Complex Langevin Simulations: Reliability and applications to full QCD at non-zero density

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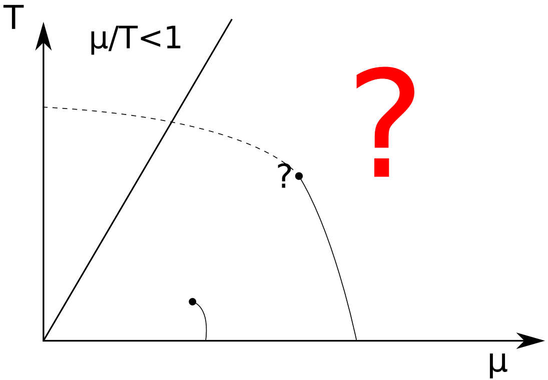
The QCD phase diagram



Reminder: Complex Langevin (CL)

- We want to sample the path integral $Z = \int e^{-S(\phi)} d\phi$ with S taking values in $\mathbb{C}$
- Langevin process $\dot{\phi} = -\frac{\partial S}{\partial \phi} + \eta$ with Gaussian noise η yields correct distribution $\rho(\phi) = e^{-S(\phi)}$ in the real case $\rightarrow$ stochastic quantization.
- For the complex case split into complex and real part

$$\partial_\tau \text{Re } \phi = -\text{Re } \frac{\partial S}{\partial \phi} + \eta \ \& \ \partial_\tau \text{Im } \phi = -\text{Im } \frac{\partial S}{\partial \phi}$$

  which yield some combined distribution $P(\text{Re}\phi, \text{Im}\phi)$
- The process yields the correct physics, if $\langle \mathcal{O} \rangle_\rho = \langle \mathcal{O} \rangle_P$, which can be proven under certain conditions (Aarts et al arXiv:0912.3360, Aarts et al arXiv:1101.3270, Nagata et al arXiv:1606.07627)
- Hope: Distribution stays close to the real axis such that the correct physics is sampled.

Boundary terms from the proof for correctness

- Possible failure if: Non-ergodicity, poles, **boundary terms**
- Interpolating quantity between $\langle \mathcal{O} \rangle_\rho$ (what we want) and $\langle \mathcal{O} \rangle_P$ (what we have): $F(t, \tau)$
- Boundary term is given by (Scherzer et al arXiv:1808.05187):

$$B(Y,t) = -\int_{|\vec{y}|<Y} \left(L^T P(t) \right) \mathcal{O}(0) \big) \, d^N x d^N y + \int_{|\vec{y}|<Y} P(t) (L_c \mathcal{O}(0)) d^N x d^N y$$

- We want $Y \to \infty$ and $t \to \infty$

Explicit computation of boundary terms: 2 variants

- Boundary term can be computed as a **surface integral**
  $B(Y,t) = \int_{|\vec{y}|<Y} \nabla_y \cdot \left(\vec{K}_y \mathcal{O}(0) P(t)\right) d^N x d^N y$
  (see Scherzer et al arXiv:1808.05187 for a derivation)
  $= \int_{|\vec{y}|=Y} \vec{n} \cdot \left(\vec{K}_y P(t) \mathcal{O}(0)\right) d^N x \, dS$

- Or alternatively as a **volume integral** from
  $B(Y,\infty) = \int_{|\vec{y}|<Y} P(t)(L_c \mathcal{O}(0)) d^N x d^N y = \langle L_c \mathcal{O} \rangle_Y$
  (Since $L^T P = \dot{P} = 0$ as $t \to \infty$)

- $L_c = (D_i + K_i)\, D_i$
- Mind the order of the limits in both cases!
- There is freedom in the choice of Y, e.g. unitarity norm for lattice models.

Simple example: The holomorphic Polyakov chain

- Model: Chain of $SL(3,\mathbb{C})$ matrices with $-S = c_+ \mathrm{Tr}\mathcal{L} + c_- \mathrm{Tr}\mathcal{L}^{-1}$, where $\mathcal{L}$ is the Polyakov loop and $c_\pm = \beta + \kappa \exp(\pm\mu)$, gauge fixed and diag. (2 d.o.f.)

