Complex Langevin and the sign problem in QCD

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Advances in Monte Carlo Techniques for Many-Body Quantum Systems
(INT-18-2b)
2018-08-27

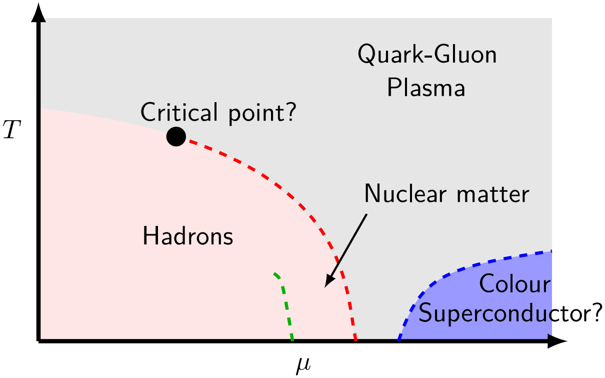
CLE: Motivation

Outline

- Motivation
- (Brief) Review of lattice QCD
- Stochastic quantisation and complex Langevin
- Results
- Summary

CLE: Motivation

Description of QCD under different thermodynamical conditions



- Experimental investigations in progress (LHC, RHIC) and planned (FAIR)
- Perturbation theory only applicable at high temperature/density (asymptotic freedom)
- Full exploration requires non-perturbative (e.g. lattice) methods

Standard Monte Carlo methods

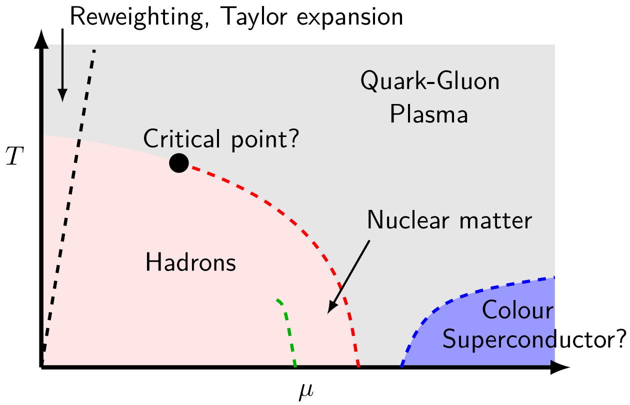
Monte Carlo at $\mu = 0$

- Theory is simulated on Euclidean spacetime
- Path integral weight e^{iS} becomes $e^{-S_E} \geq 0$
- Vacuum expectation values via path integrals
  - Configurations generated with probability proportional to e^{-S_E}

Monte Carlo at $\mu > 0$

- At $\mu > 0$ the Euclidean action S_E is no longer real (Sign Problem)
- For QCD, the fermion determinant acquires a complex phase
- e^{-S_E} cannot be interpreted as probability distribution
- Results from some techniques (e.g., reweighting, Taylor expansion) are not reliable when $\mu/T \gtrsim 1$

QCD phase diagram



Standard Monte Carlo methods cannot probe far into the phase diagram

Lattice QCD

Wilson gauge action

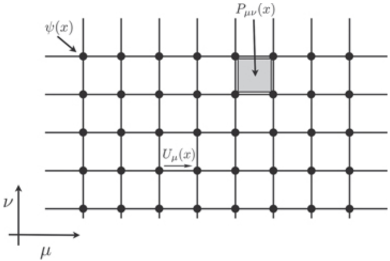
[Wilson 1974 *Phys. Rev. D* **10** 2445]

