Lattice QCD at nonzero baryon number

XIII Hadron Physics

III: complex Langevin dynamics

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Where are we?

complex weight:

- straightforward importance sampling not possible
- overlap problem

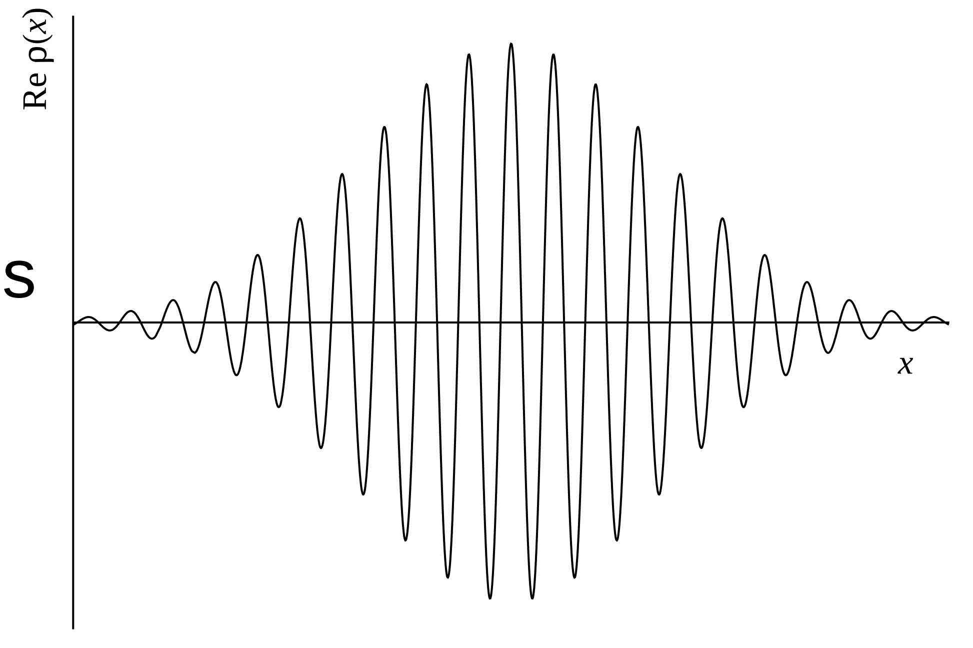
various possibilities:

- preserve overlap as best as possible
- use approximate methods at small μ
- do something radical:
  - rewrite partition function in other dof
  - explore field space in a different way
  - . . .

Overlap problem

- configurations differ in an essential way from those obtained at $\mu = 0$ or with $|\det M|$
- cancelation between configurations with 'positive' and 'negative' weight

dominant configurations in the path integral?



Complex integrals

- consider simple integral

$$Z(a,b) = \int_{-\infty}^{\infty} dx\, e^{-S(x)} \qquad S(x) = \frac{1}{2}ax^2 + ibx$$

- complete the square/saddle point approximation:

into complex plane

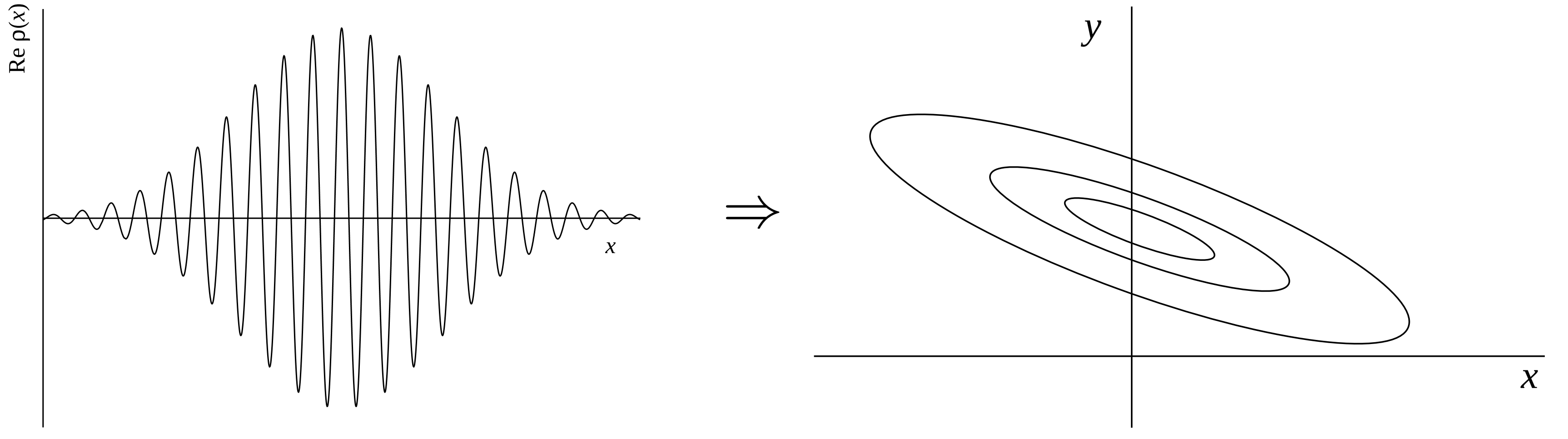
- lesson: don't be real(istic), be more imaginative

radically different approach:

- complexify all degrees of freedom $x \to z = x + iy$
- enlarged complexified space
- new directions to explore

Complexified field space

dominant configurations in the path integral?



real and positive distribution $P(x, y)$: how to obtain it?

$\Rightarrow$ solution of stochastic process

complex Langevin dynamics

Parisi 83, Klauder 83

Gaussian integral

- consider complex Gaussian integral

$$Z(a,b) = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2 - ibx} \qquad \left(= \sqrt{\frac{2\pi}{a}} e^{-\frac{1}{2}b^2/a} \right)$$

complex action $S^*(b) = S(-b^*)$ [assume $a > 0$ and real]

- phase quenched theory

$$Z_{\rm pq} = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}ax^2} = Z(a,0) = \sqrt{\frac{2\pi}{a}}$$

- sign problem: average phase factor

$$\langle e^{-ibx} \rangle_{\rm pq} = \frac{Z(a,b)}{Z(a,0)} = e^{-\frac{1}{2}b^2/a}$$

Gaussian integral

$$Z(a,b) = \int dx\, e^{-\frac{1}{2}ax^2 - ibx} \qquad \langle x^2 \rangle = -2\frac{\partial \ln Z}{\partial a} = \frac{a-b^2}{a^2}$$

goal: compute numerically without importance sampling

first take $b = 0$:

- use analogy with Brownian motion

  Parisi & Wu 81

  particle in a fluid: friction (a) and kicks (η)

- Langevin equation

$$\frac{d}{dt}x(t) = -ax(t) + \eta(t) \qquad \langle \eta(t)\eta(t') \rangle = 2\delta(t-t')$$

Gaussian integral

- Langevin equation $\dot{x}(t) = -ax(t) + \eta(t)$
- analytical solution

$$x(t) = e^{-at}x(0) + \int_0^t ds\, \eta(s) e^{-a(t-s)}$$

- correlator [take $x(0) = 0$, no i.c. dependence]

$$\langle x^2(t) \rangle = \int_0^t ds \int_0^t ds' \, \langle \eta(s)\eta(s') \rangle e^{-a(2t-s-s')}$$

- noise averaged correlator, use $\langle \eta(s)\eta(s') \rangle = 2\delta(s-s')$

$$\lim_{t\to\infty} \langle x^2(t) \rangle = \frac{1}{a}$$

- no importance sampling, solution of stochastic process

Fokker-Planck equation

- associated distribution $\rho(x,t)$

$$\langle O(x(t)\rangle_\eta = \int dx\, \rho(x,t) O(x)$$

noise average   distribution average

- Langevin eq for $x(t)$ $\Leftrightarrow$ Fokker-Planck eq for $\rho(x,t)$

$$\dot\rho(x,t) = \partial_x \left(\partial_x + S'(x)\right) \rho(x,t)$$

- stationary solution: $\rho(x) \sim e^{-S(x)}$
- typically reached exponentially fast

review: Damgaard & Hüffel 87

Complex Gaussian integral

$$Z(a,b) = \int dx\, e^{-S(x)} \qquad\qquad S(x) = \frac{1}{2}ax^2 + ibx$$

$b \neq 0$:

- analytically: complete the square

  shift in the complex plane $x \to x - i\frac{b}{a}$

- achieve the same with Langevin equation

  "complexify" $x \to z = x + iy$

$$\begin{aligned}
\dot{x} &= -\mathrm{Re}\,\partial_z S(z) + \eta = -ax + \eta \\
\dot{y} &= -\mathrm{Im}\,\partial_z S(z) \qquad = -ay - b
\end{aligned}$$

with $S(z) = S(x + iy)$

Complex Gaussian integral

- solution: $$x(t) = x(0)e^{-at} + \int_0^t ds\, e^{-a(t-s)}\eta(s)$$
$$y(t) = [y(0) + b/a]e^{-at} - b/a$$

- correlators:

$$\begin{aligned}
\langle x^2(t)\rangle &= x^2(0)e^{-2at} + \left(1 - e^{-2at}\right)/a &\to& \quad 1/a \\
\langle x(t)y(t)\rangle &= x(0)e^{-at}\left([y(0) + b/a]e^{-at} - b/a\right) &\to& \quad 0 \\
\langle y^2(t)\rangle &= \left([y(0) + b/a]e^{-at} - b/a\right)^2 &\to& \quad b^2/a^2
\end{aligned}$$

- combination $x \to x + iy$:

$$\lim_{t\to\infty}\langle[x(t) + iy(t)]^2\rangle = \langle x^2 - y^2 + 2ixy\rangle = \frac{1}{a} - \frac{b^2}{a^2} = \frac{a - b^2}{a^2}$$

correct!

Distribution

associated distribution $P(x, y; t)$ in complex plane

- real and positive distribution (if it exists)

$$\langle O(x+iy)(t)\rangle \quad = \quad \int dxdy\, P(x,y;t) O(x+iy)$$

Langevin eq
for $x(t)$ and $y(t)$

Fokker-Planck eq
for $P(x, y; t)$

- Fokker-Planck equation:

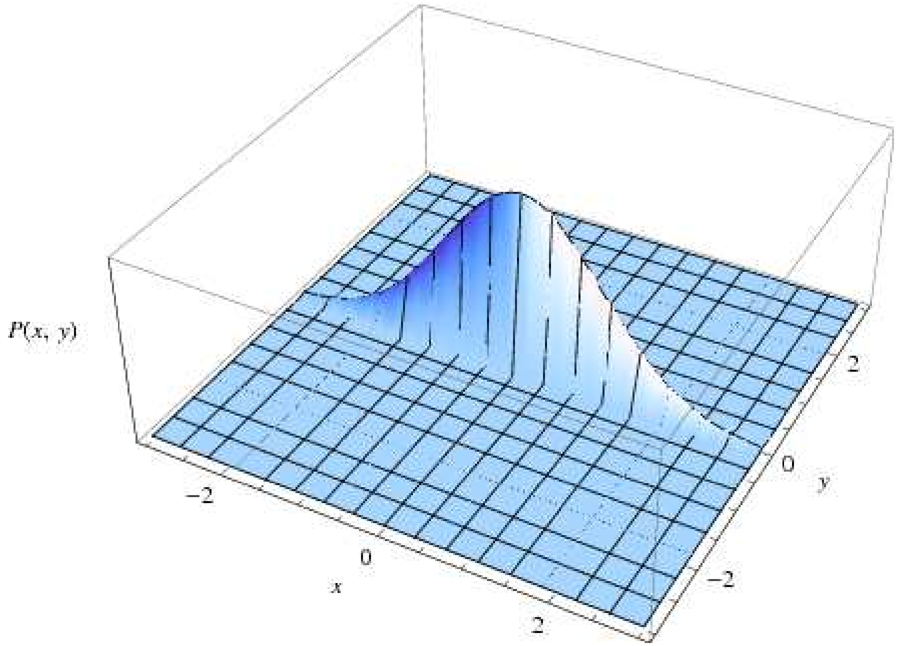
$$\dot{P}(x,y;t) = \left[\partial_x \left(\partial_x + \text{Re}\ \partial_z S\right) + \partial_y \text{Im}\ \partial_z S\right] P(x,y;t)$$

- solvable in Gaussian models (like here)
- no generic solutions known

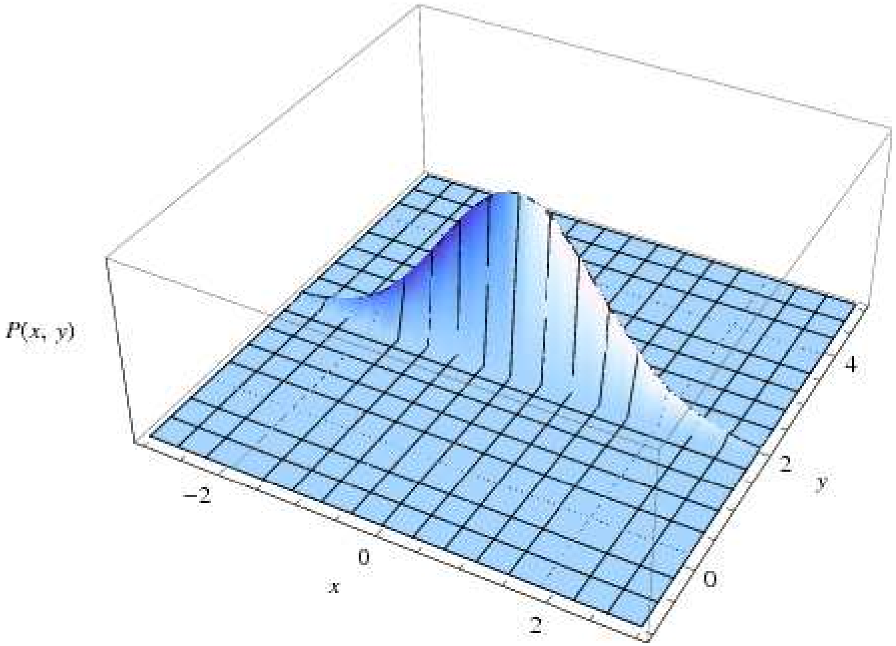
Distribution

distribution $P(x, y)$ in the complex plane

$b = 0$



$b = -2$



shift in the complex plane: $y \to -b/a$

Langevin process
"finds" distribution:

$$P(x, y) \sim e^{-ax^2/2} \delta(y + b/a)$$

More interesting Gaussian integral

final Gaussian example:

- $S = \frac{1}{2}(a+ib)x^2$ $\qquad\qquad$ $\langle x^2 \rangle = \frac{1}{a+ib}$
- coupled Langevin equations

$$\dot{x} = -ax + by + \eta \qquad\qquad \dot{y} = -ay - bx$$

- solve and find correlators when $t \to \infty$

$$\langle x^2 \rangle = \frac{1}{2a}\frac{2a^2+b^2}{a^2+b^2} \qquad \langle y^2 \rangle = \frac{1}{2a}\frac{b^2}{a^2+b^2} \qquad \langle xy \rangle = -\frac{1}{2}\frac{b}{a^2+b^2}$$

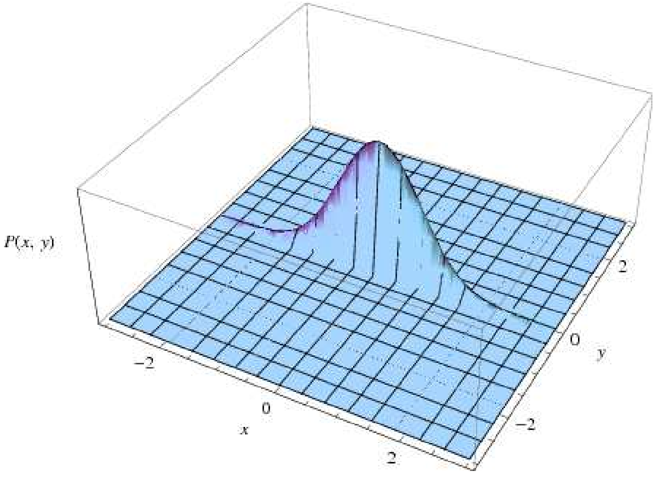
- correlator $\langle z^2 \rangle = \langle x^2 - y^2 + 2ixy \rangle = \dfrac{a-ib}{a^2+b^2} = \dfrac{1}{a+ib}$

correct!

