Finite Temperature Lattice QCD

Introduction
The QCD transition
The transition temperature
The Equation of State
Screening masses

finite density → Ch. Schmidt
topological aspects

→ M. Müller-Preußker
asymptotic freedom $\alpha_s(Q \to \infty) = 0$, at finite $T$: $Q \sim T$

- universe $n_B/n_\gamma \approx 10^{-9} \rightarrow$ cosmology

- at high density
  - probably rich phase structure
    (color superconductivity, color-flavor locking ...)
  - neutron stars $\rightarrow$ astrophysics
  - difficult for the lattice (sign problem)
    $\rightarrow$ lectures by G. Aarts, Ch. Schmidt

- heavy ion collisions (LHC, RHIC, FAIR)
  - FAIR: $N_B/S \approx 0.03, \mu_B/T \approx 2.5$
  - RHIC: $N_B/S \approx 0.003, \mu_B/T \approx 0.25$
– at mid rapidity, baryon density is small
– short equilibration time $\tau_{\text{equi}} \lesssim 1 \text{ fm}$ (strong interaction !)
– expansion is described by hydrodynamics $\longrightarrow$ Equation of State
estimates from a simple model: bag model

\[
p_H = d_H \frac{\pi^2}{90} T^4 \\
d_H = \# \text{d.o.f.} = 3 \quad (\pi^\pm, \pi^0)
\]

hadron view

\[
p_P = d_P \frac{\pi^2}{90} T^4 - B
\]

quark-gluon view

\[
d_P = 2 \cdot 8 + \frac{7}{8} \cdot 2 \cdot 2 \cdot 3 \cdot N_F (G, q)
\]

at \( T \neq 0 \), instead of energy \( E \), free energy

\[
F = E - TS = -pV \quad \text{minimal}
\]

\[\Rightarrow \text{here 1st order phase transition}\]

since \( \epsilon = \frac{E}{V} \sim T^2 \partial (p/T) / \partial T \)

has a discontinuity

\[
p_H(T_c) = p_P(T_c) \iff T_c = \left( \frac{90}{\pi^2(d_P - d_H)} \right)^{1/4} B^{1/4} \approx 0.7 B^{1/4} \approx 140 \text{ MeV}
\]

NOTE: we have a scale here, the temperature \( T \)

\[
M_H = \frac{16\pi}{3} R^3 B
\]
Quantum statistics in equilibrium:

the central quantity is the **partition function** \( Z = \text{tr}\{\exp(-\hat{H}/T)\} = \sum_n \langle n | \exp(-\hat{H}/T) | n \rangle \) (at \( \mu = 0 \))

compare with time evolution operator \( \exp(-it\hat{H}) \)

- (inverse) temperature direction \( \equiv \) imaginary time \( \tau = it \)
- temporal extent limited by \( 0 \leq \tau \leq 1/T \)
- trace requests periodic b.c. in time for bosons \( \phi(\tau = 1/T) = \phi(0) \) (commutators)
  anti-periodic b.c. in time for fermions \( \psi(\tau = 1/T) = -\psi(0) \) (anti-commutators)

\[ \rightarrow \text{Feynman path integral} \]

\[ Z(T, V) = \int_{\text{periodic}} D\phi(\vec{x}, \tau) \exp\left\{ - \int_0^{1/T} d\tau \int_V d^3\vec{x} \mathcal{L}_E[\phi(\vec{x}, \tau)] \right\} \]

where \( \mathcal{L}_E \) is the euclidean Lagrange density

apply standard thermodynamic relations, e.g. energy density \( \epsilon = \frac{T^2 \partial \ln Z}{V \frac{\partial T}{V}} \)

specific heat \( c_V = \frac{1}{VT^2} \frac{\partial^2 \ln Z}{\partial (1/T)^2} \)

on the lattice as at zero temperature, but

\[ a(\beta)T = \frac{1}{N_\tau} \quad \text{and} \quad LT = \frac{N_\sigma}{N_\tau} \]
• charm at $m_c/T_c = \mathcal{O}(10)$ presumably too heavy for the dynamics at $T_c$

• leaves light $m_u \simeq m_d \equiv m_l$ and strange $m_s$ quark

• the nature of the transition is expected to depend strongly on $m_l$ and $m_s$:
Pure gauge, $m_{l,s} \rightarrow \infty$

- the action is invariant under the global transformation $U_\tau(\vec{x}, \tau = N_\tau) \rightarrow z U_\tau(\vec{x}, \tau = N_\tau)$
  with $z \in Z(3) = \{\exp(in2\pi/3), n = 0, 1, 2\}$, the center group of $SU(3)$
- the Polyakov loop $L(\vec{x}) = tr \prod_\tau U_\tau(\vec{x}, \tau)$ is not

