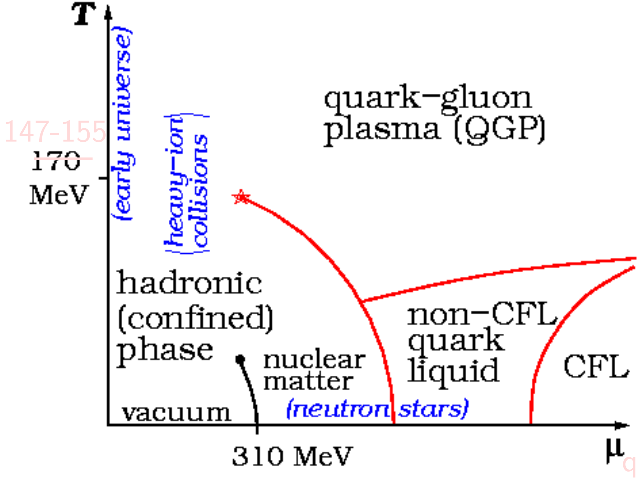
The phase diagram of QCD - a lattice perspective

Attila Pásztor

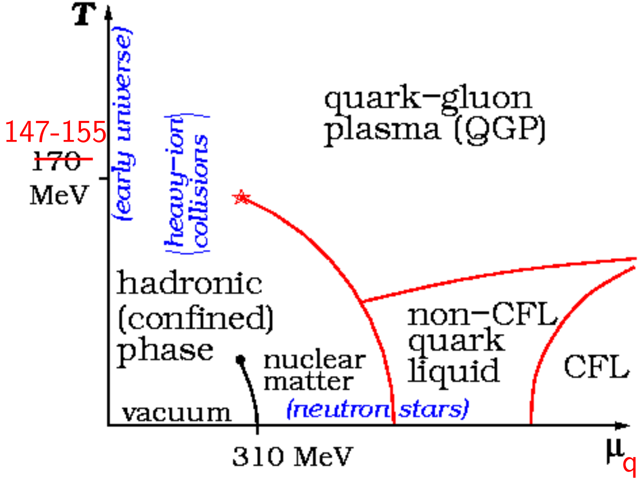
University of Wuppertal
Wuppertal-Budapest Collaboration

FAIRNESS 2017
June 1st 2017, Sitges, Spain

The phase diagram of QCD according to Wikipedia

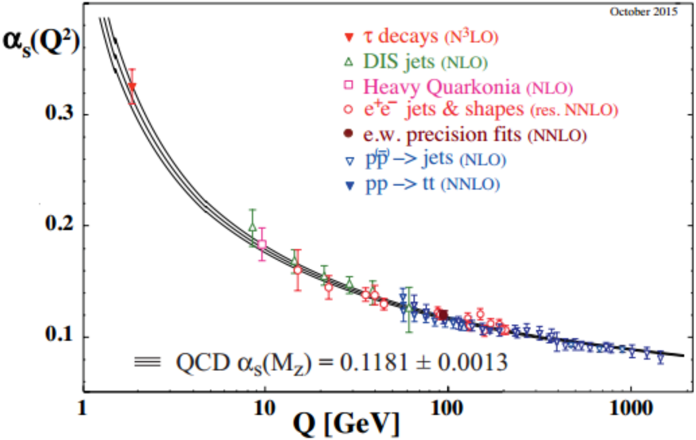


The phase diagram of QCD according to Wikipedia

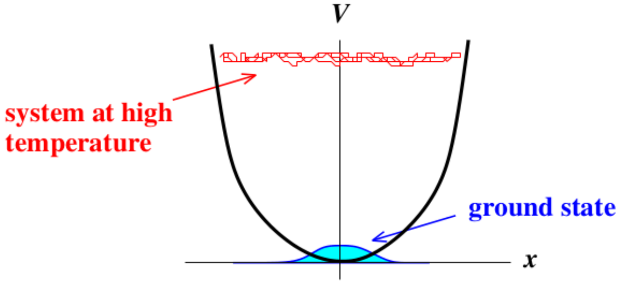


Why lattice QCD?

The Strong Coupling Constant (PDG)

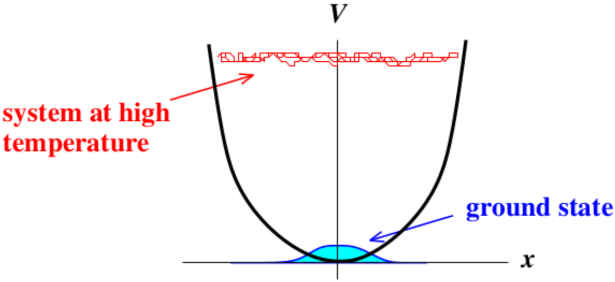


Finite temperature



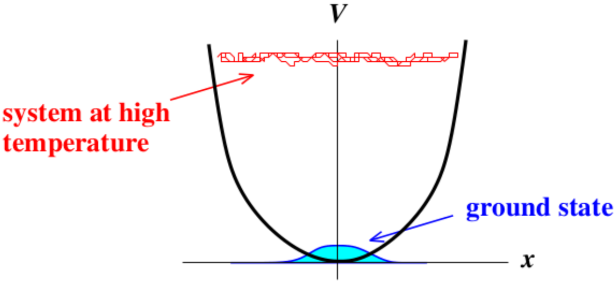
At finite T naive perturbation theory breaks down, even for small g. To illustrate: Imagine a particle moving in a slightly anharmonic potential $V(x) \sim \omega_0^2 x^2 + g x^4$ (mass term + coupling term)

Finite temperature



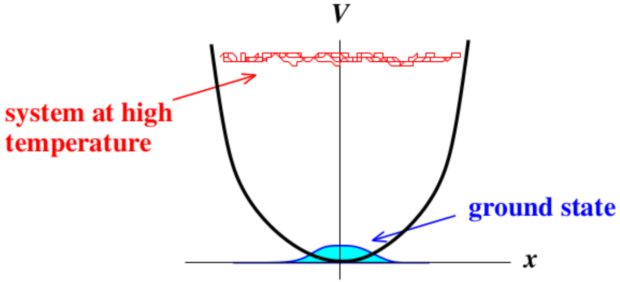
If we ask questions about the ground state, we can approximate the potential by a harmonic oscillator and treat the quartic piece as a perturbation, since the ground state wave function will only extend over a range of x where gx^4 is small compared to $\omega_0^2 x^2$.

