Fighting the sign problem with contour deformations

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What is the sign problem?

Grand canonical partition function of QCD:

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

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;
- real time dynamics $\sim \langle f|e^{-iH}|i\rangle = \int \mathcal{D}x\; e^{iS[x]}$ (see previous talk by Paul Hotzy);
- etc.

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 ($r[U]$ real and positive):

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

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:

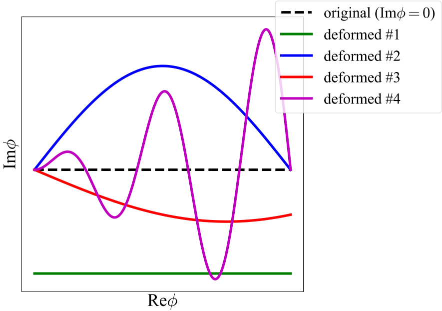
$$\left\langle \frac{w}{r} \right\rangle_r = \frac{\mathcal{Z}_w}{\mathcal{Z}_r} \qquad \Longrightarrow \qquad \begin{cases} 1 & \sim \text{perfect!} \\ \approx 0 & \sim \text{not so much\dots} \end{cases}$$

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

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. integral over 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 $\{p\}$:

$$\mathcal{Z} = \int\limits_{\mathcal{M}_{\rm def}} \mathcal{D}U_{\rm def}\; w[U_{\rm def}] = \int\limits_{\mathcal{M}_{\rm def}} \mathcal{D}X\; \det \mathcal{J}(X) w[U_{\rm def}(X)]\;.$$

In this case the phase quenched partition function:

$$\mathcal{Z}_{\rm PQ}^{\rm def}(\{p\}) = \int\limits_{\mathcal{M}_{\rm def}} \mathcal{D}X \left| \det \mathcal{J}(X) w[U_{\rm def}(X)] \right| ,$$

hence the severity of the sign problem:

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

Integration manifold optimisation ∼ machine learning

The sign problem is milder if

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

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

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

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

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

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

Application: Stephanov model

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

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

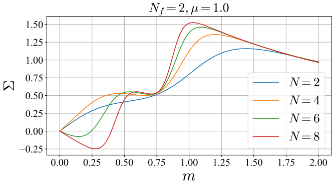
where:

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

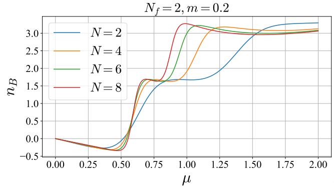
$$D = \begin{pmatrix} 0 & iW + \mu \\ iW^\dagger + \mu & 0 \end{pmatrix} \in \mathbb{C}^{2N\times 2N}$$

[arXiv:hep-ph/0003017]

- chiral condensate $\Sigma(m,\mu) \propto \partial \log \mathcal{Z}/\partial m$



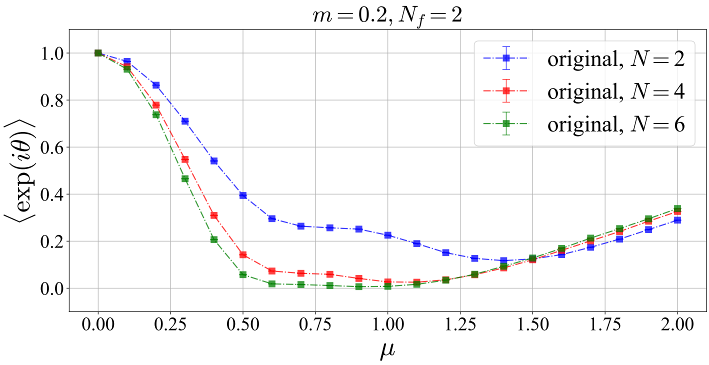
- baryon number density $n_B \propto \partial \log \mathcal{Z}/\partial \mu$



Application: Stephanov model and its sign problem at finite μ

Severity of the sign problem (average phase):

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



Complex Langevin method does not work for this model:
J. Bloch et. al `arXiv:hep-lat/1712.07514`.

Application: complexification and deformation *ansätze*

- Complexification:

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

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

α, β parameterised by A, B with 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!

- Motivation:

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

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

$$\Downarrow$$

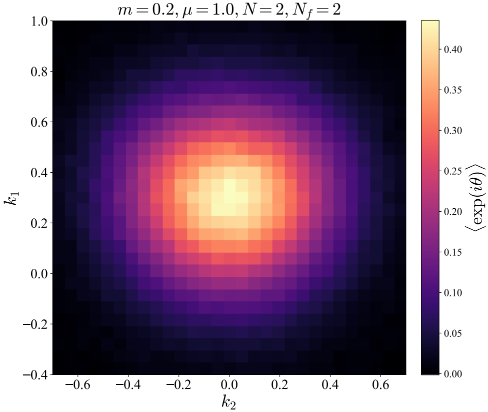
The *ansatz*:

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

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

Example result: constant shift *ansatz*

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

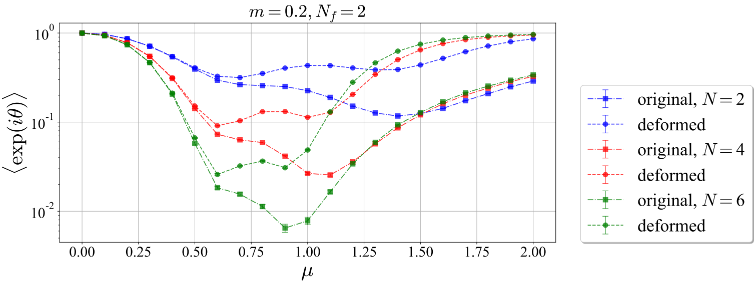


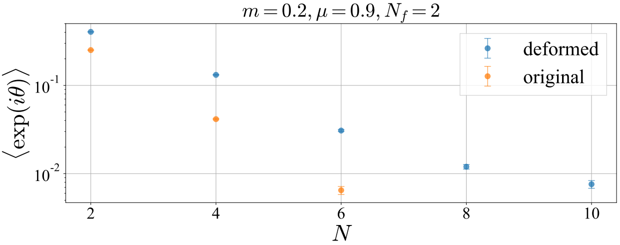
- Only relevant parameter is k_1.
- Same result emerges from 20-parameter linear *ansatz* ($\text{Im}a = k_1$):

$$\alpha = (a + b\text{Tr}A + c\text{Tr}B)\text{id} + (1 + d)A + eB$$

$$\beta = (f + g\text{Tr}A + h\text{Tr}B)\text{id} + jA + (1 + k)B$$

Example result: μ- and N-dependence





Example result: piecewise optimisation of the trace

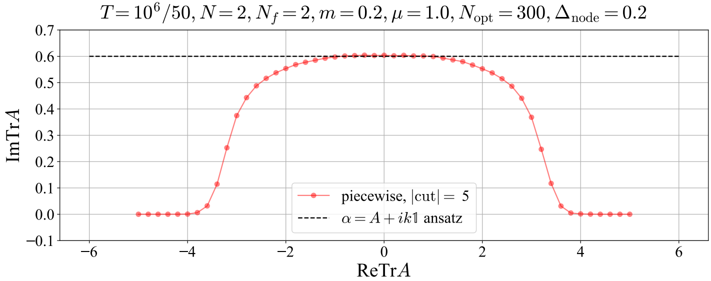
$\sim$ deforming only $t = \mathrm{Tr}A$.

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.

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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