$\Rightarrow \langle L(\vec{x}) \rangle$ is an order parameter for the spontaneous breakdown of the $Z(3)$ symmetry

- the rise of $L$ signals a phase transition
- the susceptibility $\chi_L \sim \langle L^2 \rangle - \langle L \rangle^2$
  measures thermal fluctuations which grow large at $T_c$

i.e. in pure Yang-Mills, $\langle L \rangle$ detects the confinement - deconfinement transition

measures the free energy of static quarks at separation $r$

$F_{QQ}(r \rightarrow \infty) \rightarrow \infty$ for $T < T_c$

$F_{QQ}(r \rightarrow \infty) \rightarrow$ finite for $T > T_c$

with fermions, $\langle L \rangle$ is not an order parameter, $Z(3)$ broken by fermion action
Universality in a nutshell

Introduction

• at and in the vicinity of a phase transition thermal fluctuations grow large or diverge
• i.e. correlation lengths ξ become large or diverge
• in this limit microscopic interaction details don’t matter \( \rightarrow \) series of “spin blockings” and RG flow
• what counts are global symmetries and the dimension

a universality class consists of all those models which flow into the same critical fixed point under repeated renormalization group transformations
\( \rightarrow \) hence the same critical behavior in terms of scaling with universal critical exponents and certain other universal quantities/functions

• equilibrium QCD (Yang-Mills) at high T is expected to be 3 dimensional generically: \( \phi(\tau) = \sum_n \phi(\omega_n) \exp(i\omega_n \tau) \) with \( \omega_n = 2\pi T n \) \( \rightarrow \) only static modes \( (n = 0) \) survive
\( \Rightarrow \) compare with (classical) 3d systems with the same global symmetries,

• pure \( SU(3) \) Yang-Mills: the same universality class as the 3d \( Z(3) \) (3-state) Potts spin model (weakly) 1st order

* the theory behind this is Wilson’s renormalization group
there is a huge condensed matter literature
for introductory lectures see e.g. J. Engels at

http://www.physik.uni-bielefeld.de/igs/schools/Fall2006/phase.html
the free energy density $f = -\frac{T}{V} \ln Z$ consists of a regular and a singular part, $f = f_{\text{reg}} + f_{\text{sing}}$, where $f_{\text{sing}}$ develops the singularities which drive the transition.

scaling: in the vicinity of a critical point $(T_c, H = 0)$, under an arbitrary scale change $b$

$$f_{\text{sing}}(t, h) = b^{-d} f_{\text{sing}}(b^{y_t} t, b^{y_h} h)$$

where $y_t, y_h$ are universal critical exponents

$$t = \frac{1}{t_0} \frac{T - T_c}{T_c}$$  \quad \text{(normalized) reduced temperature}$$

$$h = \frac{1}{h_0} H$$  \quad \text{(normalized) external symmetry breaking, e.g. magnetic field, } m_q \text{ in QCD}$$

$t_0, h_0$ non-universal metric factors i.e. need to be adjusted for each model
\[ f_{\text{sing}}(t, h) = b^{-d} f_{\text{sing}}(b^{yt} t, b^{y_h} h) \]

- choose \( b = |t|^{-1/y_t} \): 
  \[ f_{\text{sing}}(t, h) = |t|^{d/y_t} f_{\text{sing}}(\pm 1, |t|^{-y_h/y_t} h) \]
  
  \( \Rightarrow \) for magnetization \( M = -\partial f / \partial H \) find at \( t < 0, H = 0 \): 
  \[ M \sim (-t)^{\beta} \text{ with } \beta = (d - y_h)/y_t \]
  
  \( \Rightarrow \) for susceptibility \( \chi = \partial M / \partial H \sim \langle (\delta M)^2 \rangle \) find at \( H = 0 \): 
  \[ \chi \sim |t|^{-\gamma} \text{ with } \gamma = (2y_h - d)/y_t \]

- choose \( b = |h|^{-1/y_h} \): 
  \[ f_{\text{sing}}(t, h) = |h|^{d/y_h} f_{\text{sing}}(t|h|^{-y_t/y_h}, \pm 1) \]
  
  \( \Rightarrow \) for magnetization find at \( t = 0 \): 
  \[ M \sim |h|^{1/\delta} \text{ with } 1/\delta = d/y_h - 1 \]
  
