The QCD Phase Diagram at zero and small Baryon Densities

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- The expected qualitative picture and computational methods
- The activities in the last year ⇒systematics!
- A non-standard scenario
- Conclusions
The expected phase diagram:

Non-pert. problem $\Rightarrow$ Lattice 1975-2001: $\mu \neq 0$ impossible $\Rightarrow$ sign problem!

Where does this picture come from?

- Simulations on $T$-axis (light quarks only now)
- models for $T = 0, \mu \neq 0$

Take more general view $\Rightarrow$ parameter space $\{m_{u,d}, m_s, T, \mu\}$
$N_f = 2$: 

$\mu, m = 0$ : \[ SU(2)_V \times SU(2)_A \rightarrow SU(2)_V \]

true order parameter $\langle \bar{\psi} \psi \rangle \Rightarrow$ separate phases  

**if** second order **then** $\Rightarrow O(4)$

---

N.B. $m=0$: 1.O. all the way also possible

*$N_f = 3$:*

$\mu = 0, m < m_c$ first order  

$\mu = 0, m > m_c$ crossover

**⇒ standard scenario:** $\mu_c$ increases with $m$  

$(\mu = 0, T = 0$ transitions connected)
Full phase diagram 3d: $\{m, T, \mu\}$

e.g. $N_f = 3$:

- Confined/deconfined $\Rightarrow$ pseudo-critical surface $T_0(\mu, m)$ (from susceptibilities)
- 1.O./crossover $\Rightarrow$ line of critical points $T^E(\mu) = T_0(\mu, m_c(\mu))$ (from FSS)

Projection onto (pseudo-) critical surface:

$\Rightarrow \mu^c(m)$ or $m_c(\mu)$
The case \( N_f = 2 + 1, \mu = 0 \):

\[ \Rightarrow m_c(\mu = 0) \text{ (unimproved KS)} \]

Bielefeld; Columbia; de Forcrand, O.P.

universality: 3d Ising

Bielefeld

N.B: \( m_c \) has cut-off effects!

(factor 1/4?)

Bielefeld, MILC

Finite density, \( \mu \neq 0 \)
Lattice QCD at finite temperature and density

Difficult (impossible?): sign problem of lattice QCD

\[ Z = \int DU \left[ \det M(\mu) \right] f e^{-S_g[U]} , \quad S_f = \sum_f \bar{\psi} M \psi \]

\[ \det(M) \] complex for SU(3), \( \mu = \mu_B/3 \neq 0 \Rightarrow \) no Monte Carlo importance sampling

Evading the sign problem:

I. Two-parameter reweighting in \((\mu, \beta)\)

\[ Z = \left\langle \frac{e^{-S_g(\beta)} \det(M(\mu))}{e^{-S_g(\beta_0)} \det(M(\mu = 0))} \right\rangle_{\mu=0,\beta_0} \]

idea: simulate at \( \beta_0 = \beta_c(0) \), better overlap by sampling both phases; errors? ovlp.?

I.a Reweighting + density of states

\( \Rightarrow \) larger \( \mu \), low \( T \), Fodor, Katz, Schmidt, Lat05

Fodor, Katz
II. Taylor expansion

idea: for small $\mu/T$, compute coeffs. of Taylor series $\Rightarrow$ local ops. $\Rightarrow$ gain V
convergence?

III.a Imaginary $\mu$ + analytic continuation

fermion determinant positive $\Rightarrow$ no sign problem

idea: for small $\mu/T$, fit full simulation results of imag. $\mu$ by Taylor series

• vary two parameters $(\mu, T) \Rightarrow$ controlled continuation?

III.b Imaginary $\mu$ + Fourier transformation

idea: canonical partition function at fixed baryon density

• no analytic continuation, but determinant needed $\Rightarrow$ thermodynamic limit?

IV. Theories without sign prob.: finite isospin density

idea: no sign problem, reproduces baryon chem. pot. for small $\mu/T$?

All agree on $T_0(m, \mu)$!!! $(\mu/T \lesssim 1)$
$N_f = 2, \mu = 0, m = 0$: is it O(4)? (or O(2) for finite a)

- previous evidence inconclusive  
  cf. old proceedings

**New investigation:**

D'Elia, Di Giacomo, Pica

FSS on $L^3 \times 4$, $L = 16 - 32$, standard staggered Fermions, R-algorithm, $m/T \gtrsim 0.055$

In critical region:

⇒ spec. heat : $C_V - C_0 \simeq L^{\alpha/\nu} f_c \left( \tau L^{1/\nu}, am L^{y_h} \right)$ \quad $\tau = 1 - T/T_c$

⇒ suscept. of order param. : $\chi \simeq L^{\gamma/\nu} f_\chi \left( \tau L^{1/\nu}, am L^{y_h} \right)$  

and others...

