Reweighting Methods for Finite Density QCD

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First LatticeNET workshop
on challenges in Lattice field theory

Benasque
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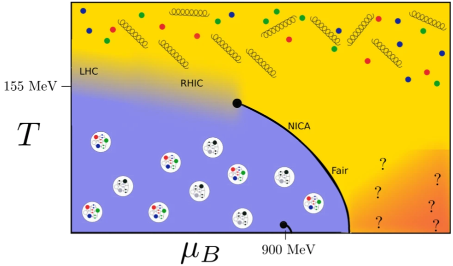
Based on work with Sz. Borsányi, Z. Fodor, J. N. Guenther, K. Kapás, S. D. Katz, D. Nógrádi, A. Pásztor, Z. Tulipánt, C. H. Wong

Lattice QCD at Finite Density

NP problem: phase diagram of QCD at finite temperature and density

Rich structure expected from effective models, chPT

Figure from [Guenther (2021)]



Lattice QCD allows for numerical first-principle NP studies of QCD – if adequate numerical techniques are available

Finite T, $\mu_B = 0$: $\det(\not{D} + m) \in \mathbb{R}^+$

- posdef Boltzmann weight $\rightarrow$ standard methods:
  $\Rightarrow$ crossover at $T \simeq 155$ MeV [Borsányi *et al.* (2010), Bazavov *et al.* (2016)]

Finite T, $\mu_B \neq 0$: $\det(\not{D} + m + \mu\gamma^0) \in \mathbb{C}$

- complex Boltzmann weights $\rightarrow$ importance sampling unavailable:
  $\Rightarrow$ sign problem

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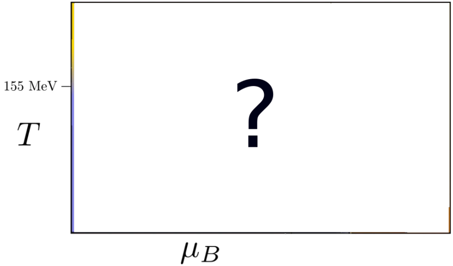

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Approaches to the Sign Problem

Elegant approach: **solve the sign problem**

- reformulation in different variables (e.g., duality, worm algorithms. . .) – not available for QCD
- complex Langevin [Seiler, Sexty, and Stamatescu (2013)] – convergence issues (convergence itself, and to what)

Poor man's approach: **bypass the sign problem**

- several methods available
- all come with side effects

Approaches to the Sign Problem

Reconstruct from theories without a sign problem

- reweighting from zero baryochemical potential
  [Hasenfratz and Toussaint (1992), Barbour *et al.* (1998), Fodor and Katz (2002, 2004)]
  – overlap problem
- imaginary chemical potential [de Forcrand and Philipsen (2002)]
  – analytic continuation problem
- Taylor expansion around $\mu_B = 0$ [Gavai and Gupta (2003)]
  – analytic continuation problem
- density of states
  [Fodor, Katz, and Schmidt (2007), Langfeld, Lucini and Rago (2014)]
  – hard residual sign problem

Change path-integration contour to reduce the sign problem

- Lefschetz thimbles [Cristoforetti, Di Renzo, and Scorzato (2012)]
  – identification of thimbles, residual sign problem
- contour deformation [Mori, Kashiwa, and Ohnishi (2017)]
  – how to identify convenient paths?

Reweighting

Simplest solution: reweighting from sign-problem-free theory

- exact in principle

$$Z = \int D\phi\, e^{-S[\phi,\mu]} \qquad e^{-S} \text{ generally complex}$$

$$Z_0 = \int D\phi\, e^{-S[\phi,0]} \qquad S[\phi,\mu=0] \text{ real}$$

$$\langle O \rangle = \frac{\langle O\, e^{-(S[\phi,\mu]-S[\phi,0])}\rangle_0}{\langle e^{-(S[\phi,\mu]-S[\phi,0])}\rangle_0} = \frac{\langle O\, e^{-(S[\phi,\mu]-S[\phi,0])}\rangle_0}{Z/Z_0}$$