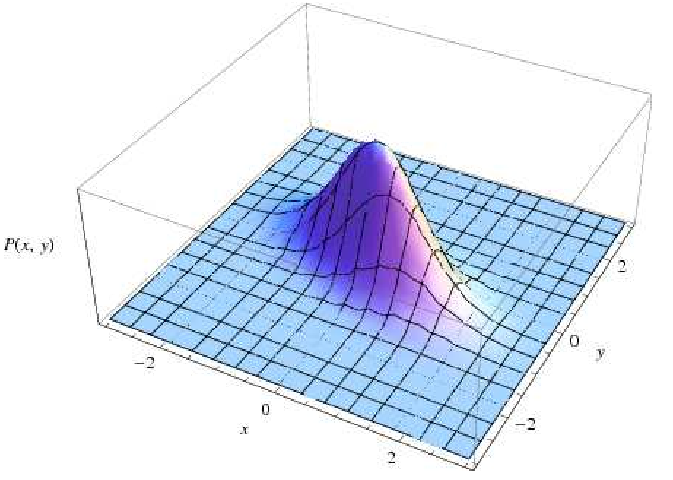
More interesting Gaussian integral

distribution $P(x, y)$ in the complex plane

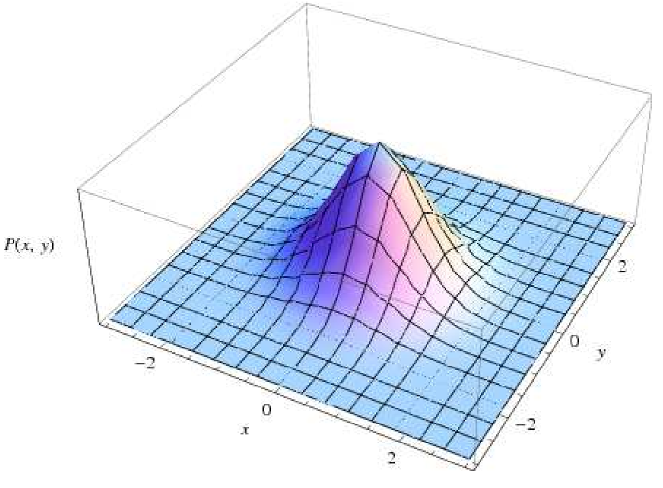
$b = 0.01$



$b = 1$



$b = 10$



Langevin process “finds” this distribution

original weight e^{-S} is complex

this distribution is real and positive

Complex Langevin dynamics: basics

partition function $Z = \int dx\, e^{-S(x)}$ $\qquad S(x) \in \mathbb{C}$

- reach equilibrium distribution à la Brownian motion
- no importance sampling, instead stochastic process

$$\dot{x} = -\mathrm{Re}\,\partial_z S(z) + \eta \qquad \langle \eta(t)\eta(t')\rangle = 2\delta(t-t')$$
$$\dot{y} = -\mathrm{Im}\,\partial_z S(z) \qquad S(z) = S(x+iy)$$

- associated distribution $P(x,y;t)$

$$\langle O(x+iy)(t)\rangle = \int dxdy\, P(x,y;t) O(x+iy)$$

- $x(t), y(t)$ Langevin eq $\Leftrightarrow$ $P(x,y;t)$ Fokker-Planck eq

$$\dot{P}(x,y;t) = \left[\partial_x \left(\partial_x + \mathrm{Re}\,\partial_z S\right) + \partial_y \mathrm{Im}\,\partial_z S\right] P(x,y;t)$$

Discretization

most cases not analytically solvable

numerical solution of Langevin equation

- discretize stochastic equation (Itō calculus)

$$x_{n+1} = x_n + \epsilon K_n^{\rm R} + \sqrt{\epsilon}\eta_n$$
$$y_{n+1} = y_n + \epsilon K_n^{\rm I}$$

- drift terms

$$K_n^{\rm R} = -{\rm Re}\,\frac{\partial S}{\partial z} \qquad K_n^{\rm I} = -{\rm Im}\,\frac{\partial S}{\partial z}$$

- noise $\langle \eta_n \eta_{n'} \rangle = \delta_{nn'}$
- use adaptive stepsize if necessary

Field theory

adapt to field theory: stochastic quantisation

Parisi & Wu 81, Parisi, Klauder 83

- path integral $Z = \int D\phi \, e^{-S}$
- Langevin dynamics in “fifth” time direction

$$\frac{\partial \phi(x,t)}{\partial t} = -\frac{\delta S[\phi]}{\delta \phi(x,t)} + \eta(x,t)$$

- Gaussian noise

$$\langle \eta(x,t) \rangle = 0 \qquad \langle \eta(x,t)\eta(x',t') \rangle = 2\delta(x-x')\delta(t-t')$$

- compute expectation values $\langle \phi(x,t)\phi(x',t) \rangle$, etc
- study converge as $t \to \infty$

Complex Langevin dynamics

does it work?

- for real actions: stochastic quantisation   Parisi & Wu 81
- equivalent to path integral quantisation
- for complex actions: formal proof was notably absent

recent progress:

- theoretical foundation given[1]
- practical criteria for correctness formulated[2]
- severe sign and Silver Blaze problems solved[3]
- first results for gauge theories[4] and even full QCD[5]

[1] 0912.3360 [1,2] 1101.3270 1306.3075 [3] 0810.2089 1006.0332

[4] 0807.1597 1211.3709 [5] 1307.7748 1408.3770 $+\ldots$

Localised distributions

crucial role played by distribution $P(x, y)$

if

- the action is holomorphic (no $\log \det$!)

and

- the distribution is localised, i.e.

$$P(x, y) = 0 \text{ for } |y| > y_{\max} \text{ [or } P(x, y) \to 0 \text{ fast enough]}$$

then

- correct result is obtained GA, Seiler & Stamatescu 0912.3360

for meromorphic drifts – with poles –, problems *may* appear (e.g. due to a $\log \det$ in the action) but not necessarily so

Mollgaard & Splittorff 1309.4335, Greensite 1406.4558

Gauge theories

in collaboration with

Nucu Stamatescu, Erhard Seiler, Dénes Sexty

Pietro Giudice, Benjamin Jäger, Jan Pawlowski

Frank James, Lorenzo Bongiovanni, Felipe Attanasio

Gauge theories

SU(N) gauge theory: complexification to SL($N, \mathbb{C}$)

- links $U \in$ SU(N): complex Langevin update

$$U(n{+}1) = R(n)\, U(n) \qquad\qquad R = \exp\left[i\lambda_a \left(\epsilon K_a + \sqrt{\epsilon}\eta_a\right)\right]$$

Gell-Mann matrices λ_a ($a = 1, \ldots N^2 - 1$)

- drift: $K_a = -D_a(S_{\rm YM} + S_{\rm F}) \qquad S_{\rm F} = -\ln\det M$

Gauge theories

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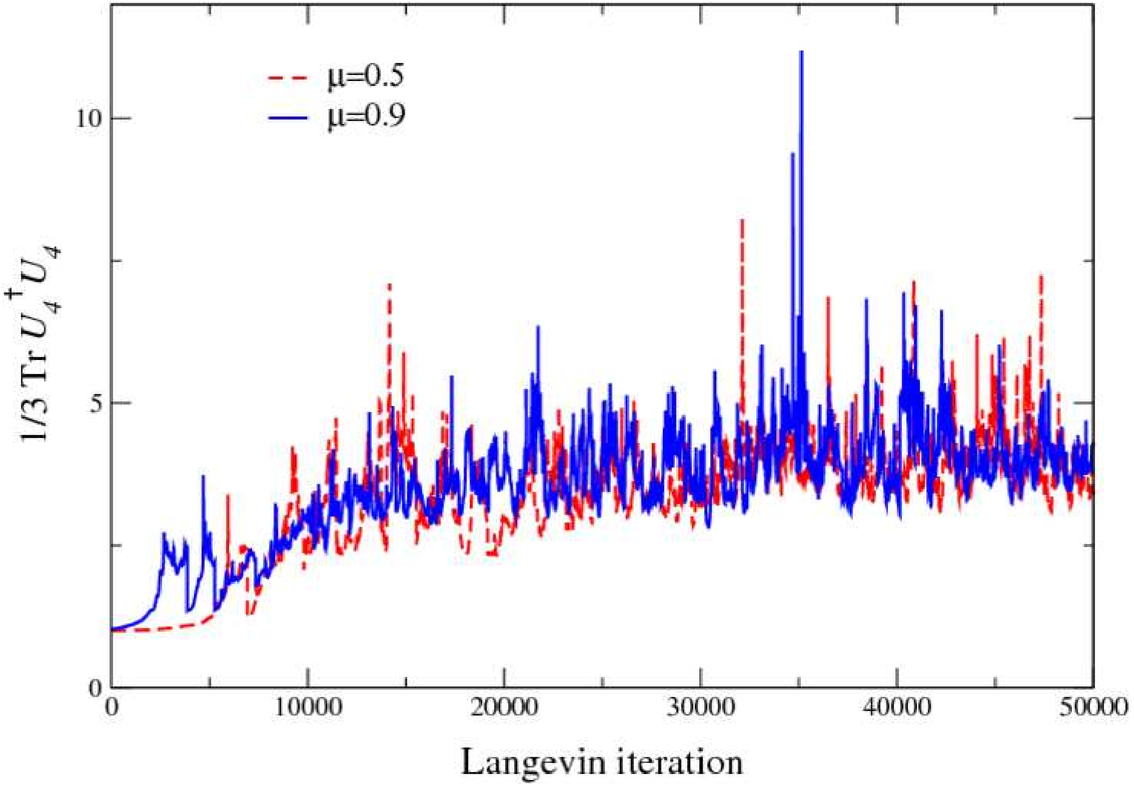
Gell-Mann matrices λ_a ($a = 1, \ldots N^2-1$)