**Strategy:**

- Fix $y_h$ to O(4) value
- choose $L, am$ to keep $am L^{y_h}$ fixed⇒ one variable only, inf. $V \Rightarrow am = 0.$

⇒ check consistency with scaling
similar: keeping $\tau L^{1/\nu}$ fixed, check of 1st order:
But no metastability in plaquette distributions

⇒ still not conclusive!
  • scaling window very small ?
  • fermion formulation? (Wilson sees $O(4)$)
  • cut-off effects ?

⇒ $N_t = 6$ study promised;

Suggestions:
  • FSS at fixed $am$
  • Binder cumulants
  • exact algorithm
Finite density by Taylor expansion, $N_f = 2$:

Finite $V$: $Z(m > 0, \mu, T)$ analytic in entire parameter space

CP-Symmetry: $Z(\mu) = Z(-\mu) \Rightarrow$ all observables have Taylor series in $(\mu/T)^2$

Pressure density: $p(T, \mu) = \left(\frac{T}{V}\right) \log Z(T, \mu), \quad \frac{p}{T^4} = \sum_{n=0}^{\infty} c_{2n}(T) \left(\frac{\mu}{T}\right)^{2n}$

Coefficients: generalized quark number suscept. at $\mu = 0 \Rightarrow$ measurable!

$V \rightarrow \infty$: phase transitions $\Rightarrow$ singularities in pressure

Radius of convergence $\equiv$ distance to nearest singularity;

E.g.: $\rho_n = \left| \frac{c_0}{c_{2n}} \right|^{1/2n}, \quad r_n = \left| \frac{c_{2n}}{c_{2n+2}} \right|^{1/2}, \quad \rho, r = \lim_{n \rightarrow \infty} \rho_n, r_n$

If singularity on real axis (asymptotically all coeffs. positive) $\Rightarrow$ critical point
Technicalities:

\[ \mu \text{-dependence in } \det M \Rightarrow \frac{\partial \ln \det M}{\partial \mu} = \text{tr} \left( M^{-1} \frac{\partial M}{\partial \mu} \right) \text{ etc.} \]

\Rightarrow \text{traces of composite local ops., Gaussian noise vectors } \sim O(10^{-100})

non-trivial FSS of susceptibilities \Rightarrow \text{delicate cancellations for large } V

Quark number susceptibility to order \( \mu^6 \)

Gavai, Gupta

Lattices \( L^3 \times 4, \ L = 8 - 24 \), standard staggered, R-algorithm, \( m/T_0 = 0.1 \)

Strategy: compute coeffs. at different \( T/T_0 = 0.75 - 2.15 \Rightarrow \text{extrapolate to finite } \mu \)

\[ T \]

\[ \mu \]

\[ V_1 \]

\[ V_2 \]
$T/T_0 = 0.95$, convergence radius vs. order $n$:

\[ \rho_n \text{ on } 8^3, 24^3 \]

\[ r_n \text{ on } 8^3, 24^3 \]

⇒ **strong volume dependence!**

⇒ need \( L m_{\pi} \gtrsim 5 - 6 \) \( (L \gtrsim 16 - 18) \)

⇒ need more terms for larger $V$

⇒ quoted result:

\[
\frac{\mu_B^c}{T} = 1.1 \pm 0.2
\]

\[
\frac{T}{T_0} = 0.95
\]
The pressure to order $\mu^6$

Lattice $16^3 \times 4$, Symanzik improved Wilson, p4-improved staggered fermions, R-algorithm, $m/T_0 \approx 0.4$

Comparisons with $(\mu/T)$-expansions of

- high $T$ pert. theory
- hadron resonance gas (HRG) model

coefficients in different orders:

$c_6 \ll c_4 \ll c_2 \Rightarrow$ coeffs. $\sim O(1)$ for "natural" expansion parameter $\frac{\mu}{\pi T}$

de Forcrand, O.P.
radius of convergence:

\[ n_q/\chi_q = \frac{\partial p}{\partial n_q} (= 0 \text{ for 2.O.}) \]

lines: coeffs. from HRG model: \( c_4/c_2 = 3/4 \)