Finite temperature



At high temperature states probe a large range of x. No matter how small g is, gx^4 will always be bigger than $\omega_0^2 x^2$ for large enough x. So at high enough T, a perturbative treatment in g breaks down.

Finite temperature

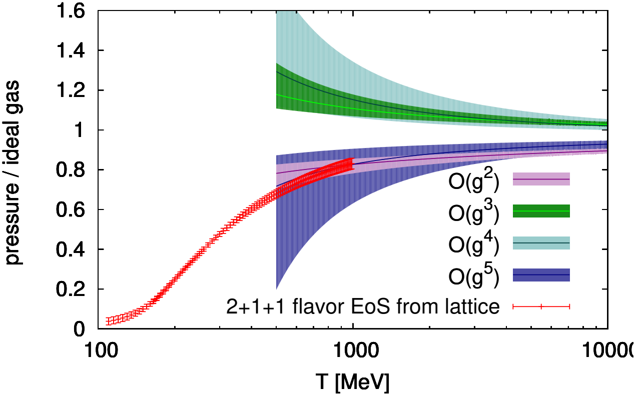


In the example, I phrased the problem as one of high T for fixed potential $V(x)$. However, I would have encountered the same problem if I had held T and g fixed but decreased ω_0 ($\rightarrow$ this is analogous to gauge theories at finite temperature)

The pressure in perturbative QCD

lQCD : WB: Nature 539 (2016) no.7627, 69-71

pQCD: Kajantie et al: PRD67 (2003) 105008



What is lattice gauge theory?

α_s

Lattice field theory is a non-perturbative regularization scheme of Euclidean quantum field theory.

Lattice $\to$ UV cutoff $\sim \pi/a$

Imaginary time: $t = -i\tau$

Discretize Euclidean space-time domain on a $N_s^3 \times N_\tau$ spacetime lattice.
Most commonly with periodic boundary conditions.

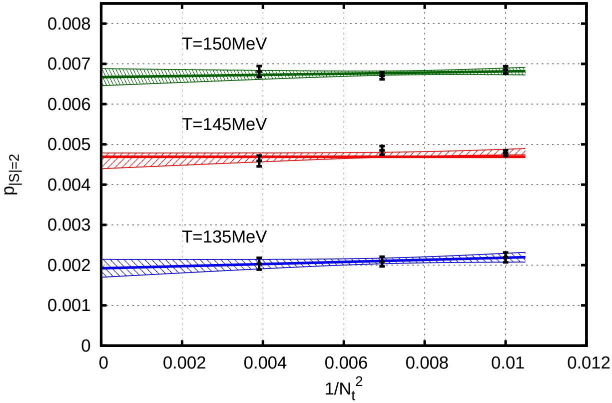
Finite temperature $T = \frac{1}{N_t a}$

Also important: renormalization and continuum limit.

For T fixed, $1/N_t \sim a$.

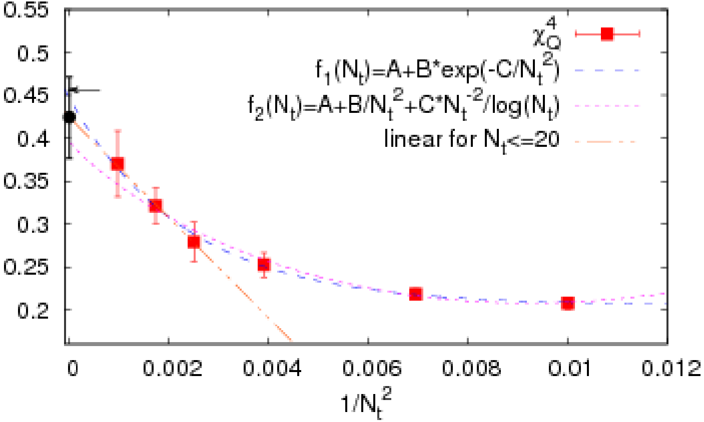
The continuum limit is important!!!

Cut-off effects can be mild. E.g. the $S = 2$ partial pressure



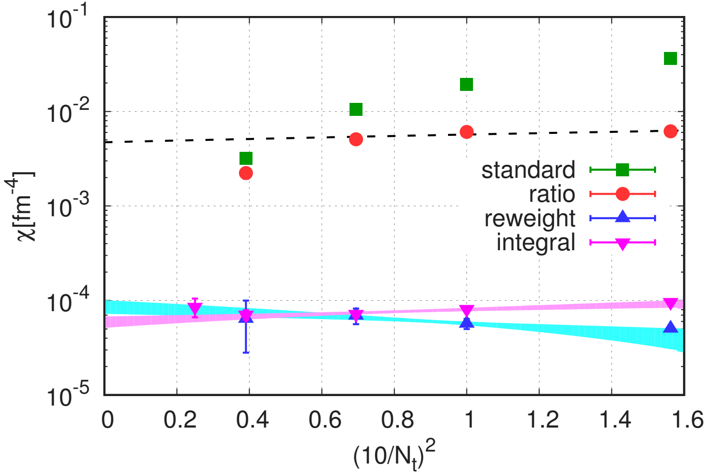
The continuum limit is important!!!

Cut-off effects can be big. E.g. charge fluctuations



The continuum limit is important!!!

Cut-off effects can be enormous. Example: Topological susceptibility



QCD thermodynamics at $\mu_B = 0$
The QCD transition

Deconfinement: Polyakov loop

- We consider a system of QCD matter and put an infinite mass static quark in it as a probe

$$\langle \Phi \rangle \sim e^{-F_Q/T}$$

- Excess free energy F_Q from putting the probe in the system
- Finite free energy $\rightarrow$ no confinement
- Infinite free energy $\rightarrow$ confinement

Confined: $\langle \Phi \rangle = 0$ Deconfined: $\langle \Phi \rangle \neq 0$

Polyakov loop: order parameter for confinement

Indeed, for pure gauge theory, without dynamical quarks (quenched) there is a first order phase transition and the Polyakov loop is an order parameter.