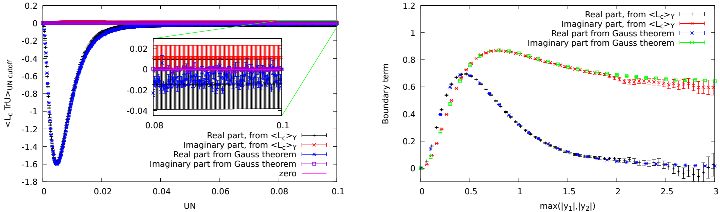


Figure: Left: CLE works!, $\beta = 2$, $\kappa = 0.1$, $\mu = 1$. Right: CLE fails!, $\beta = i$, $\kappa = 0 = \mu$

- Note: Large stepsize in the volume integral version leads to deviations from zero even if CLE is correct!
- Volume integral: Large Y have low statistics, errorbars increase. Look for plateau.

The XY model 1

- CLE famously fails here for even small imaginary parts in the action (Aarts, James arXiv:1005.3468)

$$S = -\beta \sum_{x} \sum_{\nu=0}^{2} cos(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,0})$$

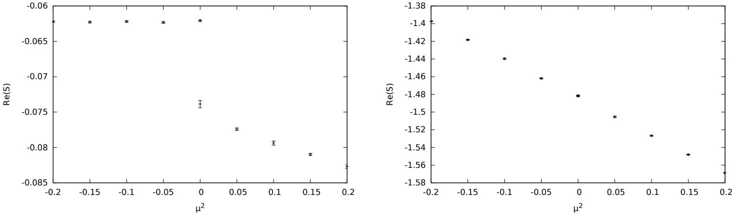


Figure: Left: $\beta = 0.2$, Right: $\beta = 0.7$

The XY model 2

- Boundary terms via volume integral with $Y = max(Im(\phi)^2)$

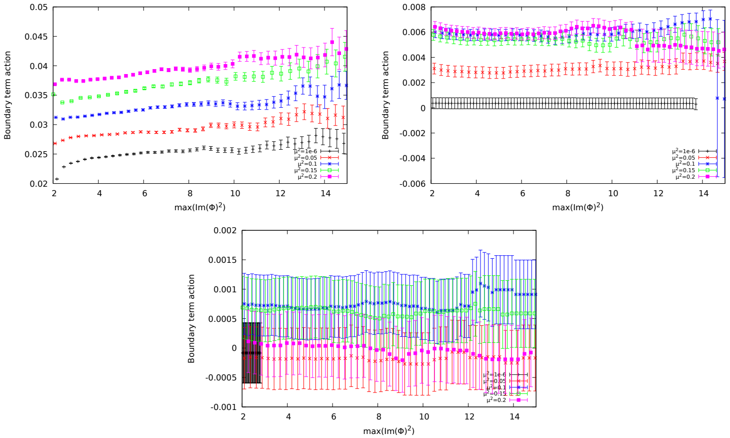


Figure: Top Left: $\beta = 0.2$, Top Right: $\beta = 0.7$, Bottom: $\beta = 0.9$

The XY model 3

- Drift criterion (Nagata et al arXiv:1606.07627)

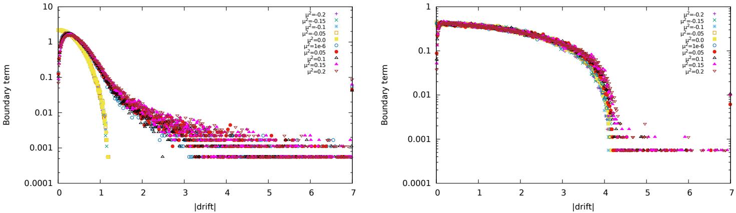
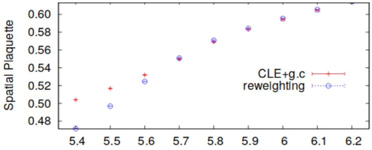
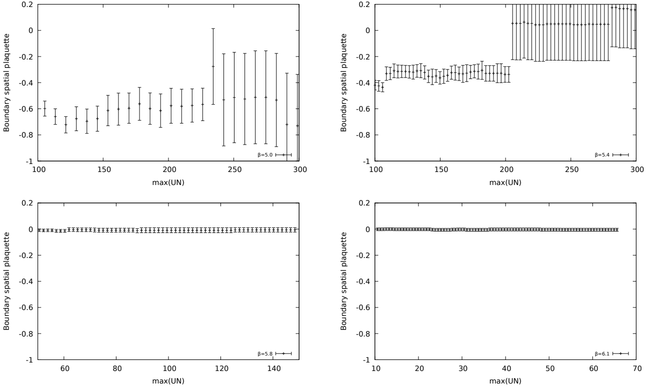


