Lattice QCD at finite T and μ, phase diagram and the critical point

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1. Introduction
2. Overlap improving multi-parameter reweighting
3. Phase diagram, critical endpoint in n_f=2+1 dynamical QCD
4. Taylor expansion, imaginary chemical potential methods
5. The density of states method at larger μ
6. Summary

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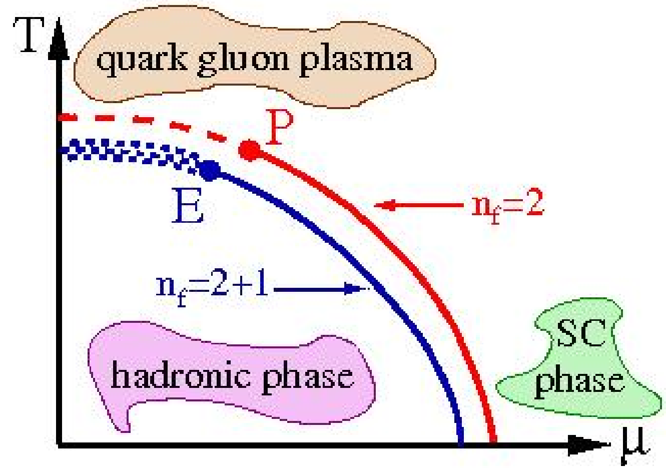
Introduction, experimental motivation



- Chiral phase transition (PT)

$n_f = 2$ with $m_q = 0$ at $\mu = 0 \Rightarrow 2^{nd}$ order PT
$n_f = 2$ with $m_q = 0$ at $T = 0 \Rightarrow 1^{st}$ order PT
$n_f = 2$ with $m_q = 0 \Rightarrow$ tricritical point (P) at μ,T≠0

$n_f = 3$ with $m_q = 0$ at $\mu = 0 \Rightarrow 1^{st}$ order PT
increasing m_s weakens the 1^{st} order PT $\Rightarrow$ cross-over

$n_f = 2+1$ with physical m_q at $\mu = 0 \Rightarrow$ cross-over
$n_f = 2+1$ with physical m_q at $T = 0 \Rightarrow 1^{st}$ order PT
$n_f = 2+1$ with physical $m_q \Rightarrow$ critical endpoint (E) at μ,T≠0

"If and when the critical point E is discovered, it will appear prominently on the map of the phase diagram featured in any future textbook of QCD." (F. Wilczek)

- location of the endpoint: nonperturbative prediction of QCD

lattice gauge theory: serious problems at $\mu \neq 0$

measure (Dirac determinant) complex $\Rightarrow$ no importance sampling

I.M. Barbour et al., Nucl. Phys. B (Proc. Supl.) 60A, 220 (1998)

Glasgow method: μ reweighting based on an ensemble at $\mu = 0$

after collecting 20 million configurations only unphysical results

$T = \mu = 0$ ensemble does not overlap with the transition states

M.A. Halasz et al., Phys. Rev. D58, 096007 (1998)

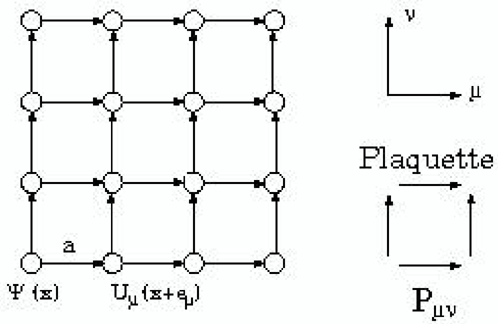
random matrix model for the Dirac operator can be solved

$\Rightarrow T_E \approx 120$ MeV and $\mu_E \approx 700$ MeV, can be off by a factor of 2-3