- consistency with hadron resonance gas
- no evidence for critical point
- Not in conflict with Gavai, Gupta (different action, larger \( m \))
- but different conclusion than at \( \mu^4 \)!
- previous experience (spin models, strong coupling series), use many terms (10-20)

\[ \mu/T = 0.4 \quad \mu/T = 0.8 \]

\[ 0.8 \quad 1 \quad 1.2 \quad 1.4 \]

\[ 0 \quad 0.2 \quad 0.4 \quad 0.6 \quad 0.8 \quad 1 \]

\[ T/T_c \]

\[ n_q/(\mu_q \chi_q) \]

\[ T/T_0 \]

e.g. Itzykson, Drouffe
Systematics of reweighting and Taylor expansion

\[ \langle O \rangle_{(\beta, \mu)} = \frac{\langle O e^{\frac{n_f}{4} \Delta \ln \det M} e^{-\Delta S_g} \rangle_{(\beta_0, 0)}}{\langle e^{\frac{n_f}{4} \Delta \ln \det M} e^{-\Delta S_g} \rangle_{(\beta_0, 0)}} \sim e^{-V \Delta F} \]

\[ \det M = | \det M | e^{i \theta} \]

⇒ **Breakdown of reweighting** for \( \langle \cos \theta \rangle \ll 1 \)

or \( \sigma(\theta) = \sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} > \pi/2 \)

⇒ **compute variance from Taylor coeffs.**

Bielefeld-Swansea

\[ \theta^{(n)} = \frac{n_f}{4} \Im \sum_{j=1}^{n} \frac{\mu^{2j-1}}{(2j-1)!} \frac{\partial^{2j-1} \ln \det M}{\partial \mu^{2j-1}} \]

Contours of \( \sigma(\theta) \): (fixed \( V = 16^3 \))
Observation: LYZ competing with noise of $\det M$

$$Z_{\text{norm}}(\beta_{\text{Re}}, \beta_{\text{Im}}, \mu) = \left\langle e^{6 i \beta_{\text{Im}} N_{\text{site}} \Delta P e^{i \theta}} \left| e^{(N_f/4)(\ln \det M(\mu) - \ln \det M(0))} \right\rangle_{(\beta_{\text{Re}}, 0, 0)} \right|$$

⇒ doesn’t work at infinite $V$ (not surprising...)

In practice: • enough statistics for a given volume? • errors reliable?
QCD at finite isospin density

Son, Stephanov

Opposite chemical potentials for u,d-quarks:
\[ \mu_u = -\mu_d = \mu \Rightarrow \mu_I \equiv (\mu_u - \mu_d) = 2\mu \]

\[ \Rightarrow \text{phases of determinants cancel} \]

\[ Z = \int DU \left| \det M(\mu) \right|^{N_f} e^{-S_g[U]} \]

Pion condensate \( \neq \) QCD, but for \( \mu_I < m_\pi \) recover QCD:

\[ \langle O \rangle_\mu = \frac{\langle e^{i\theta} O \rangle_{\mu_I=2\mu}}{\langle e^{i\theta} \rangle_{\mu_I=2\mu}} \]

consider \( O \) probing p.t.

for \( \langle \cos \theta \rangle_{\mu_I} \sim 1, O' = e^{i\theta} O \) shows same transition!

Numerically verified for \( T_0(\mu, m), \quad N_f = 2, 3 \):

• in Taylor expansion (Bielefeld-Swansea)
• simulations at \( \mu_I \) (Kogut, Sinclair) and \( \mu_i \) (de Forcrand, O.P.)
Phase of the determinant and phase-quenched QCD

\( \sigma(\theta) \) and the transition to a pion condensate at finite isospin:

⇒ related, since

phase of \( \det M \)'"destroys" pion condensate

boundary for reweighting?

observation:

FK-points both lie on boundary ⇒...

similarly for Taylor exp.
QCD at complex $\mu$: general properties

$$Z(V, \mu, T) = \text{Tr} \left( e^{-\left(\hat{H} - \mu \hat{Q}\right)/T} \right); \quad \mu = \mu_r + i \mu_i; \quad \bar{\mu} = \mu/T$$

exact symmetries: $\mu$-reflection and $\mu_i$-periodicity

Roberge, Weiss

$$Z(\bar{\mu}) = Z(-\bar{\mu}), \quad Z(\bar{\mu}_r, \bar{\mu}_i) = Z(\bar{\mu}_r, \bar{\mu}_i + 2\pi/N_c)$$

