The Severity of the Sign Problem in Different Regions of the QCD Phase Diagram

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Sign Problems and Complex Actions
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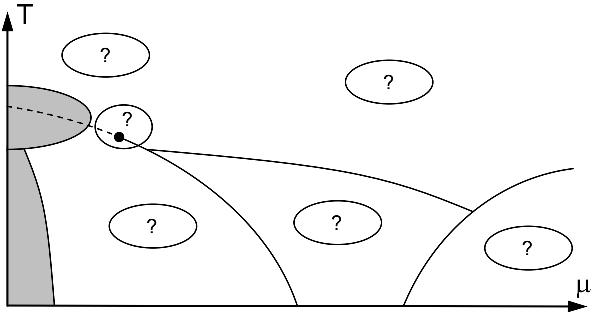
- arXiv:0808.2987 "On the sign problem in dense QCD" with Stephen Hsu (University of Oregon)

What's the question?

Strongest evidence about severity of sign problem in the QCD phase diagram ?

Quantify/define degree of severity of sign problem ?



- later: focus on phase transition region
- from insights gained: suggest Z_{new} method; "typicality" problems

Outline

1. Introduction
   - sign problem in dense QCD
   - split into two positive ensembles Z_+, Z_-
2. Free energies and analyticity
   - severity of the sign problem
3. Regions of the QCD phase diagram
   - hadronic phase, quark-gluon plasma, CSC phase
   - general considerations
4. Monte-Carlo methods
   - degrees of severity of sign problem
   - the $|\mathrm{Re}\det M(A)|$ method; typicality
   - comparision with reweighting and quenching methods
5. Conclusions & Questions

The sign problem in dense QCD

Partition function of grand canonical ensemble:

$$\begin{aligned} Z(\beta,\mu) &= \mathrm{Tr}\, e^{-\beta(\mathcal{H}-\mu\mathcal{N})} && \text{real and positive } (\mu\in\mathbb{R}) \\ &= \sum_{\{\Psi[\phi(x)]\}} \langle\Psi| e^{-\beta(\mathcal{H}-\mu\mathcal{N})} |\Psi\rangle && \text{sum of pos. terms, } \textit{typicality} \end{aligned}$$

vastness of Hilbert space $\{\Psi\}$
$\rightarrow$ Euclidean functional integral over *classical* field configurations

$$\begin{aligned} Z &= \int \mathcal{D}A \int \mathcal{D}\psi\mathcal{D}\overline{\psi}\; e^{-\int_0^\beta dx^4 \int d^3x\; \{\overline{\psi}(\not{D}(A)-m-\mu\gamma_4)\psi+\frac{1}{4g^2}F^a_{\mu\nu}F^{a\mu\nu}\}} \\ &= \int \mathcal{D}A\; (\det M(A))\; e^{-\int_0^\beta dx^4 \int d^3x\; \frac{1}{4g^2}F^a_{\mu\nu}F^{a\mu\nu}} \end{aligned}$$

with $M(A) = \not{D}(A) - m - \mu\gamma_4$ not (similar to) Hermitian

The sign problem in dense QCD

$$\Rightarrow \quad Z(\beta,\mu) = \int \mathcal{D}A \; (\det M(A)) \; e^{-S_G(A)} \quad \in \mathbb{R}^+ \; ,$$

although $\det M(A) \in \mathbb{C}$ for generic A.

No probability interpretation for $(\det M(A))\, e^{-S_G(A)}$
$\rightarrow$ sign problem or phase problem: importance sampling?

Idea: lump phase into observable $\mathcal{O}$

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A \; |\det M(A)| \; e^{-S_G(A)} \;\; \mathcal{O}(A) e^{i\theta(A)}}{\int \mathcal{D}A \; |\det M(A)| \; e^{-S_G(A)} \;\; e^{i\theta(A)}}$$

and sample with measure $|\det M(A)|\, e^{-S_G(A)}$

$\rightarrow$ phase/sign fluctuations in denominator/numerator; poor overlap?

