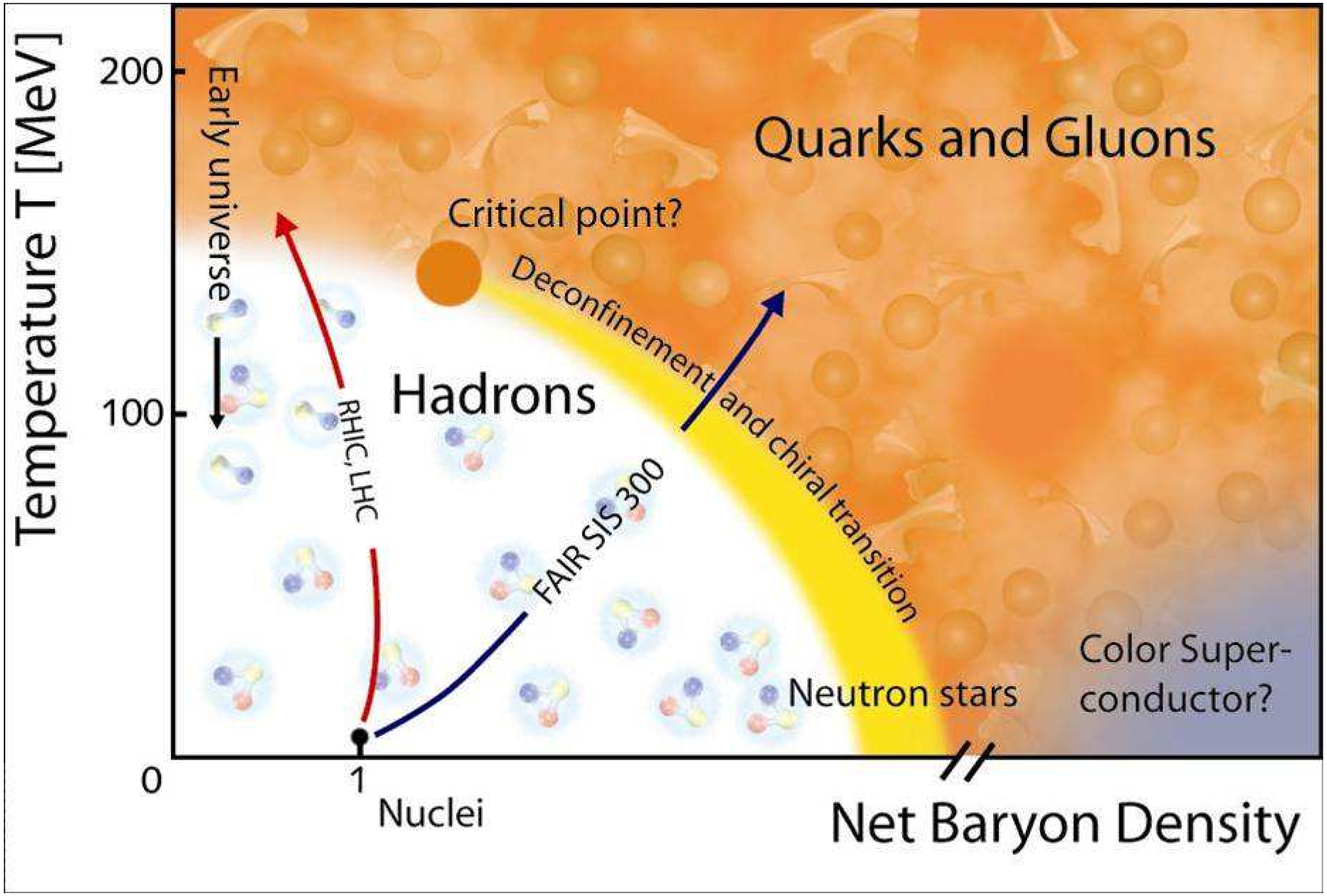
Lattice QCD at nonzero baryon density

Gert Aarts

Swansea University
Prifysgol Abertawe

QCD phase diagram



a well-known possibility

Lattice QCD at nonzero chemical potential

- partition function/euclidean path integral

$$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_{\rm YM}} \det M$$

- fermion determinant is complex

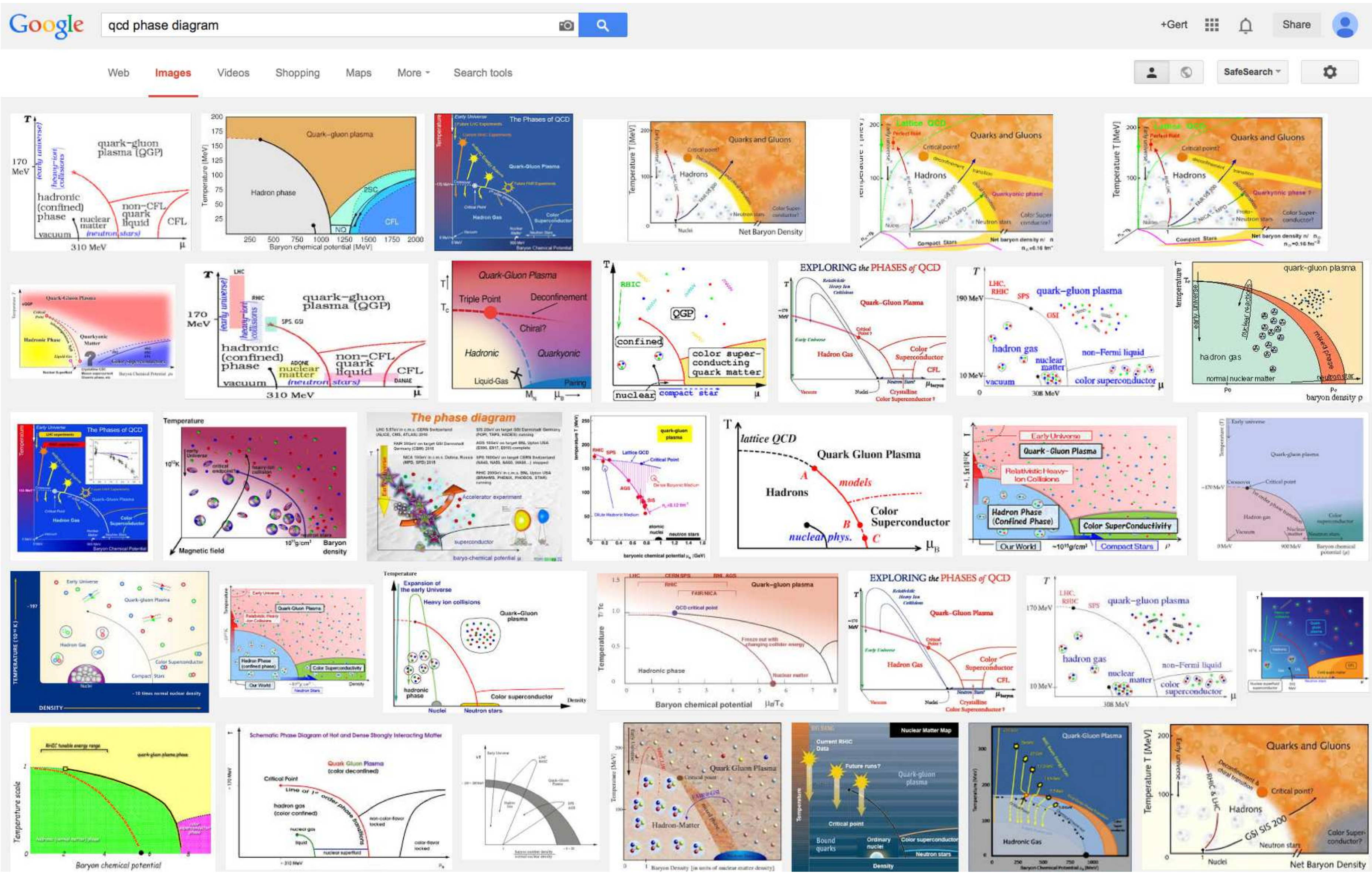
$$[\det M(\mu)]^* = \det M(-\mu^*) \in \mathbb{C}$$

- no positive weight in path integral
- standard numerical methods based on importance sampling not applicable

$\Rightarrow$ sign problem

$\Rightarrow$ phase diagram not yet determined

Many QCD phase diagrams



Outline

- lattice QCD and chemical potential
- sign problem
- some recent advances
  - density of states
  - into the complex plane
  - complex Langevin dynamics
  - Lefschetz thimbles
- QCD with heavy quarks

for review and references (and exercises!), see

Introductory lectures on lattice QCD at nonzero baryon number

`J. Phys. Conf. Ser. 706 (2016) 022004 [arXiv:1512.05145 [hep-lat]]`

Lattice QCD

nonperturbative regularisation of QCD

$$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_{\rm YM}} \det M$$

- define partition function on spacetime lattice
- gluons (U) live on links, quarks ($\psi, \bar{\psi}$) on vertices
- Wick rotation to euclidean time $iS \to -S$
- SU(3) gauge symmetry at *finite* lattice spacing
- recover Lorentz invariance in continuum limit