J. Berges, K. Rajagopal, Nucl. Phys. B538, 215 (1999)

Nambu-Jona-Lasinio model, $T - \mu$ phase diagram

lattice action of QCD and Monte-Carlo techniques



$$\mathscr{L} = -\frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \bar{\psi}(D_\mu \gamma^\mu + m)\psi$$

anti-commuting $\psi(x)$ quark fields live on the sites

gluon fields, $A^a_\mu(x)$ are used as links and plaquettes

$$U(x,y) = \exp(ig_s \int_x^y dx'^\mu A^a_\mu(x')\lambda_a/2)$$

$$P_{\mu\nu}(n) = U_\mu(n) U_\nu(n+e_\mu) U^\dagger_\mu(n+e_\nu) U^\dagger_\nu(n)$$

$S = S_g + S_f$ consists of the pure gluonic and the fermionic parts

$$S_g = 6/g_s^2 \cdot \Sigma_{n,\mu,\nu} \left[1 - \mathrm{Re}(P_{\mu\nu}(n))\right]$$

quark differencing scheme:

$$\bar\psi(x)\gamma^\mu \partial_\mu \psi(x) \to \bar\psi_n \gamma^\mu (\psi_{n+e_\mu} - \psi_{n-e_\mu})$$
$$\bar\psi(x)\gamma^\mu D_\mu \psi(x) \to \bar\psi_n \gamma^\mu U_\mu(n) \psi_{n+e_\mu} + \ldots$$

in continuum the chemical potential acts: $\mu a \bar\psi_x \gamma_4 \psi_x$

fourth component of an imaginary(!), constant vector potential

fermionic part as a bilinear expression: $S_f = \bar\psi_n M_{nm} \psi_m$

Euclidean partition function gives Boltzman weights

$$Z = \int \prod_{n,\mu} [dU_\mu(x)][d\bar\psi_n][d\psi_n] e^{-S_g - S_f} = \int \prod_{n,\mu} [dU_\mu(n)] e^{-S_g} \det(M[U])$$

Metropolis step for importance sampling:

$$P(U \to U') = \min\left[1, \exp(-\Delta S_g) \det(M[U'])/\det(M[U])\right]$$

for μ=0 the determinant is positive, for $\mu \neq 0$ it is complex

$\Rightarrow$ no probability interpretation, no Monte-Carlo method

Overlap improving multi-parameter reweighting

Z. Fodor and S.D. Katz, Phys. Lett. B534 (2002) 87

$$Z(m,\mu,\beta) = \int \mathcal{D}U \exp[-S_g(\beta,U)] \det M(m,\mu,U) =$$

$$\int \mathcal{D}U \exp[-S_g(\beta_0,U)] \det M(m_0,\mu=0,U)$$

$$\left\{ \exp[-S_g(\beta,U)+S_g(\beta_0,U)] \frac{\det M(m,\mu,U)}{\det M(m_0,\mu=0,U)} \right\}$$

first line = measure, field configurations of the Monte-Carlo

curly bracket = can be measured on each configuration, weight

expectation value of an observable O:

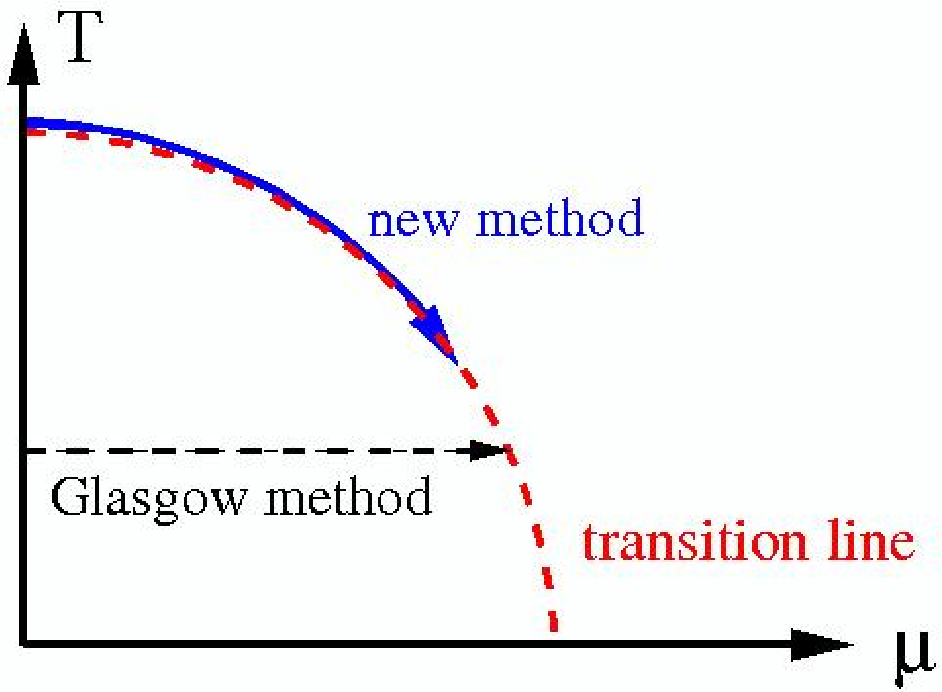
$$\langle 0 \rangle_{\beta,\mu,m} = \frac{\sum w(\beta,\mu,m) O(\mu,m)}{\sum w(\beta,\mu,m)}$$