  \( \Rightarrow \) note that \( \beta + \gamma = y_h/y_t = \beta \delta \) “hyperscaling relation”
  
  \( \Rightarrow \) at \( t \approx 0 \): 
  \[ M(t, h) = |h|^{1/\delta} f_G(z) \text{ with } f_G(z) = f_{\text{sing}}(z) + z f'_{\text{sing}}(z) \text{ universal and } z = t|h|^{-1/\beta \delta} \]

- similarly, e.g. the so-called Binder cumulant \( B_4 = \frac{\langle (\delta M)^4 \rangle}{\langle (\delta M)^2 \rangle^2} \) with \( \delta M = M - \langle M \rangle \) is a universal number

- keep in mind though that corrections to scaling might be important, and there are also the regular terms
The QCD transition

conjectured landscape of transitions

arising from the chiral symmetry of QCD at $m_q = 0$

$SU_L(N_f) \times SU_R(N_f) \times U_A(1)$

− its spontaneous breakdown at low $T$
− its restoration at high $T$
− and its modelling by $\sigma$ models
  (universality)
− note: $U_A(1)$ broken by triangle anomaly
  but could be effectively restored at high $T$
  (no topologically non-trivial configurations)

$N_F = 2$  Wilczek, Pisarski
− if $U_A(1)$ effectively restored then 1st order
− if 2nd order then in $SU(2) \times SU(2) \simeq O(4)$ class

$N_F = 3$  Wilczek, Pisarski
− 1st order
− at critical end point: $Z(2)$ class  Gavin et al.
$N_F = 2$

- conflicting results for critical behavior of $M = \langle \bar{q}q \rangle$, all from coarse lattices with un-improved actions
  - Wilson $M$ scales $\sim O(4)$ in $m \sim H$ at $T > T_c$ [Iwasaki et al.]
  - staggered $\chi_m, \chi_t$ do not scale $\sim O(4)$ in $m$ [Karsch,EL; JLQCD; MILC]
  - staggered $M$ scales $\sim O(4)$ in $L$ [Engels et al.]
  - staggered $c_V$ scales as 1st order [Di Giacomo et al.]
  - staggered $M$ is as in $O(2)$ at finite $L$ [Kogut, Sinclair]

- $U_A(1)$:
  - if effectively restored, then degeneracy in 2-point function (mass spectrum) [Shuryak; Cohen et al.; ...]

- current projects with Wilson-type quarks [QCDSF-DIK,tmfT,WHOT] have not yet addressed this question
\( N_F = 3 \)

Binder cumulant \( B_4 \)

- intersection for various \( V \)
  - yields critical value of \( m \)
- value of \( B_4 \) is universal
- corrections from \( V \) finite and ‘order parameter not matched correctly’

\[
\begin{align*}
\text{standard action} & \quad m_c \simeq 4 m_u^{\text{phys}} \iff m_{PS} \simeq 290 \text{ MeV} \\
\text{[Bielefeld; deForcrand, Philipsen]} & \quad \text{but: – } m_c \text{ not universal} \\
& \quad \text{– improved action: } m_{PS} \simeq 70 \text{ MeV}
\end{align*}
\]

magnetization-like order parameter \( \mathcal{M} \)
not identical with chiral condensate \( \langle \bar{q}q \rangle \)
(chiral symmetry broken by \( m_q \neq 0 \) anyway)

\[
\mathcal{M} = \langle \bar{q}q \rangle + s S
\]
$N_F = 2 + 1$

Recent projects all use improved staggered quarks (p4fat3, asqtad, stout, HISQ) *

At finite lattice spacing: taste violations $O(a^2 \alpha_s)$

⇒ the pion 16-multiplet → 8 different representations, *staggχPT*: 5 different reps.

Only 1 pion is true Goldstone boson also at $a \neq 0$: $m_{\gamma_5}^2 = m_G^2 \sim m_q$ in chiral limit

⇒ the expected $O(4)$ for 2 light flavors in the limit $m_l \rightarrow 0$ goes over into $O(2)$ at $a \neq 0$

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* First results from DWF fermions, not yet on the nature of the transition [Christ, Karsch et al.]