Reality of Z

First: make $Z \in \mathbb{R}$ more manifest:

$$\begin{aligned} Z &= \text{Re}\ Z = \int \mathcal{D}A\ \text{Re}\left(\det M(A)\ e^{-S_G(A)}\right) \\ &= \int \mathcal{D}A\ \left(\text{Re} \det M(A)\right)\ e^{-S_G(A)} \end{aligned}$$

physical reason:

a) $\det M(A') = (\det M(A))^*$ for PC-conj. $A'_\mu\left(\vec{x}, x^4\right) \equiv A^*_\mu\left(-\vec{x}, x^4\right)$
(and $\psi'\left(\vec{x}, x^4\right) = \gamma_5 \gamma_2 \psi^*\left(-\vec{x}, x^4\right)$)

b) in lattice formulation of gauge theories:
links $U \to U^* \Rightarrow \det M(U^*) = (\det M(U))^*$ and $S_G(U^*) = S_G(U)$

Two positive ensembles: Z_+ and Z_-

$$Z \;=\; \int \mathcal{D}A \;\left(\mathrm{Re}\det M(A)\right)\; e^{-S_G(A)}$$

$\{+\}$: set of configurations $A^a_\mu(x)$ with $\mathrm{Re}\det M(A) \;>\; 0$
$\{-\}$: $\mathrm{Re}\det M(A) \;<\; 0$

$$\begin{aligned} Z \;&=\; \sum_{\{+\}} |\mathrm{Re}\det M| e^{-S_G(A;\,\beta)} \;-\; \sum_{\{-\}} |\mathrm{Re}\det M| e^{-S_G(A;\,\beta)} \\ &\equiv \qquad\qquad Z_+ \qquad\qquad\quad - \qquad\qquad\quad Z_- \end{aligned}$$

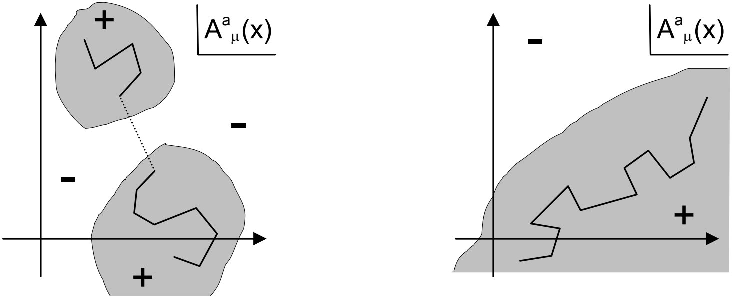
- $Z_+ \;>\; Z_- \;\geq\; 0$
- Z_+, Z_- partition functions of fictitious 4+1 dim systems?
  "potential" $V_{4+1}(A) = S_G(A) - \ln|\mathrm{Re}\det M(A)|$

Independent ensembles?

Fictitious Hamiltonian(s) ($\rightarrow$ molecular dynamics algorithm):

$$H_{4+1}[A,\pi;\beta] = \sum_i \frac{1}{2}\pi_i^2 \; + \; \left\{ S_G(A;\beta) - \ln\left|\mathrm{Re}\det M(A)\right| \right\}$$

Potential barrier $V_{4+1} = +\infty$ between $\{+\}$ and $\{-\}$.



- If connected & ergodic, sampling with H-equations (in principle)

Assumption – two *separate* ensembles

Assumption for the next part of this talk:

Z_+, Z_- are sensible ensembles on their own,
i.e. each is connected and allows for ergodic sampling

- $Z = Z_+ - Z_-$: important split for following part of talk
- useful to characterize severity of sign problem? $\longrightarrow$ later

Free energies

Free energy densities F_+, F_-: $\quad Z_\pm(\mu,\,\beta;\,V) \equiv \exp\left(-V\,F_\pm(\mu,\,\beta)\right)$

actually: $F_\pm$ are the *intensive* parts, but $\exists$ volume dependence

$$Z_+(\mu,\,\beta;\,V) \equiv \exp\left(-V\,f_+(\mu,\,\beta;\,V)\right)$$

$\rightarrow$ then define: $F_+(\mu,\beta) \equiv \lim_{V\to\infty} f_+(\mu,\beta,V)$

but finite-volume corrections: $f_+(V) = F_+ + \hat{f}_+(V)$

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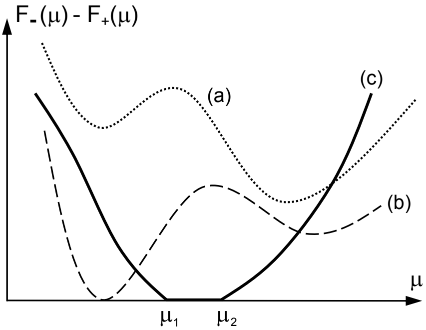
a) $F_+ < F_- \;\Rightarrow\; Z_+$ dominates Z_- exponentially at large V
$\rightarrow$ MILD sign problem: $Z_-/Z_+ \rightarrow 0$ for $V \rightarrow \infty$

b) $F_+ = F_- \;\Rightarrow\; Z_+$ and Z_- generically of same size
$\rightarrow$ SEVERE sign problem: $Z_-/Z_+ > 0$ at $V \rightarrow \infty$
(if $\hat{f}_-(V) - \hat{f}_+(V) > 1/V \;\rightarrow$ MILD sign problem)