- numerically extremely challenging (exponentially hard in V, μ)

$$\frac{Z}{Z_0} = e^{-V(F-F_0)} \underset{V\to\infty}{\to} 0 \text{ or } \infty$$

- the distribution we sample is far from the distribution we want: tails of the weight distribution sampled poorly (overlap problem)

Easing up reweighting

Brute force approach, better to ease up how demanding it is:

1. minimise the cost of fermions

   $\Rightarrow$ rooted staggered fermions $\rightarrow$ **geometric matching**

2. minimise the overlap problem

   $\Rightarrow$ compact range of weights (no tails) $\rightarrow$ **phase or sign quenching**

3. minimise the sign problem

   $\Rightarrow$ wise choice of simulated theory $\rightarrow$ **contour deformation**

Part I: Geometric matching

Rooted staggered fermions

Best choice for brute-force approach: rooted staggered fermions

$$D_{\rm stag}[U;\mu] = \frac{1}{2}\sum_{\alpha=1}^{4} \eta_\alpha \left(e^{\delta_{\alpha,4}\mu} U_\alpha \mathcal{T}_\alpha - e^{-\delta_{\alpha,4}\mu} \mathcal{T}_\alpha^\dagger U_\alpha^\dagger \right)$$

$$(\mathcal{T}_\alpha)_{x,y} = \delta_{x+\hat{\alpha},y} \qquad (\eta_\alpha)_{x,y} = (-1)^{\sum_{\nu<\alpha} x_\nu} \delta_{x,y}$$

In the continuum limit $\det(D_{\rm stag} + m)$ describes four degenerate "tastes" of fermions $\rightarrow [\det(D_{\rm stag} + m)]^{\frac{1}{4}}$ describes one taste only (rooting trick)

Numerically cheap, no additive mass renormalisation

Conceptually controversial but phenomenologically satisfactory at $\mu = 0$

Rooted staggered fermions at finite μ

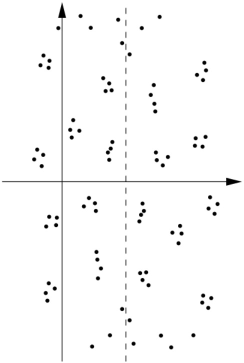
Rooting introduces further problems originating from taste breaking:

- ambiguous definition of the fourth root
- spurious branch-point singularities in the rooted determinant
- near-zero eigenmode quartets introduce large cutoff effects

Problems should go away as $a \to 0$, but should be cured already at finite a to avoid dangerous analyticity issues and reduce discretisation effects

Prescription [Golterman, Shamir, Svetitsky (2006)]:

- identify quartets of near-degenerate staggered modes $i\lambda_n + m$
- replace them with fourth root of their product



Analyticity issues fixed, cutoff effects reduced compared to other prescriptions

Implemented in practice with doublets ($N_f = 2$ light quarks, $\mu_s = 0$) using the reduced matrix formalism [arXiv:1911.00043]

Reduced matrix formalism

Unrooted staggered fermions ($\hat{\mu} = \frac{\mu}{T}$)

$$Z(\beta, \mu) = \int DU\, e^{-S_g[U;\beta]} \det M[U; \hat{\mu}] \qquad M[U; \hat{\mu}] = D_{\rm stag}[U; \mu] + m$$

Reduced matrix [Hasenfratz and Toussaint (1992)]

$$\det M[U; \hat{\mu}] = e^{3V\hat{\mu}} \det(P[U] - e^{-\hat{\mu}}) = e^{3V\hat{\mu}} \prod_n (\xi_n[U] - e^{-\hat{\mu}})$$

Temporal gauge $U_4(t, \vec{x}) = 1$ for $0 \leq t < N_t - 1$

$$P = -\begin{pmatrix} B_0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} B_1 & 1 \\ 1 & 0 \end{pmatrix} \dots \begin{pmatrix} B_{N_t-1} & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} U_4 & 0 \\ 0 & U_4 \end{pmatrix} \Bigg|_{t=N_t-1}$$

$$B_i = 2\eta_4 (D^{(3)}_{\rm stag} + m)|_{t=i}$$

Reduced matrix formalism

$$Z(\beta, \mu) = e^{3V\hat{\mu}} \int DU\, e^{-S_g[U;\beta]} \det(P[U] - e^{-\hat{\mu}})$$

Reduced matrix P is μ-independent, convenient for reweighting

$P \neq P^\dagger$, generally complex eigenvalues

Properties of eigenvalues...

