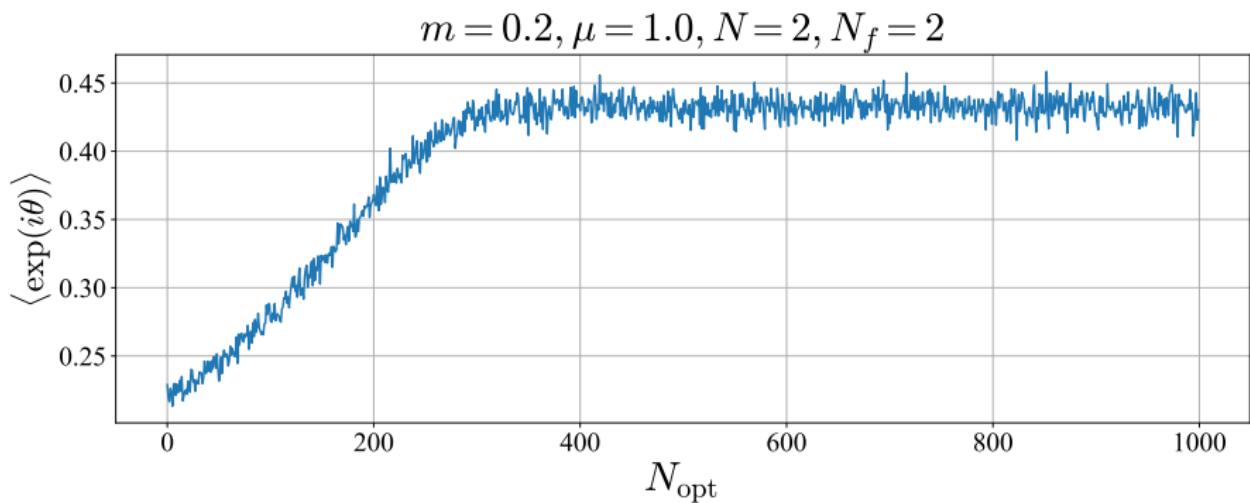


$$\text{Im}(a) = k_1 = p_1$$

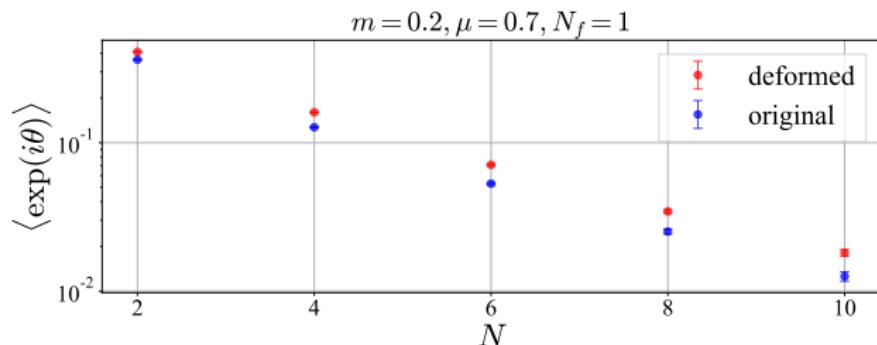
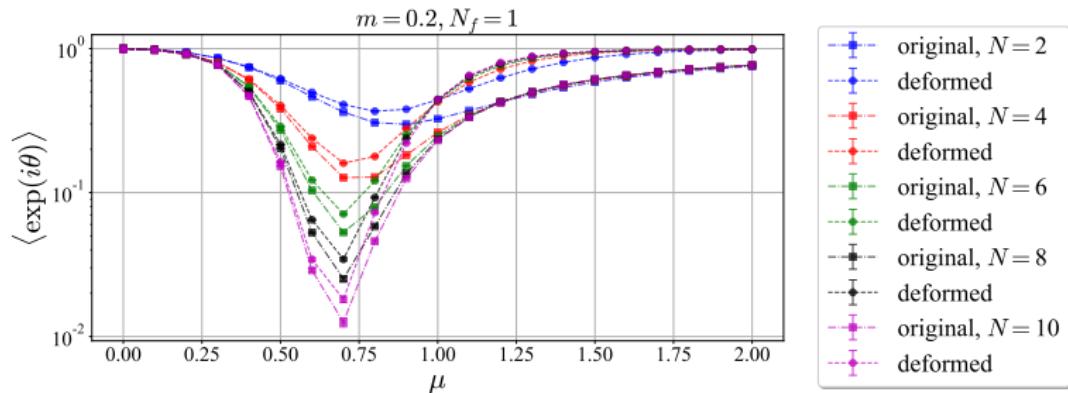