observables to get the transition points at $\mu \neq 0$ (susceptibilities)

simultaneously changing several parameters: better overlap

e.g. transition configurations are mapped to transition ones

Comparison with the Glasgow method



one parameter reweighting	New method
single parameter (μ)	two parameters (μ and β)
purely hadronic configurations	transition configurations

QCD with n_f=2+1 dynamical staggered fermions

Z. Fodor, S. D. Katz, hep-lat/0106002 (JHEP 03 (2002) 014)

- partition function with multi-parameter reweighting

$$Z(\alpha) = \int \mathcal{D}\phi \, \exp[-S_{bos}(\alpha_0,\phi)][\det M(\phi,\alpha_0)]^{n_f/4}$$
$$\{\exp[-S_{bos}(\alpha,\phi) + S_{bos}(\alpha_0,\phi)][\det M(\phi,\alpha)/\det M(\phi,\alpha_0)]^{n_f/4}\}$$

we measure fractional powers of the complex determinants
⇒ choose among the possible Riemann-sheets

a. gauge fix to $A_0 = 0$ on all but the last timeslice
b. multiply the j-th row/column by $e^{\pm j\mu}$
c. rearrange the columns of the matrix
d. L_t-2 Gauss elimination step gives a $6L_s^3 \times 6L_s^3$ matrix

$$\det M(\mu) = e^{-3V\mu} \prod_{i=1}^{6L_s^3} (e^{L_t\mu} - \lambda_i)$$

⇒ gives Z for "arbitrary" μ and β

Lee-Yang zeros of the partition function

C.N. Yang and T.D. Lee, Phys. Rev. 87, 404 (1952)

• distinguish between a crossover and a 1^{st} order PT

1^{st} order PT: free energy $\propto \log Z(\beta)$ non-analytic
PT appears not at finite V, but only at V$\to \infty$
Z has zeros even at finite V, at complex parameters (β)
Re(β_0), zero with smallest imaginary part: transition point

for 1^{st} order PT: zeros approach the real axis
$1/V$ scaling in the V$\to \infty$ limit
generates the non-analiticity of the free energy

crossover: zeros do not approach the real axis

• illustration with Lee-Yang zeros

in $V \to \infty$ limit the partition function has the form

$$Z = Z_a + Z_b = e^{-Vf_a} + e^{-Vf_b}$$

free-energy densities coincide at T_c: $f_b = f_a + \alpha(T - T_c) + ...$

$$Z = 2\exp[-V(f_a + f_b)(T - T_c)/2] \cosh[-V\alpha(T - T_c)]$$

for complex T values (controlled by β) there are zeros of Z

$$Im(T_0) = \pi \cdot (n - 1/2)/(V\alpha)$$

with integer numbers of n and $Re(T) \approx T_c$

1/V scaling expected $V \to \infty$ limit (α depends on V)
for rapid cross-over (no phase transition scenario)
finite value is obtained in the $V \to \infty$ limit