- $(P^\dagger)^{-1} = \Sigma_2 P \Sigma_2 \Rightarrow$ eigenvalues come in pairs $(\xi_n, \frac{1}{\xi_n^*})$
- $\det P = \prod_n \xi_n = 1$
- $\prod_{n, |\xi_n|<1} \xi_n$ real positive

...imply properties of Z:

- CP symmetry, $Z(\mu) = Z(-\mu)$
- Z real analytic, $Z(\mu^*) = Z(\mu)^*$
- $Z(\mu) \neq 0$ for μ real positive or purely imaginary

Partition function zeros and critical points

$$Z(\beta,\mu) = e^{3V\hat{\mu}} \int DU\, e^{-S_g[U;\beta]} \det(P[U] - e^{-\hat{\mu}})$$

- entire function of $\beta \Rightarrow$ zeros $\times$ nonvanishing (Weierstrass)

$$Z = e^{h(z)} \prod_{n=1}^{\infty} (\beta - \beta_n) \to \text{Fisher zero: } Z(\beta_{\rm F}(\mu),\mu) = 0$$

- $e^{3V\hat{\mu}} \times$ polynomial in $e^{-\hat{\mu}} \Rightarrow$ precisely $6V$ zeros

$$Z = e^{3V\hat{\mu}} \sum_{n=0}^{6V} \mathcal{P}_n(\beta) e^{-n\hat{\mu}} \to \text{Lee-Yang zero: } Z(\beta,\mu_{\rm LY}(\beta)) = 0$$

Critical points = singular points of $F = -\frac{1}{V}\log Z$ = accumulation points of complex $Z(\beta,\mu)$ zeros on real β or μ axis in the infinite-volume limit

Volume scaling of zero closest to real axis $\sim$ nature of critical point:

- $\beta_{\rm F}, \mu_{\rm LY}|_{V\to\infty} \neq 0$: crossover
- $\beta_{\rm F}, \mu_{\rm LY} \sim V^{-1}$: first order
- $\beta_{\rm F}, \mu_{\rm LY} \sim V^{-\alpha}$, $\alpha < 1$: second order

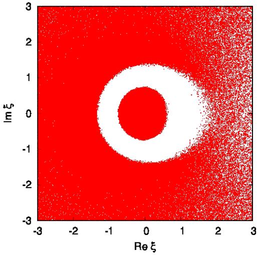
Problems with rooting

Reweighting & standard rooting [Fodor and Katz (2002, 2004)]

$$\sqrt{\frac{\det M(\hat\mu)}{\det M(0)}}\Bigg|_{\text{standard}} \equiv e^{\frac{3}{2}V\hat\mu}\prod_{n=1}^{6V}\sqrt{\frac{\xi_n - e^{-\hat\mu}}{\xi_n - 1}}$$

Root of ratio of eigenvalues, branch cut on negative real axis

- $Z(\beta,\mu)e^{-3V\hat\mu}$ not a polynomial in $e^{-\hat\mu}$ anymore
- Spurious square-root singularities at $e^{-\hat\mu} = \xi_n$ on each configuration, no cancelation mechanism
- Can mask position of the singularity closest to the origin in the complex $e^{-\hat\mu}$ plane



3000 configurations, $12^3 \times 4$, $\beta = 3.35$
tree-level Symanzik improved gauge action
2+1 2-stout improved staggered fermions,
physical quark masses