Figure: Left: $\beta = 0.2$, Right: $\beta = 0.7$

HDQCD

- Boundary terms via volume integral with unitarity norm $Y = max(U^\dagger U - \mathrm{Tr}1)$ (Figure taken from Seiler et al arXiv:1211.3709)





Complex Langevin for QCD phase transition

- Instead of $\mathbb{R}$ and $\mathbb{C}$, we have SU(3) and SL(3,$\mathbb{C}$).
- The Langevin process is formulated in the algebra and exponentiated into the group

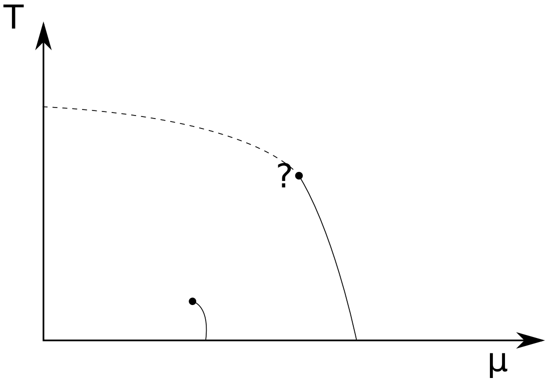
$$U_{\tau+\epsilon}(n) = \exp\left(\sum i\lambda_a \left(\epsilon(-DS)_{x,\mu,a} + \sqrt{\epsilon}\eta_{x,\mu,a}\right)\right) U_\tau(n)$$

- A priori, the process is unstable. However we can use gauge transformations to keep the process close to SU(3) where we want it to be. Seiler et al arXiv:1211.3709
- We use Wilson fermions (2 flavors)

How to scan the phase diagram?

- The chemical potential μ is a parameter of the action.
- The temperature is given by the temporal direction of the lattice, $T = 1/(aN_t)$ and can be varied either by varying the number of points N_t or the lattice spacing a.
- Typical lattice QCD setup: vary the lattice spacing (via the coupling).
- Problem: complex Langevin unstable at too large lattice spacings/too high couplings.
- Hence we vary N_t.

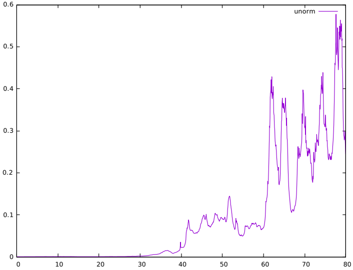
Where can we simulate?

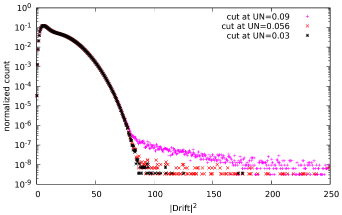


- No poles
- No runaways/boundary terms
- Reasonably fast simulation

What about boundary terms?

- We wish to stay close to SU(3), which we quantify via the unitarity norm $N_U = \mathrm{Tr}\ U^\dagger U - 3$.





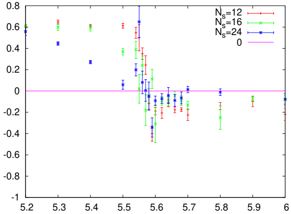
- We stop the simulation if the unitarity norm grows too large, empirically $N_U \approx 0.1$, otherwise boundary terms start to occur (drift criterion already shows negligible deviation).
- If the observables of interest thermalize before the norm becomes too large, we can take measurements.

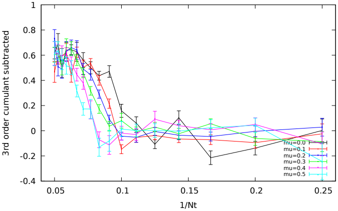
How to detect the phase transition?