Chiral symmetry

For massless quarks, the QCD Lagrangian:

$$\mathcal{L} = \bar{\Psi}_a(i\partial_\mu - gA_\mu)\Psi_a + \dots$$

$$\left.\begin{array}{l}\Psi \to e^{i\gamma_5\phi}\Psi \\ \Psi \to e^{i\gamma_5\vec{\tau}\cdot\vec{\phi}}\Psi\end{array}\right\}$$ is invariant to axial and iso-axial rotations

Noethers theorem leads to conserved currents:

~~$j_5^\mu = \bar{\Psi}\gamma^\mu\gamma_5\Psi$~~ Destroyed by anomaly

$$j_{5a}^\mu = \bar{\Psi}\gamma^\mu\gamma_5\tau_a\Psi$$

- Spontaneously broken for $m = 0 \to$ Chiral condesate

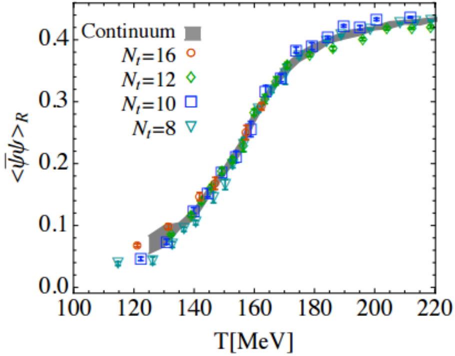
$$\left\langle\bar{\Psi}\Psi\right\rangle = \frac{T}{V}\frac{\partial \log Z}{\partial m_q} \neq 0$$

- Explicitly broken for $m > 0$

Chiral condensate: order parameter for the chiral transition

Chiral vs deconfinement transition

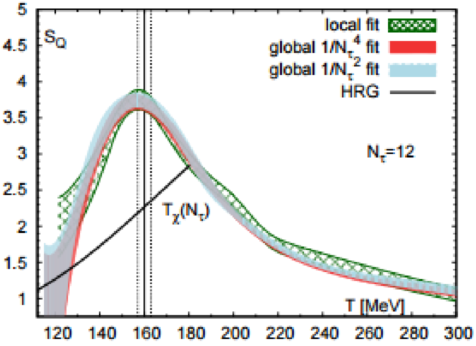
- There is no true phase transition in QCD, only a crossover.
- QCD explicity breaks both center and chiral symmetry.
- We use both the Polyakov loop or the chiral condensate the crossover $\rightarrow T_c$ values overlap



Wuppertal-Budapest: JHEP 1009 (2010) 073

Chiral vs deconfinement transition

- There is no true phase transition in QCD, only a crossover.
- QCD explicity breaks both center and chiral symmetry.
- We use both the Polyakov loop or the chiral condensate the crossover $\rightarrow T_c$ values overlap

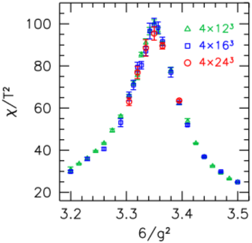


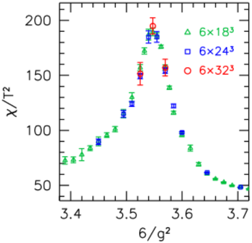
BNL-Bielefeld: PRD93 (2016) no.11, 114502

Finite size scaling

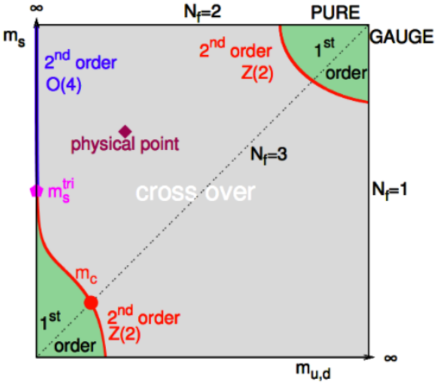
Proof for crossover? $\rightarrow$ Finite site scaling (with continuum limit extrapolation)

- In a finite volume there are no phase transitions
- In 2nd order transitions, finite size scaling depends on critical exponents.
- In 1st order transitions, the peak of the susceptibility diverges as $\propto V$
- A crossover means there is no finite size scaling. $\rightarrow$ QCD (Nature 443 (2006) 675-678)





The Columbia plot

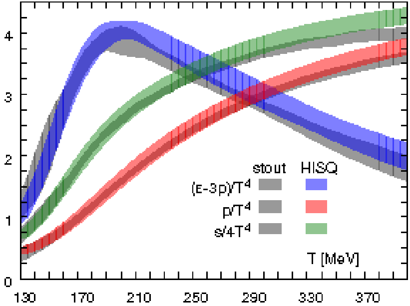


- Pure gauge
  Francis et al Phys.Rev. D91 (2015)
  $T_c = 294(2)$MeV
- $N_f = 2$
  Wilson $N_\tau = 16$
  $m_\pi = 220$ MeV $\rightarrow$ $T_c = 193(7)$MeV
  Brandt et al., 1310.8326
- Physical point: staggered and Wilson (WB: PRD92 (2015) no.1, 014505)
- $N_f = 3$
  BNL-Bielefeld: $N_\tau = 6$ HISQ
  no sign of a true PT down to
  $m_\pi \sim 80$MeV

QCD thermodynamics at $\mu_B = 0$
The equation of state

Equation of state for $N_f = 2+1$

Two independent and compatible results for the $\mu = 0$ and $N_f = 2+1$

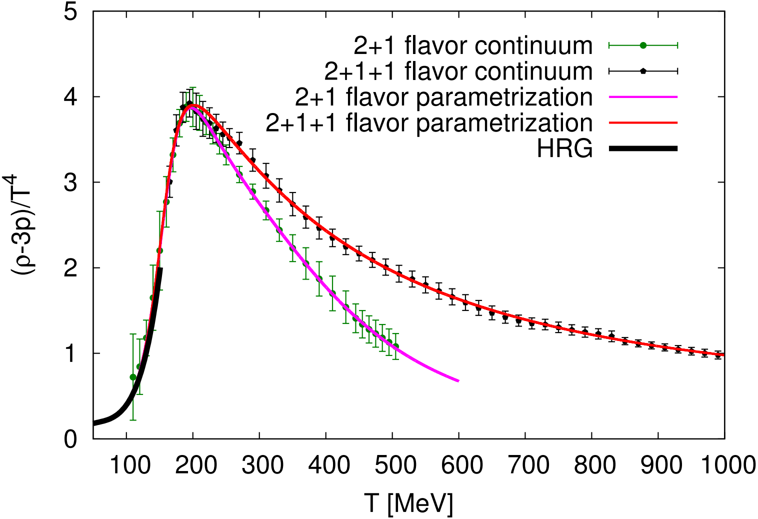


This is nice, but...