Free energy densities

Statistical Mechanics: free energy densities $F_{\pm}$ are analytic functions of their arguments (μ, β), away from phase boundaries/transitions

- $F_{+} = F_{-}$ in open set $\Rightarrow F_{+} \equiv F_{-}$ in common domain of analyticity
- $F_{+} \neq F_{-}$ in open set $\Rightarrow F_{+} = F_{-}$ at most on submanifold



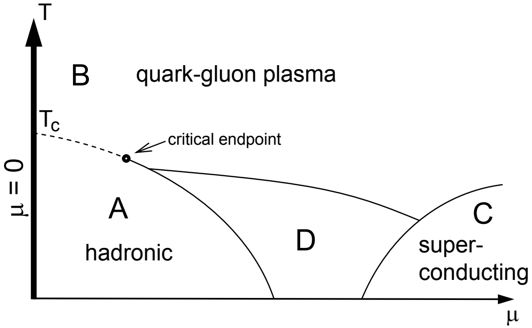
Severe sign problem at (potentially) $F_{+}(\mu) = F_{-}(\mu)$

Sign problem in the QCD phase diagram

Example: $\mu = 0$

$Z_- = 0,\ Z_+ = Z > 0$

$\rightarrow F_+ < F_- = +\infty$



Now: • examine different regions (A, B, C) of QCD phase diagram

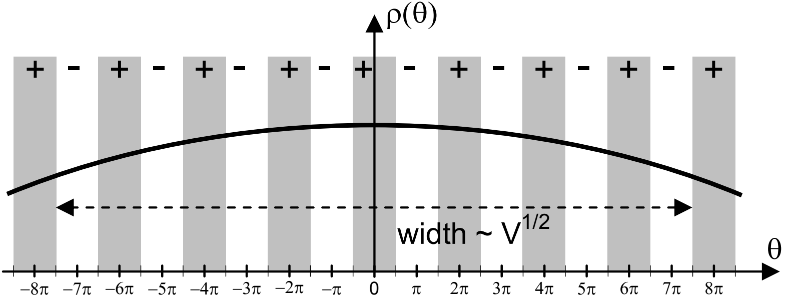
• apply analyticity reasoning

A: hadronic phase

phase of quark matrix: $\det M(A) = |\det M(A)|\ e^{i\theta(A)}$

chiral perturbation theory at low μ, T (Splittorff & Verbaarschot):

θ has Gaussian distribution $\rho(\theta)$, width $= \sqrt{\langle\theta^2\rangle - \langle\theta\rangle^2} \sim V^{1/2}$



So: $Z_-/Z_+ \to 1$ as $V \to \infty$, i.e. in particular $F_+ = F_-$
(see also: $Z_+ > Z_-$)

A: hadronic phase

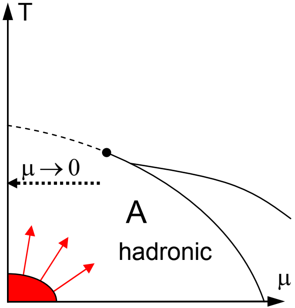
$F_+ = F_-$ in open region of small μ, small T

analyticity $\Rightarrow F_+ \equiv F_-$ in entire phase: SEVERE SIGN PROBLEM

at least for small (μ, T): if V large enough $\rightarrow$ $Z_+/Z_- \approx 1$
$\rightarrow$ how can sampling at finite V give reliable results for $V = \infty$?