Results: many-parameter *ansätze*

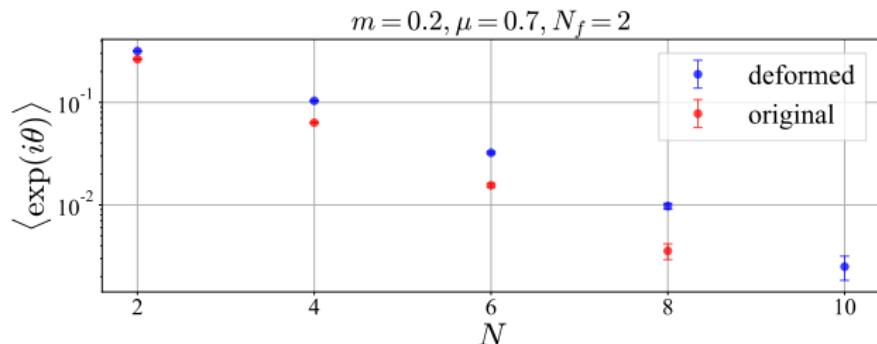
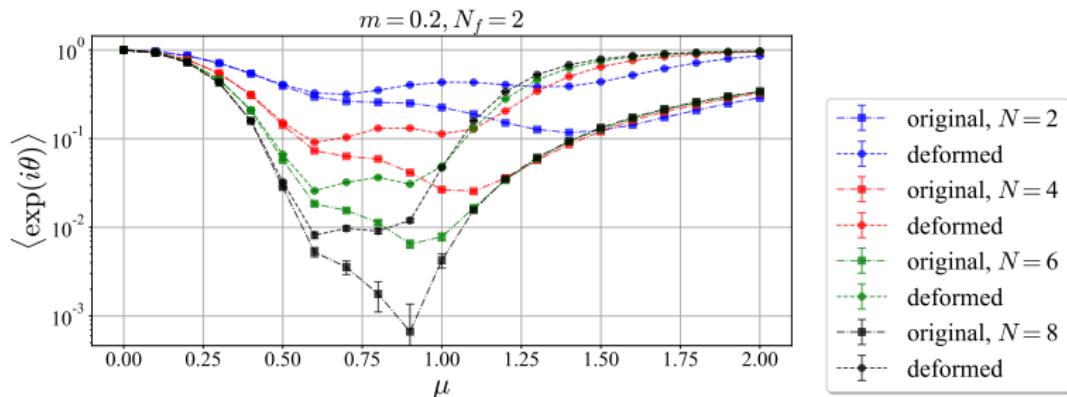
Visible improvement in the sign problem:



Results: μ and N-dependence at $N_f = 1$ ($\text{Im}(a) = k_1 = p_1$)

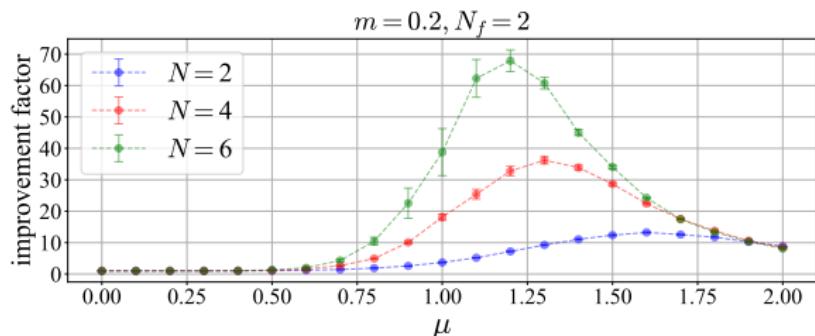
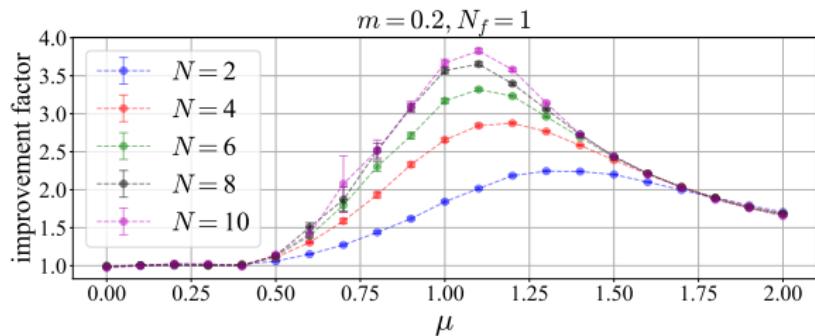


Results: μ - and N -dependence at $N_f = 2$ ($\text{Im}(a) = k_1 = p_1$)