- *Gauge links* $U_{x\mu} = \exp\left(iaA_{x\mu}\right) \in \mathrm{SU}(3)$ "transport" the gauge fields between x and $x+\hat{\mu}$ and have the desired gauge transformation behaviour
- Simplest gauge invariant objects on the lattice: Plaquettes

$$U_{x,\mu\nu} = U_{x\mu}U_{x+\hat{\mu},\nu}U^{\dagger}_{x+\hat{\nu},\mu}U^{\dagger}_{x\nu} = \exp\left(ia^2F_{x,\mu\nu} + \mathcal{O}(a^3)\right)$$

$$S[U] = \frac{\beta}{3}\sum_x\sum_{\mu<\nu}\mathrm{ReTr}\left[\mathbb{1} - U_{x,\mu\nu}\right]$$
$$= \frac{\beta}{3}\sum_x\sum_{\mu<\nu}\mathrm{Tr}\left[\mathbb{1} - \frac{1}{2}\left(U_{x,\mu\nu} + U^{\dagger}_{x,\mu\nu}\right)\right]$$

with $\beta = 6/g^2$



[Beane et al 2015 *J. Phys. G: Nucl. Part. Phys.* **42** 034022]

Lattice QCD

Fermi action (naïve)

$$S_F = \overline{\psi}_x \left[\frac{\gamma_\nu}{2} \left(e^{\mu \delta_{\nu,4}} U_{x\nu} \psi_{x+\hat{\nu}} - e^{-\mu \delta_{\nu,4}} U_{x,-\nu} \psi_{x-\hat{\nu}} \right) + m \psi_x \right] = \sum_{x,y} \overline{\psi}_x M_{x,y} \psi_y$$

Path integral

- Vacuum expectation values via path integration

$$\langle \mathcal{O} \rangle = \int \mathcal{D}U \mathcal{D}\overline{\psi} \mathcal{D}\psi \, \mathcal{O} \, e^{-S-S_F} = \int \mathcal{D}U \det(M) \, e^{-S} = \int \mathcal{D}U \, e^{-S+\ln \det M}$$

- M depends on the gauge links U and chemical potential μ
- Sign problem: $(\det M(U,\mu))^* = \det M(U,-\mu^*)$

Stochastic quantization

Stochastic quantization

[Damgaard and Hüffel, Physics Reports]

- Add fictitious time dimension θ to dynamical variables
- Evolve them according to a Langevin equation

$$\frac{\partial x(\theta)}{\partial \theta} = -\frac{\delta S}{\delta x(\theta)} + \eta(\theta)\,,$$

where S is the action and $\eta(\theta)$ are white noise fields satisfying

$$\langle \eta(\theta) \rangle = 0\,, \quad \langle \eta(\theta)\eta(\theta') \rangle = 2\delta(\theta - \theta')\,,$$

- Quantum expectation values are computed as averages over the Langevin time θ after the system reaches equilibrium at $\theta = \theta_0$

$$\langle \mathcal{O} \rangle \equiv \int \mathcal{D}x\, \mathcal{O}\, e^{-S} \equiv \lim_{\theta' \to \infty} \frac{1}{\theta' - \theta_0} \int_{\theta_0}^{\theta'} \mathcal{O}(\theta) d\theta$$

Complex Langevin method

Complex Langevin

[Parisi, Phys. Lett. B131 (1983)]
[Klauder, Acta Phys. Austriaca Suppl. 25 251 (1983)]

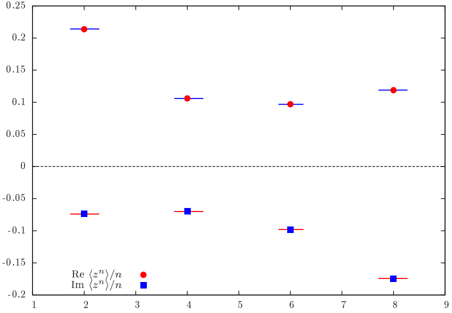
- Complexify the fields, i.e., give each component an imaginary part ($x \to z = x + iy$)
- Rewrite action and observables in term of new fields
- It circumvents the sign problem by deforming the path integral into the complex plane