Order of limits to get ordinary QCD:

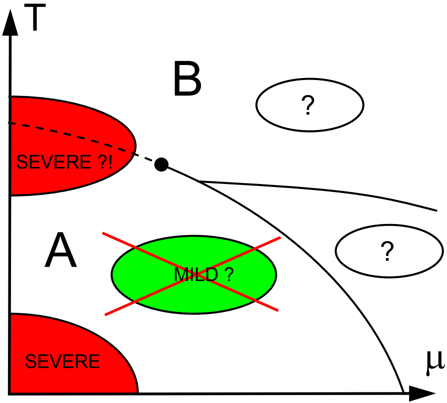
- $V \rightarrow \infty$ first, then $\mu \rightarrow 0$:
  $\lim_{\mu \rightarrow 0} F_-(\mu) < \infty$
- $\mu = 0$ at any V:
  $F_-(\mu = 0, V) = +\infty$



The reasoning

What's the strongest argument for SEVERE sign problem in all of A?

In all of the phase diagram?



B: quark-gluon plasma phase

- N quark flavors with μ:
  $Z_N = \int \mathcal{D}A \; \det M(A) \; e^{-S_G(A)}$
- $N/2$ flavors with $+\mu$, $N/2$ flavors with $-\mu$:
  $Z_{|N|} = \int \mathcal{D}A \; |\det M(A)| \; e^{-S_G(A)}$

$$\Rightarrow \qquad Z_N \leq Z_{|N|} \qquad \text{and} \qquad \frac{Z_N}{Z_{|N|}} = \frac{\exp(-VF_N)}{\exp(-VF_{|N|})}$$

a) models have different physics (pion condensation in $Z_{|N|}$)

b) F_N, $F_{|N|}$ perturbatively for large T, small μ/T (Vuorinen):
$\rightarrow$ terms linear in flavor chemical potentials $\Rightarrow \quad F_N > F_{|N|}$

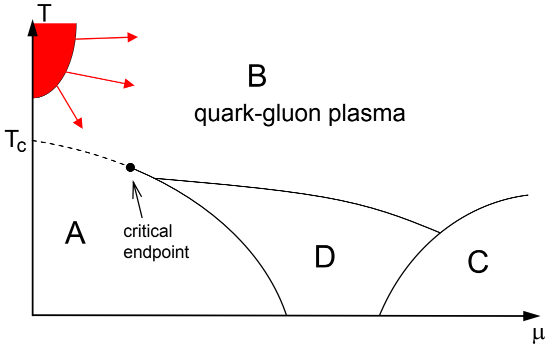
B: quark-gluon plasma phase

$$\Rightarrow \quad \frac{\exp(-VF_N)}{\exp(-VF_{|N|})} = \frac{Z_N}{Z_{|N|}} = \int d\theta\ \rho(\theta)\cos(\theta)\ \rightarrow\ 0 \qquad (V \rightarrow \infty)$$

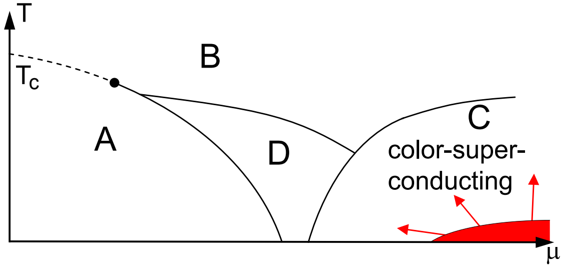
So: a) $\rho(\theta)$ peaked at $\theta = (n + 1/2)\pi$, i.e. $\det M$ imaginary $\rightarrow$ NO

b) $\rho(\theta)$ smooth with large width: $Z_{N-}/Z_{N+}\ \rightarrow\ 1\ \ (V \rightarrow \infty)$

$\rightarrow$ SEVERE SIGN PROBLEM in all of B by analyticity



C: CSC phase



- if no severe sign problem: QCD inequalities apply
  – rely on positive measure $d\mu = \mathcal{D}A^a_\mu \; e^{-S_G(A)} \; \det M(A)$
- Vafa & Witten: NO spontaneous breaking of vector symmetries (e.g., baryon number)
- but: explicit calculations in far CSC phase show breaking (Hong & Hsu; valid in $\mu \to \infty$, $T/\mu \to 0$)

$\Rightarrow$ SEVERE SIGN PROBLEM in all of CSC phase

D: other phases

Possible reasonings about severity of sign problem:

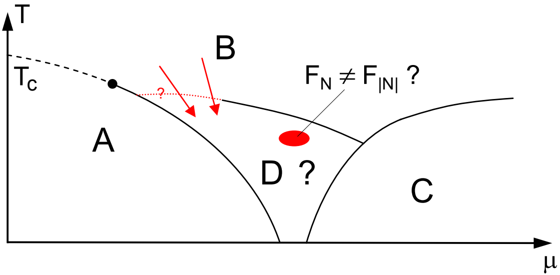
- analytic (crossover) or no phase transitions/boundaries
  $\Rightarrow$ analyticity suggests severe/mild sign problem

  A $\leftrightarrow$ B transition?