- drift: $K_a = -D_a(S_{\rm YM} + S_{\rm F}) \qquad S_{\rm F} = -\ln\det M$
- complex action: $K^\dagger \neq K \Leftrightarrow U \in$ SL($N,\mathbb{C}$)
- deviation from SU(N): unitarity norms

$$\frac{1}{N}\mathrm{Tr}\,\left(UU^\dagger - 1\!\!1\right) \geq 0 \qquad\qquad \frac{1}{N}\mathrm{Tr}\,\left(UU^\dagger - 1\!\!1\right)^2 \geq 0$$

Gauge theories

deviation from SU(3): unitarity norm $$\frac{1}{3}\mathrm{Tr}\,UU^\dagger \geq 1$$



heavy dense QCD, 4^4 lattice with $\beta = 5.6$, $\kappa = 0.12$, $N_f = 3$

GA & Stamatescu 0807.1597

Gauge theories

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

Gauge theories

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

in practice this is not the case

$\Rightarrow$ unitary submanifold is unstable!

- process will not stay close to SU(N)
- distributions not localised
- wrong results in practice, non-analytic around $\mu^2 \sim 0$

Unstable gauge theories

what is the origin? can this be fixed?

- gauge freedom: link at site k

$$U_k \to \Omega_k U_k \Omega_{k+1}^{-1} \qquad \Omega_k = e^{i\omega_a^k \lambda_a}$$

in SU(N): $\omega_a^k \in \mathbb{R}$ $\Rightarrow$ in SL($N, \mathbb{C}$): $\omega_a^k \in \mathbb{C}$

- uncontrolled dynamics in gauge directions
- unitarity norms grow exponentially
- control those with gauge cooling

Seiler, Sexty & Stamatescu 1211.3709

see also GA, Bongiovanni, Seiler, Sexty & Stamatescu 1303.6425

$$U_k \to \Omega_k U_k \Omega_{k+1}^{-1} \qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad \alpha > 0$$

Gauge cooling

cooling update at site k $\qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad \alpha > 0$

$$U_k \to \Omega_k U_k \qquad U_{k-1} \to U_{k-1}\Omega_k^{-1}$$

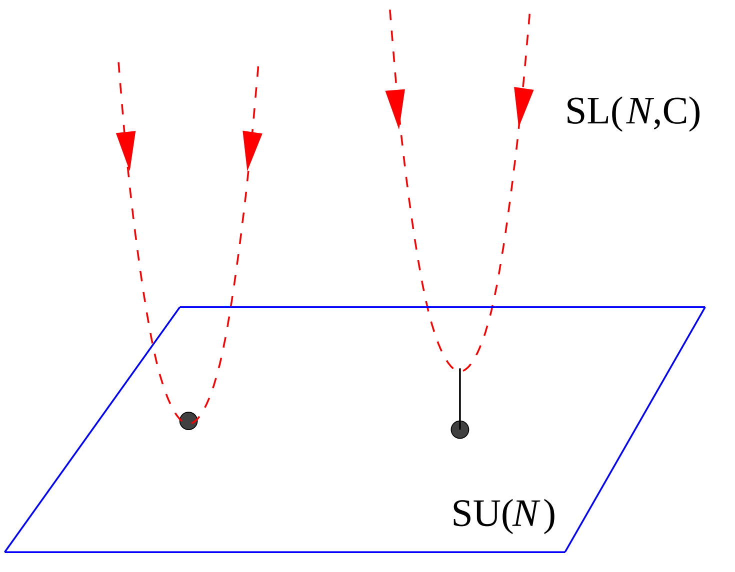
unitarity norm: distance $\qquad \mathrm{d} = \sum_k \frac{1}{N}\mathrm{Tr}\left(U_k U_k^\dagger - 1\!\!1\right)$

after one update, $\mathrm{d} \to \mathrm{d}'$

linearise

$$\mathrm{d}' - \mathrm{d} = -\frac{\alpha}{N}(f_a^k)^2 + \mathcal{O}(\alpha^2) \leq 0$$

reduce distance from SU(N)



Gauge cooling

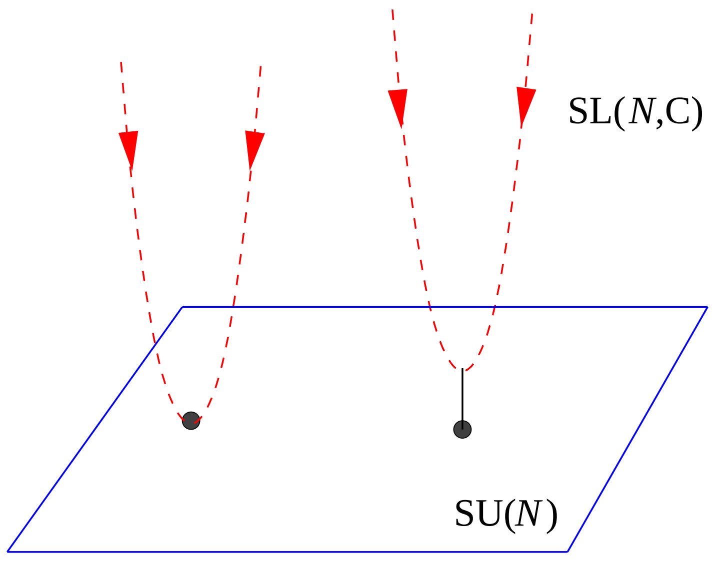
what is f_a^k? $\qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad d' - d = -\alpha/N(f_a^k)^2 + \dots$

- choose f_a^k as the gradient of the unitarity norm

$$f_a^k = 2\mathrm{Tr}\,\lambda_a\left(U_k U_k^\dagger - U_{k-1}^\dagger U_{k-1}\right)$$

- if $U \in$ SU(N): $f_a^k = 0$, $d = 0$, no effect

cooling brings the links as close as possible to SU(N)



Gauge cooling

- simple example: one-link model

$$S = \frac{1}{N}\mathrm{Tr}\, U \qquad\qquad U \to \Omega U \Omega^{-1}$$

$$\mathrm{d} = \frac{1}{N}\mathrm{Tr}\, \left(UU^\dagger - 1\!\!1\right) \qquad\qquad f_a = 2\mathrm{Tr}\, \lambda_a \left(UU^\dagger - U^\dagger U\right)$$

- note: $c = \mathrm{Tr}\, U/N, \;\; c^* = \mathrm{Tr}\, U^\dagger/N$ invariant under cooling

- cooling dynamics:

$$\mathrm{d}' - \mathrm{d} \equiv \dot{\mathrm{d}} = -\frac{\alpha}{N} f_a^2 = -\frac{16\alpha}{N}\mathrm{Tr}\, UU^\dagger[U, U^\dagger]$$

- in SU(2)/SL(2,$\mathbb{C}$):

$$\dot{\mathrm{d}} = -8\alpha\left(\mathrm{d}^2 + 2\left(1 - |c|^2\right)\mathrm{d} + c^2 + c^{*2} - 2|c|^2\right)$$