Simple toy model: Anharmonic oscillator with complex mass

$$H = \frac{p^2}{2m} + \frac{1}{2}\omega x^2 + \frac{1}{4}\lambda x^4$$

Exact partition function:

$$Z \propto \sqrt{\frac{4\xi}{\omega}} e^{\xi} K_{-\frac{1}{4}}(\xi)\,, \quad \xi = \frac{\omega^2}{8\lambda}$$



CLE: Complexification

When can it be trusted? [Aarts, Seiler, Stamatescu, Phys.Rev. **D81** (2010) 054508]

- Sampling a *complex* weight $\rho(x)$ of real x using a *real* weight $P(x,y)$ of $z = x + iy$
- For S and $\mathcal{O}$ holomorphic

$$\langle \mathcal{O} \rangle_\rho = \langle \mathcal{O} \rangle_P$$

$$\int dz\, \mathcal{O}(z)\rho(z) = \int dx\, dy\, \mathcal{O}(x,y)P(x,y)$$

- Sufficient conditions:
  - Fast falloff in imaginary direction ($y \to \infty$) of $P(x,y)$
  - $\langle \tilde{L}\mathcal{O} \rangle = 0$ for *all* $\mathcal{O}$, with $\tilde{L} = [\partial_z - (\partial_z S)]\,\partial_z$

Stochastic quantization (gauge theories)

Lattice gauge theories

[Damgaard and Hüffel, Physics Reports]

- Evolve gauge links according to the Langevin equation

$$U_{x\mu}(\theta+\varepsilon) = \exp\left[X_{x\mu}\right] U_{x\mu}(\theta)\,,$$

where

$$X_{x\mu} = i\lambda^a(-\varepsilon D^a_{x\mu} S\left[U(\theta)\right] + \sqrt{\varepsilon}\,\eta^a_{x\mu}(\theta))\,,$$

λ^a are the Gell-Mann matrices, ε is the step size, $\eta^a_{x\mu}$ are white noise fields satisfying

$$\langle \eta^a_{x\mu}\rangle = 0\,, \quad \langle \eta^a_{x\mu}\eta^b_{y\nu}\rangle = 2\delta^{ab}\delta_{xy}\delta_{\mu\nu}\,,$$

S is the QCD action and $D^a_{x\mu}$ is defined as

$$D^a_{x\mu} f(U) = \left.\frac{\partial}{\partial\alpha} f(e^{i\alpha\lambda^a} U_{x\mu})\right|_{\alpha=0}$$

CLE: Complexification (gauge theories)

Complexification

[Aarts, Stamatescu, JHEP **09** (2008) 018]

- Allow gauge links to be non-unitary: SU$(3) \ni U_{x\mu} \to U_{x\mu} \in$ SL$(3, \mathbb{C})$
- Use $U_{x\mu}^{-1}$ instead of $U_{x\mu}^{\dagger}$ as
  - it keeps the action holomorphic;
  - they coincide on SU(3) but on SL$(3, \mathbb{C})$ it is U^{-1} that represents the backwards-pointing link.
- That means the plaquette is now

$$U_{x,\mu\nu} = U_{x\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu}^{-1} U_{x\nu}^{-1} \, ,$$

and the Wilson action reads

$$S[U] = \frac{\beta}{3} \sum_{x} \sum_{\mu<\nu} \mathbf{Tr} \left[\mathbb{1} - \frac{1}{2} \left(U_{x,\mu\nu} + U_{x,\mu\nu}^{-1} \right) \right]$$

CLE: Complexification (gauge theories)

Gauge cooling

[Seiler, Sexty, Stamatescu, Phys.Lett. **B723** (2013) 213-216]

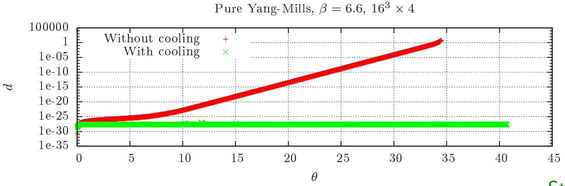
- SL$(3,\mathbb{C})$ is not compact $\Rightarrow$ gauge links can get arbitrarily far from SU(3)
- During simulations monitor the distance from the unitary manifold with