Geometric matching

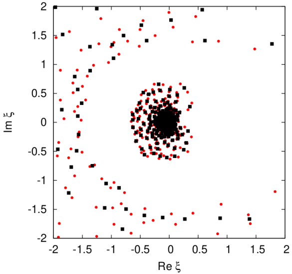
Geometric matching [arXiv:1911.00043]: for 2+1 flavours, $\mu_{u,d} = \mu_q$, $\mu_s = 0$

- identify nearby doublets (ξ_1, ξ_2)

  Minimise the total sum of the distances within pairs (Blossom algorithm)
- $(\xi_1, \xi_2) \to \tilde{\xi} = \sqrt{\xi_1 \xi_2}$ (closest root)
- correct by small phase to preserve $\prod_{n,|\xi_n|<1} \tilde{\xi}_n$ real positive

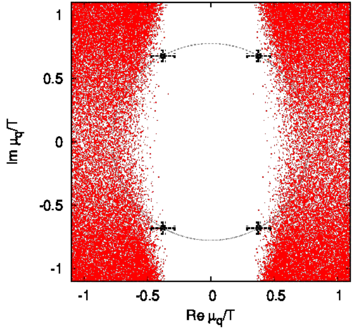
$$\left. \sqrt{\frac{\det M(\hat{\mu})}{\det M(0)}} \right|_{\text{geom}} \equiv e^{\frac{3}{2}V\hat{\mu}} \prod_{n=1}^{3V} \frac{\tilde{\xi}_n - e^{-\hat{\mu}}}{\tilde{\xi}_n - 1}$$

- $Z(\beta, \mu) e^{-3V\hat{\mu}}$ again a polynomial, with $3V$ zeros
- Properties of P (and Z) preserved
- Spurious singularities removed on each configuration
- Correct pairing in the continuum



Radius of convergence and spurious singularities

Log of eigenvalues of P vs. Lee-Yang zeros closest to $\mu = 0$



3000 configs, $12^3 \times 4$, $\beta = 3.35$ tree-level Symanzik improved gauge action
2+1 2-stout improved staggered fermions, physical quark masses

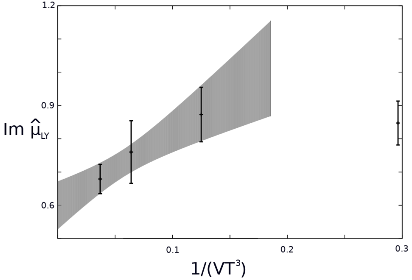
Spurious singularities inside the true radius of convergence (= distance of closest singularity) $\rightarrow$ underestimated without matching

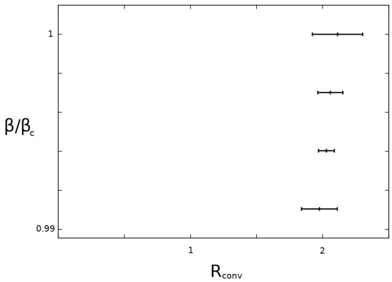
Radius of convergence

Small ($L = 8, 10, 12$) and coarse ($N_t = 4$) lattices

but Symanzik-improved + 2stout smeared

Distance of closest LY zero from the origin = radius of convergence in $\hat{\mu}$





- Finite $\lim_{V\to\infty} \mathrm{Im}\hat{\mu}_{\mathrm{LY}} \Rightarrow$ crossover
- Radius of convergence quite insensitive to β near β_c

Part II: Sign quenching

Optimising the simulated theory: sign quenching

Freedom to choose the simulated theory $\det M = |\det M| e^{i\theta}$

$$Z_{\mathrm{simulation}} = \int DU \, e^{-S_g} |\det M| f(\theta) \qquad f \geq 0$$

Optimal choice to minimise sign problem for partition function:

$$f(\theta) = |\cos\theta|$$

Minimise fluctuations of reweighting factors
[de Forcrand, Kim, and Takaishi (2003)]