Gauge cooling

SU(2)/SL(2,$\mathbb{C}$) one-link model

$$\dot{\mathrm{d}} = -8\alpha\left(\mathrm{d}^2 + 2\left(1 - |c|^2\right)\mathrm{d} + c^2 + c^{*2} - 2|c|^2\right)$$

- $c = \frac{1}{2}\mathrm{Tr}\,U, \quad c^* = \frac{1}{2}\mathrm{Tr}\,U^\dagger$ invariant under cooling
- if $c = c^*$: U gauge equivalent to SU(2) matrix

$$\dot{\mathrm{d}} = 8\alpha(\mathrm{d} + 2 - 2c^2)\mathrm{d} \qquad\qquad \mathrm{d}(t) \sim e^{-16\alpha(1-c^2)t} \to 0$$

- if $c \neq c^*$: U not gauge equivalent to SU(2) matrix

$$\mathrm{d}(t) \to \mathrm{d}_0 = |c|^2 - 1 + \sqrt{1 - c^2 - c^{*2} + |c|^4} > 0$$

minimal distance from SU(2)
reached exponentially fast
power law in case of many links

Langevin with gauge cooling

in QCD:

- unitary submanifold very unstable
- gauge cooling essential
- alternate Langevin updates with cooling updates

recent and new results for

- heavy dense QCD
- full QCD
- hopping parameter expansion to all orders
- SU(3) with a θ-term (not shown here)

Heavy dense QCD

Benjamin Jäger, Felipe Attanasio, GA, Stamatescu, Sexty, Seiler 1411.2632

Heavy dense QCD

consider static quarks: fermion determinant simplifies

$$\det M = \prod_{\mathbf{x}} \det\left(1 + he^{\mu/T}\mathcal{P}_{\mathbf{x}}\right)^2 \det\left(1 + he^{-\mu/T}\mathcal{P}_{\mathbf{x}}^{-1}\right)^2$$

with $h = (2\kappa)^{N_\tau}$ and $\mathcal{P}^{(-1)}$ (conjugate) Polyakov loops

- full Wilson gauge action is included
- nontrivial phase diagram:
  - thermal deconfinement transition (as in pure glue)
  - μ-driven transition at $\mu_c \sim -\ln(2\kappa)$

test case for full QCD

Heavy dense QCD

consider static quarks: fermion determinant simplifies

$$\det M = \prod_{\mathbf{x}} \det\left(1 + he^{\mu/T}\mathcal{P}_{\mathbf{x}}\right)^2 \det\left(1 + he^{-\mu/T}\mathcal{P}_{\mathbf{x}}^{-1}\right)^2$$

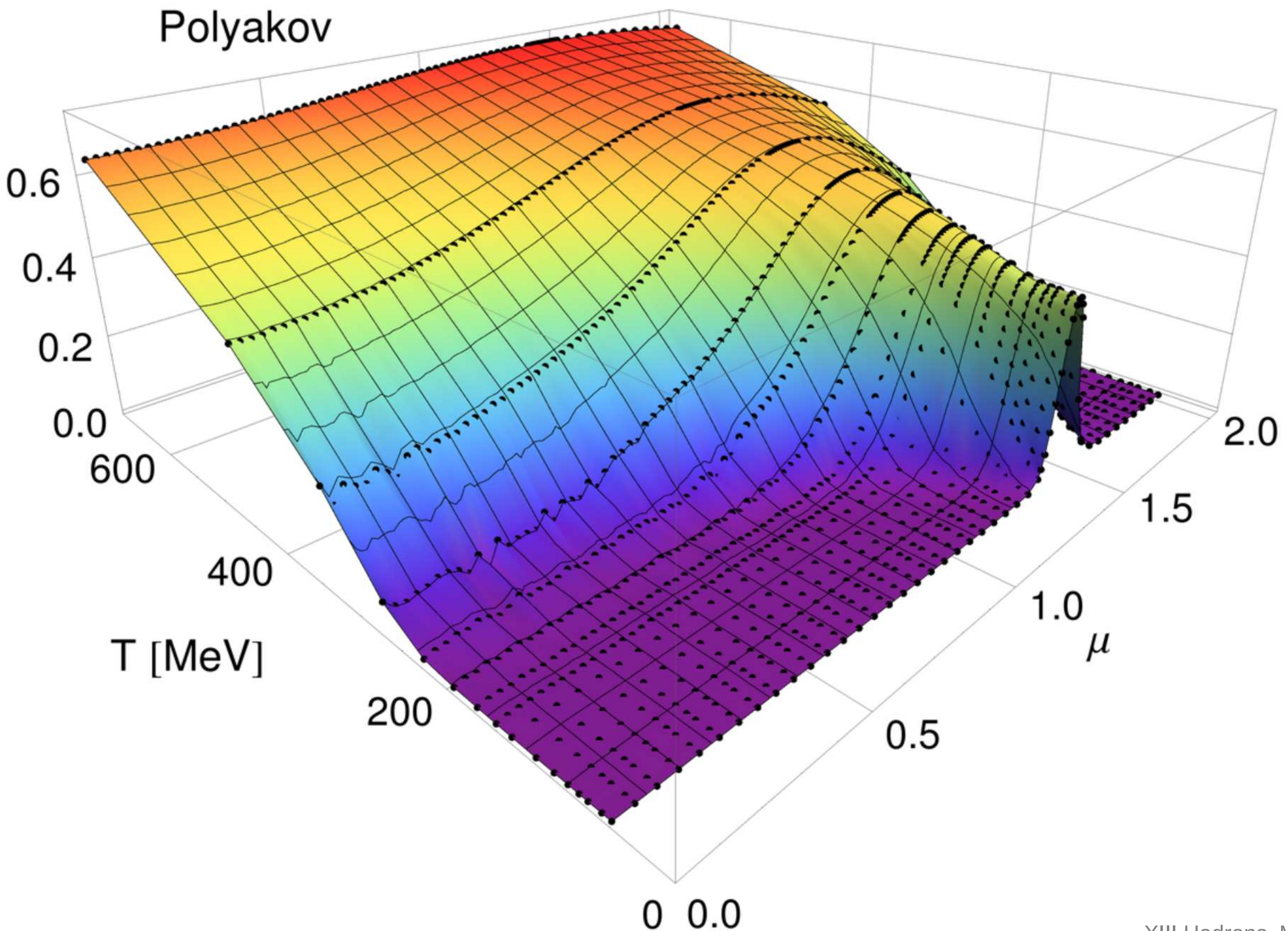
with $h = (2\kappa)^{N_\tau}$ and $\mathcal{P}^{(-1)}$ (conjugate) Polyakov loops

preliminary results for Polyakov loop and density
and their susceptibilities

- $\beta = 5.8$ ($a \sim 0.15$ fm)
- $\kappa = 0.12$ ($\mu_c \sim -\ln(2\kappa) = 1.43$)
- volume $8^3 \times N_\tau$
- $N_\tau = 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 18\ 20\ 22\ 24\ 26\ 28$