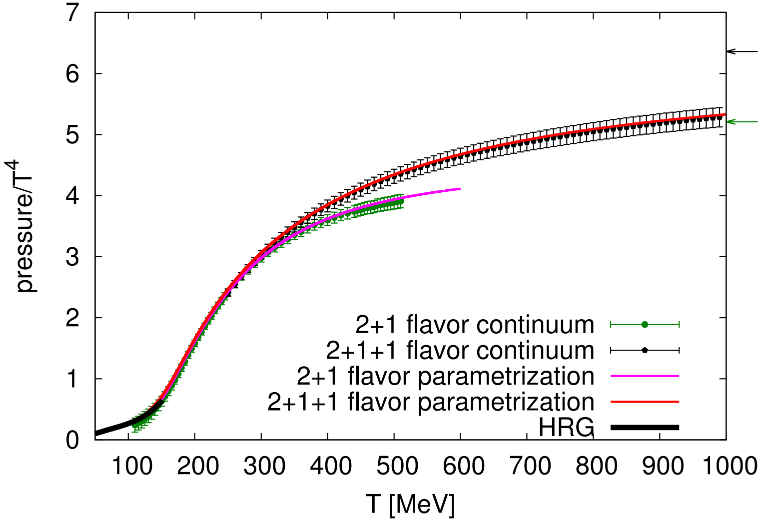
(1) Heavy ion physics: needs $\mu > 0$

(2) Cosmology: needs higher temperature, therefore more quark flavours

Equation of state with dynamical charm



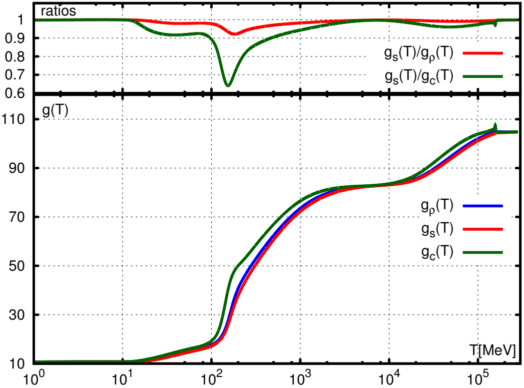
Equation of state with dynamical charm



Effect of charm quark is described well by a tree level perturbative

The full cosmological equation of state

WB: Nature 539 (2016) no.7627, 69-71



Electroweak contribution: Laine, Meyer 1503.04935, JCAP 1507 (2015)

Energy d. $\rho = g_\rho \frac{\pi^2}{30} T^4$ entropy d. $s = g_s \frac{2\pi^2}{45} T^3$ heat cap. $c = g_c \frac{2\pi^2}{15} T^3$

Cooling rate in the early universe: $\frac{dT}{dt} = -\frac{T^3}{M_{\rm Pl}} \frac{2\pi^{3/2}}{3\sqrt{5}} \frac{\sqrt{g_\rho} g_s}{g_c}$

Finite baryon density

QCD in the grand canonical ensemble

Grand canonical partition function:

$$e^{-F/T} = \mathcal{Z}(T;\mu_u,\mu_d,\mu_s) = \mathrm{Tr}\left(e^{-\beta(H-\mu_u N_u-\mu_d N_d-\mu_s N_s)}\right)$$

$\Longrightarrow$ 4D phase diagram.

$$\begin{aligned}
\text{Quark number density} \qquad \langle n_q\rangle &= \frac{T}{V}\frac{\partial \log \mathcal{Z}}{\partial \mu_q} \\
\text{Baryon number density} \qquad \langle n_B\rangle &= \frac{1}{3}\left(\langle n_u\rangle + \langle n_d\rangle + \langle n_s\rangle\right) \\
\text{Isospin density} \qquad \langle n_I\rangle &= \frac{1}{2}\left(\langle n_u\rangle - \langle n_d\rangle\right) \\
\text{Electric charge} \qquad \langle n_Q\rangle &= \frac{2}{3}\langle n_u\rangle - \frac{1}{3}\langle n_d\rangle - \frac{1}{3}\langle n_s\rangle
\end{aligned}$$

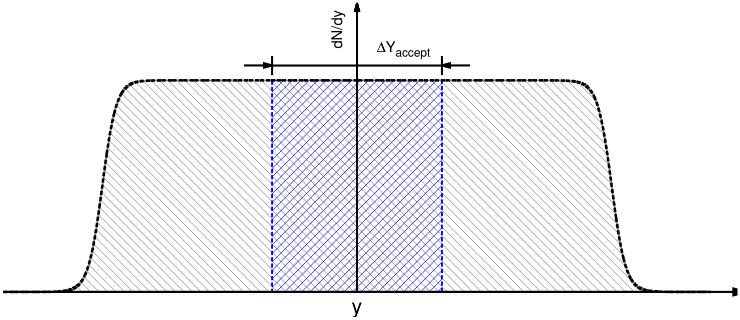
Both for heavy ion physics and neutron star physics, we need:

- $\langle n_I\rangle < 0$ not a problem
- $\langle n_B\rangle > 0$ complex action problem

} I will shortly review why

Do conserved charges fluctuate in HIC?