Sign quenched ensemble

$$Z_{\mathrm{SQ}} = \int DU \, e^{-S_g} |\mathrm{Re} \det M| = \int DU \, e^{-S_g} |\det M| \, |\cos\theta|$$

$$Z = \int DU \, e^{-S_g} \det M = \int DU \, e^{-S_g} \mathrm{Re} \det M = Z_{\mathrm{SQ}} \langle \mathrm{sign}(\mathrm{Re} \det M) \rangle_{\mathrm{SQ}}$$

Overlap problem

$$Z_{\mathrm{SQ}} = \int DU\, e^{-S_g} |\det M|\, |\cos\theta\,|$$

Pro:

- $\mathrm{sign}(\mathrm{Re}\det M) = \pm 1$ takes values in a finite set, no overlap problem

Con:

- $\mathrm{Re}\det M$ nonlocal, numerically expensive

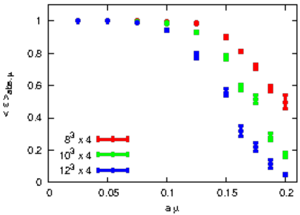
More precisely: no tails of the weight distribution, any sampling problem should show up in the error bars of the average sign $\langle \mathrm{sign}(\mathrm{Re}\det M)\rangle_{\mathrm{SQ}}$

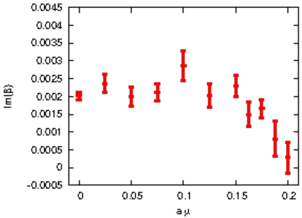
Overlap problem under control: as long as average sign is accurate, estimates are reliable

$$\langle O \rangle = \frac{\langle O\, \mathrm{sign}(\mathrm{Re}\det M)\rangle_{\mathrm{SQ}}}{\langle \mathrm{sign}(\mathrm{Re}\det M)\rangle_{\mathrm{SQ}}}$$

Testing the sign quenched ensemble

$N_f = 2+1$ unimproved staggered fermions, $N_t = 4$, physical masses, $\mu_u = \mu_d$, $\mu_s = 0$ [arXiv:2004.10800]

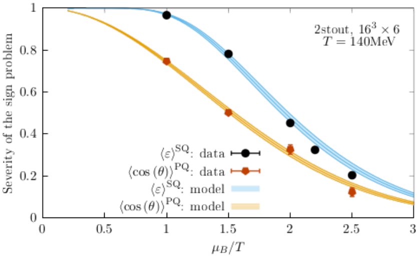




- average sign under control up to $a\mu \simeq 0.2$
- no geometric matching, use Fisher zeros
- fit $\mathrm{Im}\,\beta_{\mathrm{F}} = A + B/V$, first order transition when $A = 0$
- critical endpoint at $\mu/T_c \sim 0.8$, agrees with [Fodor and Katz (2002, 2004)]

Finite-density QCD with the sign quenched ensemble

$N_f = 2+1$ tree-level Symanzik improvement, 2stout smearing, $N_t = 6$
physical masses, $\mu_u = \mu_d$, $\mu_s = 0$ [arXiv:2108.09213]



Model for severity of sign problem :

- $\langle\cos\theta\rangle^{\mathrm{PQ}} \simeq e^{-\frac{1}{2}\langle\theta^2\rangle^{\mathrm{PQ}}}$
- $\langle\theta^2\rangle^{\mathrm{PQ}} \simeq 4\mu^2 VT\chi_{11}^{ud} = 4\hat{\mu}^2(LT)^3\chi_{11}^{ud}$
- wrapped Gaussian for pdf of phases $\langle\varepsilon\rangle^{\mathrm{SQ}} = \frac{\langle\cos\theta\rangle^{\mathrm{PQ}}}{\langle|\cos\theta|\rangle^{\mathrm{PQ}}} \left(\geq \langle\cos\theta\rangle^{\mathrm{PQ}}\right)$
- at asymptotically large μ or $V \to$ uniform pdf, $\langle\varepsilon\rangle^{\mathrm{SQ}}/\langle\cos\theta\rangle^{\mathrm{PQ}} \to \frac{\pi}{2}$