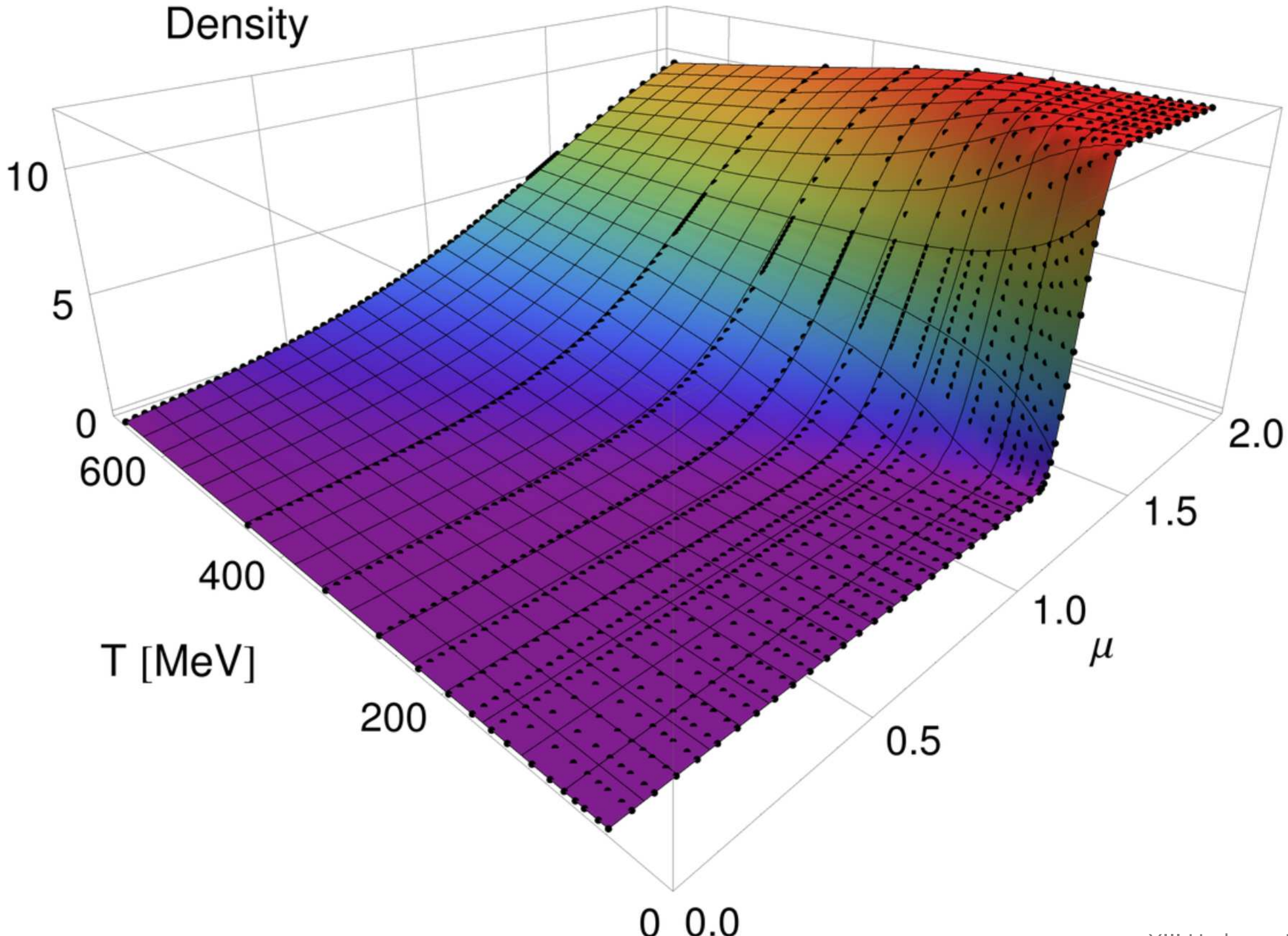
Heavy dense QCD

Polyakov loop



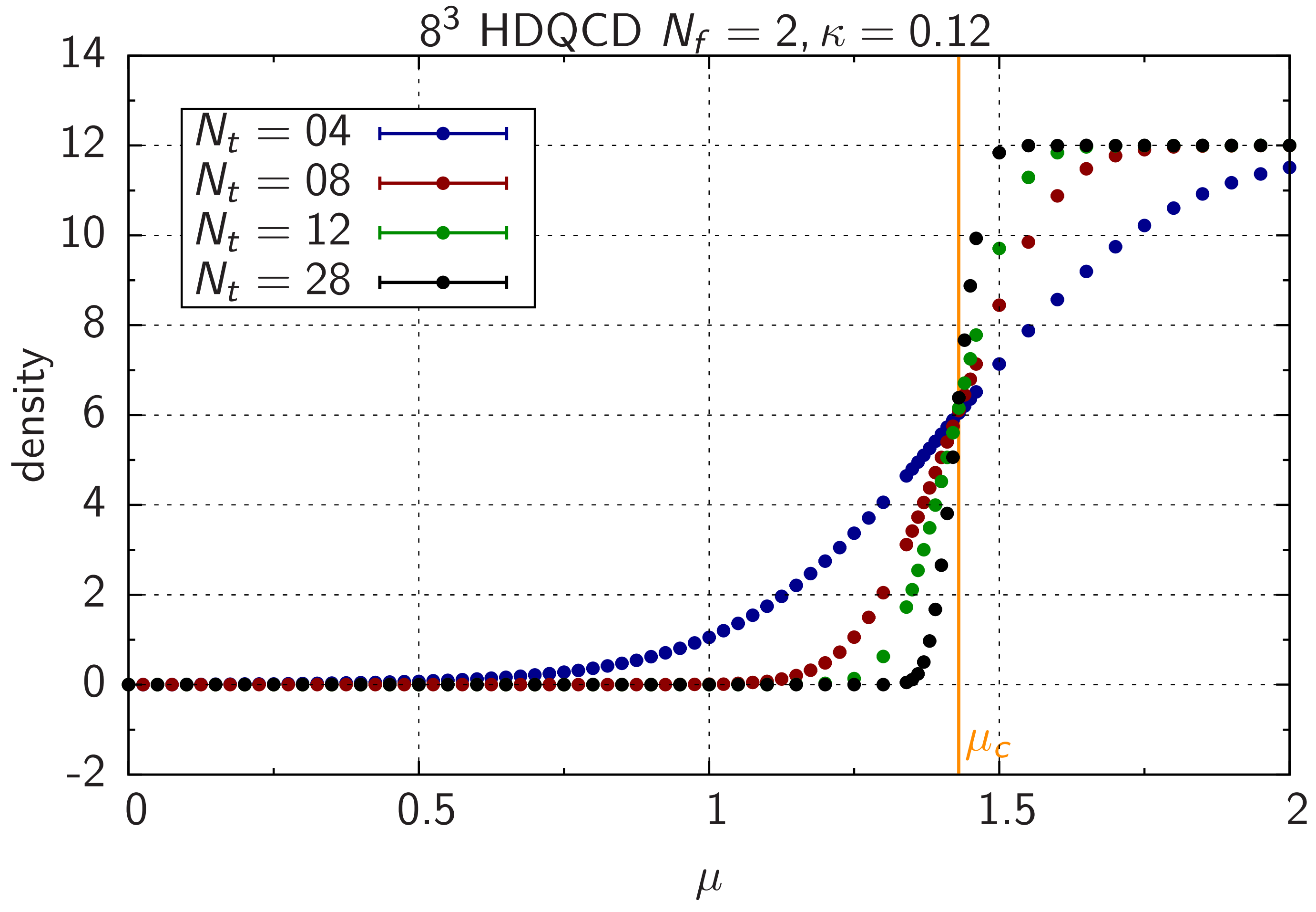
Heavy dense QCD

density



Heavy dense QCD

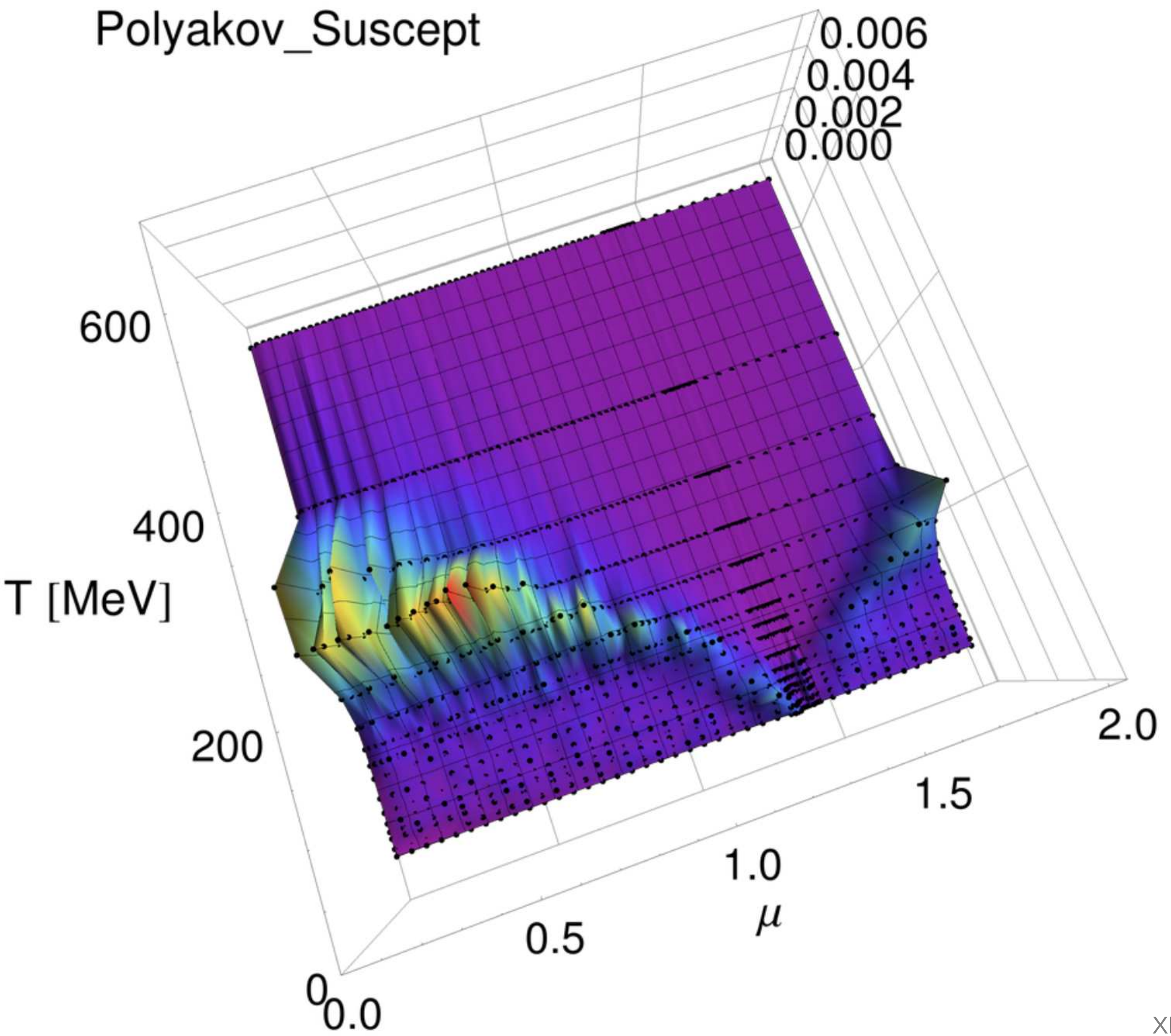
density $\mu_c = -\ln(2\kappa) = 1.43$ $n_{\rm sat} = 12$