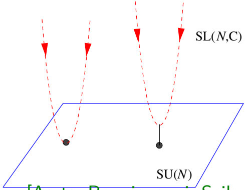
$$d = \frac{1}{N_s^3 N_\tau} \sum_{x,\mu} \mathbf{Tr}\left[U_{x\mu}U_{x\mu}^\dagger - \mathbb{1}\right]^2 \geq 0$$

- Use gauge transformations to decrease d

$$U_{x\mu} \to \Lambda_x U_{x\mu} \Lambda_{x+\mu}^{-1}$$

necessary, but not always sufficient





[Aarts, Bongiovanni, Seiler, Sexty, Stamatescu, hep-lat/1303.6425]

Results

Observables considered

- Polyakov loop: order parameter for confinement in pure Yang-Mills

$$P = \frac{1}{N_s^3} \sum_{\vec{x}} \langle \mathcal{P}_{\vec{x}} \rangle \,, \quad \mathcal{P}_{\vec{x}} = \prod_{\tau} U_4(\vec{x}, \tau)$$

- Spatial plaquette:

$$\frac{1}{3N_s^3 N_\tau} \sum_x \sum_{1<\mu<\nu<3} \langle U_{x,\mu\nu} \rangle \,, \quad U_{x,\mu\nu} = U_{x\mu} U_{x+\hat{\mu},\nu} U^{-1}_{x+\hat{\nu},\mu} U^{-1}_{x\nu}$$

- Chiral condensate: order parameter for confinement for massless quarks

$$\langle \overline{\psi} \psi \rangle = \frac{\partial}{\partial m} \ln Z$$

Heavy-dense QCD

Heavy-dense approximation

[Bender et al, Nucl. Phys. Proc. Suppl. **46** (1992) 323]

- Heavy quarks → quarks evolve only in Euclidean time direction:

$$\det M(U,\mu) = \prod_{\vec{x}} \left\{ \det\left[1 + (2\kappa e^{\mu})^{N_\tau} \mathcal{P}_{\vec{x}}\right]^2 \det\left[1 + \left(2\kappa e^{-\mu}\right)^{N_\tau} \mathcal{P}_{\vec{x}}^{-1}\right]^2 \right\}$$

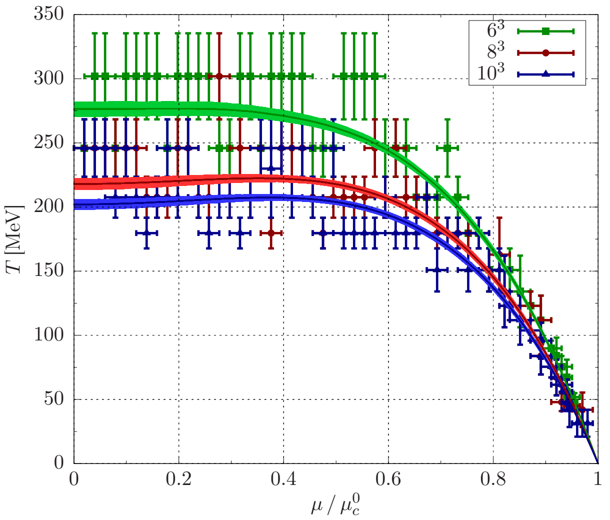
- Polyakov loop

$$\mathcal{P}_{\vec{x}} = \prod_{\tau} U_4(\vec{x},\tau)$$

- Exhibits the sign problem: $[\det M(U,\mu)]^* = \det M(U,-\mu^*)$
- Siver-blaze problem at $T = 0$