ALICEnext

Endpoint with physical quark masses on $L_t = 4$ lattices

Z.Fodor, S.D.Katz, hep-lat/0402006, JHEP 04 (2004) 050

- three basic steps of the analysis

m_s=0.25, m_{ud}=0.0092: physical ones, T=0 measurements show

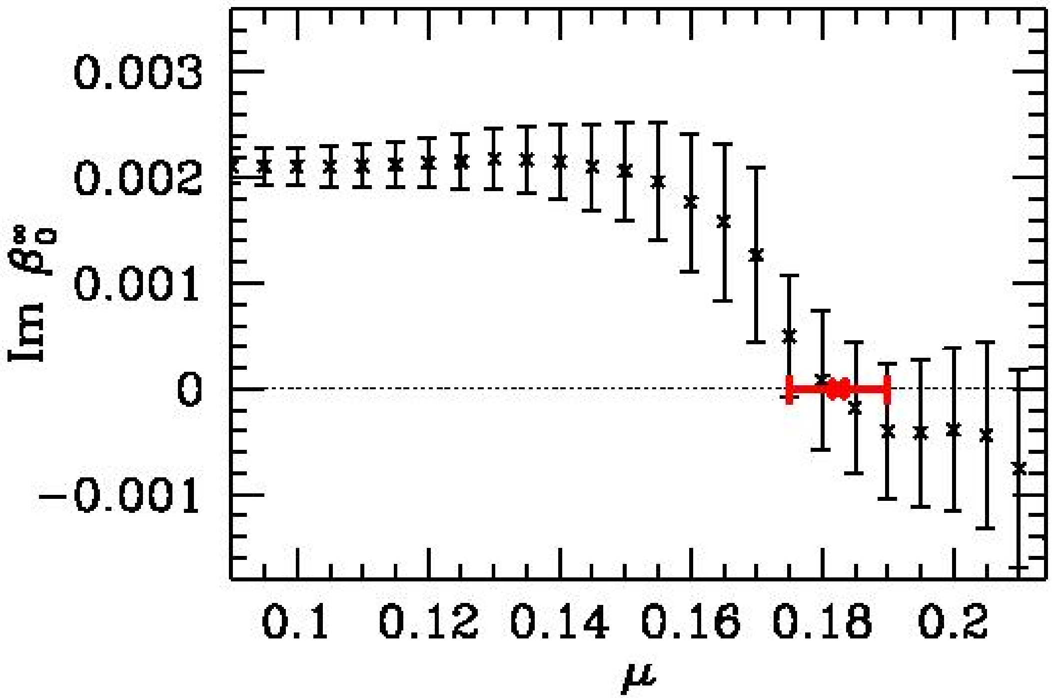
a. determine the transition points, Re(β_0), on L_s=6,8,10,12
β_c as a function of μ by the Lee-Yang zeros
for $\mu \neq 0$ overlap improving multi-parameter reweighting
100k,100k,100k,150k configurations, respectively
every 50th configuration treated as independent (few thousend)

b. by inspecting the $V \to \infty$ limit of Im(β_0)
separate the crossover and the 1^{st} order PT regions in μ

c. connect μ=T=0 lattice parameters with observables:
physical scale by R_0 (1/403 MeV) and m_ρ (770 MeV)
(3×3000 configurations on $12^3 \cdot 24$ lattices)