first order transition at $T = 0$ (expected) Silver Blaze

Heavy dense QCD

Polyakov loop susceptibility



Full QCD at nonzero density

Dénes Sexty 1307.7748

Full QCD

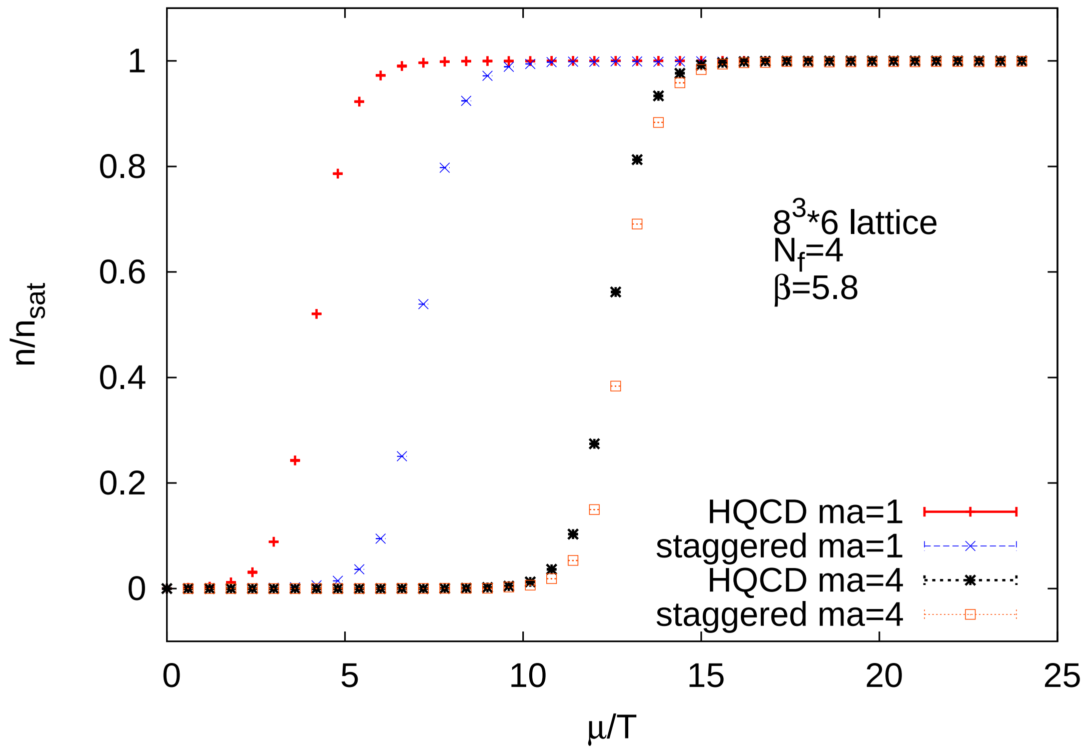
first application to full QCD

- fermion determinant: additional drift term in CLE
- requires inversion of fermion matrix
- stochastic inversion using conjugate gradient

staggered fermions with 4 flavours
(Wilson fermions as well)

- monitor unitarity norm, log det, distributions, . . .
- compare with HDQCD for heavy quarks and reweighting for light quarks