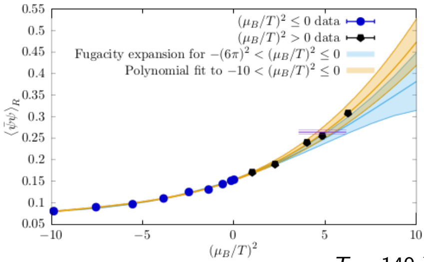
Finite-density QCD with the sign quenched ensemble

- Renormalised chiral condensate

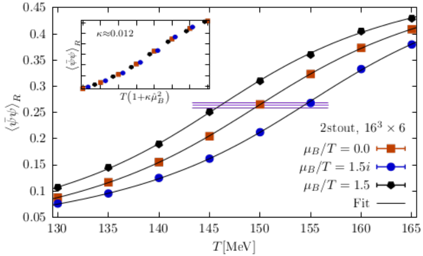
$$\langle\bar\psi\psi\rangle_R(T,\mu) = -\frac{m_{ud}}{f_\pi^4}\left(\langle\bar\psi\psi\rangle_{T,\mu} - \langle\bar\psi\psi\rangle_{0,\mu}\right)$$

- Can reach $\hat\mu_B = \frac{\mu_B}{T} = 2.5$ where extrapolations fail, covering RHIC BES range
- No sign of transition along T getting stronger
- Chiral condensate shows approximate scaling

$$\langle\bar\psi\psi\rangle_R(T,\mu) \simeq f(T(1+\kappa\hat\mu^2))$$



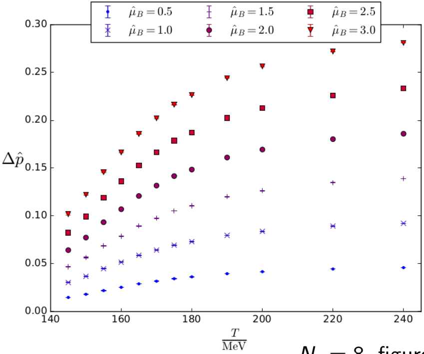
$T = 140$ MeV



Figures from [arXiv:2108.09213]

Equation of state from phase quenched ensemble

$Z_{\mathrm{PQ}} = \int DU\, e^{-S_g} |\det M|$ also free from overlap problem (?)



$N_t = 8$, figure from [arXiv:2208.05398]

$$\Delta\hat{p} = \frac{1}{T^4}\left[p(T,\mu_B) - p(T,0)\right] = \frac{1}{(LT)^3}\log\frac{Z(T,\mu_B)}{Z(T,0)}$$

$$= \frac{1}{T^4}\int_0^{\mu_B} d\hat{\mu}_I\, n_I(\hat{\mu}_I) + \frac{1}{(LT)^3}\log\langle e^{i\theta}\rangle_{\mathrm{PQ}}$$

Part III: Contour deformation

Optimising the simulated theory: path deformation

Path integral is over real variables (gauge fields), but this may not be the best choice

Example: U(1) theory with staggered fermions + chemical potential

$$
\begin{aligned}
D_{\rm stag} &= \frac{1}{2}\eta_4 \left(e^{\mu} U_4 \mathcal{T}_4 - e^{-\mu} \mathcal{T}_4^{\dagger} U_4^{*} \right) + \dots \\
&= \frac{1}{2}\eta_4 \left(e^{i(\varphi_4 - i\mu)} \mathcal{T}_4 - \mathcal{T}_4^{\dagger} e^{-i(\varphi_4 - i\mu)} \right) + \dots
\end{aligned}
$$

$Z =$ integral of analytic function of φ_4, use Cauchy theorem

$$
\begin{aligned}
\int_{-\pi}^{\pi} d\varphi_4\, f(\varphi_4 - i\mu) &\underset{\substack{\text{shift}\\ \text{contour}}}{=} \int_{-\pi+i\mu}^{\pi+i\mu} dz_4\, f(z_4 - i\mu) \\
&= \int_{-\pi}^{\pi} dx_4\, f(x_4 + i\mu - i\mu) = \int_{-\pi}^{\pi} dx_4\, f(x_4)
\end{aligned}
$$

