Bulk QCD Thermodynamics on the lattice

- I Phase diagram at $\mu = 0$
- II Equation of state at $\mu = 0$
- III Phase diagram at $\mu \neq 0$
- IV Equation of state at $\mu \neq 0$

numerical treatment of QCD \Rightarrow discretize (Euclidean) space-time



$$Z(T,V) = \int \prod_{i=1}^{N_{ au}N_{\sigma}^3} d\phi(x_i) \exp\left\{-S[\phi(x_i)]
ight\}$$

finite yet high-dimensional path integral

\rightarrow Monte Carlo

- thermodynamic limit, IR cut-off effects
- \bullet continuum limit, UV cut-off effects
- chiral limit

numerical effort $\sim (1/m)^p$

$$LT = \frac{N_{\sigma}}{N_{\tau}} \to \infty$$
$$aT = \frac{1}{N_{\tau}} \to 0$$

$$m \rightarrow m_{\rm phys} \simeq 0$$

I Phase diagram at $\mu = 0$

Localisation of the phase transition

• order parameter

1.) **Polyakov loop** $L(\vec{x}) = \frac{1}{3} \operatorname{tr} \prod_{\tau} U_{\tau}(\vec{x}, \tau)$

- sensitive on Z(3) symmetry (pure gauge theory only) - measures free energy of an isolated quark $\langle L\rangle\sim e^{-F_{\rm quark}/T}$

hadron phase

plasma phase

 $F_{\text{quark}} \to \infty$ $\langle L \rangle = 0$ $F_{\text{quark}} \text{ endlich}$ $\langle L \rangle \neq 0$

2.) chiral condensate

- sensitive on chiral symmetry $(m \rightarrow 0)$

hadron phase	$\langle \bar{q}q \rangle \neq 0$
plasma phase	$\langle \bar{q}q \rangle = 0$

• susceptibilities

e.g. chiral susceptibility - measures fluctuations

$$\chi_m \sim \frac{\partial^2 \ln Z}{\partial m^2} \sim \langle (\overline{q}q)^2 \rangle - \langle \overline{q}q \rangle^2$$



critical temperature T_c

$$T_c = \frac{1}{N_\tau \, a(g_c)}$$

at T = 0, same (bare) coupling g_c , measure e.g. string tension $\sigma \Rightarrow : \sqrt{\sigma} a(g_c) = number$ \Rightarrow dimension less ratio $T = 1 \qquad q(a)$

$$\frac{I_c}{\sqrt{\sigma}} = \frac{1}{N_\tau a(g_c)} \star \frac{a(g_c)}{number} = \frac{1}{N_\tau \star number}$$

 $\sqrt{\sigma}$ only weakly affected by quark mass



new results: $N_F = 2 + 1$, $N_\tau = 4, 6$, exact algorithm (RHMC)



combined continuum/chiral extrapolation (d = 1.08 for O(4), d = 2 for first order)

$$(T_c r_0)_{m_l, N_\tau} = T_c r_0 + A(m_{PS} r_0)^d + B/N_\tau^2$$

chiral limit $T_c r_0 = 0.444(6)_{-2}^{+12}$ $T_c/\sqrt{\sigma} = 0.399(5)_{-1}^{+10}$ phys. point $T_c r_0 = 0.456(7)_{-1}^{+3}$ $T_c/\sqrt{\sigma} = 0.408(7)_{-1}^{+3}$

with new T = 0 MILC (lattice) results for $r_0 = 0.469(7)$ fm obtain: $T_c = 192(5)(4)$ MeV

nature of the phase transition (at $\mu = 0$) expected

• $\Phi(\tau) = \sum_n \exp\{i\omega_n\tau\} \Phi(\omega_n)$ with Matsubara frequencies $\omega_n = \begin{cases} 2\pi Tn & \text{bosons} \\ \pi T(2n+1) & \text{fermions} \end{cases}$

 \rightarrow for high temperatures static boson-modes only

- \rightarrow three-dimensional effective theory
- long range correlations
 - \rightarrow global symmetries count, microscopic details don't (universality)
 - \rightarrow here: chiral symmetries, σ models

 $\Rightarrow N_F = 2$

- if phase transition continuous (2nd order), then $SU_R(2) \otimes SU_L(2) \simeq O(4)$
- if $U_A(1)$ effectively restored (no non-trivial topological configurations at T_c^{chiral}), then phase transition discontinuous (1st order).