Lattice QCD

nonperturbative regularisation of QCD

$$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_{\rm YM}} \det M$$

- define partition function on spacetime lattice
- gluons (U) live on links, quarks ($\psi, \bar{\psi}$) on vertices
- Wick rotation to euclidean time $iS \to -S$
- SU(3) gauge symmetry at *finite* lattice spacing
- recover Lorentz invariance in continuum limit
- integrate out fermions by hand: determinant
- 'solve' remaining gluonic integral
- amenable to numerical computation

Lattice QCD

nonperturbative regularisation of QCD

$$Z = \int DU\,D\bar{\psi}D\psi\,e^{-S} = \int DU\,e^{-S_{\rm YM}}\,\det M$$

- amenable to numerical computation
- finite volume: $N_s^3 \times N_\tau$ with $T = 1/aN_\tau$
- real and positive weight

$$0 < e^{-S_{\rm YM}}\,\det M < \infty$$

- use importance sampling to approximate integral
- requires use of large scale numerical facilities
- well-controlled approach to thermodynamics

Chemical potential

- phase diagram: introduce chemical potential μ
- couples to conserved charge (baryon number)

$$n \sim \psi^\dagger \psi = \bar{\psi}\gamma_4\psi = j_4$$

- temporal component of current $j_\nu = \bar{\psi}\gamma_\nu\psi$

on the lattice: fermion hopping terms $j_\nu \sim \kappa\bar{\psi}_x\gamma_\nu\psi_{x+\nu}$

modify temporal hopping terms:

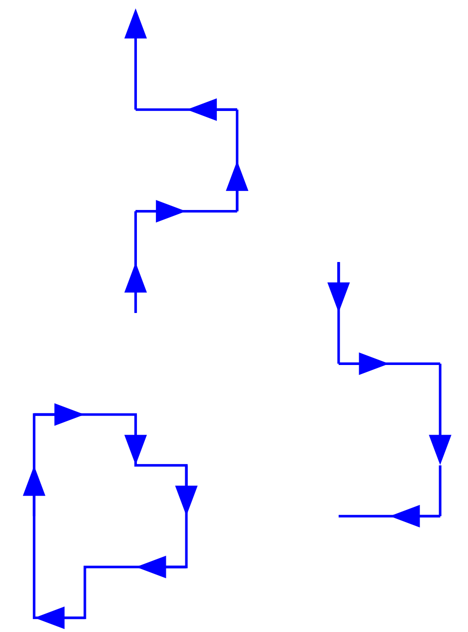
- forward hopping: κe^{μ}
- backward hopping: $\kappa e^{-\mu}$

$\Rightarrow$ exactly conserved (Noether) charge at *finite* lattice spacing

Hasenfratz & Karsch 83

Chemical potential on the lattice

chemical potential introduces an imbalance between forward and backward hopping



- forward hopping (quark)
  $\Rightarrow$ favoured as $e^{\mu n_\tau}$
- backward hopping (anti-quark)
  $\Rightarrow$ disfavoured as $e^{-\mu n_\tau}$
- closed worldline
  $\Rightarrow$ μ dependence cancels exactly

μ dependence only remains when worldline wraps around time direction

$$e^{\mu N_\tau} = e^{\mu/T}$$

$$e^{-\mu N_\tau} = e^{-\mu/T}$$

Chemical potential on the lattice

imbalance leads to fundamental issue: sign problem!

at $\mu = 0$: quark matrix M

$$\det M^\dagger = \det(\gamma_5 M \gamma_5) = \det M = (\det M)^*$$

- real determinant

at $\mu \neq 0$:

$$\det M^\dagger(\mu) = \det \gamma_5 M(-\mu^*)\gamma_5 = \det M(-\mu^*) = [\det M(\mu)]^*$$

- complex determinant
- no real weight: numerical methods break down

note: real determinant for imaginary chemical potential

Roberge & Weiss 86, Lombardo 00, de Forcrand & Philipsen 03-12

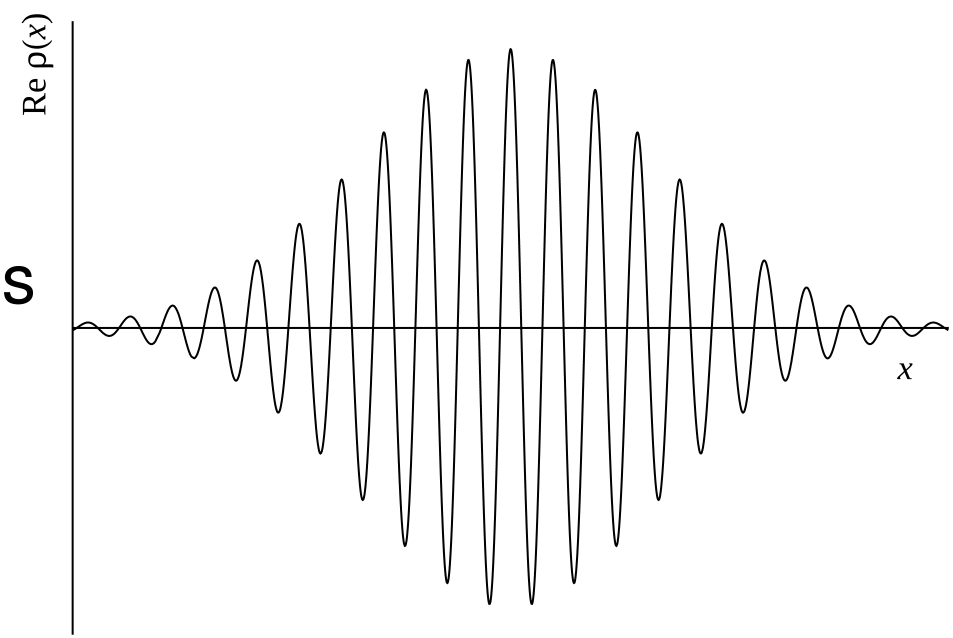
Sign problem

- complex weight is a hard problem: cannot be ignored

$$\det M(\mu) = |\det M(\mu)| e^{i\theta}$$

- correct physics easily destroyed
  (e.g. by ignoring the phase)

dominant configurations
in the path integral?



Sign problem

sign problem not specific for QCD

- appears generically in theories with imbalance
- in both fermionic and bosonic theories
  i.e. not due to anti-commuting nature of fermions
- also in condensed-matter models, e.g. Hubbard model away from half-filling

understanding of sign problem relevant across physics

generic solution to sign problem not expected: NP hard

`Troyer & Wiese 04`

more and more solutions to specific theories available

`SIGN 2017, INT Seattle, March 20-24 2107`

Evading the sign problem

a (personal) selection of solutions to various theories:

- density of states
- complex excursions
  - complex Langevin (CL) dynamics
  - Lefschetz thimbles
- application of complex Langevin to heavy dense QCD

Density of states

Density of states

basic idea:

- do path integral $Z = \int DU\, w(U)$ in two steps, using constrained simulations
- density of states for operator x

$$\rho(x) = \int DU\, w(U)\delta\left[x - x(U)\right]$$

- observables depending on x can be constructed

$$\langle O(x)\rangle = \frac{\int dx\, \rho(x)O(x)}{\int dx\, \rho(x)}$$

- histogram method, factorisation, Wang-Landau, ...

Goksch 1988, Anagnostopoulos & Nishimura 02

Fodor, Katz & Schmidt 07, Ejiri 08, ...

Density of states

main issues:

- constrained integral should have positive weight
- $\rho(x)$ computable to very high relative precision

Density of states

main issues:

- constrained integral should have positive weight
- $\rho(x)$ computable to very high relative precision

theories with a sign problem: $w(U) = |w(U)|e^{i\theta}$

- assume $\theta(n)$ depends only on net density $n(U)$
- positive density of states

$$\rho(x) = \int DU\, |w(U)|\, \delta\left[x - n(U)\right]$$

- observables and partition function

$$\langle O(n)\rangle = \frac{1}{Z}\int dx\, \rho(x) e^{i\theta(x)} O(x) \qquad Z = \int dx\, \rho(x) e^{i\theta(x)}$$

Density of states

$$\langle O(n) \rangle = \frac{1}{Z} \int dx\, \rho(x) e^{i\theta(x)} O(x) \qquad\qquad Z = \int dx\, \rho(x) e^{i\theta(x)}$$

if $\rho(x)$ can be determined to very high precision:

- sign problem isolated in remaining single integral
- cancelations under better control
- precise integration over oscillating function $\rho(x) e^{i\theta(x)}$