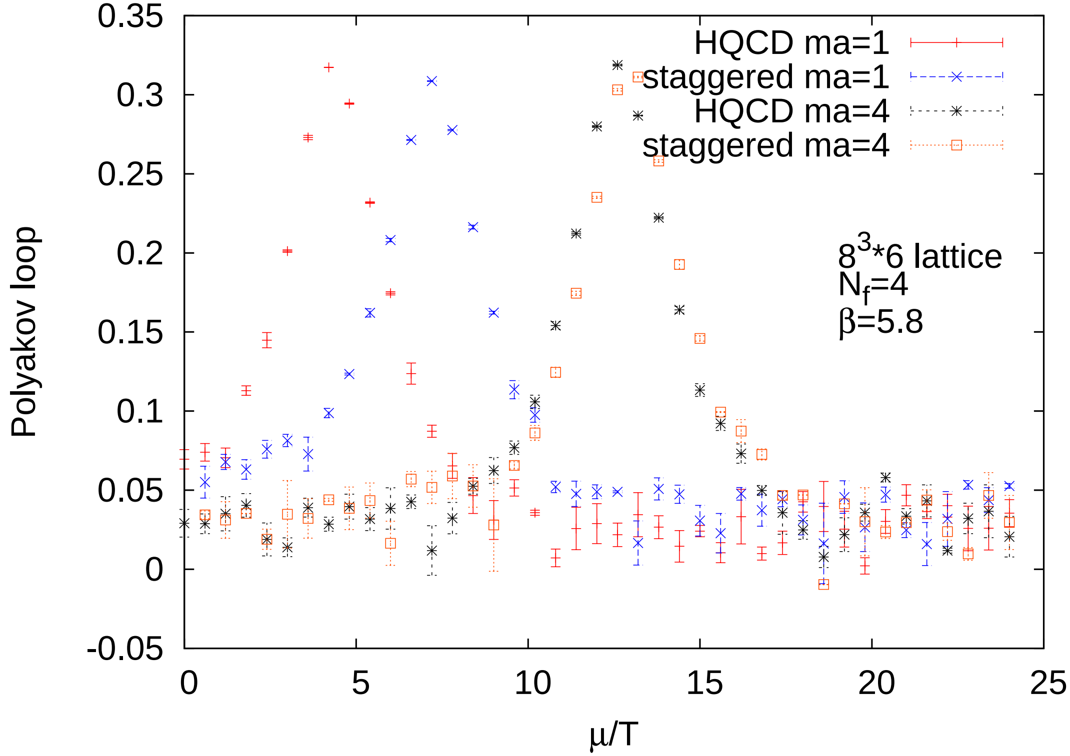
Full QCD



density / density$_{\rm sat}$ vs μ/T

- for heavier quarks and lighter quarks
- comparison with HDQCD

Full QCD

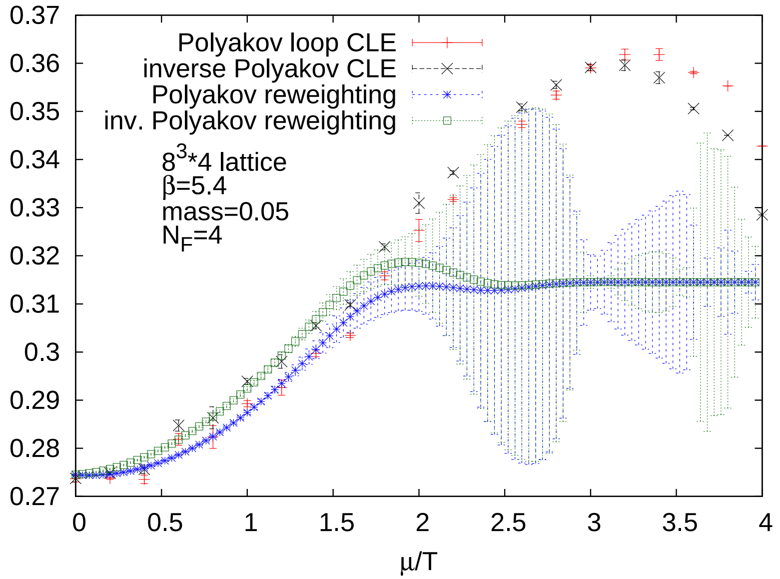


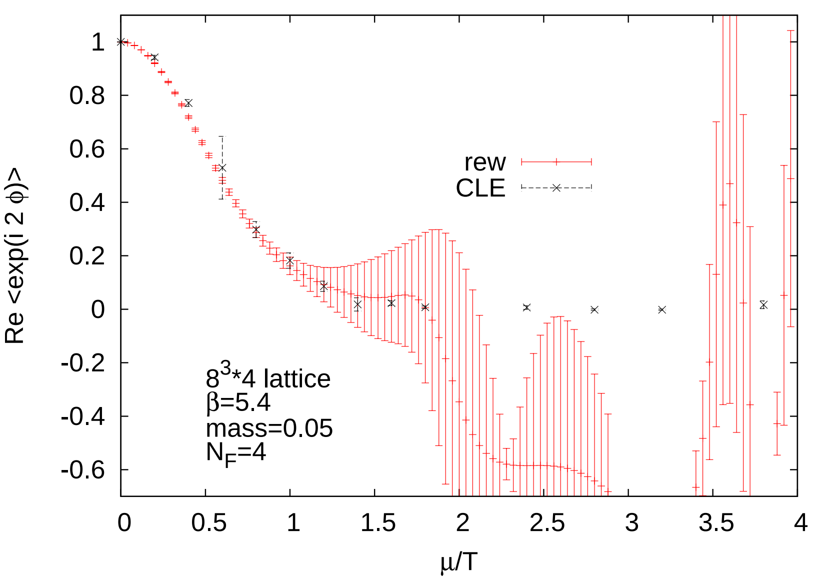
Polyakov loop vs μ/T

- for heavier quarks and lighter quarks
- comparison with HDQCD

Full QCD

comparison with reweighting





Polyakov loop vs μ/T average sign

- for light quarks
- agreement until reweighting breaks down

Fodor, Katz & Sexty in prep

From HDQCD to full QCD:

hopping parameter expansion to all orders

Dénes Sexty, GA, Seiler, Stamatescu 1408.3770

From HDQCD to full QCD

heavy dense QCD

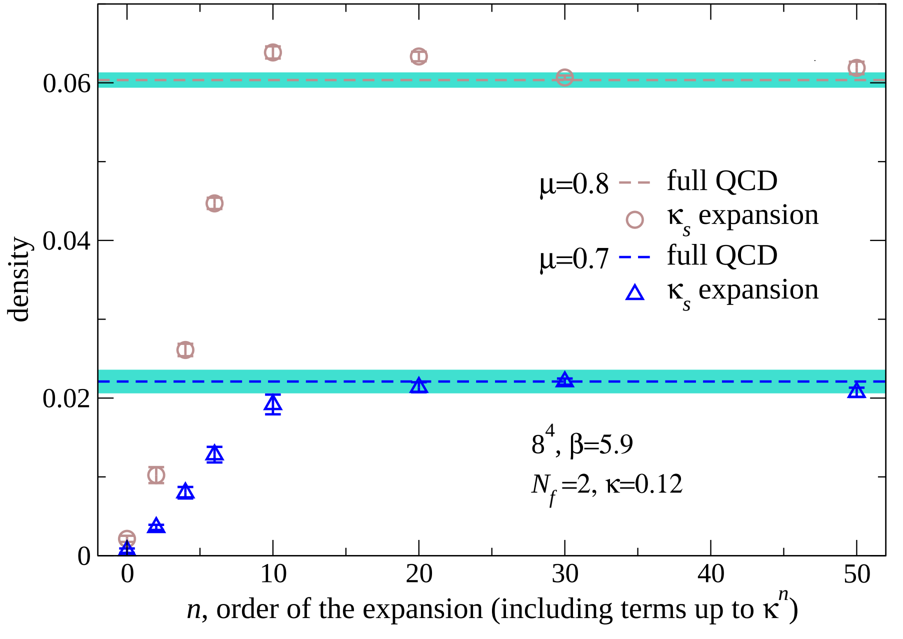
- leading order term in expansion in inverse quark kinetic mass: static limit
- several shortcomings: e.g. $m_B/3 = m_\pi/2 = m_q$, immediate saturation after onset

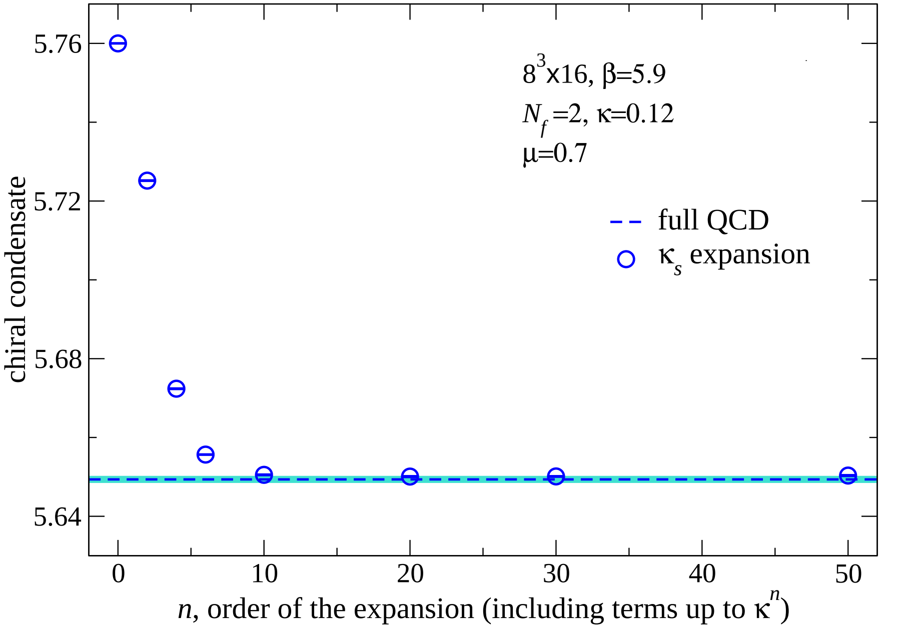
improve and make connection with full QCD

- systematic expansion of quark determinant to all orders in spatial hopping parameter κ_s
- truncate at high order, up to $\mathcal{O}(\kappa_s^{50})$
- determinant still complex: simulate with Langevin
- compare with full QCD results for Wilson fermions

From HDQCD to full QCD

convergence of hopping parameter expansion





density (8^4) chiral condensate ($8^3 \times 16$)

- agreement between expansion and full result
- important cross check
- implies $\log\det$ not a problem

Outlook

QCD at nonzero μ $\quad\Leftrightarrow\quad$ sign problem

relevant for QCD phase diagram, heavy-ion collisions, dense objects, ...

- sign problem has been studied from many perspectives
- 'well understood' (overlap, Silver Blaze, ...)
- towards a solution for QCD

sign problem appears not only in QCD

also in many (lower-dimensional, condensed matter) theories

$\Rightarrow$ learn from those models as well

Outlook

some approaches with (limited) applicability in full QCD:

- overlap preserving reweighting
- Taylor series
- imaginary μ and analytical continuation
- ...

partial or full solutions in not quite QCD (not discussed):

- strong coupling QCD
- flux representations in spin models
- density of states
- ...

at this stage: complex Langevin most promising

Outlook

at this stage: complex Langevin most promising

but...

lots of work to be done!

Where is Swansea?

in Wales, United Kingdom
about three hours from London by direct train

Swansea University

university campus next to the beach

Swansea and the Gower

many beautiful beaches, considerably colder than here!