$$\Rightarrow N_F = 3$$
 [Wilczek, Pisarski]

- phase transition discontinuous \rightarrow even at $m \leq m_c \neq 0$
- at critical end point m_c : Z(2) Ising universality

 $\Rightarrow N_F = 2 + 1$

- depending on quark masses $m_{u,d}, m_s$

[Wilczek, Pisarski]

[Gavin,Gocksch,Pisarski]

expected phase diagram in the $m_{u,d} - m_s$ plane ($\mu = 0$)



critical behavior

in the vicinity of a phase transition: correlation length $\rightarrow\infty$

 \Rightarrow scaling behavior of the free energy density

 $f(t, m, L) = b^{-d} f(b^{y_t} t, b^{y_h} m, L/b)$ with reduced temperature $t = \frac{|T - T_c|}{T_c}$

 \Rightarrow scaling laws, e.g.

$$\langle M \rangle \sim m^{1/\delta}$$

$$\chi_m \sim L^{\gamma/\nu}$$

$$B_4 = \frac{\langle (\delta M)^4 \rangle}{\langle (\delta M)^2 \rangle^2}$$
 (here: $\delta M = M - \langle M \rangle, M \simeq \overline{q}q \rangle$

with critical exponents $\delta, \gamma, \nu, \dots$ und Binder-cumulant B_4 universal

	Z(2)	O(2)	O(4)
γ/ν	1.963(3)	1.962(5)	1.975(4)
B_4	1.604(1)	1.242(2)	1.092(3)

 $N_F = 2$

- conflicting results for critical behavior
 - Wilson $\langle M \rangle$ scales ~ O(4) in m
 - staggered χ_m, χ_t does not scale ~ O(4) in m
 - staggered $\langle M \rangle$ scales ~ O(4) in L
 - staggered c_V scales as 1st order
 - staggered $\langle M \rangle$ is as in O(2) at finite L

• $U_A(1)$:

- if effectively restored, then mass spectrum degeneracy



[Iwasaki et al.] [Karsch,EL; JLQCD; MILC] [Engels et al.] [Di Giacomo et al.]

[Kogut, Sinclair]

[Shuryak; Cohen et al;, ...]

screening masses in accord with theoretical expectation



$N_F = 3$

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'



[Bielefeld; deForcrand, Philipsen]

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

 $\mathcal{M} = \langle \overline{q}q \rangle + sS$



improved action: 'reweighting' in quark mass (see later)







1st order at physical point unlikely









• old results: $16^3 \times 4$, $m_{\pi}/m_{\rho} \simeq 0.7$ [Karsch, EL, Peikert]



quark masses seem to not matter too much – controlling/reducing UV effects important

expected properties :





the problem :

$$Z_{GC}(T, V, \boldsymbol{\mu}) = \int \mathcal{D}U_{\mu} \, \mathcal{D}q \, \mathcal{D}\overline{q} \, \exp\left\{-S_{G}(U) + \overline{q}M(\boldsymbol{\mu})q\right\}$$

integrate over quark fields

$$Z_{GC}(T, V, \mu) = \int \mathcal{D}U_{\mu} \det M(\mu) \exp \{-S_G(U)\}$$

- for $\mu \neq 0$: det $M(\mu)$ complex \Rightarrow can not be used as statistical weight in Monte Carlo
- reformulate: det $M(\mu) = |\det M(\mu)| e^{i\Theta}$ and use phase Θ as (part of the) observable: $\langle \mathcal{O} \rangle_{\det M} = \langle \mathcal{O} e^{i\Theta} \rangle_{|\det M|} / \langle e^{i\Theta} \rangle_{|\det M|}$
- but : $\langle e^{i\Theta} \rangle_{|\det M|} \sim e^{-V}$ 'sign problem'

* 'Reweighting'

simulate at parameters $p_0 = (g, m, \mu)_0$ and reweight to $p = (g, m, \mu)$

 $\mathcal{D}Ue^{-S_G(p)} \det M(p) = \frac{\mathcal{D}Ue^{-S_G(p_0)} \det M(p_0) \star e^{-[S_G(p) - S_G(p_0)]} \frac{\det M(p)}{\det M(p_0)}}{\text{simulation}}$

• limited by overlap

* 'Taylor-expansion'

* 'imaginary μ '