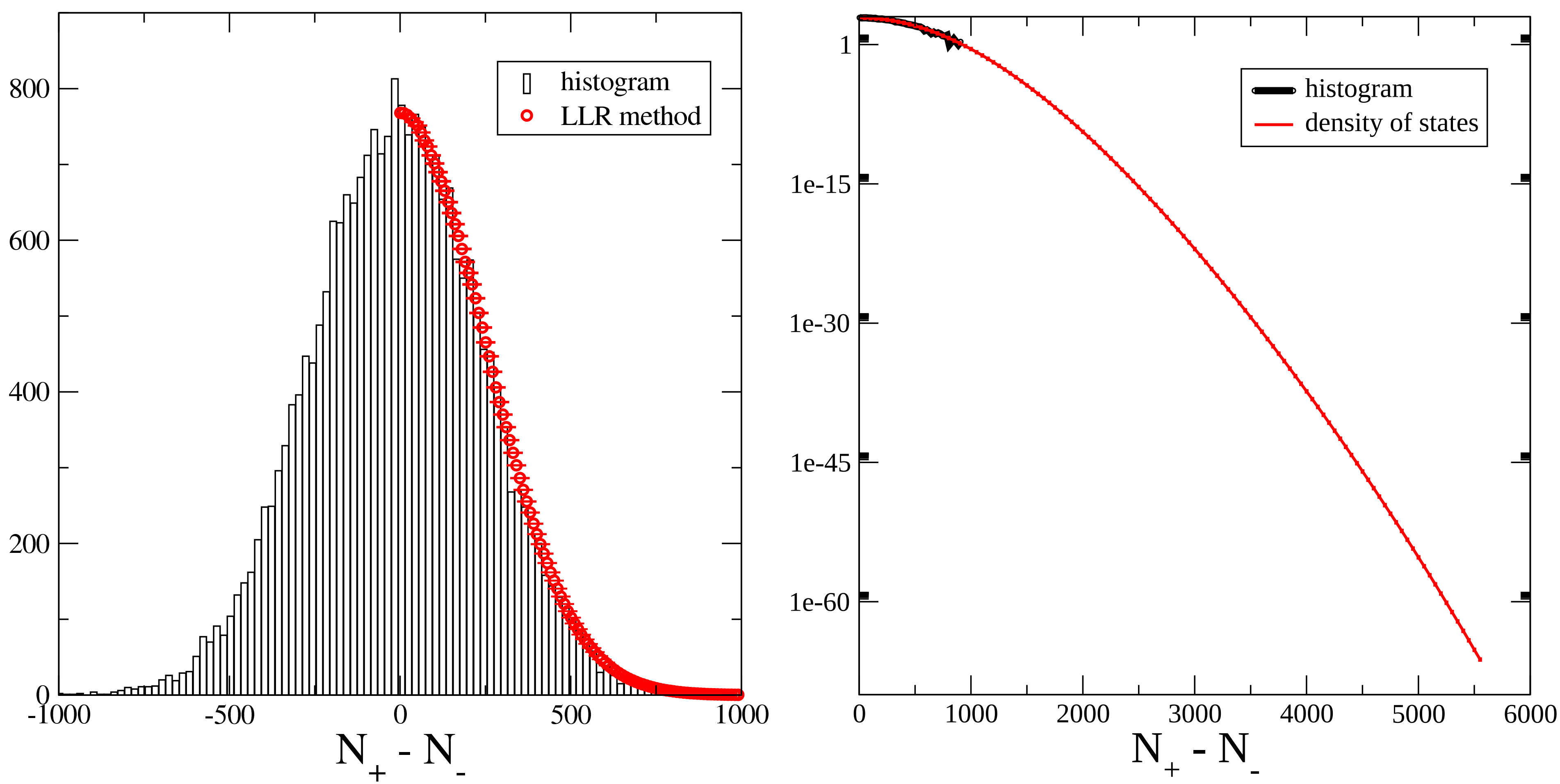
la prova è nel pudding

promising reincarnation: Local Linear Relaxation (LLR)

Langfeld, Lucini & Rago 12

- Z(3) spin model — Lucini & Langfeld 14
- heavy dense QCD — Garron & Langfeld 16

Density of states



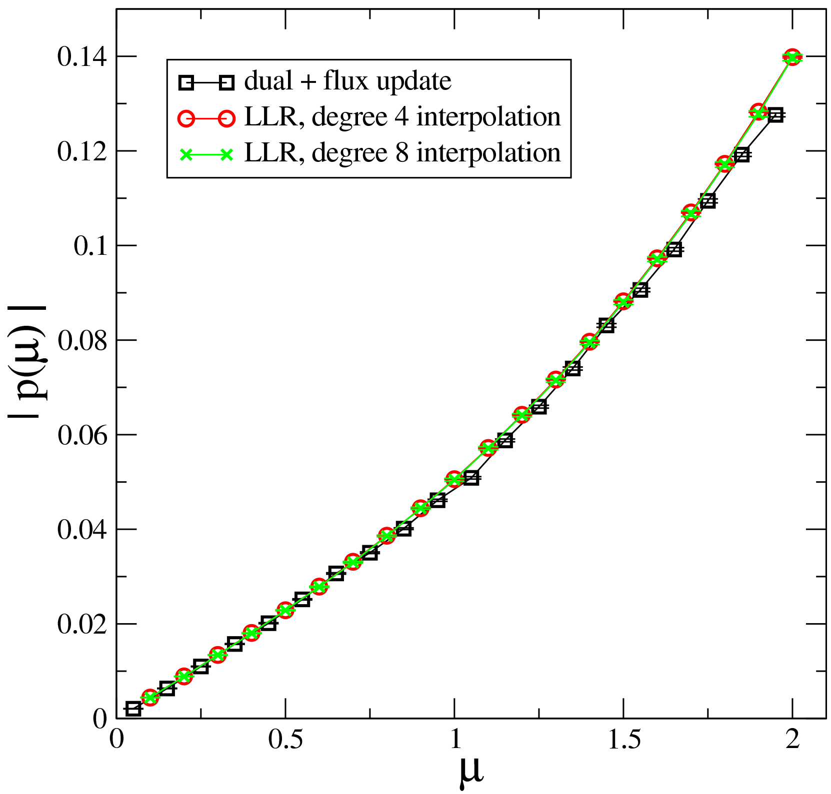
histogram vs. density of states ($x = N_+ - N_-$)

density of states extends over more than 60 orders of magnitude

Density of states

comparison with alternative approach: dual formulation

Gattringer et al 12



- extreme precision needed to carry out remaining oscillatory integral
- agrees with dual method
- potential problems at large μ or at the transition
- under investigation

- improvement on older histogram methods
- extension to gauge theories

Langfeld (Lattice 2016)

Lucini (XQCD 2016)

Complex excursions

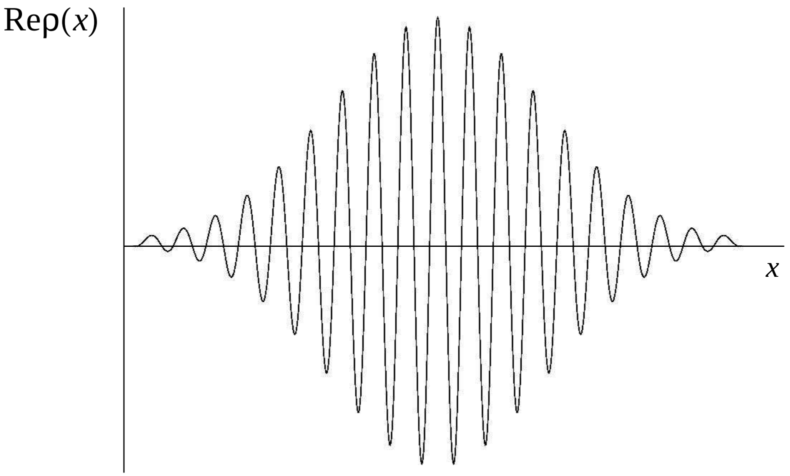
Complex measure

- complex weight

$$\det M(\mu) = |\det M(\mu)|e^{i\theta}$$

- cancelation between configurations with ‘positive’ and ‘negative’ weight

dominant configurations in the path integral?



- take the complexity seriously!