- If we look at the entire system, none of the conserved charges will fluctuate
- By studying a sufficiently small subsystem, the fluctuations of conserved quantities become meaningful
- This choice of a subsystem in the experiment is implemented by and acceptance cut in rapidity and transverse momentum



Finite baryon density
II. Complex action problems at finite density

Euclidean path integral

Start with a grand canonical partition function: $Z = \mathrm{Tr}\left(e^{-(H-\mu N)/T}\right)$
Notation: $H - \mu N \to H$ for simplicity

The partition function $Z = \mathrm{Tr}\left(e^{-H/T}\right)$ written as a path integral:

$$Z = \sum_{c_1, c_2, \ldots} \left\langle c_1 | e^{-aH} | c_2 \right\rangle \left\langle c_2 | e^{-aH} | c_3 \right\rangle \ldots \left\langle c_{n-1} | e^{-aH} | c_1 \right\rangle =: \sum_{[c]} w[c]$$

- Maps the quantum system to a classical system, with configurations c
- $w(c) =$ weight of a configuration c
- $w(c) \geq 0 \implies$ can use Monte Carlo
- $w(c)$ can be negative or complex $\implies$ sign or complex action problem
- Sign problem property of the system **AND** the basis we used

Quantum Field Theory

$$\mathcal{Z} = \int \mathcal{D}\Phi \; e^{-S_E} = \sum_{[c]} w[c]$$

Bosonic and fermionic example with a sign problem:

- Charged scalar field:

$$S = \int d^4x \left[-\Phi^* \Delta \Phi + (m^2 - \mu^2)|\Phi|^2 + 2i\mu \, \mathrm{Im} \, \Phi^* \partial_0 \Phi \right]$$

- QCD with the fermions integrated out:

$$S = S_{\mathrm{YM}} - \sum_{q=1}^{N_f} \ln \det M(m_q, \mu_q)$$

$$\det M(m_q, \mu_q) \in \mathbb{C} \text{ if } \mu_{\mathrm{q}} > 0$$

Complex action appears when we have particle-antiparticle asymmetry!

What does it mean to solve a sign problem?

Given a quantum system, with $Z = \mathrm{Tr}\, e^{-H/T} = \mathrm{Tr}\, e^{-(H_0 - \mu N)/T}$,
there is a path integral representation:

$$Z = \sum_{c_1,\ldots,c_{n-1}} \left\langle c_1 | e^{-aH} | c_2 \right\rangle \left\langle c_2 | e^{-aH} | c_3 \right\rangle \ldots \left\langle c_{n-1} | e^{-aH} | c_1 \right\rangle =: \sum_{[c]} w(c)$$

Here $w(c)$ = weight of classical configurations. We say that:

- The quantum system suffers a sign problem if there are negative or complex weights $w(c)$ in the classical representation.
- An algorithm is of polynomial complexity if the computational time needed to arrive at a given accuracy for an observable scales polynomially with the system size (volume).
- An algorithm that is of polynomial complexity for the related classical system is called a **solution of the sign problem for the given system**.

M. Troyer, U.-J. Wiese, cond-mat/0408370

Non-example: Reweighting

$$\langle O \rangle_w = \frac{\int \mathcal{D}U O[U] w[U]}{\int \mathcal{D}U w[U]} = \frac{\int \mathcal{D}U O[U] \frac{w[U]}{r[U]} r[U]}{\int \mathcal{D}U \frac{w[U]}{r[U]} r[U]} = \frac{\left\langle O \frac{w}{r} \right\rangle_r}{\left\langle \frac{w}{r} \right\rangle_r}$$

If the new weight r is real, we can use importance sampling. The reweighting factor:

$$\left\langle \frac{w}{r} \right\rangle_r = \frac{Z_w}{Z_r} = e^{-\frac{V}{T}\Delta f} \qquad \Delta f = f_w - f_r$$

exponantially goes to 0 in the infinite volume limit. This is called the **overlap problem**: $< O >_w \rightarrow 0/0$.
Say I chose $r = |w|$, then $\left\langle \frac{w}{r} \right\rangle_r = \left\langle e^{i\phi} \right\rangle = e^{-\frac{V}{T}(f_w - f_{|w|})}$ illustrates the sign problem nicely.

The best one can do is make Δf small (e.g. Z. Fodor, S.D. Katz, JHEP 0404 (2004) 050), but the overlap problem is still an exp. in V

Example: Dual variables

We had in general the path integral representation:

$$Z = \sum_{c_1,\dots,c_{n-1}} \left\langle c_1 | e^{-aH} | c_2 \right\rangle \left\langle c_2 | e^{-aH} | c_3 \right\rangle \dots \left\langle c_{n-1} | e^{-aH} | c_1 \right\rangle =: \sum_{[c]} w(c)$$

Lots of freedom in the choice of the c_i. So why not change basis?
If a representation $[c]$ can be found where:

- $W([c]) \geq 0$
- $W([c])$ can be computed in polynomial time

then the sign problem is solved (by changing variables in the path integral)
Such a change of variables is known for:

- Charged scalar fields: C. Gattringer, T. Kloiber, NPB 869, 2013
- Abelian Higgs model: Y. D. Mercado, C. Gattringer, A. Schmidt, PRL111, 2013
- Yukawa model: S. Chandrasekharan, 2013
- $\dots$
- But not for QCD.

Finite baryon density
III. Small μ physics

Fluctuations in the grand canonical ensemble

The expectation value of a conserved charge:

$$\langle N_q \rangle = T \frac{\partial \log \mathcal{Z}}{\partial \mu_q}$$

The response to μ_q is given by the fluctuations of the conserved charge:

$$\frac{\partial \langle N_i \rangle}{\partial \mu_j} = T \frac{\partial^2 \log \mathcal{Z}}{\partial \mu_i \partial \mu_j} = \frac{1}{T} \left(\langle N_i N_j \rangle - \langle N_i \rangle \langle N_j \rangle \right)$$

The higher order susceptibilities:

$$\chi^{u,d,s,c}_{i,j,k,l} = \frac{\partial^{i+j+k+l} \left(p/T^4 \right)}{(\partial \hat{\mu}_u)^i (\partial \hat{\mu}_d)^j (\partial \hat{\mu}_s)^k (\partial \hat{\mu}_c)^l} \text{ where } \hat{\mu} = \mu/\mathrm{T}$$

To change the variables one can use:

$$\mu_u = \frac{1}{3}\mu_B + \frac{2}{3}\mu_Q \qquad \mu_d = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q \qquad \mu_s = \frac{1}{3}\mu_B - \frac{1}{3}\mu_Q - \mu_S$$

To write the $\chi^{B,Q,S}_{i,j,k}$s as linear combinations of $\chi^{u,d,s}_{i,j,k}$.