[Bielefeld-Swansea; Gavai,Gupta]

$$\langle \mathcal{O} \rangle \left(\frac{\mu}{T}\right) = \langle \mathcal{O} \rangle_{\mu=0} + \langle \tilde{\mathcal{O}}_2 \rangle_{\mu=0} \star \left(\frac{\mu}{T}\right)^2 + \langle \tilde{\mathcal{O}}_4 \rangle_{\mu=0} \star \left(\frac{\mu}{T}\right)^4 + \dots \quad \text{with}$$

h
$$\tilde{\mathcal{O}}_k = \frac{1}{k!} \frac{\partial^k \mathcal{O} \det N}{\partial \mu^k}$$

Glasgow

[Forcrand,Philipsen; D'Elia,Lombardo]

- $\mu = i\mu_I \Rightarrow \det M$ real and positive
- analytic continuation to real μ

• limited by convergence radius

• limited by $Z(\mu_I/T) = Z(\mu_I/T + 2\pi/3)$



μ

New

* 'canonical'

[Forcrand,Kratochvila]

$$Z_C(B) = \frac{1}{2\pi} \int d\left(\frac{\mu_I}{T}\right) \exp\left\{-i3B\frac{\mu_I}{T}\right\} Z_{GC}(\mu = \mu_I)$$

- sample at fixed μ_I
- Fourier transform each determinant \rightarrow work $\sim N_{\sigma}^9 \times N_{\tau}$
- combine with reweighting in μ_I
- back to $Z_{GC}(\mu)$ by $\Sigma_B \exp\left\{+3B\frac{\mu}{T}\right\} Z_C(B)$

Simulations at finite μ Is the future canonical? Conclusions

Simulation method Canonical vs grand canonical Results Maxy

Phase Diagram $T - \mu$: comparing apples with apples



see hep-lat/0602024canonical partition fct. $N_F = 4$ small lattices

taken from Forcrand

agreement at small μ/T seems to hold also at

- $N_F < 4$
- bigger lattices

i) reweighting becomes unreliable

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Ph. de Forcrand
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- applicable at small values for μ in the phenomenologically relevant range for RHIC, LHC
- first, exploratory results in qualitative agreement, further systematic investigations required
- in particular at smaller quark masses :



- considerable quark mass dependence

 $N_F = 3$, improved action

$$\frac{T_c(\mu)}{T_c(0)} = 1 - 0.025(6) \left(\frac{\mu}{T_c(0)}\right)^2$$

$$\frac{T_c(\mu)}{T_c(0)} = 1 - 0.114(46) \left(\frac{\mu}{T_c(0)}\right)^2$$

(perturbative β -function $d\beta_c/d\ln a$)

pressure $(\mu = (\mu_u, \mu_d, \ldots))$

Observables

with

$$\frac{p}{T^4} = \Omega(T,\mu) = \frac{1}{VT^3} \ln Z(T,\mu) = \sum_{n=0}^{\infty} c_n(T,m_q) \left(\frac{\mu}{T}\right)^n$$

$$c_n(T, m_q) = \frac{1}{n!} \frac{1}{VT^3} \frac{\partial^n \ln Z(T, \mu)}{\partial (\mu/T)^n} |_{\mu=0}$$

number density

$$\frac{n_q}{T^3} = \frac{1}{VT^3} \frac{\partial \ln Z(T,\mu)}{\partial (\mu/T)} = \sum_{n=2}^{\infty} nc_n(T,m_q) \left(\frac{\mu}{T}\right)^{n-1}$$

interaction measure

$$\frac{\epsilon - 3p}{T^4} = \sum_{n=0}^{\infty} c'_n(T, m_q) \left(\frac{\mu}{T}\right)^n$$

with

$$c'_n(T, m_q) = T \frac{dc_n(T, m_q)}{dT}$$

from those, energy density

$$\frac{\epsilon}{T^4} = \sum_{n=0}^{\infty} (3c_n(T, m_q) + c'_n(T, m_q)) \left(\frac{\mu}{T}\right)^n$$

and entropy density

$$\frac{s}{T^3} = \frac{\epsilon + p - \mu n_q}{T^4} = \sum_{n=0}^{\infty} ((4 - n)c_n(T, m_q) + c'_n(T, m_q)) \left(\frac{\mu}{T}\right)^n$$