Complex integrals

- consider simple integral

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

- complete the square/saddle point approximation:

  into complex plane

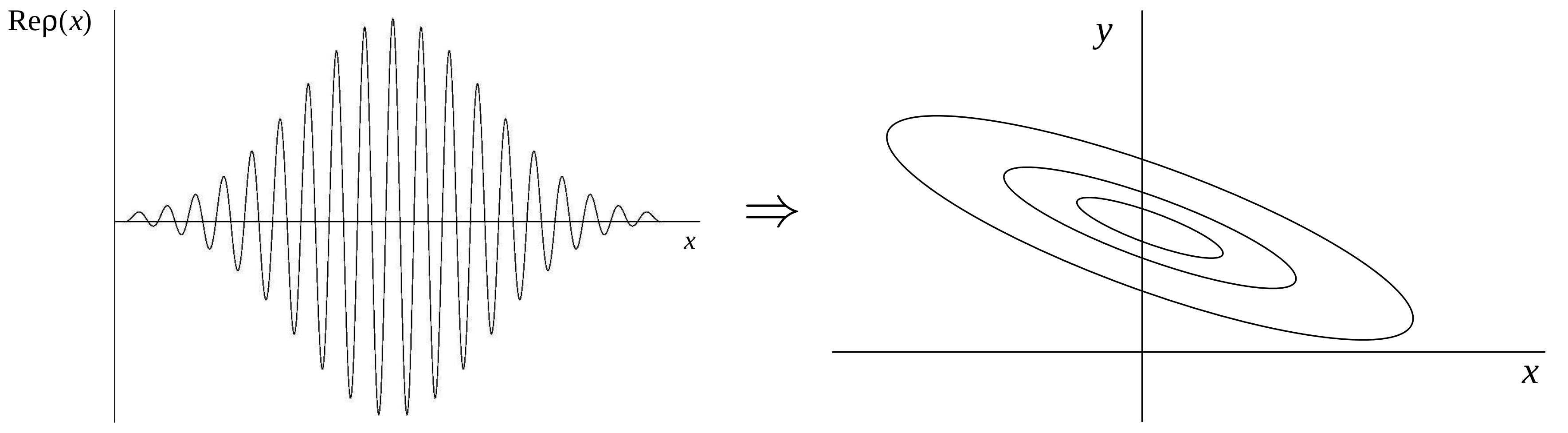
- lesson: don't be real(istic), be more imaginative

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 $P(x, y)$: complex Langevin

Parisi 83, Klauder 83

- deformation of integration contour: Lefschetz thimbles

Airy 1838, Witten 10

Complex Langevin dynamics

with Nucu Stamatescu, Erhard Seiler, Dénes Sexty

Benjamin Jäger, Pietro Giudice, Jan Pawlowski

Lorenzo Bongiovanni, Felipe Attanasio, Frank James, ...

since 2008

Complex Langevin dynamics

main idea:

- generate field configurations using stochastic process

$$\dot{z} = -\partial_z S + \eta \qquad\qquad \langle \eta(t)\eta(t')\rangle = 2\delta(t-t')$$

- reach equilibrium distribution à la Brownian motion
- no importance sampling required

Langevin drift $K = -\partial_z S$ derived from complex weight:

explore complexified configurations

- one degree of freedom: $z \to x + iy$
- real scalar field: $\phi(x) \to \phi_{\mathrm{R}}(x) + i\phi_{\mathrm{I}}(x)$
- gauge link U: SU(3) $\Rightarrow$ SL(3,$\mathbb{C}$)

rely on holomorphicity

Complex Langevin dynamics

applicability for holomorphic actions:

- check criteria a posteriori GA, Seiler & Stamatescu 09
- gauge cooling essential Seiler, Sexty & Stamatescu 12

successful applications to various models, including with phase transitions and severe sign problems

but success not guaranteed (criteria)

open question: meromorphic drift

- with weight $\det M$: drift contains $\mathrm{Tr}\, M^{-1}$
- poles: problems *may* appear Mollgaard & Splittorff 13
- ongoing work GA, Seiler, Sexty & Stamatescu
  Nagata, Nishimura & Shimasaki 16, ...

Lefschetz thimbles

Lefschetz thimbles

- explore complexified field configurations with more analytical control

Lefschetz thimbles: generalised saddle point expansion

- integrate along lines of steepest descent
- keep sign problem under control
- implemented in various models

Christoforetti, di Renzo, Mukherjee, Scorzato, Schmidt et al 12–16

Fujii, Kikukawa, Tanizaki et al 13–16

- comparison with complex Langevin dynamics

GA 13, GA, Bongiovanni, Seiler & Sexty 14

- relax conditions of strict thimble integration

Alexandru, Bedaque et al 15–16

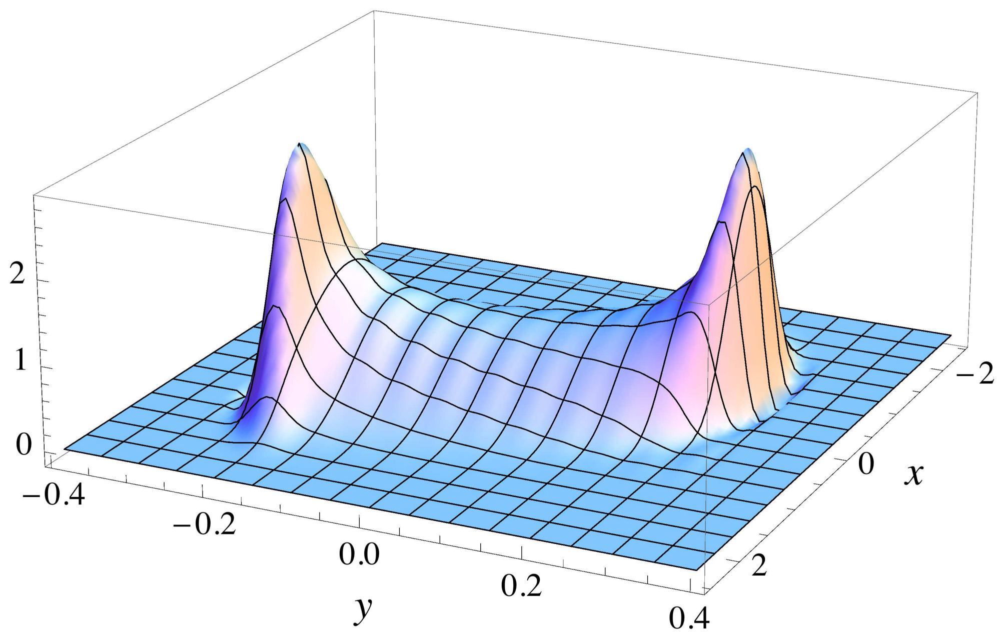
Example: Quartic model

$$Z = \int_{-\infty}^{\infty} dx\, e^{-S} \qquad\qquad S(x) = \frac{\sigma}{2}x^2 + \frac{\lambda}{4}x^4$$

complex mass parameter $\sigma = A + iB$, $\lambda \in \mathbb{R}$

often used toy model Ambjorn & Yang 85, Klauder & Petersen 85, Okamoto et al 89, Duncan & Niedermaier 12

real and positive distribution sampled in CL dynamics



essentially analytical proof for CL: GA, Giudice & Seiler 13

Example: Quartic model

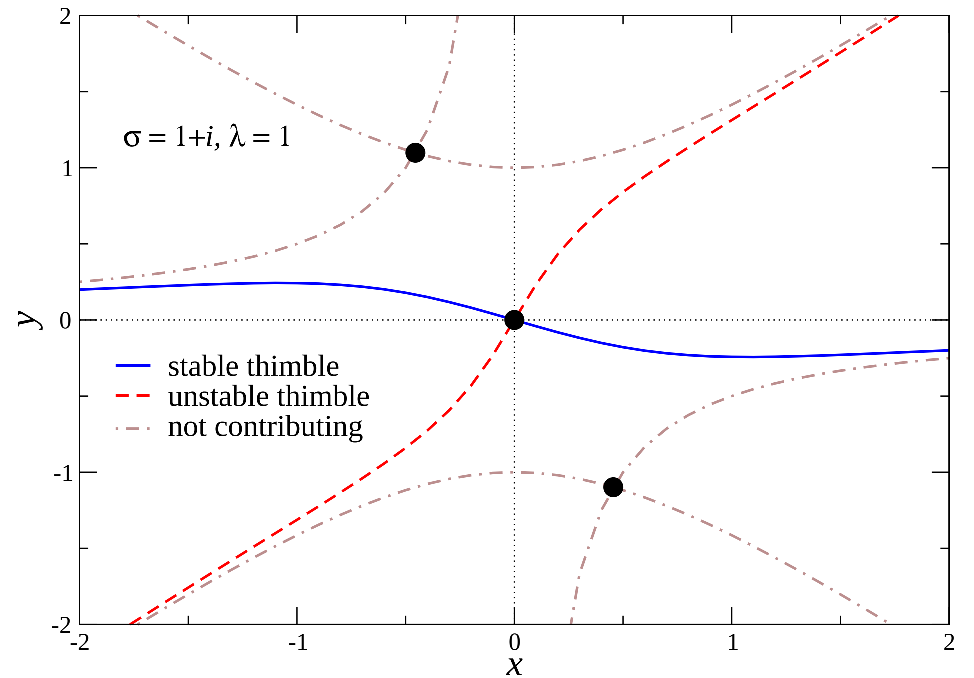
Lefschetz thimbles: saddle point expansion through stationary (critical) points