• separate the crossover and the 1^{st} order PT

$V \to \infty$ limit of Im(β_0) as a function of μ



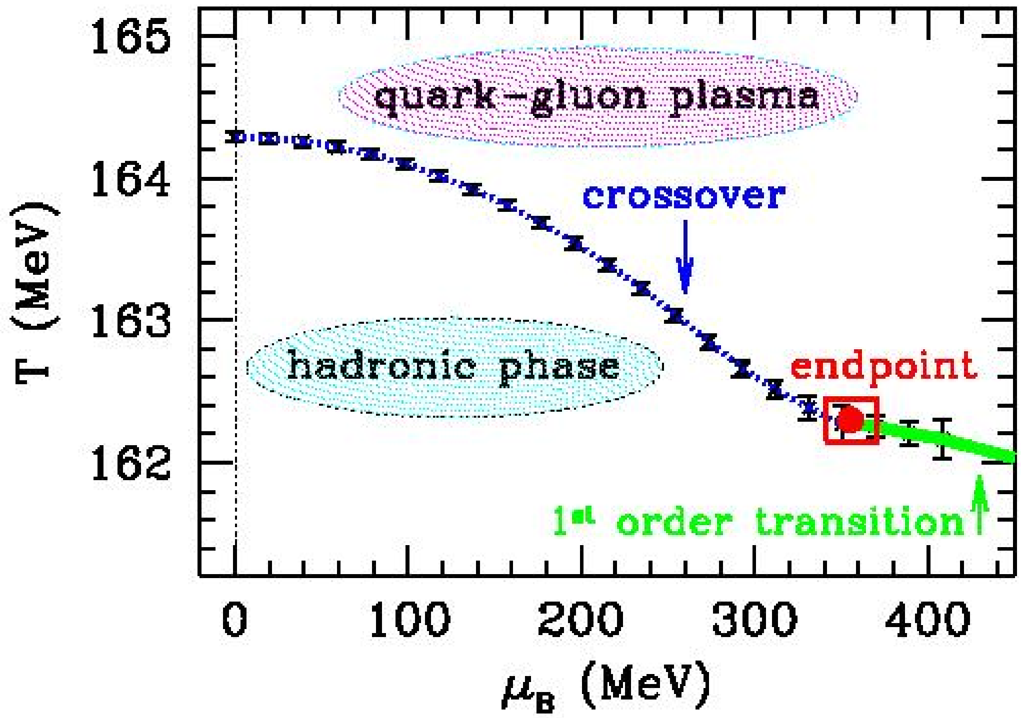
small μ: Im(β_0^∞) inconsistent with 0 $\Rightarrow$ crossover

increasing μ: Im(β_0^∞) decreases $\Rightarrow$

transition becomes consistent with a 1^{st} order PT

endpoint chemical potential: $\mu_{end} = 0.183(8)$

- T as a function of the baryonic chemical potential μ_B



- lattice result for physical quark masses at $L_t = 4$

endpoint: $T_E = 162 \pm 2$ MeV, $\mu_E = 360 \pm 40$ MeV

at μ_B=0 transition temperature: $T_c = 164 \pm 2$ MeV.

$T/T_c = 1 - C\mu_B^2/T_c^2$ wit C=0.0032(1)

$\mu \neq 0$ multi-parameter reweighting with Taylor expansion

C.R. Allton et al., Phys. Rev. D66 074507,'02, D68 014507,'03

$$Z(m,\mu,\beta) = \int \mathcal{D}U \exp[-S_g(\beta,U)] \det M(m,\mu,U) =$$

$$\int \mathcal{D}U \exp[-S_g(\beta_0,U)] \det M(m_0,\mu=0,U)$$

$$\left\{ \exp[-S_g(\beta,U) + S_g(\beta_0,U)] \frac{\det M(m,\mu,U)}{\det M(m_0,\mu=0,U)} \right\}$$

instead of evaulating determinants expand them in μ or exp(μ):

$$\ln\left(\frac{\det M(\mu)}{\det M(0)}\right) = \sum_{n=1}^{\infty} \frac{\mu^n}{n!} \frac{\partial^n \ln \det M(0)}{\partial \mu^n} \equiv \sum_{n=1}^{\infty} R_n \mu^n$$