 $\frac{\chi_{ff}(T,\mu)}{T^2} = \frac{\partial^2 \Omega(T,\mu)}{\partial (\mu_f/T)^2}$ diagonal and off-diagonal susceptibilities $\frac{\chi_{fk}(T,\mu)}{T^2} = \frac{\partial^2 \Omega(T,\mu)}{\partial (\mu_k/T)\partial (\mu_k/T)}$ with $\mu_q = \frac{1}{2}(\mu_u + \mu_d)$ and $\mu_I = \frac{1}{2}(\mu_u - \mu_d)$ $\frac{\chi_q(T,\mu)}{T^2} = \frac{\partial^2 \Omega(T,\mu)}{\partial (\mu_a/T)^2} = 2\left(\chi_{uu} + \chi_{ud}\right)$ quark number susceptibility $\frac{\chi_I(T,\mu)}{T^2} = \frac{\partial^2 \Omega(T,\mu)}{\partial (\mu_I/T)^2} = 2(\chi_{uu} - \chi_{ud})$ isovector susceptibility charge susceptibility $\frac{\chi_Q(T,\mu)}{T^2} = \frac{\partial^2 \Omega(T,\mu)}{\partial (\mu_Q/T)^2} = \frac{1}{9} (5\chi_{uu} - 4\chi_{ud})$

and higher moments/derivatives

[Vuorinen]

What is known analytically

(A) high temperature : perturbation theory

 $\Omega(T,\mu) = \Omega^{(0)}(T,\mu) + g^2 \ \Omega^{(2)}(T,\mu) + g^3 \ \Omega^{(3)}(T,\mu) + \mathcal{O}(g^4)$

with <u>Stefan-Boltzmann</u> (free gas) limit

$$\frac{p_{SB}}{T^4} = \Omega^{(0)}(T,\mu) = \frac{8\pi^2}{45} + \sum_{f=u,d,\dots} \left[\frac{7\pi^2}{60} + \frac{1}{2}\left(\frac{\mu_f}{T}\right)^2 + \frac{1}{4\pi^2}\left(\frac{\mu_f}{T}\right)^4\right]$$

diagonal suscept.

off-diagonal suscept.

$$\frac{\chi_{ff}(T,\mu)}{T^2} = 1 + \frac{3}{\pi^2} \left(\frac{\mu_f}{T}\right)^2 + \mathcal{O}(g^2)$$
$$\frac{\chi_{fk}(T,\mu)}{T^2} = g^3 \kappa \frac{\mu_f}{T} \frac{\mu_k}{T} + \mathcal{O}(g^4)$$
$$\frac{\chi_{fk}(T,0)}{T^2} = -\frac{5}{144\pi^6} g^6 \ln 1/g$$

(B) low temperature : hadron resonance gas model

$$\Omega_{HRG}(T,\mu_q,\mu_I) = \sum_{i \in mesons} \Omega^M_{m_i}(T,\mu_q,\mu_I) + \sum_{i \in baryons} \Omega^B_{m_i}(T,\mu_q,\mu_I)$$

where

$$\Omega_{m_i}^{M/B} = \frac{1}{2\pi^2} \left(\frac{m_i}{T}\right)^2 \sum_{\ell=1}^{\infty} \left\{\frac{1}{(-1)^{\ell+1}}\right\} \ell^{-2} K_2 \left(\frac{\ell m_i}{T}\right) z_i^{\ell} \quad \text{with} \ z_i = \exp((3B_i \mu_q + 2I_{3i} \mu_I)/T)$$
fugacities

• for baryons, $\ell \geq 2$ terms can safely be neglected¹ \Rightarrow at $\mu_I = 0$:

$$\frac{p(T, \mu_q, \mu_I = 0)}{T^4} \simeq G(T) + F(T) \cosh\left(\frac{3\mu_q}{T}\right) \qquad \Rightarrow \qquad \frac{\chi_q}{T^2} = 9F(T) \cosh\left(\frac{3\mu_q}{T}\right)$$
likewise,
$$\frac{\chi_I(T, \mu_q, \mu_I = 0)}{T^2} \simeq G^I(T) + F^I(T) \cosh\left(\frac{3\mu_q}{T}\right)$$

• For all quantities X of the form $X = G^X(T) + F^X(T) \cosh(3\mu_q/T)$:

$$X = \sum_{n=0}^{\infty} c_n^X(T) \left(\mu_q / T \right)^n \qquad \text{with} \qquad \frac{c_{2n+2}^X}{c_{2n}^X} = \frac{9}{(2n+2)(2n+1)} \quad \text{for } n \ge 1$$

¹ $K_2(x) \sim e^{-x}(1 + P(1/x))/\sqrt{x}$

pressure

quark number

q number suscept.