- critical points:

$$z_0 = 0$$
$$z_\pm = \pm i\sqrt{\sigma/\lambda}$$

- thimbles can be computed analytically

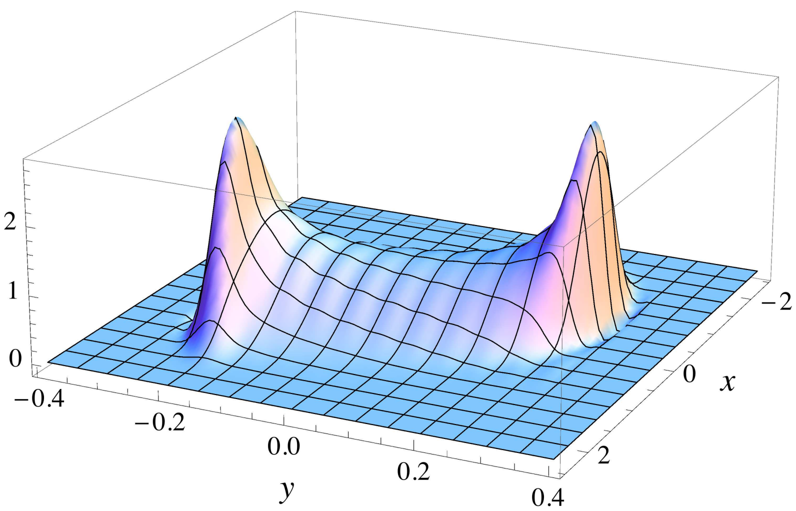
$$\mathrm{Im}S(z_0) = 0$$
$$\mathrm{Im}S(z_\pm) = -AB/2\lambda$$

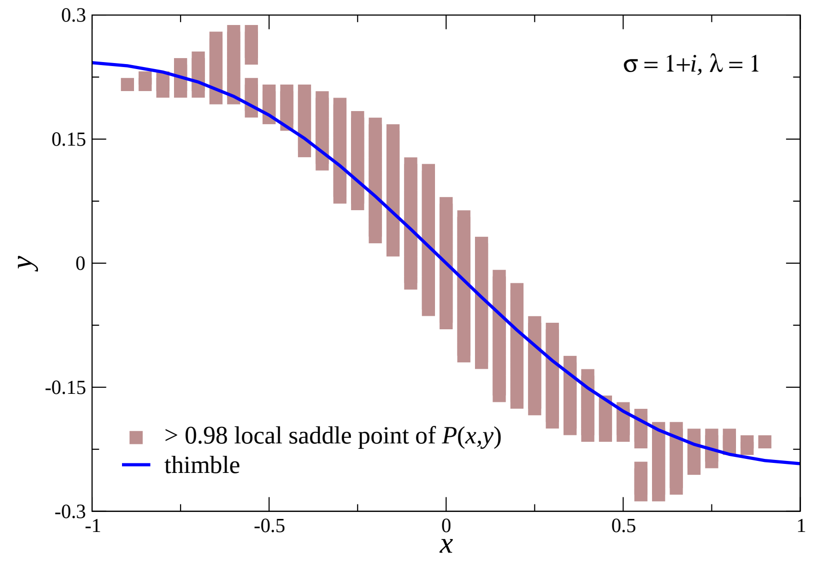


- for $A > 0$: only 1 thimble contributes
- integrating along thimble gives correct result, with inclusion of complex Jacobian

Langevin versus Lefschetz

compare thimble and Langevin distribution





- thimble and CL distribution follow each other
- however, weight distribution quite different

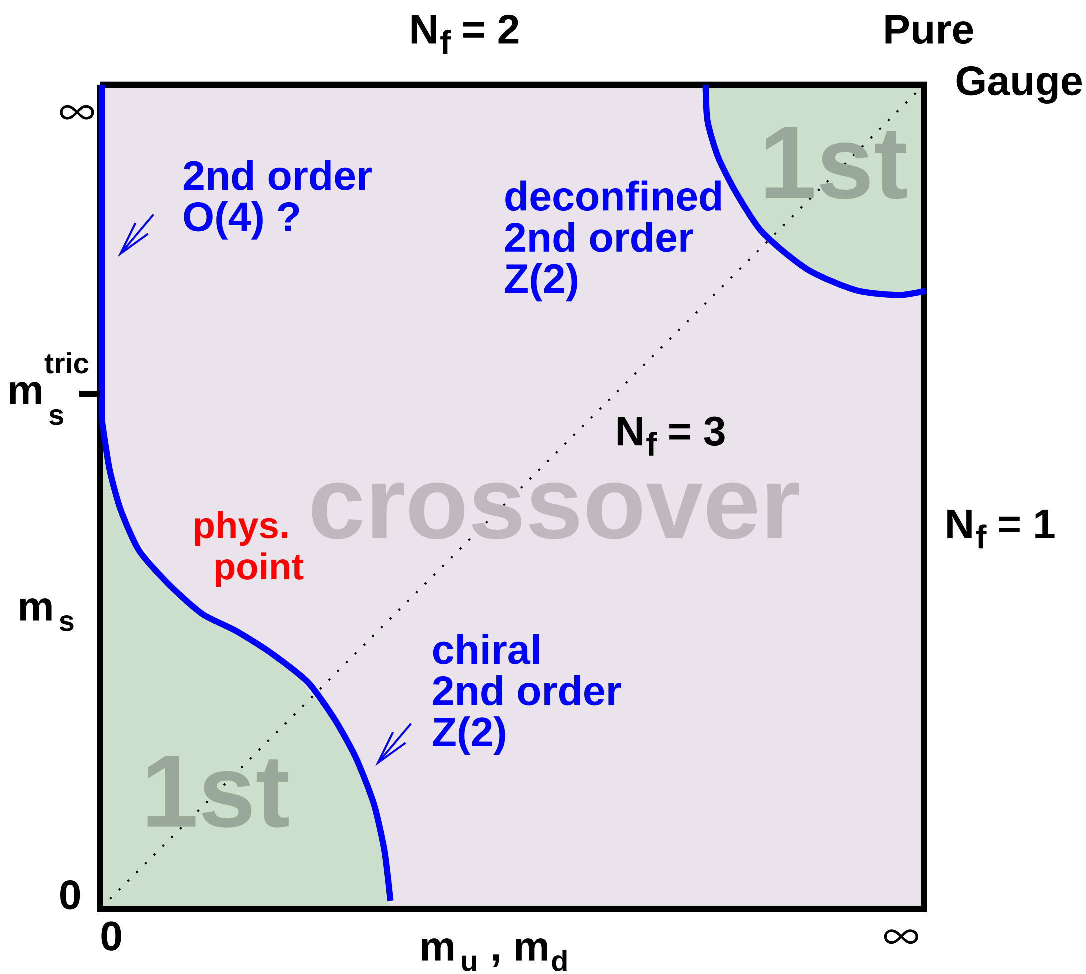
intriguing result: going into the complex plane can evade sign problem in several ways

QCD with heavy quarks

Complex Langevin dynamics

QCD phase structure

Columbia plot: order of thermal transition at $\mu = 0$



QCD with heavy quarks

heavy quark corner of Columbia plot

- first order transition to deconfined phase
- Polyakov loop order parameter
- quark determinant simplifies considerably
- hopping expansion (LO): only straight quark world lines
- fermion determinant

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

$\mathcal{P}_{\mathbf{x}} =$ untraced Polyakov loop $\qquad h = (2\kappa)^{N_\tau}$

- determine phase diagram in heavy quark sector

widely used limit of QCD to test methods

QCD with heavy quarks

expectations for phase diagram

two transitions:

- full Wilson gauge action is included
- thermal deconfinement transition (as in pure glue)

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

- μ-driven transition: $2\kappa e^{\mu} \gtrless 1$
- critical chemical potential for onset at $\mu_c = -\ln(2\kappa)$

determine phase diagram by direct simulation in $T - \mu$ plane

test case for full QCD

Complex Langevin dynamics

QCD with static quarks or heavy dense QCD (HDQCD)

GA, Attanasio, Jäger, Seiler, Sexty & Stamatescu 08-16
GA, Attanasio, Jäger & Sexty, JHEP [arXiv:1606.05561 [hep-lat]]