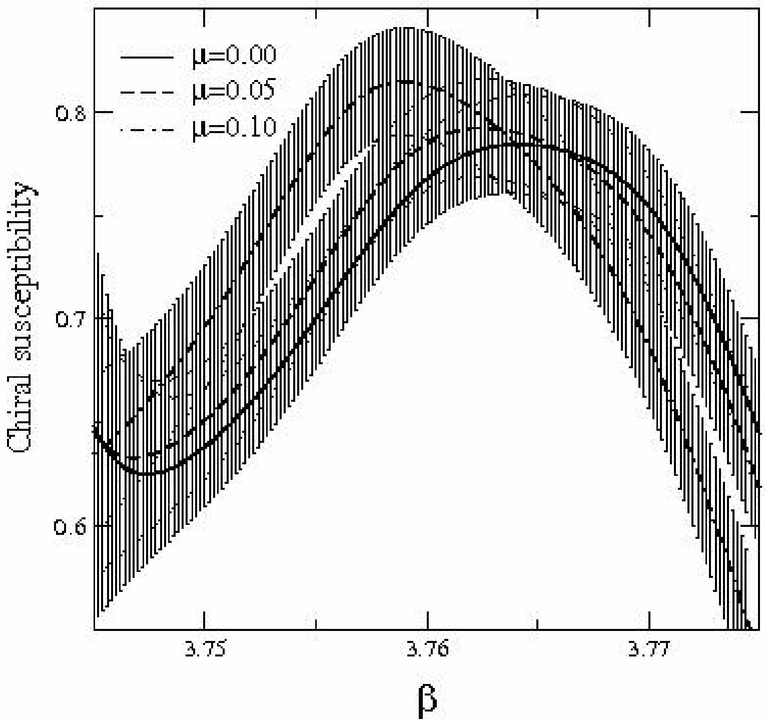
faster than the complete evaluation of the determinants

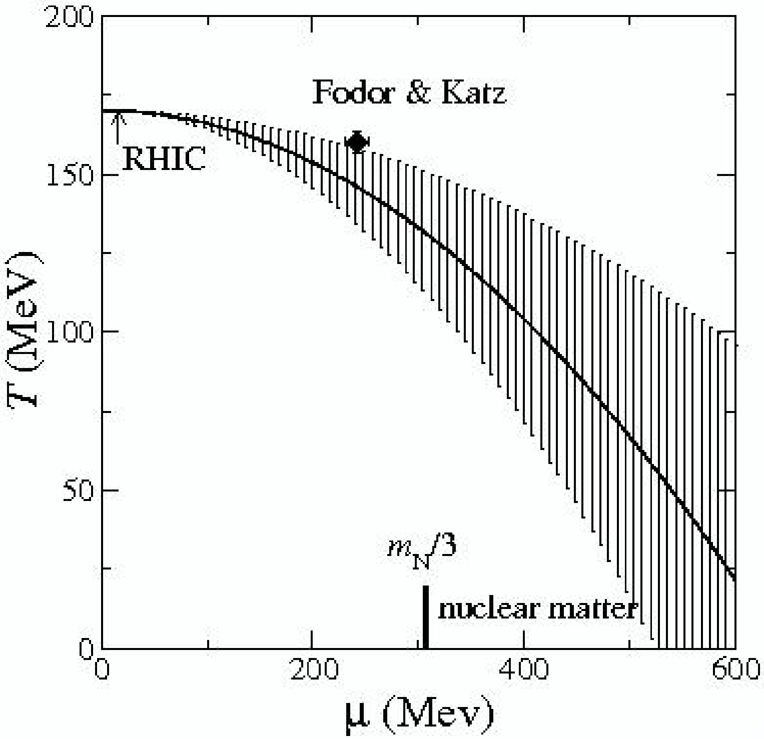
only valid for somewhat smaller μ values than the full technique

• trace out the transition points $\beta_c(\mu)$ in 2 flavour QCD

by looking for the susceptibility peaks of Polyakov or $\langle\bar{\psi}\psi\rangle$

convert it into physical units (T and μ_B in MeV)





⇒ curvature is consistent with other results

presence of higher order terems in the Taylor expansion

⇒ uncertainties at small T and large μ

• radius of convergence

true phase transitions: non-analiticity in the pressure

expand around μ=0 and look for the convergence radius

many terms and infinite volume limit must be taken

radius of convergence shows critical singularity

if all coefficients are positive (infinite volume)

$\Rightarrow$ singularity is on the real axis

$$r_n = (c_{2n}/c_{2n+2})^{1/2}$$

spin models: upto 20 different terms in the series

some models give good predicitions others fail

comment: convergence radius is always finite

there are singularities on the complex plane

even in the absence of a critical point:

$\Longrightarrow$ lower limit

- standard action, 4 terms in the pressure

R.V. Gavai and S. Gupta, PRD71 (2005) 114014

two flavours with a bit large quark masses: m/T_c=0.1

volume dependence: 4$\cdot L^3$ lattices with L=8–24

Taylor coefficients of the pressure (4 terms, 3 ratios)