Imaginary $\mu$ phase diagram:

$Z(3)$-transitions: $\bar{\mu}_i^c = \frac{2\pi}{3} \left( n + \frac{1}{2} \right)$

1st order for high $T$, crossover for low $T$

analytic continuation within arc:

$|\mu|/T \leq \pi/3 \Rightarrow \mu_B \lesssim 550\text{MeV}$

$$\langle O \rangle = \sum_{n}^{N} c_n \bar{\mu}_i^{2n} \Rightarrow \mu_i \longrightarrow i \mu_i$$

Pade approximants? (Lombardo, Lat05)
A generalized imaginary $\mu$-approach

Azcoiti, Di Carlo, Galante, Laliena

Reformulation of staggered action, chemical potential term

$$\frac{1}{2} \sum_n \bar{\psi}_n \eta_0(n) \left( e^{\mu a} U_{n,0} \psi_{n+0} - e^{-\mu a} U_{n-0,0}^\dagger \psi_{n-0} \right)$$

Hasenfratz, Karsch

$$\rightarrow x \frac{1}{2} \sum_n \bar{\psi}_n \eta_0(n) \left( U_{n,0} \psi_{n+0} - U_{n-0,0}^\dagger \psi_{n-0} \right)$$

$$+ y \frac{1}{2} \sum_n \bar{\psi}_n \eta_0(n) \left( U_{n,0} \psi_{n+0} + U_{n-0,0}^\dagger \psi_{n-0} \right), \quad x = \cosh(a\mu), \ y = \sinh(a\mu)$$

solid line: phase transitions
dotted line: physical line $x^2 - y^2 = 1$

Sign problem $\Rightarrow$ simulations at imaginary $y = i\bar{y}$

possible improvement: simulations at different $x, y$,
lower temperatures
better control of continuation?
**Numerical results, $N_f = 4$**

$8^3 \times 4$, standard staggered, R-algorithm, $m/T \approx 0.2$

Fitting to $\beta_c(\bar y) = \beta_0 + \beta_1 \bar y^2$ plus continuation:

- works at least as well as standard imag. $\mu$, more expensive
- can it be made to work better? control of errors beyond $\mu/T > 1$?
- $N_f = 2$ in progress, preliminary evidence for critical point

$\beta = \beta_0 + \beta_1 \bar y^2$

point of departure for reweighting, improved range?

Laliena, Lat05
QCD at fixed baryon number

Fix baryon number $B$: $\Rightarrow \delta(3B - \int d^3x \, \bar{\psi} \gamma_0 \psi)$

$$Z_C(B) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\left(\frac{\mu_i}{T}\right) e^{-i3B \frac{\mu_i}{T}} Z_{GC}(\mu = i\mu_i)$$

- Sample $Z_{GC}(\mu = i\mu_{MC})$

$$\Rightarrow \frac{Z_C(B)}{Z_{GC}(i\mu_{MC})} = \left\langle \frac{1}{\det(i\mu_{MC})} \int d\mu_i \exp\left(i3B \frac{\mu_i}{T}\right) \det(i\mu_i) \right\rangle$$

- Fourier transform each determinant exactly (work $\propto L_s^9 L_t$) $\leftarrow$ low $T$

- Sign problem $\leftrightarrow$ noise in $Z_C(B) \leftarrow$ governed by $B$ (not $V$)

- Study few-baryon system at low temperature: Nuclear Physics!

preliminary results, Wilson fermions: Alexandru et al, Lat05
**Numerical results,** $N_f = 4$

$6^3 \times 4$, standard staggered, HMC-algorithm, $m/T \approx 0.2$  
(p.t. first order $\forall \mu$)

**Chemical potential versus baryon density**

$F(B) \rightarrow \mu$ transformation via saddle point approximation:

$$Z_{GC}(\mu) = \int d\rho \exp \left( -\frac{V}{T}(f(\rho)) + \mu \rho \right) \implies \mu \approx f'(\rho) \approx \frac{F(B+1)-F(B)}{3}$$