Taylor expansion of the pressure

Suppose we either:

- fix $\mu_S = 0 = \mu_Q$ for simplicity
- fix $\langle S \rangle = 0$ and $\langle Q \rangle = 0.4 \langle B \rangle$ for HIC

The pressure is now:

$$\frac{P}{T^4} = P(T, \mu = 0) + \sum_{k=1}^{\infty} c_{2k} \left(\frac{\mu_B}{T} \right)^{2k}$$

Alternatively, I can fix nothing and calculate the 3 variable Taylor expansion. The coefficients contain lots of info:

- $T_c(\mu)$
- EoS
- Lower limit on location of critical point
- ...

Complexity of the Taylor expansion approach

$$\mathcal{Z} = \int \mathcal{D}U e^{-S_{YM}[U]} \det M[U; m_u, \mu_u) \det M[U; m_d, \mu_d) \det M[U; m_s, \mu_s)$$

$$P = -\ \log \mathcal{Z}$$

$$\frac{P}{T^4} = P(T, \mu = 0) + \sum_{k=1}^{\infty} c_{2k} \left(\frac{\mu_B}{T}\right)^{2k}$$

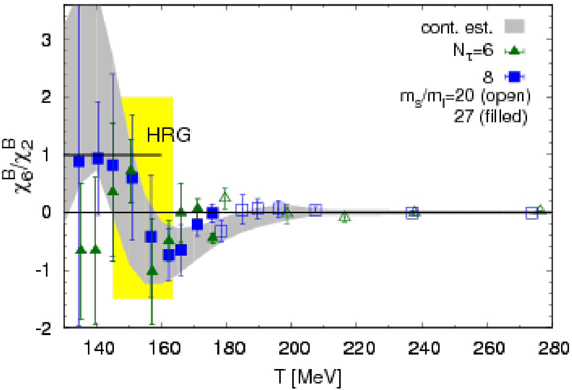
$$c_{2k} \sim \left\langle \mathrm{Tr}\left(\text{order 2k polynomial in } \mathrm{M}^{-1} \text{ and } \mu \text{ derivatives of M}\right)\right\rangle_{\mu=0}$$

- Number of terms grows exponentially with order
- Cancellations: c_{2k} finite as $V \to \infty$, but sum of terms scaling with $\mathcal{O}(V^{k-1})$

$\Longrightarrow$ The sign problem strikes back.

Complexity of the Taylor expansion method

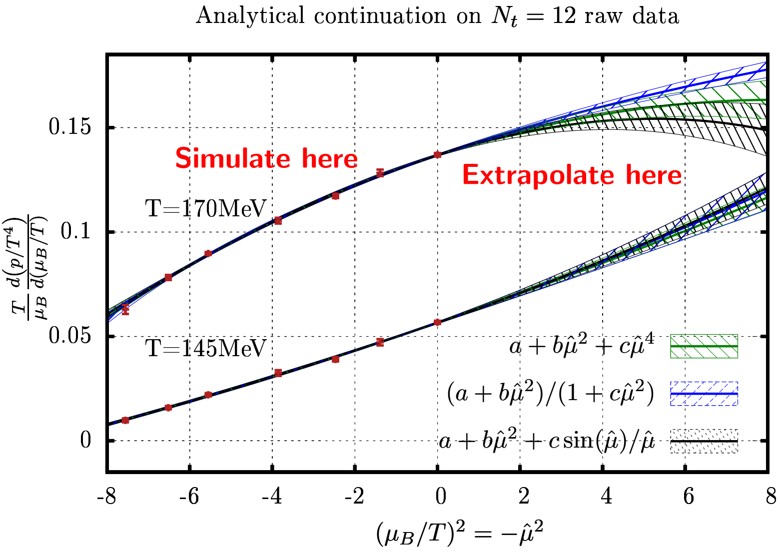
$\Longrightarrow$ The sign problem strikes back. The result is that after years of runs:



BNL-Bielefeld-CCNU: hep-lat/1701.04325

To reliably constrain the critical point, much higher order is needed.

Analytical continuation



Analytical continuation vs Taylor expansion

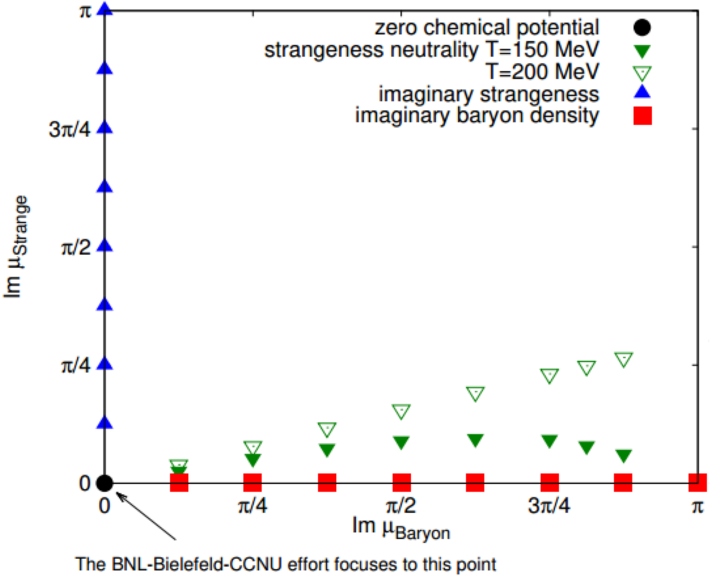
If we just restrict ourselves to calculating Taylor coefficients:

- Since I am fitting the dependence in $\mathrm{Im}\,\mu$ I have to take less derivatives
- So I have a volume factor less of cancellations, I win in statistics
- The price I pay is the systematic error coming from the extrapolation

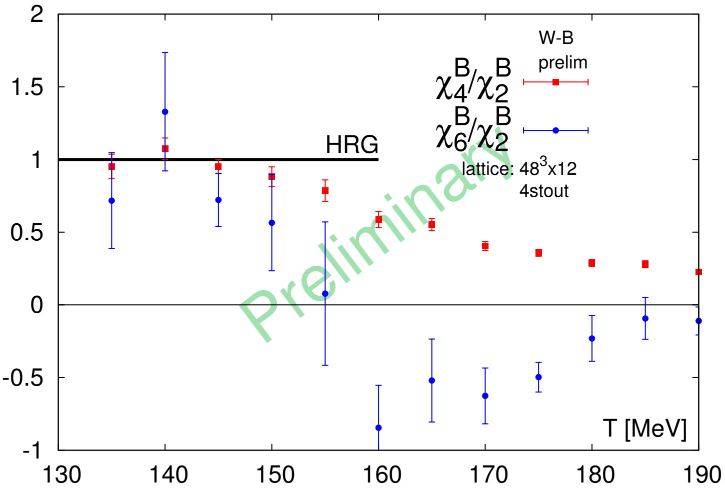
BUT

There are also other uses of imaginary μ (I will talk about hadron chemistry)

Simulation landscape with imaginary μ_B

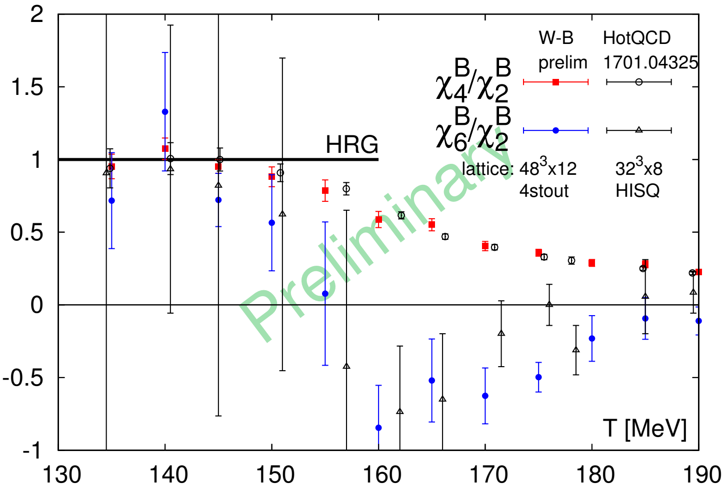


The power of the method: χ_6^B/χ_2^B



See also D'Elia et al 1611.08285; Datta et al 1612.06673 ; BNL-Bielefeld-CCNU: 1701.04325

The power of the method: χ_6^B/χ_2^B

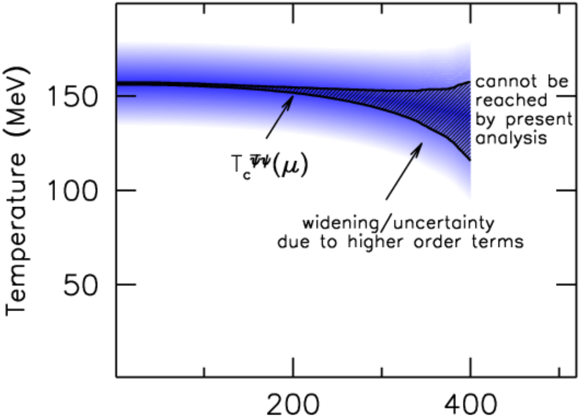


See also D'Elia et al 1611.08285; Datta et al 1612.06673 ; BNL-Bielefeld-CCNU: 1701.04325

The crossover line from analytical continuation

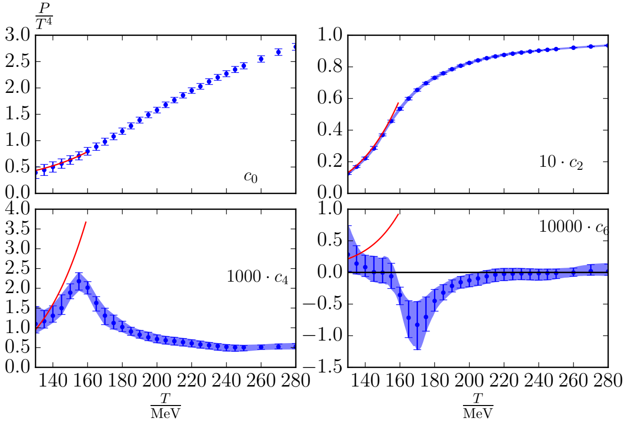
$$\frac{T_c(\mu_B)}{T_c(0)} = 1 - \kappa\,(\mu_B/T_c(\mu_B))^2 \qquad \kappa = 0.0149(21)$$

WB: hep-lat/1507.07510 μ_S and μ_Q from $\langle S\rangle = 0$ and $\langle Q\rangle = 0.5\,\langle B\rangle$



Equation of state from analytical continuation

WB: hep-lat/1507.07510 μ_S and μ_Q from $\langle S \rangle = 0$ and $\langle Q \rangle = 0.4 \langle B \rangle$