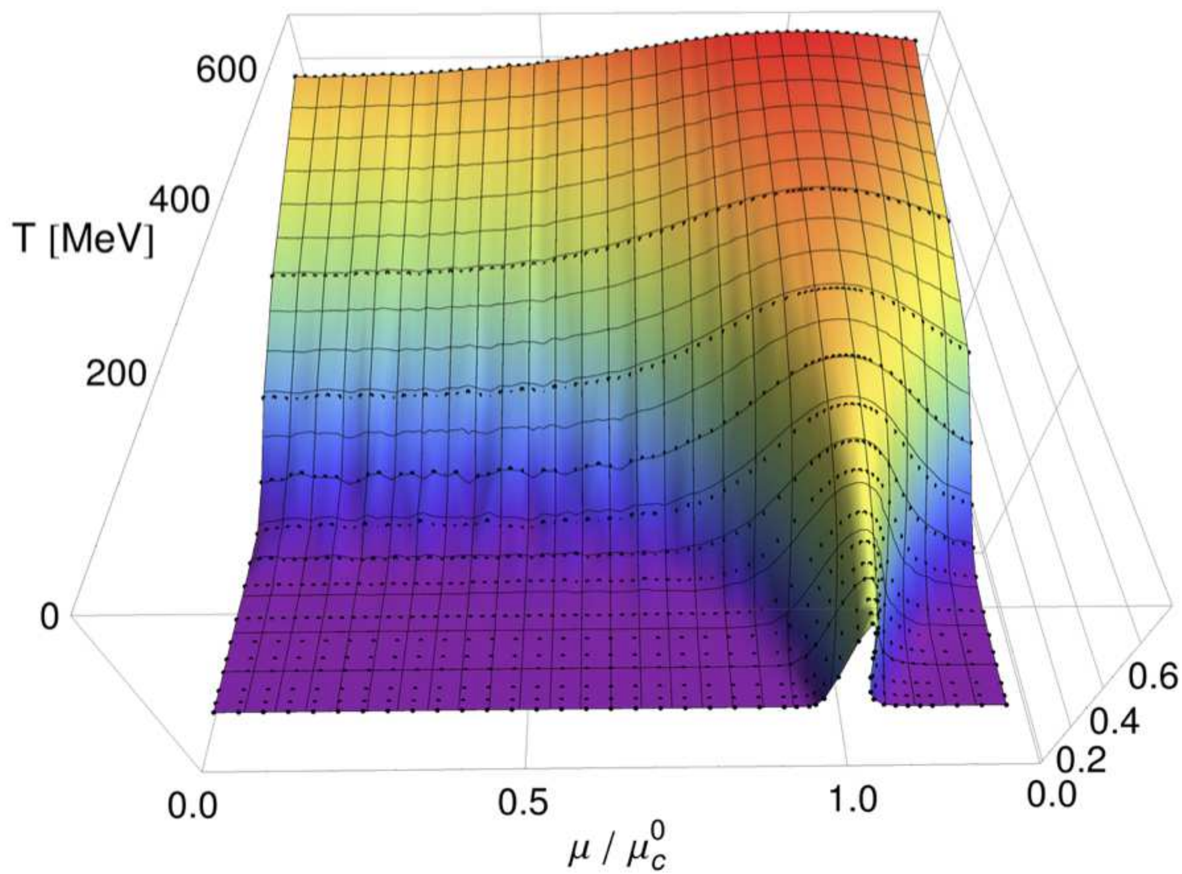
simulation details

- lattice coupling/spacing: $\beta = 5.8 \qquad a \sim 0.15$ fm
- hopping parameter: $\kappa = 0.04 \qquad \mu_c^0 = -\ln(2\kappa) = 2.53$
- spatial volume $6^3, 8^3, 10^3$
- $N_\tau = 2\ 3\ 4\ 5\ 6\ 7\ 8\ 9\ 10\ 11\ 12\ 13\ 14\ 15\ 16\ 18\ 20\ 24\ 28$
- $T \sim 48 \ldots 671$ MeV
- direct simulation in $T - \mu$ plane ($\sim$ 880 parameter combinations)

observables: Polyakov loop, quark density

Heavy dense QCD

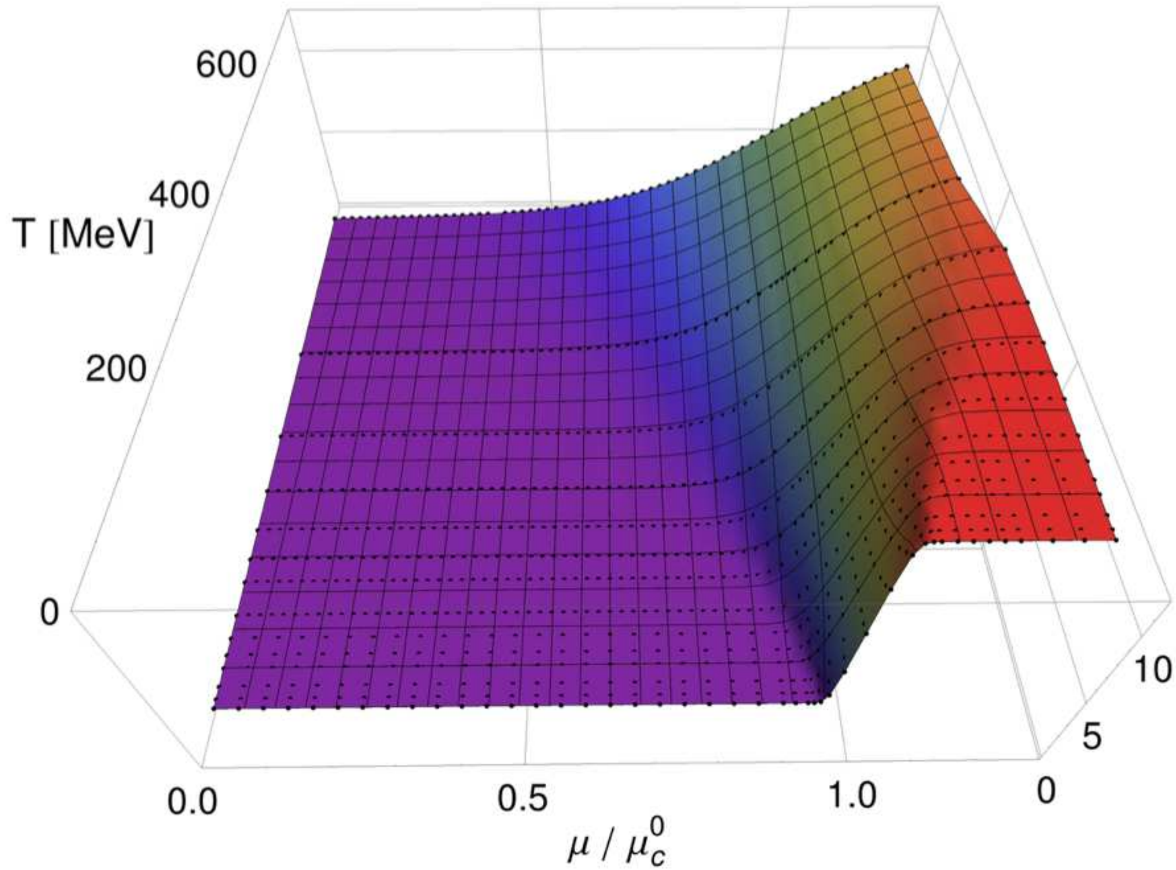
Polyakov loop



- $\langle P \rangle = 0$ at low T, μ: confinement
- $\langle P \rangle \neq 0$ at high T, μ: deconfinement
- $\mu > \mu_c^0$ at $T = 0$: saturation, lattice artefact, unphysical