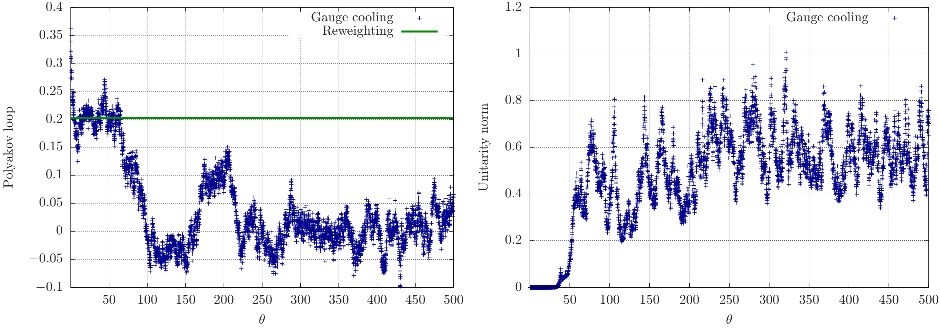
Phase boundary of HDQCD

[Aarts, Attanasio, Jäger, Sexty, JHEP **09** (2016) 087]



CLE: Instabilities

Gauge cooling (mild sign problem)



Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm ("large" but under control)

CLE: Dynamic stabilisation

Dynamic stabilisation

[Attanasio, Jäger, hep-lat/1808.04400]

- New term in the drift to reduce the non-unitarity of $U_{x,\nu}$

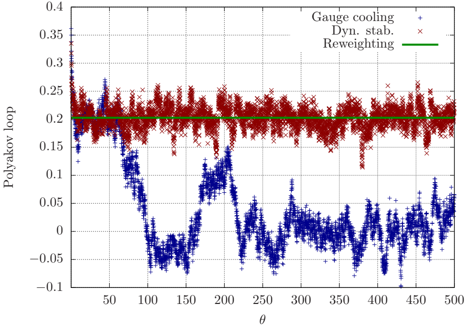
$$X_{x\nu} = i\lambda^a \left(-\epsilon D^a_{x,\nu} S - \epsilon \alpha_{\mathrm{DS}} M^a_x + \sqrt{\epsilon}\, \eta^a_{x,\nu}\right) \, .$$

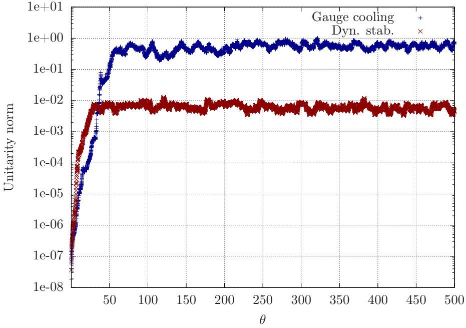
with α_{DS} being a control coefficient

- M^a_x: constructed to be irrelevant in the continuum limit
- M^a_x only depends on $U_{x,\nu} U^\dagger_{x,\nu}$ (non-unitary part)

CLE: Dynamic stabilisation

Dynamic stabilisation (mild sign problem)

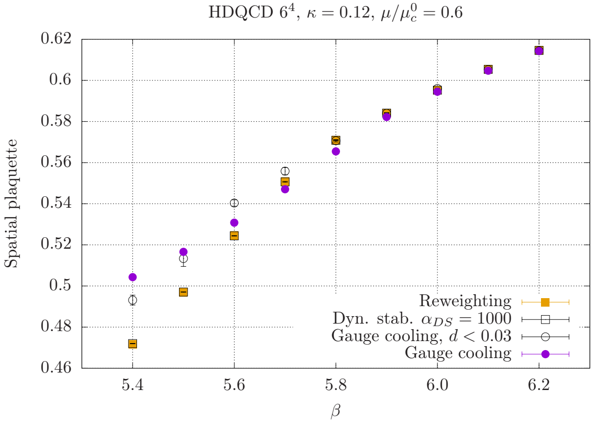




Left: Langevin time history of Polyakov loop
Right: Langevin time history of unitarity norm (notice log scale!)