$\Rightarrow$ no μ dependence

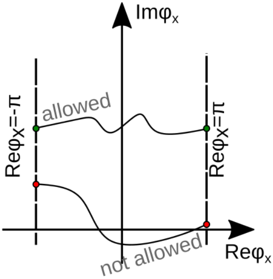
Contour deformation

Z = integral of analytic function on real manifold

Change the integration manifold to reduce severity of the sign problem
[Mori, Kashiwa, and Ohnishi (2017)]

Deforming the integration contour in the complex plane does not change Z if the endpoints are kept fixed

For gauge/spin systems the integrand is periodic, we can move also the endpoints in the same way



Parameterise deformed manifold $\mathcal{M}$ as $z = z(t)$, with real variables $t \in \mathrm{M}$

$$Z = \int_{\mathcal{M}_0} D\phi \, e^{-S[\phi,\mu]} = \int_{\mathcal{M}} Dz \, e^{-S[z,\mu]} = \int_{\mathrm{M}} Dt \, \det \frac{Dz}{Dt} \, e^{-S[z(t),\mu]}$$

$$= \int_{\mathrm{M}} Dt \, e^{-S_{\mathrm{eff}}[z(t),\mu]} \equiv Z_{\mathcal{M}}$$

Contour deformation and sign problem

Partition function independent of deformed manifold $\mathcal{M}$, but its phase- or sign-quenched version is not

$$Z_{\mathcal{M},\,\mathrm{SQ}} = \int_{\mathrm{M}} Dt\ \left|\cos \mathrm{Im} S_{\mathrm{eff}}[z(t),\mu]\right| e^{-\mathrm{Re} S_{\mathrm{eff}}[z(t),\mu]}$$
$$\neq \int D\phi\ \left|\cos \mathrm{Im} S[\phi,\mu]\right| e^{-\mathrm{Re} S[\phi,\mu]} = Z_{\mathrm{SQ}}$$

$$\frac{Z_{\mathcal{M}}}{Z_{\mathcal{M},\,\mathrm{SQ}}} = \langle \mathrm{sign}\left(\cos \mathrm{Im} S_{\mathrm{eff}}\right)\rangle_{\mathcal{M},\,\mathrm{SQ}} = \langle \varepsilon \rangle_{\mathcal{M},\,\mathrm{SQ}}$$
$$\neq \langle \mathrm{sign}\left(\cos \mathrm{Im} S\right)\rangle_{\mathrm{SQ}} = \langle \varepsilon \rangle_{\mathrm{SQ}} = \frac{Z}{Z_{\mathrm{SQ}}}$$

Optimise contour to minimise the sign problem = maximise $\langle \varepsilon \rangle_{\mathcal{M},\,\mathrm{SQ}}$

So far used for toy models (see [Alexandru *et al.* (2018)])

XY model with chemical potential

Our toy model: XY in 2+1 D with chemical potential [arXiv:2202.07561]

$$Z = \int D\varphi \, e^{\beta \sum_x \left(\cos(\varphi_x - \varphi_{x+\hat{0}} + i\mu) + \sum_{j=1,2} \cos(\varphi_x - \varphi_{x+\hat{\jmath}}) \right)}$$

Sign problem solved using worldline formulation

$$Z = \sum_{\{k\}} \prod_x I_{k_{x,\alpha}}(\beta) e^{\mu \delta_{\alpha,0} k_{x,\alpha}} \delta \left(\sum_\alpha k_{x,\alpha} - k_{x-\hat{\alpha},\alpha} \right)$$

[Banerjee and Chandrasekharan (2010)]

Strategy:

- try simple path deformations
- optimise parameters to reduce severity of the sign problem

Contour deformation for the XY model

Main parameterisation:

$$\varphi_x(t_x) = t_x + i \sum_{k=1}^{K} A_k(x^0) \cos[k(t_x - t_{x+\hat{0}})] + B_k(x^0) \sin[k(t_x - t_{x+\hat{0}})]$$