First results from improved Wilson quarks, mainly equation of state [WHOT]
in $O(N)$ spin models

\[ M(t, h) = h^{1/\delta} f_G(z) \]

with $z = t/h^{1/\beta \delta}$ and $f_G$ universal

\[ M \sim (-t)^\beta \text{ at } h = 0, t < 0 \]
\[ M \sim h^{1/\delta} \text{ at } t = 0 \]
\[ M \simeq h^{1/\delta} (-z)^\beta [1 + \tilde{c}_2 \beta (-z)^{-\beta \delta / 2} + \ldots] = M(t, 0) + c(t) \sqrt{h} + \ldots \text{ at } z \to -\infty \quad \text{Zia, Wallace} \]

$\sqrt{h}$ behavior is known as Goldstone effect in $d=3$ ($\sim h \ln h$ in $d=4$) Gasser, Leutwyler, Hasenfratz

critical exponents $\beta, \delta$ and $f_G(z)$ known
from spin model simulations [Engels et al.]

<table>
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<tr>
<th>$N$</th>
<th>$\beta$</th>
<th>$\delta$</th>
<th>$\tilde{c}_2$</th>
<th>$z_p$</th>
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<td>1.56(10)</td>
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<td>0.380</td>
<td>4.824(9)</td>
<td>0.666(6)</td>
<td>1.33(5)</td>
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</tbody>
</table>
The QCD transition

the chiral condensate $\langle \bar{q}q \rangle \sim \langle \text{Tr} D_q^{-1} \rangle$

is the order parameter in the limit $m_l \to 0$, i.e. takes the role of the magnetization $M$

complications: – needs multiplicative renormalization $\langle \bar{q}q \rangle^R = Z_m^{-1} \langle \bar{q}q \rangle$

where $Z_m$ is mass renormalization $m^R_q = Z_m m_q$

– away from chiral limit receives additive power divergence $\langle \bar{q}q \rangle(m_q) = \langle \bar{q}q \rangle(0) + m_q / a^2$

$\sim$ subtracted condensate $M = m_s [\langle \bar{l}l \rangle - \frac{m_l}{m_s} \langle \bar{s}s \rangle]$ , difference to $M_b = m_s \langle \bar{l}l \rangle$ small and vanishing

fit data to the scaling function $f_G$ with 3 unknowns: $t_0, h_0$, the metric constants

$T_c$, the critical temperature in the chiral limit

\[ \text{data is well described by } O(2) \text{ scaling} \]

\[ \text{note: } (m_l/m_s)^{\text{phys}} \sim 1/27 \]
at $m_l/m_s \geq 1/10$ corrections to scaling need to be taken into account

$$M(t, h) = h^{1/\delta} f_G(t/h^{1/\beta \delta}) + a_t h + b_1 h + b_3 h^3 + b_5 h^5$$

$b_1 \simeq 0$ for (subtracted) $M$
the chiral susceptibility $\chi_M$ is now fixed completely

$$\chi_M(t, h) = \frac{\partial M}{\partial H} = \frac{1}{h_0} h^{1/\delta - 1} f_\chi(z) \quad \text{with} \quad f_\chi(z) = \frac{1}{\delta} \left( f_G(z) - \frac{z}{\beta} f'_G(z) \right)$$

v.v., reconstruct scaling fct $f_\chi$ from the data on $\chi_M$: $f_\chi = \chi_M h_0 h^{1-1/\delta}$

recall, in QCD $\langle \bar{q}q \rangle(m_q) = \langle \bar{q}q \rangle(0) + \sqrt{m_q} + m_q/a^2 + \cdots$

moreover, in QCD $\chi_M = 2\chi_{\text{dis}} + \chi_{\text{con}}$ with

$$\chi_{\text{dis}} = \frac{1}{16 N^3 \sigma N_F} \left\{ \langle (\text{Tr} D_l^{-1})^2 \rangle - \langle \text{Tr} D_l^{-1} \rangle^2 \right\} \quad \text{measures fluctuations of the chiral condensate}$$

$$\chi_{\text{con}} = \frac{1}{4} \sum_x \langle D_l^{-1}(x, 0) D_l^{-1}(0, x) \rangle \quad \text{arises from the explicit } m_q \text{ dependence of } D_q = D + m_q$$

- integral over quark-line connected correlator of the scalar isovector $a_0$

$\Rightarrow$ quadratically UV divergent $\sim a^{-2}$

- in $O(N)\chi PT$ it can be shown that $\chi_{\text{con}}$ vanishes for $N = 4$ but not for $N = 2$ [Smilga, Stern, Verbaarschot]

- in stagg$\chi PT$ taste violations lead to IR Goldstone contribution to $\chi_{\text{con}} \sim 1/\sqrt{m_q}$ [DeTar et al.]