Deconfinement in HDQCD

Good agreement with reweighting – even when GC converges to the wrong limit



Spatial plaquette as a function of the inverse coupling β for HDQCD

Dynamical fermions

Staggered quarks

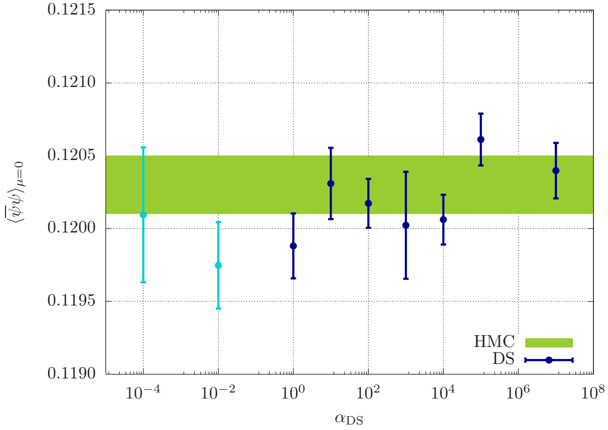
- The Langevin drift for N_f flavours of staggered quarks

$$\begin{aligned} D^a_{x,\nu} S_F &\equiv D^a_{x,\nu} \ln\det M(U,\mu) \\ &= \frac{N_F}{4} \mathrm{Tr}\left[M^{-1}(U,\mu) D^a_{x,\nu} M(U,\mu) \right] \end{aligned}$$

- Inversion is done with conjugate gradient method
- Trace is evaluated by bilinear noise scheme – introduces imaginary component even for $\mu = 0$!

Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

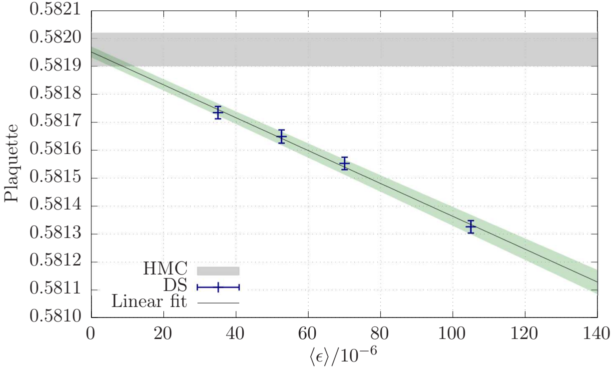
Comparison between CLE + DS runs and HMC (results by P. de Forcrand)



Green band represents results from HMC simulations
α_{DS} scan of the chiral condensate for a volume of 6^4

Staggered quarks ($\beta = 5.6,\ m = 0.025,\ N_F = 4$)

Comparison between CLE + DS runs and HMC (results by P. de Forcrand)



Grey band represents results from HMC simulations
Langevin step size extrapolation of the plaquette for a volume of 12^4

Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 4$)

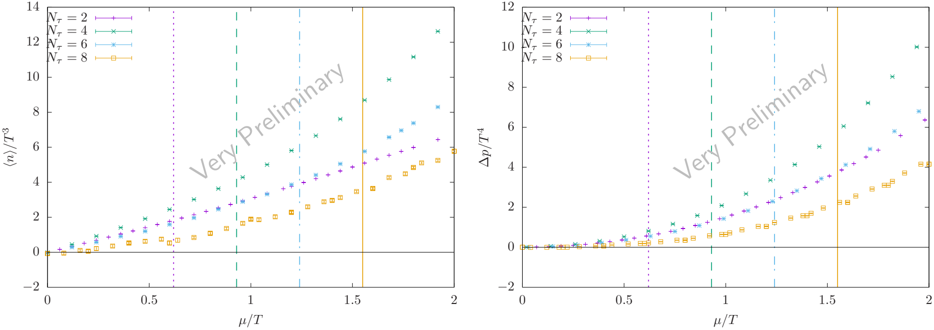
Comparison between CLE + DS runs and HMC (results by P. de Forcrand)