**Comparison of methods:**

- Weakly interacting massless gas
- Hadron Resonance Gas
- QGP
- Confined

<table>
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<th>Method</th>
<th>$\langle \mu \rangle / T$</th>
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<td>D'Elia, Lombardo, 16</td>
<td>~ 0.85(1)</td>
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<td>Azcoiti et al., 8</td>
<td>~ 0.45(5)</td>
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<td>Fodor, Katz, 6</td>
<td>~ 0.10(1)</td>
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<td>Our reweighting, 6</td>
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</table>
The critical endpoint and its quark mass dependence in $N_f = 3$

Expect: \[ \frac{m_c(\mu)}{m_c(\mu=0)} = 1 + c_1 \left( \frac{\mu}{\pi T} \right)^2 + \ldots \]

Inverted: curvature of critical surface $\mu_c(m)$
Criticality: cumulant ratios

3d Ising universality:

\[
B_4(m_c, \mu_c) = \frac{\langle (\delta \bar{\psi} \psi)^4 \rangle}{\langle (\delta \bar{\psi} \psi)^2 \rangle^2} \to 1.604, \quad V \to \infty
\]

\((B_4 = 1\) (first-order), \(3\) (crossover) for \(V = \infty\))

\[
B_4(a m, a \mu) = 1.604 + B \left( a m - a m_c(0) + A(a \mu)^2 \right) + \ldots
\]

de Forcrand, O.P.

\[
\Rightarrow \frac{m_c(\mu)}{m_c(\mu = 0)} = 1 + 0.84(36) \left( \frac{\mu}{\pi T} \right)^2 + \ldots
\]

FSS:

\[
\nu = 0.62(3)
\]

\[
\nu(\text{Ising}) = 0.63
\]
\( N_f = 3 \) at finite isospin density

Lattices \( L^3 \times 4, L = 8, 12, 16 \), standard staggered, R-algorithm, \( m \gtrsim m_c(0) \)

Finite stepsize effects change order:

Extrapolated results:

\[ dB_4/d\mu_I^2 \gtrsim 0 \], more crossover with \( \mu \)??
Redoing $N_f = 3$ with an exact algorithm

de Forcrand, O.P.

Extrapolations $dt^2 \to 0$ prohibitively expensive for small $m$

⇒ use exact algorithm here: Rational Hybrid MC

Clark, Kennedy, Lat05

Testing RHMC against $dt^2 - > 0$:

The critical mass $m_c(0)$ with RHMC:

leftmost data: RHMC

• 25% change in $m_c(0)$

• $dB_4/d\mu_f^2 \approx 0$

• consistent with finite isospin!
A non-standard scenario:

no critical point at all?

continuum conversion:

\[
\frac{m_c(\mu)}{m_c(\mu = 0)} = 1 - 0.6(2) \left( \frac{\mu}{\pi T} \right)^2
\]

Positive or negative curvature:

very high quark mass sensitivity of \( \mu_c \)!!

Can one expect a critical point at “small” \( \mu \)?

\( \mu_B^c \sim 360 \text{ MeV (FK)} \) requires

\[
1 < \frac{m}{m_c(\mu = 0)} \lesssim 1.05
\]

fine tuning of quark masses!!
Outlook: \( N_f = 2 + 1 \)

Two-step procedure:

I. \((m_s, m_u, d)\) phase-diagram at \( \mu = 0 \) \( \Rightarrow m_s^c(m_u, d) \)

II. repeat for \( \mu \neq 0 \)

If there is a tricritical point:

\[ m_s^{tric}/T_0 \approx 2.8 \]
The quenched limit: Potts model

$m \rightarrow \infty$: QCD $\rightarrow$ theory of Polyakov lines $\rightarrow$ universality class of 3d 3-state Potts model (3d Ising)

large $\mu$: cluster algorithms

small $\mu/T$: sign problem mild, doable for real $\mu$!

$\Rightarrow$ Testing ground for real vs. imaginary $\mu$:

Information on upper right corner:

$\Rightarrow$ First order region shrinks with $\mu$!
Conclusions

Physics:

• $N_f = 2$ : O(4) vs. 1st order remains open

• several groups tackling critical endpoint at finite $\mu$, no convergence yet

• strong quark mass sensitivity of $\mu_c$

Systematics:

• more methods available, more cross checks

• beginning to understand phase of $\det$, finite $V$

• use exact algorithms !!!

⇒ qualitative picture in reach

⇒ physics in the continuum still a long way......(we are at $a \sim 0.3 \, fm$) ⇒ surprises?