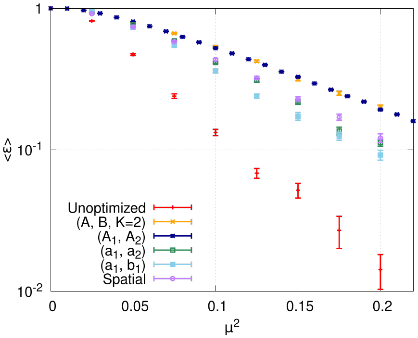
Non-mandatory restrictions:

- imaginary part is a function of the real part $t_x \in [-\pi, \pi]$
- depends only on difference of real parts at different sites

Qualitative results:

- sine terms suppressed $B_k(x^0) \approx 0$
- $A_k(x^0) \approx A_k(0)$, time-translation invariant
- including spatial neighbours or next-to-nearest temporal neighbours has little effect on the sign problem

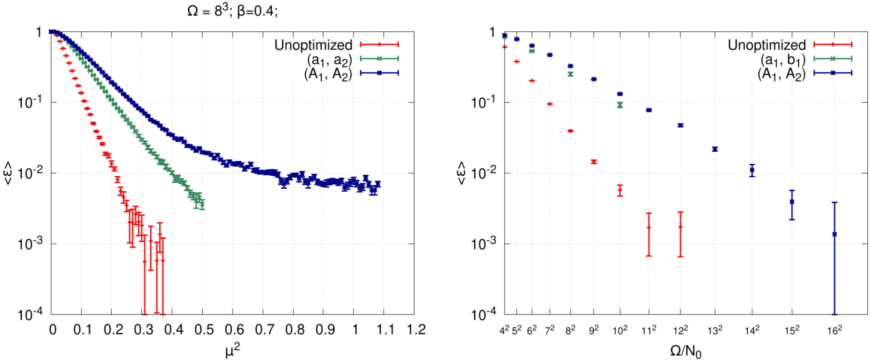
Sign problem on the deformed contour



Optimal parameterisation among those checked respects symmetries of the model (time translation, shift invariance $\varphi_x \to \varphi_x + c$)

$$(A_1, A_2): \quad \varphi_x(t_x) = t_x + i\left\{A_1 \cos[(t_x - t_{x+\hat{0}})] + A_2 \cos[2(t_x - t_{x+\hat{0}})]\right\}$$

Sign problem on the deformed contour

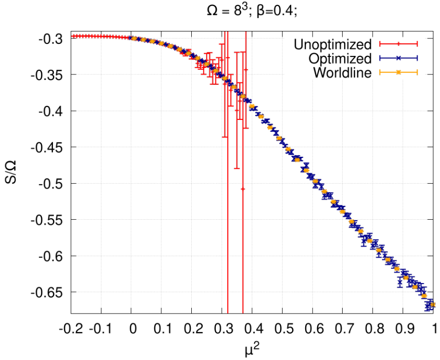


Exponential gain in severity as a function of μ^2 and $V = \Omega/N_0$

$$\langle \varepsilon \rangle \sim e^{-D\mu^2} \qquad D_{\text{undeformed}} \simeq 24 \qquad D_{\text{deformed}} \simeq 10$$

$$\langle \varepsilon \rangle \sim e^{-CV} \qquad C_{\text{undeformed}} \simeq 0.0073 \qquad C_{\text{deformed}} \simeq 0.0031$$

Undeformed vs. deformed vs. worldline



- simple sign reweighting fails at $\mu^2 \sim 0.3 \div 0.4$
- reweighting on deformed contour gives sufficient gain to reach into the ordered phase ($\mu^2 > \mu_c^2 \approx 0.54$)
- agreement with worldline (sign-problem-free) results

Summary and outlook

Improvements on reweighting methods:

- conceptual problems with rooting specific to finite μ can be dealt with (geometric matching)
- overlap problem can be avoided if weights take values in a compact domain (sign quenching)
- contour deformation effective in reducing severity of sign problem

Open issues:

- find effective contour deformations for finite-density QCD
- put everything together
- start the simulations. . .

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