- QCD with N flavors μ_1, ..., μ_N: if $F \sim \mu_i + \mu_j^3 + \mu_k^5 + \ldots$
  then $F_N > F_{|N|} \Rightarrow$ severe sign problem (via $\rho(\theta)$)

  ($F_N > F_{|N|}$ also if models have different physics)

  as before in phase B



Degrees of severity of the sign problem

So far: sign problem at $(\mu,\ T)$ SEVERE if

- $Z_-/Z_+ > 0$ for $V \to \infty$
- generically if $F_+ = F_-$

Severe only if $Z_-/Z_+ \approx 1$ for $V \to \infty$? $\to$ phases A & B

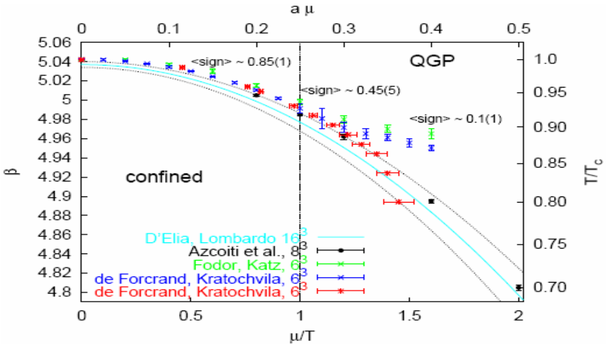
But MILD for, e.g., $Z_-/Z_+ < 0.1$ at $V \to \infty$ $(Z_- \ll Z_+)$?

$\to$ possible (only) for $F_+ = F_-$ (subleading terms in free energy)

- around high-T phase transition line from $(T_c,\ \mu = 0)$ to $\mu > 0$?

$\to$ NO analyticity arguments from now on, but split $Z_+,\ Z_-$ useful

high-T phase transition line



Good agreement at $\mu < 1.3\,T_c$ between:

- derivatives (Taylor) at $\mu = 0$
- Taylor exp. from imaginary μ
- multi-parameter reweighting

Also: $\langle\text{sign}\rangle > 10\%$
in this region
$\rightarrow$ MILD in
new definition

Now: • argue: success of reweighting related to $Z_{-} \ll Z_{+}$
• suggest Z_{new}-method

(Multi-parameter) reweighting method

$$\langle \mathcal{O} \rangle_{(\mu,\beta)} = \frac{\int \mathcal{D}A \; e^{-S_G(\beta_0)} \det M(\mu_0) \quad \frac{e^{-S_G(\beta)} \det M(\mu)}{e^{-S_G(\beta_0)} \det M(\mu_0)} \, \mathcal{O}(A)}{\int \mathcal{D}A \; e^{-S_G(\beta_0)} \det M(\mu_0) \quad \frac{e^{-S_G(\beta)} \det M(\mu)}{e^{-S_G(\beta_0)} \det M(\mu_0)}} \Bigg|_{(\mu_0,\beta_0)}$$

Difficulties for reweighting if $Z_-/Z_+ \approx 1$ at target point (μ, β):

- denominator *should* be small $\sim (Z_+ - Z_-)/(Z_+ + Z_-)$ in a *true typical* ensemble for target (μ, β)
  $\rightarrow$ sign problem: numerical uncertainties (also in numerator)
  - even if denominator small and uncertainties under control: ensemble typical for *target* (μ, β) ???
- if (somehow) only small uncertainties due to denominator: Is there good overlap between (μ_0, β_0) and target (μ, β) ?

$\rightarrow$ overlap problem more generally: typicality for $\mathbb{C}$-measure at all?

- $Z_- \ll Z_+$ seems *necessary* for reweighting to work, not *sufficient*

Z_{new} method

MC method for whose success $Z_- \ll Z_+$ is also *sufficient*: Use

$$Z_{\text{new}} \equiv Z_+ + Z_- = \sum_{\{+\}} |\mathrm{Re}\det M| e^{-S_G} + \sum_{\{-\}} |\mathrm{Re}\det M| e^{-S_G}$$

$$= \int \mathcal{D}A \, |\mathrm{Re}\det M(A)| \; e^{-S_G(A)}$$

for sampling.