$\Longrightarrow$ critical point at μ_B/T=1.1 and T/T_c=0.95

- p4 action, 3 terms in the pressure

C.R. Allton et al, PRD71 (2005) 054508

two flavours with quite large quark masses: m/T_c=0.4

Taylor coefficients of the pressure (3 terms, 2 ratios)

$\Longrightarrow$ analytic behaviour, no critical point

the two groups had different actions and quark masses

more terms of the series are needed for a conclusive result

QCD phase diagram from imaginary chemical potential

P.deForcrand, O.Philipsen, Nucl. Phys. B642 290,'02; B673 170, '03

fermion determinant: real for imaginary chemical potential (μ_I)
$\Rightarrow$ no sign problem, no need for reweighting

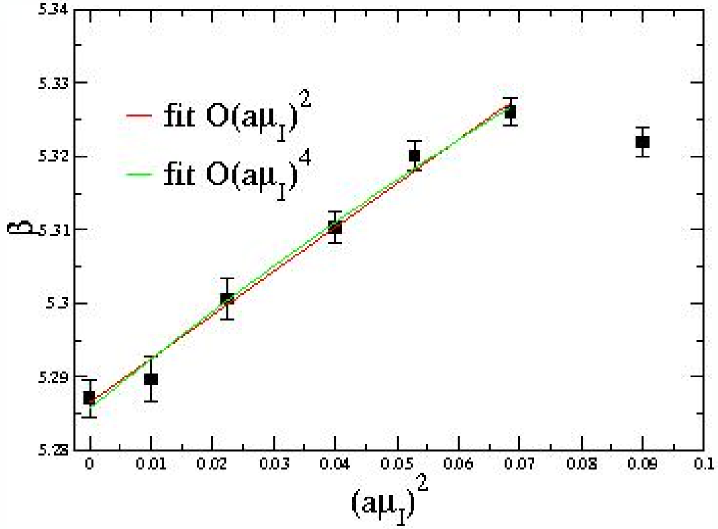
directly obtain the (β_c,μ_I) transition line
analytically continue it to get the physical (β_c,μ) line

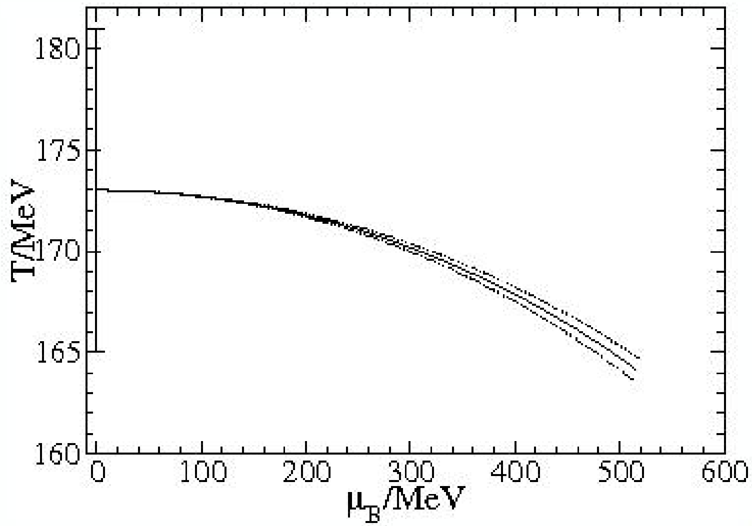
transition line (β_c, μ_I) is given by the susceptibility-peak

$$\chi = VN_t\langle(\mathscr{O} - \langle\mathscr{O}\rangle)^2\rangle, \qquad \partial\chi/\partial\beta = 0 \qquad \partial^2\chi/\partial\beta^2 < 0$$

on finite V the analytic $\chi(\mu_I, \beta)$ can be measured
using the implicitely given $\beta_c(\mu_I)$ one gets

$$\partial\beta_c/\partial\mu = -i\partial\beta_c/\partial\mu_I$$





- curvature is consistent with other results

$$T_c(\mu)/T_c(0) = 1 - 0.500(67)(\mu/\pi T_c)^2$$

- mass dependence in n_f=3 QCD for the critical endpoint:

$$m_c(\mu)/m_c(0) = 1 + 0.84(36)(\mu/\pi T_c)^2$$

- the equation of state can be determined, too

Density of states (DOS) method

Constrained simulations:

Force some observable to have a given value

this way configurations with all values of the observable present

overlap problem not so serious

For any observable:

$$< O >= \int dx \, \langle O f(U) \rangle_x \, \rho(x) \Big/ \int dx \, \langle f(U) \rangle_x \, \rho(x)$$

ρ, the density of states is the constrained partition function

for some observable ϕ

$$\rho(x) \equiv Z_\phi(x) = \int \mathcal{D}U \, g(U) \, \delta(\phi - x).$$

Possible choices for ϕ:

ϕ =PI (Bhanot et.al, '87; Karliner et.al,'88; Azooiti et.al,'90; Luo, '01; Takaishi, '04)

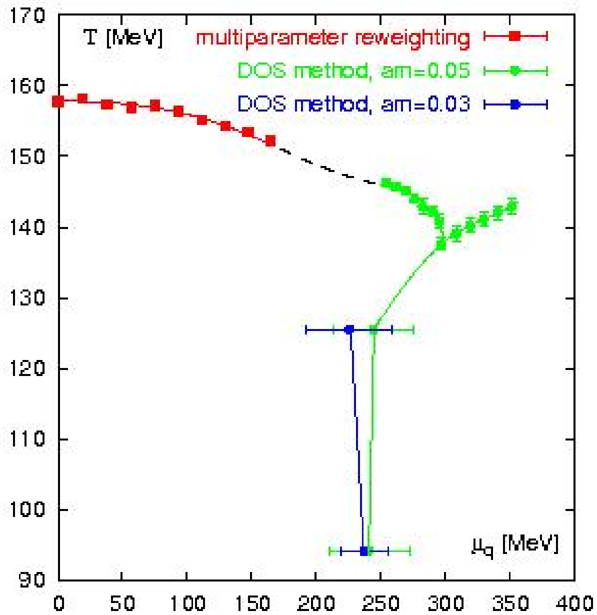
$\phi = \Theta$ (complex phase) (Gocksch, '88)

$\Phi = n_q$ (Ambjorn et. al., '02)

Results for QCD at large μ

Z. Fodor, S.D. Katz, C. Schmidt, hep-lat/0510087

$N_f = 4$ staggered QCD on 6^4, $8 \cdot 6^3$ lattices



existence of a triple point around $\mu_q \approx$ 300 MeV and T $\lesssim$ 135 MeV

Note, L_t=6 lattices: smalles T is 73 MeV (if m_ρ fixes the scale)

Mass dependence checked:

small T transition point does not depend on pion mass

Summary, outlook

• critical endpoint in the μ-T plane: unambiguous, non-perturbative prediction of the QCD Lagrangian $\Rightarrow$ important experimental consequences for heavy ion collisions

• lattice QCD at finite μ is an old, unsolved problem
recent method: overlap improving multi-parameter reweighting
presumably good enough to locate the above endpoint

• overlap improving multi-parameter reweighting:
standard importance sampling with reweighting in β, m and μ
maps transition ensemble to a transition ensemble
(or hadronic/QGP ones to hadronic/QGP ones)

• can be applied to any number of Wilson or staggered quarks

• T=0 and T≠0 simulations in QCD with n_f=2+1 quarks
infinite volume behavior of the Lee-Yang zeros
tells the difference between a 1^{st} order PT and a crossover

physical quark masses on L_t=4 lattices:

endpoint: $T_E = 162 \pm 2$ MeV, $\mu_E = 360 \pm 40$ MeV
at μ_B=0 transition temperature: $T_c = 164 \pm 2$ MeV.

• equation of state is obtained at finite temperature
(T=0.8 ... 3$\cdot T_c$) and chemical potential (μ_B=0...500 MeV)

• several other new ideas and techniques:
Taylor expansion in the chemical potential
analytic continuation from imaginary chemical potential
density of state method for large μ