$\chi_{\text{con}}$ does not contribute to $f_\chi$ in the chiral limit because of $h^{1-1/\delta}$ and $\delta > 2$
the chiral susceptibility $\chi_M$ is now fixed completely
\[
\chi_M(t, h) = \frac{\partial M}{\partial H} = \frac{1}{h_0^\delta} h^{1/\delta - 1} f_\chi(z) \quad \text{with} \quad f_\chi(z) = \frac{1}{\delta} \left( f_G(z) - \frac{z}{\beta} f'_G(z) \right)
\]
v.v., reconstruct scaling fct $f_\chi$ from the data on $\chi_M$: $f_\chi = \chi_M h_0 h^{1-1/\delta}$
and compare with $f_\chi$ from the $O(N)$ models:

peaks in $\chi_M$ at pseudocritical temperatures $T_p$ are caused by the peak in $f_\chi$ at $z = z_p$

\[
\frac{t_p}{h^{1/\beta\delta}} = \frac{1}{t_0} \frac{T_p - T_c}{H_{h_0}^{1/\beta\delta}} = z_p \quad \Rightarrow \quad \frac{T_p(H) - T_c}{T_c} = z_p \frac{H^{1/\beta\delta}}{h_0^{1/\beta\delta}} \frac{t_0}{t_0} \quad \rightarrow \text{predict } T_p \text{ from } \langle \bar{q}q \rangle
The transition temperature

- scan through $\beta \rightarrow a(\beta) \rightarrow T = 1/N_\tau a(\beta)$
- $T = 0$ scale taken from $\Upsilon 2S - 1S$ splitting [A. Gray et al.] via the heavy quark potential $V(r)$

$$r_{0,1}/a \quad \text{from} \quad r^2 \frac{dV(r)}{dr} \bigg|_{r=r_{0,1}} = 1.65(1.0)$$

for absolute values (in MeV) we use $r_0 = 0.469(7)$ fm [A. Gray et al.]

- fine tune $\hat{m}_{l,s}(\beta)$ such that $m_{\pi,K} = \text{const}$

plots for p4fat3 action at $m_l/m_s = 0.1$

similar for other actions, different $m_l/m_s$ may take other scale setting quantity e.g. $f_K$
investigate quantities sensitive to the transition

renormalized chiral condensate

\[ \Delta_{l,s}(T) = \frac{\langle \bar{\psi}\psi \rangle_{l,T} - \frac{m_l}{m_s} \langle \bar{\psi}\psi \rangle_{s,T}}{\langle \bar{\psi}\psi \rangle_{l,0} - \frac{m_l}{m_s} \langle \bar{\psi}\psi \rangle_{s,0}} \]

subtracting power-law additive and cancelling multiplicative UV divergencies

strange number susceptibility

\[ \frac{\chi_s(T)}{T^2} \sim \langle n_s^2 \rangle - \langle n_s \rangle^2 \]

measures strangeness fluctuations indicative of deconfinement and depends on \( f_{\text{sing}} \)

\( N_T = 8 \)

\( m_l/m_s \)

\( 0.1 \)

\( 0.05 \)

location of (rapid) change in both variables moves to lower \( T \) when \( m_l \) is decreased
similarly, location of (rapid) change in both variables moves to lower $T$ when $a$ is decreased

difficult to identify a transition temperature e.g. by locating an inflection point:

\[ \text{curvature} = \text{2nd derivative changes sign} \implies \text{1st one has maximum} \]
situation may look better when a different quantity is used to set the T scale

\[ r_{0,1} \text{ scale} \]

\[ f_K \text{ scale} \]

explanation: \( f_K \) is affected by taste violations roughly in the same way as \( \Delta_{l,s} \)

\[ r_i \text{ i.e. static quark potential much less sensitive} \rightarrow \text{in principle more reliable} \]

in any case, a continuum extrapolation is needed, and a better way to locate the transition
determine \( T_p(m_l, N_\tau) \) from the location of peaks of the susceptibility \( \chi_{dis} \), and compare with predictions from \( O(N) \) scaling fits to \( \langle \bar{q}q \rangle \).
extrapolation to continuum limit at physical mass $m_l/m_s = 1/27$

\[
T_c = 157 \quad (4 \text{ stat}) \quad (3 \text{ extrapolation}) \quad (1 \text{ scale}) \quad \text{MeV} \quad \text{asqtad, HISQ}
\]

\[
T_c = 147 \quad (2 \text{ stat}) \quad (3 \text{ syst}) \quad \text{MeV} \quad \text{stout} \chi_M
\]

\[
T_c = 155 \quad (3 \text{ stat}) \quad (3 \text{ syst}) \quad \text{MeV} \quad \text{stout} \Delta_{l,s}
\]