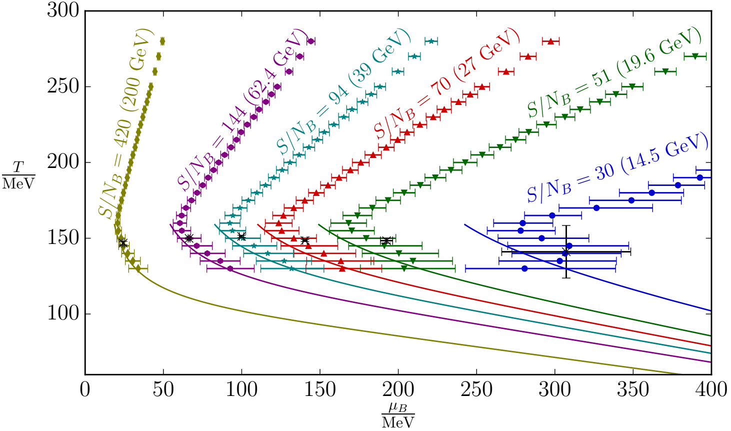


It appears Taylor expansion is under control for $\mu_B/T \leq 2$. This is not so bad. It means it can be used for RHIC energies:

$$\sqrt{s} = 200,\ 62.4,\ 39,\ 27,\ 19.6,\ 14.5\mathrm{GeV}$$

Isentropic trajectories from analytical continuation

WB: hep-lat/1507.07510 μ_S and μ_Q from $\langle S \rangle = 0$ and $\langle Q \rangle = 0.4 \langle B \rangle$



Black freeze-out parameters: Alba et al, 2014

Finite baryon density
IV. Hadron chemistry

Hadron thermodynamics from the virial expansion

- Virial Expansion: Expansion of p in fugacity $e^{\mu/T}$
- This is the natural expansion to compute with imaginary chemical potentials, since $\cosh(i\mu_I/T) = \cos(\mu_I/T)$: the virial coefficients become Fourier coefficients
- Dashen, Bernstein, Ma '69 Dashen, Rajaraman '75 $\implies$ if the interactions are dominated by narrow resonant scattering, the thermodynamics looks like a bunch of free particles
- Hadron Resonance Gas Model:

$$\frac{p^{\mathrm{HRG}}}{T^4} = \frac{1}{VT^3}\Big(\sum_{i\in\mathrm{mesons}} \log \mathcal{Z}^M\left(T, V, m_i, \{\mu\}\right) + \sum_{i\in\mathrm{baryons}} \log \mathcal{Z}^B\left(T, V, m_i, \{\mu\}\right) \Big)$$

- HRG is very commonly used in heavy ion phenomenology, e.g. to extract chemical freezeout curves

Hadron thermodynamics from the virial expansion

Allows for the separation of channels with different quantum numbers.
One chemical potential:

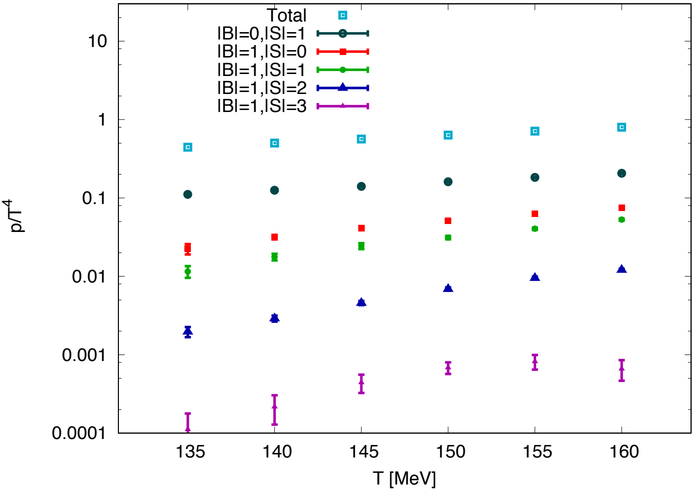
$$P(\hat{\mu}_B, \hat{\mu}_S = 0, \hat{\mu}_Q = 0) = P_0^B + P_1^B \cosh(\hat{\mu}_B) + P_2^B \cosh(2\hat{\mu}_B) + \ldots$$

Two chemical potentials:

$$\begin{aligned} P(\hat{\mu}_B, \hat{\mu}_S, \hat{\mu}_Q = 0) &= P_{00}^{BS} + P_{10}^{BS} \cosh(\hat{\mu}_B) + P_{01}^{BS} \cosh(\hat{\mu}_S) \\ &+ P_{11}^{BS} \cosh(\hat{\mu}_B - \hat{\mu}_S) + P_{12}^{BS} \cosh(\hat{\mu}_B - 2\hat{\mu}_S) \\ &+ P_{13}^{BS} \cosh(\hat{\mu}_B - 3\hat{\mu}_S) + \ldots\ , \end{aligned}$$

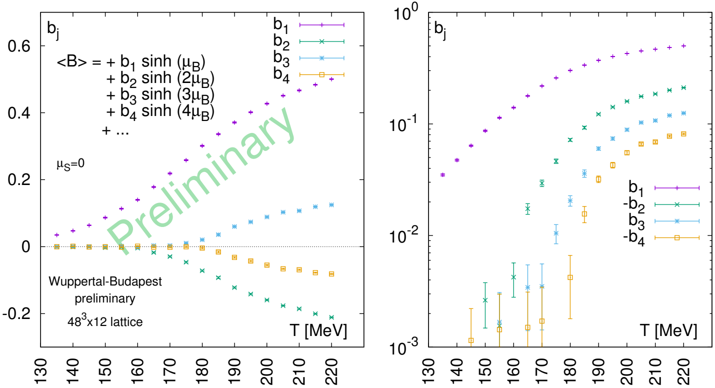
Trick: $\cosh(i\mu_I) = \cos(\mu_I) \implies$ for imaginary μ virial $\rightarrow$ Fourier

Virial coefficients → strangeness sectors



WB: 1702.01113

Virial coefficients → baryon sectors



Outlook

- For $\mu = 0$ physics there are very solid results.
- No solution for the sign problem at $\mu > 0$ is QCD. But dense QCD is important enough to keep trying.
- Progress:
  - $\mu = 0$, high T and connecting with weak coupling estimates
  - small μ physics
- There is still a lot to do even without solving the sign problem:
  - Simulations with chiral fermions
  - Columbia plot
  - Small μ physics: higher order fluctuations with high precision and in the continuum
  - Chiral vs deconfinement transition at small μ
  - Chemical freezeout

I thank my collaborators: P. Alba, R. Bellwied, Sz. Borsányi, Z. Fodor, J. Günther, C. Hoelbling, S. Katz, J. Noronha-Hostler, P. Parotto, C. Ratti, D. Sexty, K. Szabó, B. Tóth, Cs. Török

Backup