Heavy dense QCD

density

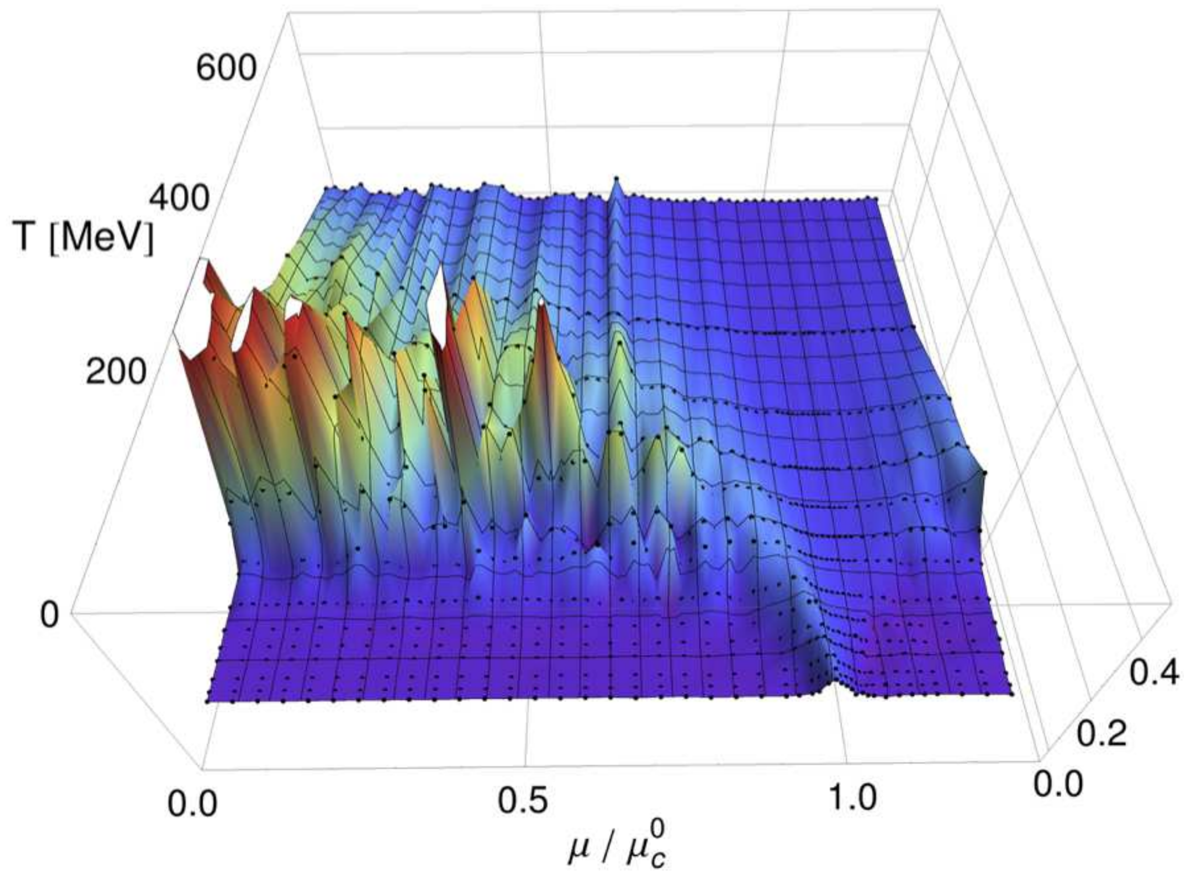


- $\langle n \rangle = 0$ at $\mu = 0$
- $\langle n \rangle$ rises slowly at high T, onset at low T
- $\mu > \mu_c^0$ at $T = 0$: saturation, lattice artefact, unphysical

Heavy dense QCD

attempt to determine the phase boundary

Polyakov loop susceptibility $\chi_P \sim \langle P^2 \rangle - \langle P \rangle^2$



signal not very clear

Heavy dense QCD

better estimate of boundary: Binder cumulant B

for order parameter O

$$B = 1 - \frac{\langle O^4 \rangle}{3\langle O^2 \rangle^2}$$

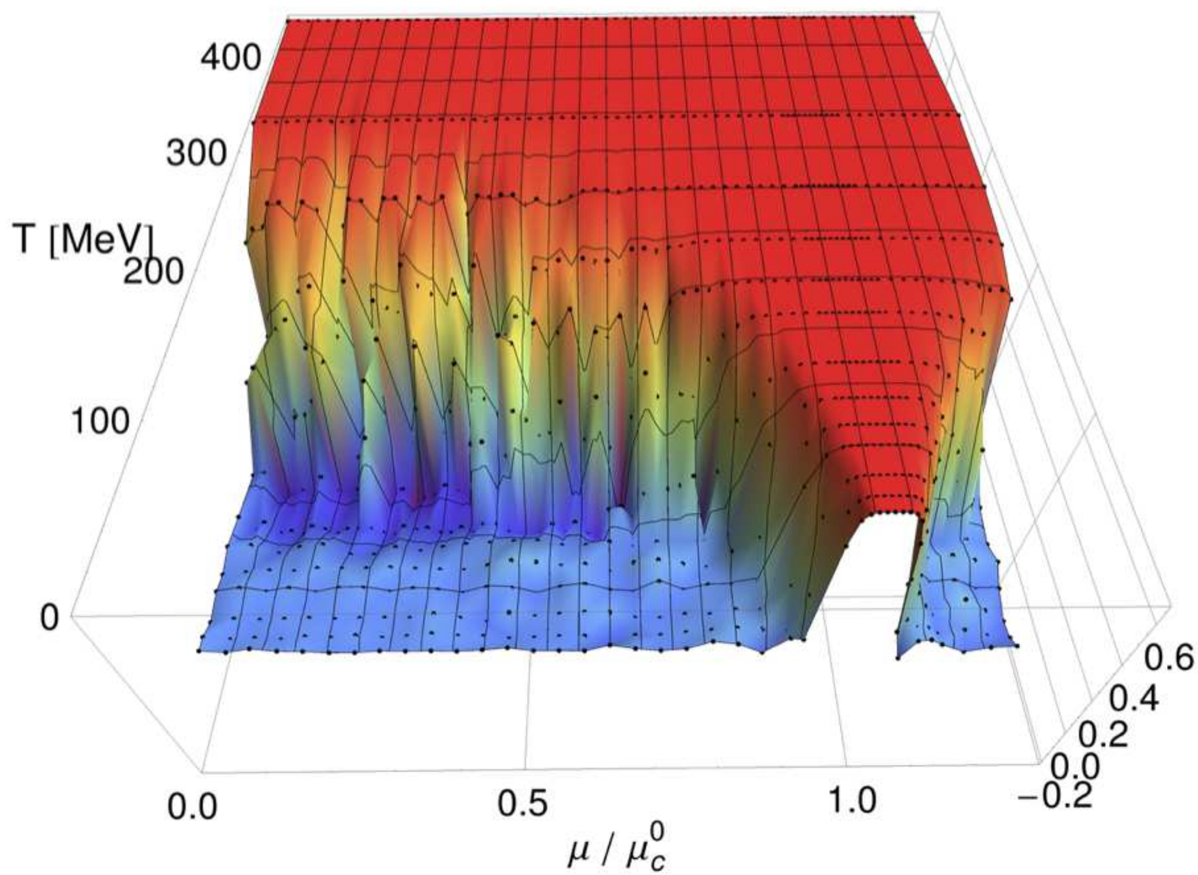
then

$$\langle O \rangle = 0 \Leftrightarrow B = 0 \qquad\qquad \langle O \rangle \neq 0 \Leftrightarrow B = \frac{2}{3}$$

(assume Gaussian fluctuations)

Heavy dense QCD

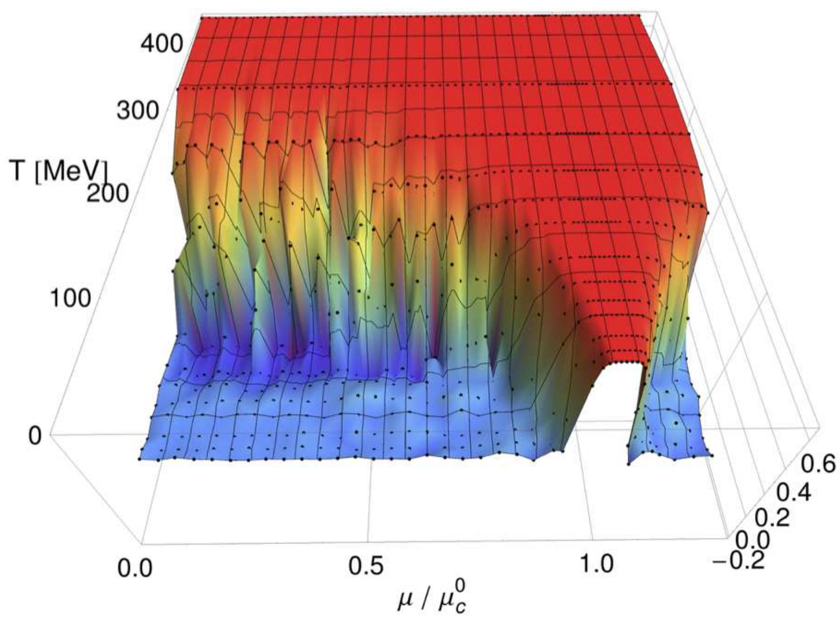
Binder cumulant

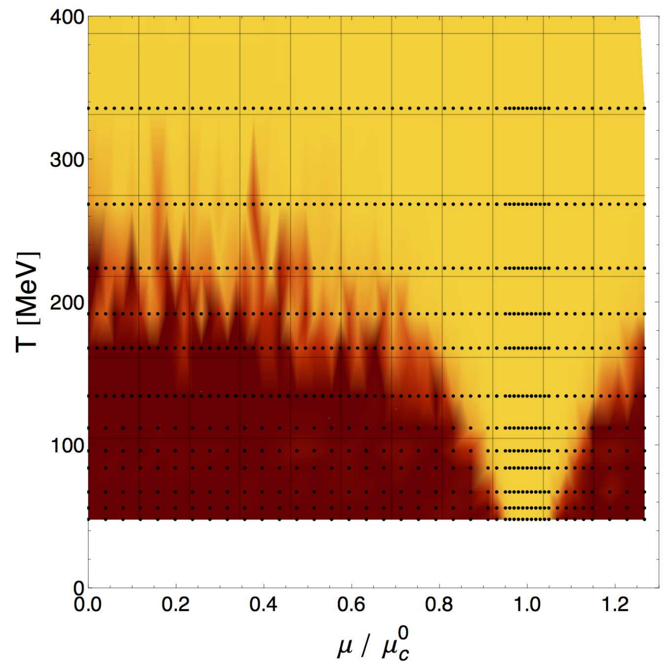


- $B \sim 0$ at low T, μ
- $B \sim 2/3$ at high T, μ

Heavy dense QCD

Binder cumulant: phase boundary





- determine boundary by $B = 1/3$
- fixed lattice spacing:
  less resolution at higher temperature $T \sim 1/N_\tau$