	Plaquette		$\overline{\psi}\psi$	
Volume	HMC	Langevin	HMC	Langevin
6^4	$0.58246(8)$	$0.582452(4)$	$0.1203(3)$	$0.1204(2)$
8^4	$0.58219(4)$	$0.582196(1)$	$0.1316(3)$	$0.1319(2)$
10^4	$0.58200(5)$	$0.58201(4)$	$0.1372(3)$	$0.1370(6)$
12^4	$0.58196(6)$	$0.58195(2)$	$0.1414(4)$	$0.1409(3)$

Expectation values for the plaquette and chiral condensate for full QCD
Langevin results have been obtained after extrapolation to zero step size

Staggered quarks ($\beta = 5.6$, $m = 0.025$, $N_F = 2$)

Preliminary results at $\mu > 0$ (not extrapolated to zero step size)



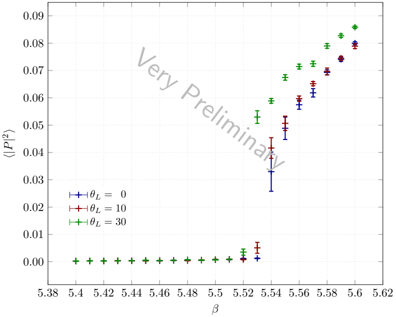
Vertical lines indicate position of critical chemical potential for each temperature
Left: Density as a function of chemical potential
Right: Pressure as a function of chemical potential

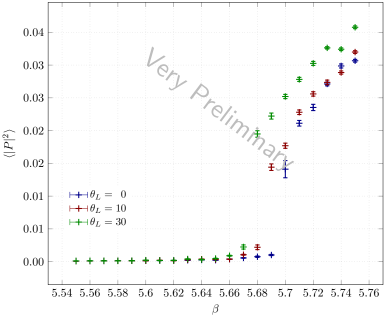
Pure Yang-Mills at $\theta^2 > 0$

- Euclidean Yang-Mills lagrangian with a topological term

$$\mathcal{L}_{\rm YM} = \frac{1}{4}{\rm Tr}[F_{\mu\nu}F_{\mu\nu}] - i\theta\frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}{\rm Tr}[F_{\mu\nu}F_{\rho\sigma}]$$

- Sign problem for real θ



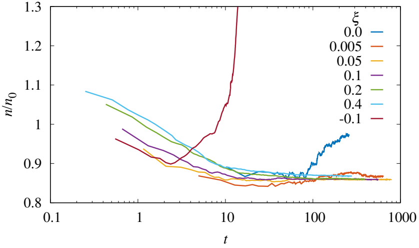


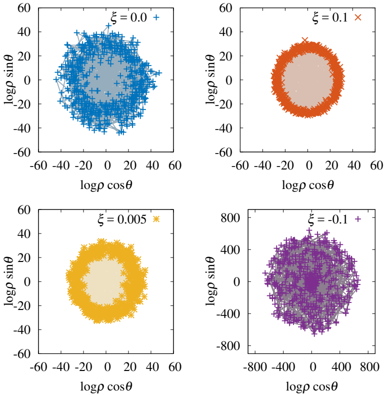
Volumes of $12^3 \times 3$ (left) and $16^3 \times 4$ (right)

Non-relativistic fermions in 1D

[Drut, Loheac, Phys.Rev. **D95** (2017) 094502]

- Sign problem for polarised systems
- Stabilisation method similar to Dynamic Stabilisation





Left: *Running* average of the density for different ξ
Right: Plot of $e^{-S} = \rho e^{i\theta}$. Each point is one snapshot of the Langevin evolution

Summary and outlook

Conclusions

- Complex Langevin provides a way of circumventing the sign problem
- Results in QCD and non-relativistic fermions possible with modified process

Future plans

- Map the phase diagram of QCD with light quarks
- Further applications in condensed matter