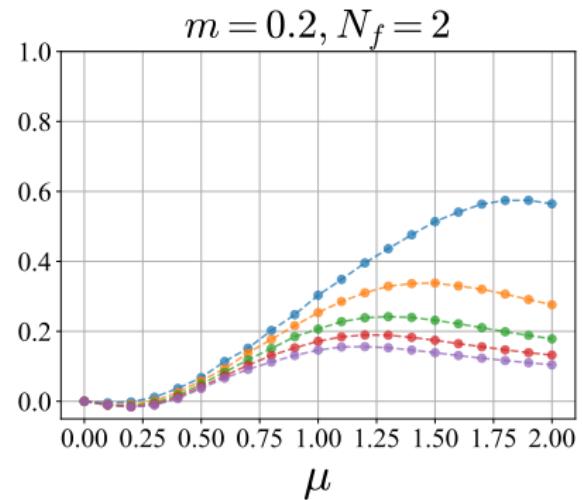
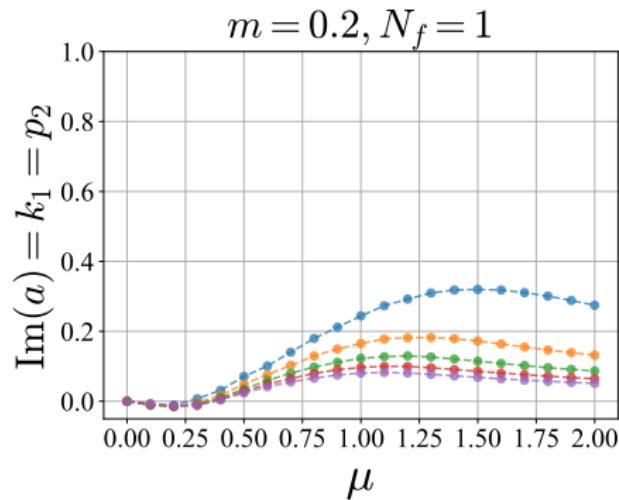
Results: improvement on the sign problem ($\text{Im}(a) = k_1 = p_1$)

Statistical improvement $\sim (\langle e^{i\theta} \rangle^{\text{def}} / \langle e^{i\theta} \rangle^{\text{original}})^2$



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

μ - and N -dependence:



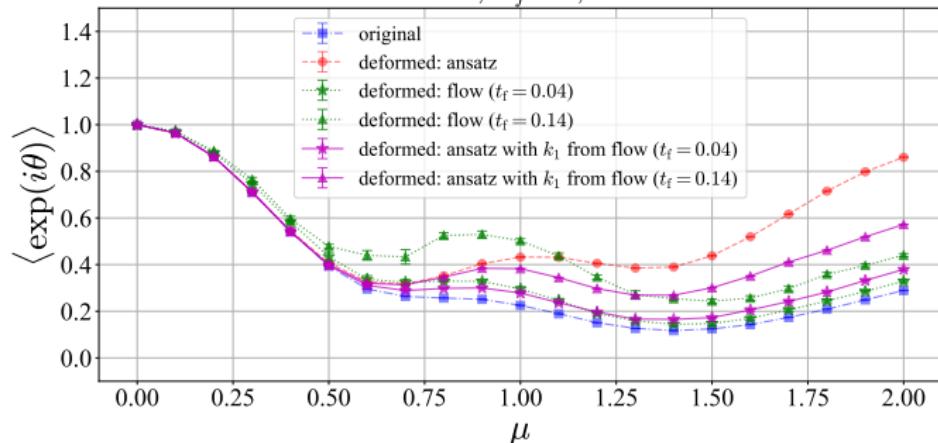
Results: holomorphic flow vs. *integration manifold optimisation*

Q: “Does the two methods find the same deformed contour?”

$$\langle \alpha_f^{ij} - A^{ij} \rangle = \langle \text{Tr}(\alpha_f - A) \rangle (t_f) \delta^{ij} \quad \longleftrightarrow \quad \langle \alpha^{ij} - A^{ij} \rangle = i k_1 N \delta^{ij}$$

hence: $k_1 = \text{Im} \langle \text{Tr}(\alpha_f - A) \rangle (t_f) / N$.

$m = 0.2, N_f = 2, N = 2$



- 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

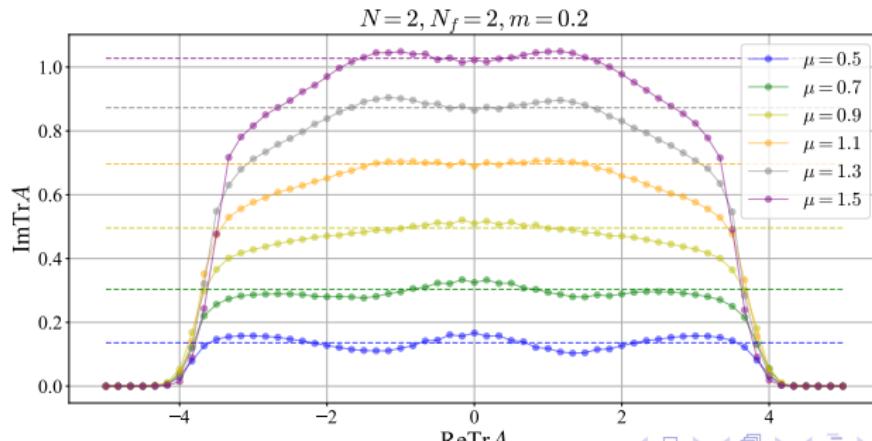
~ deforming only $t = \text{Tr}A$.

Ansatz ($\beta = B$):

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

$\text{Tr}\tilde{A} = 0$ 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 $\propto i \cdot \text{id}$) 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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