Heavy dense QCD phase diagram

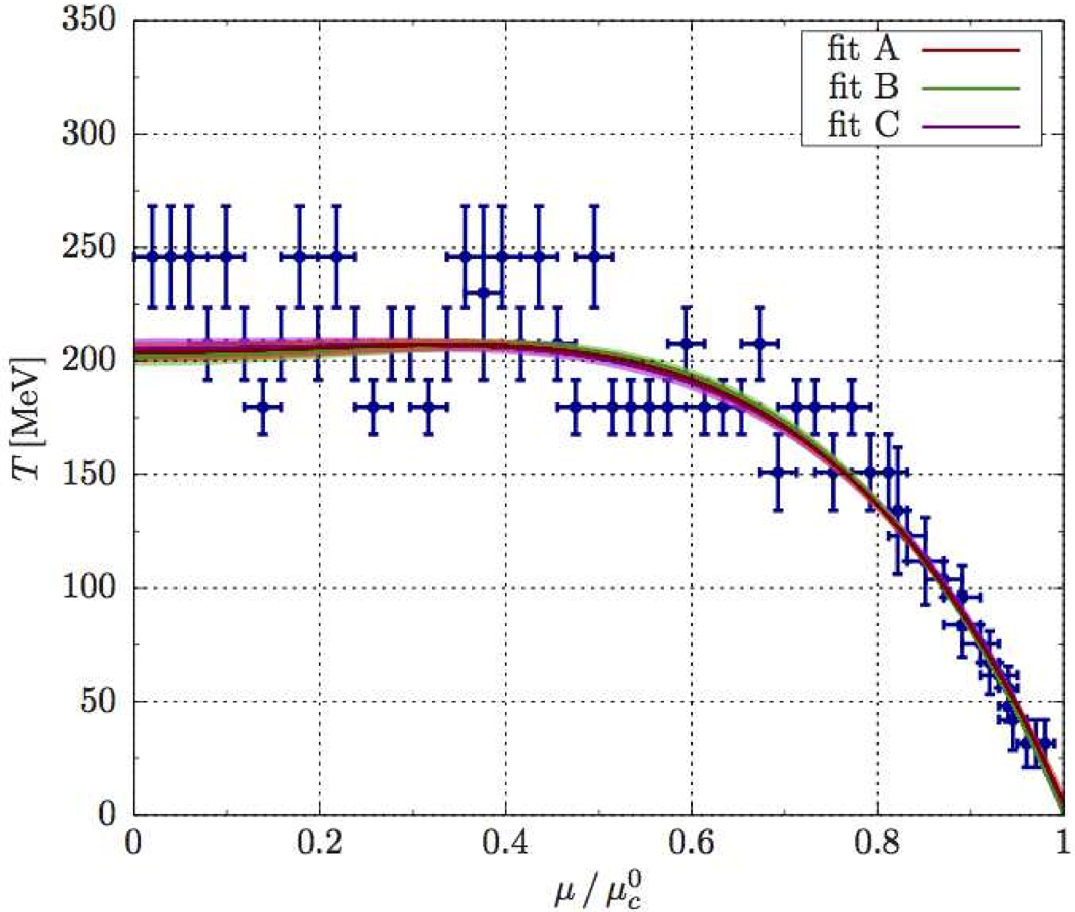
use simple Ansätze for phase boundary

$$x = \left(\mu/\mu_c^0\right)^2$$

$$A: \qquad T_c(\mu) = \sum_k a_k x^k$$

$$B: \qquad T_c(\mu) = \sum_k b_k (1-x)^k$$

$$C: \qquad T_c(\mu) = B + c_0 (1-x)^\alpha$$



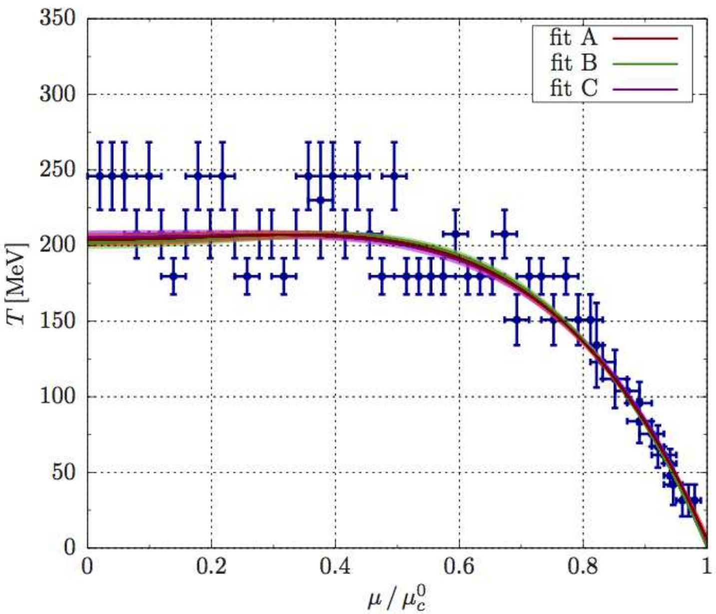
- simple fits up to μ^4 (2 parameters) are sufficient
- no sign for nonanalyticity at $T = 0$ from data yet

Heavy dense QCD phase diagram

possible to determine and parametrise boundary

many things to improve

- fixed lattice spacing
- affects thermal transition
- order of transition
- vary κ: critical endpoints
- beyond LO Philipsen et al, 10–16



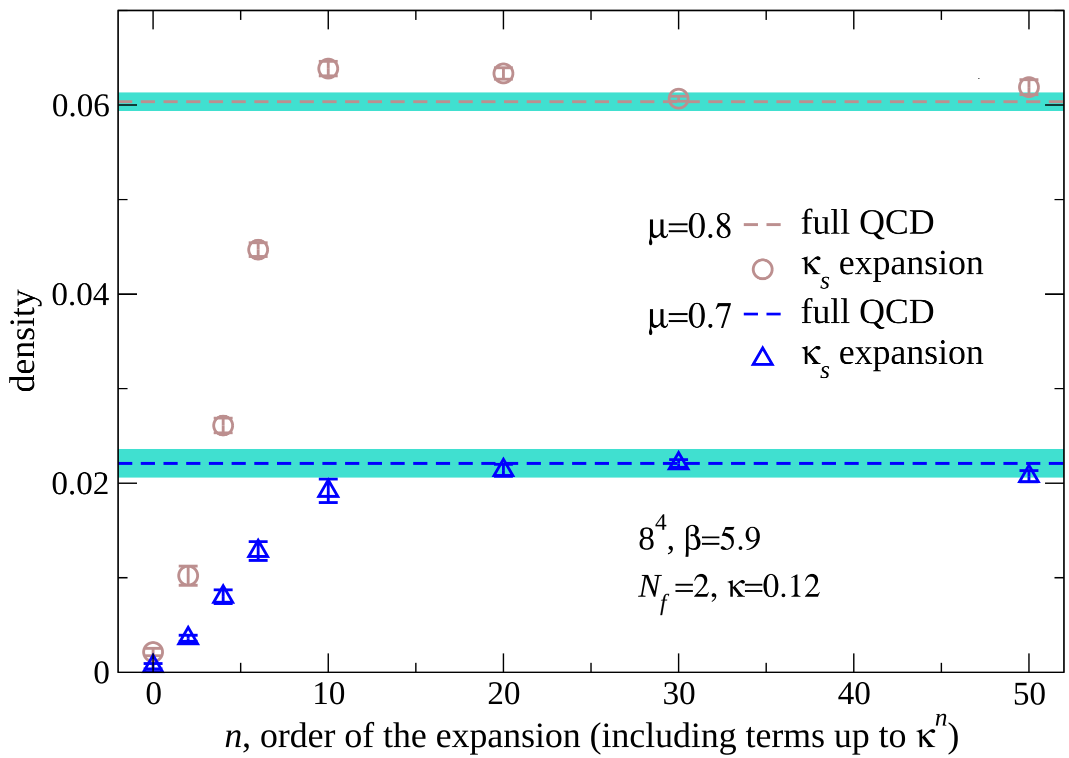
- extension to dynamical quarks Sexty 13

  GA, Seiler, Sexty & Stamatescu 14, + Attanasio, Jäger 14–16

Complex Langevin dynamics: Full QCD

- implementation of hopping parameter expansion to high order $\mathcal{O}(\kappa^{50})$ and comparison with full QCD

  Sexty 13 GA, Seiler, Sexty & Stamatescu 14



open questions related to Langevin:

drift with poles (lack of holomorphicity)

stabilisation

- more groups at Lattice2016: Kogut & Sinclair, Nagata, Nishimura & Shimasaki, GA, Attanasio, Jäger, et al

Outlook

towards the phase diagram of QCD from the lattice

- various ideas under investigation
- new algorithms: implementation in simpler models

for full QCD most promising avenues:

- density of states
- into complex plane
  - complex Langevin dynamics: first full QCD results
  - considerable activity in thimbles