Isovector suscept.







• comparison: up to $\mathcal{O}(\mu^4)$ (dashed) with up to $\mathcal{O}(\mu^6)$ (full) suggests rapid convergence

• contribution to total p is small: $p(\mu = 0)/T^4 \simeq \mathcal{O}(4)$



0.8

1.2

1.4

1.0

1.8

1.6

2.0

together with the c'_n coefficients ...

Lines of fixed entropy over baryon number

it is generally believed that the fireball expansion follows a line of fixed S/N_B



in the ideal gas limit

$$\frac{S}{N_B} = 3\frac{\frac{37\pi^2}{45} + (\frac{\mu_q}{T})^2}{\frac{\mu_q}{T} + \frac{1}{\pi^2}(\frac{\mu_q}{T})^3} \qquad \Rightarrow \frac{\mu_q}{T} = \text{const (vertical lines)}$$

isentropic expansion lines for SPS: $S/N_B \simeq 45$

RHIC:
$$S/N_B \simeq 300$$

FAIR: $S/N_B \simeq 30$

keep in mind: feasibility study of what one can do with lattice data



Isentropic EoS

- $p(\epsilon)$ to a good approximation independent of S/N_B
- $p(\epsilon)$ well parametrized by

$$\frac{p}{\epsilon} \simeq \frac{1}{3} \left(1 - \frac{1.2}{1 + 0.5 \,\epsilon \,\mathrm{fm}^3/\mathrm{GeV}} \right)$$

Comparison with analytic results

recall: ratios $\frac{c_{2n}}{c_{2n+2}}$ allow comparison with the hadron resonance gas model fairly detail independent



- above T_0 : ratios approaching SB values
- below T_0 : ratios except those involving $c_0, c_2^I, c_0^{\bar{\psi}\psi}$ (depend on $G^X(T)$) are
 - temperature independent
 - taking hadron resonance gas values \rightarrow do not indicate critical behavior



- again comparison: up to $\mathcal{O}(\mu^4)$ (dashed) with up to $\mathcal{O}(\mu^6)$
- peak in χ_q developing with increasing μ , coming from c_4
- c_6 shifts peak in χ_q to smaller T
- \bullet peak less convincing because of error bars and dip \rightarrow more statistics needed here
- no peak in $\chi_I \longrightarrow$ strong correlations between χ_{uu} and χ_{ud}



• at $T > T_0$: χ_{uu} and χ_{ud} approach SB limit, i.e. $\chi_{ud} \to 0$

- at $T > T_0$ signs in agreement with perturbation theory [Blaizot, Iancu, Rebhan]
- at $T \lesssim T_0$: $\chi_{ud} \neq 0$
- around $T_0: c_n^{ud} \simeq c_n^{uu}$ for $n > 2 \to \text{at } \mu_q = \mu_c$, peaks in both, χ_{uu} and χ_{ud}

 \rightarrow at $\mu_q > 0$, fluctuations in different flavor channels are correlated



• χ_q rises rapidly with increasing μ_q , but rise to a large extent due to rise in pressure

- no indication of criticality
- but, for $T \leq 0.96T_c$, consistency with hadron resonance gas model (at $\mu_I = 0$)

$$\frac{n_q^{HRG}}{\mu_q \chi_q^{HRG}} = \frac{T}{3\mu_q} \tanh\left(\frac{3\mu_q}{T}\right)$$

convergence radius



critical point limits convergence radius

$$\rho = \lim_{k \to \infty} \rho_k = \lim_{k \to \infty} \sqrt{\frac{c_k}{c_{k+2}}}$$

- SB limit:
$$\rho_k = \infty$$
 for $k \ge 4$

- for T big: approaching SB limit

- at
$$T_c(\mu)$$
 : $\rho_k \simeq 1$

- $c_k > 0 \Rightarrow$ convergence radius indicates critical point

Results:

- Gavai, Gupta: $\mu_B \simeq 180 \text{MeV}$ (Taylor expansion)
- Fodor, Katz: $\mu_B \simeq 360 \text{MeV}$ (Lee-Yang zeroes)
- Bi-Swansea: LGT consistent with HRG, HRG analytic (Taylor expansion)

[deForcrand, Philipsen]



existence of a critical endpoint ?

critical region has the tendency to grow with $\mu_I \Rightarrow$ shrink with real μ



but: finer lattices/improved actions needed $N_{\tau} = 4$ here