- Physically, deconfinement and chiral symmetry breaking occurs at the crossover transition.
- Order parameter: Polyakov loop, which is related to the free energy of a heavy quark antiquark pair $\left\langle L(x)L^{\dagger}(y)\right\rangle \sim e^{-F_{q\bar{q}}}$ and is zero in the confined phase.
- Order parameter: chiral condensate $\langle\bar{\psi}\psi\rangle$, which signals the occurence of quark masses.
- We wish to use observables which do not require renormalization for simplicity

3rd order cumulant

- We look at ratios of $L_{abs} = \sqrt{LL_{inv}}$.
- 3rd order cumulant $\frac{\left\langle (L_{abs} - \langle L_{abs} \rangle)^3 \right\rangle}{\langle (L_{abs} - \langle L_{abs} \rangle)^2 \rangle^{1.5}}$





- The phase transition is given by the zero crossing point.

Curvature of the transition line

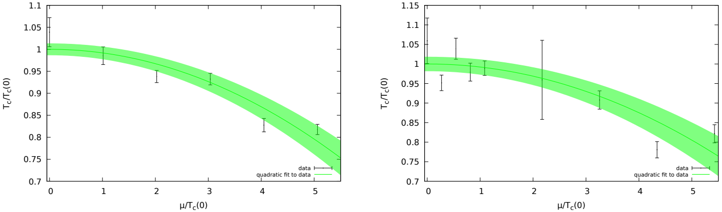
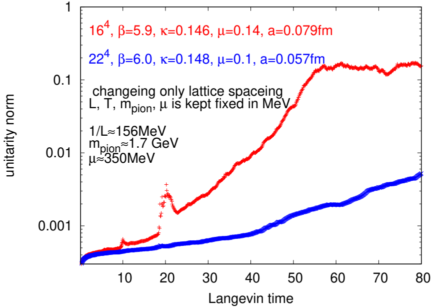
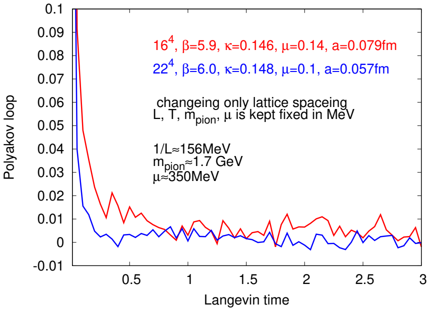


Figure: Left:$N_s = 12$, Right:$N_s = 16$

We extract the curvature of the transition line via a quadratic fit $\frac{T_c(\mu_B)}{T_c(0)} = 1 - \kappa_2 \left(\frac{\mu_B}{T_c(0)}\right)^2$ And find $\kappa_2 \approx 0.001$. Disclaimer: Still large finite size effects, its Wilson fermions!

CLE towards the continuum





Pressure

- D. Sexty, to be published
- Pressure from CLE compared to Taylor expansion (both staggered quarks)

$$\Delta\left(\frac{p}{T^4}\right) = \frac{\ln Z(\mu) - \ln Z(0)}{VT^3} = \frac{1}{VT^3}\int_0^{\mu} d\mu' \frac{\partial \ln Z(\mu')}{\partial \mu'}$$

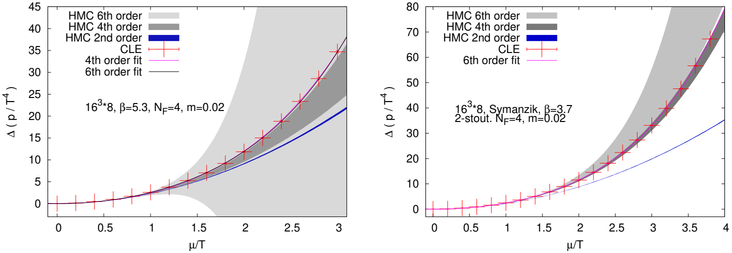


Figure: Left:no smearing, Right:stout smearing

Conclusion

- New usable criterion for failure of CLE (in case of boundary terms)
- Complex Langevin is applicable in large portions of the phase diagram, especially the transition region seems to be largely accessible
- We find that the transition line is well parametrized by a quadratic behaviour even up to $\mu/T \approx 5$