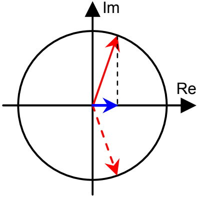
Remember: $Z = Z_+ - Z_-$ (so: $Z/Z_{\text{new}} \simeq 1$ for $F_- > F_+$)

Compute observable averages *WITH sign of real part*:

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}A \, (\mathrm{Re}\det M(A)) \, e^{-S_G(A)} \;\; \mathcal{O}(A)}{\int \mathcal{D}A \, (\mathrm{Re}\det M(A)) \, e^{-S_G(A)}}$$

Characteristics of Z_{new} method

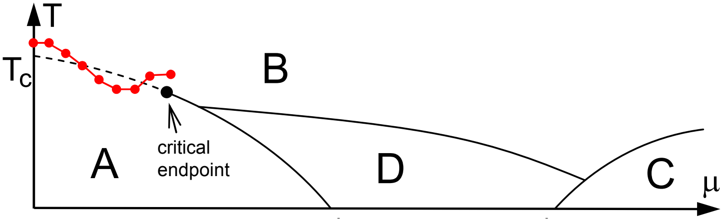
- if $Z_-/Z_+|_{(\mu,\,\beta)} \approx 1 \;\Rightarrow\;$ small denominator: sign problem
  $\rightarrow$ just as (it should be, at least) in reweighting method
- samples via $Z_{\text{new}} = Z_+ + Z_-$ likely more typical of Z than
  1. reweighting: relation $Z|_{(\mu_0,\,\beta_0)}$ vs. $Z|_{(\mu,\,\beta)}$
     Configurations sampled in $(\mu_0,\,\beta_0)$ typical of $(\mu,\,\beta)$???
  2. phase-quenched sampling: $|\det M|$ vs. $|\mathrm{Re}\det M|$
     - different *importance* for configurations on circle
     - symmetric cropping
     - modulus AND phase



- Z_{new} closest to $Z = \int \mathcal{D}A\,(\det M(A))\,e^{-S_G(A)} \rightarrow$ *biggest overlap*
- smallest possible fluctuations in reweighting factor
  (de Forcrand, Kim, Takaishi: hep-lat/0209126)

Consistency check during Z_{new} method

- start at some (μ, β) where sign problem mild (e.g., $\mu = 0$)
- slowly move in phase diagram, sampling with Z_{new}
- at each point, compare $\{-\}$ set to $\{+\}$ set: approximation still ok?
- thus: "good" overlap; control when sign problem becomes severe
  $\rightarrow$ tells where/how long the Z_{new} method can be trusted



- seems superior to (phase-)quenched or reweighting sampling

Computational cost

- probably need full computation of $\operatorname{Re}\det M$ at each microstep:
  - cannot update whole lattice at once, since no bosonic integral for $\operatorname{Re}\det M \;\rightarrow\;$ no Hybrid Monte Carlo
  - $\rightarrow$ only local link updates + Metropolis tests ?
- $\rightarrow N \times N^3$ operations for one sweep through the lattice (HMC for phase-quenched/reweighting sampling: $N^{9/4}$ for new *decorrelated* configuration; but *full* $(\det M) \sim N^3$ there)
- maybe for small μ: approximate methods to determine phase $e^{i\theta}$ $\Rightarrow \operatorname{Re}\det M$ (by Taylor expansion)
- method to try after numerics in conventional reweighting ok ? (... and still disagreement)

Conclusions & Questions

- split into two *independent* positive ensembles $Z = Z_+ - Z_-$
- analyticity reasoning for associated free energies
- examined regions of QCD phase diagram $\rightarrow$ severe sign problem
- degrees of severity of the sign problem
- "mild" sign problem around phase transition line ?
- Z_{new} method with $|\text{Re} \det M|$ sampling

- Is there meaning to "typicality" if measure $\in \mathbb{C}$? Do existing sampling methods have "good" overlap with target ensemble?
- In how far do exisiting simulations rely on $V \ll \infty$? Big finite-volume effects? Artificial results?
- In regions with maximally severe $Z_-/Z_+ \rightarrow 1$: can any sampling method ever be successful (for $V \rightarrow \infty$)?

Thank you!