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QCD at finite temperature and density on the lattice

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Thermodynamics Basics

Thermodynamical Ensembles

- Microcanonical: E, N, V fixed
- Canonical: T, N, V fixed
- Grandcanonical : T, μ , V fixed

In a GrandCanonical Ensemble define:

$$\hat{\rho} = e^{-(H-\mu\hat{N})/T}$$
$$\mathcal{Z} = Tr\hat{\rho}$$

ρ e \mathcal{Z} determine the system's state:

$$\langle O \rangle = \text{Tr} O \hat{\rho} / \mathcal{Z}$$

$$P = T \frac{\partial \ln \mathcal{Z}}{\partial V}$$

$$N = T \frac{\partial \ln \mathcal{Z}}{\partial \mu}$$

$$S = \frac{\partial T \ln \mathcal{Z}}{\partial T}$$

$$E = -PV + TS + \mu N$$

Bosons and fermions

- 1 bosonic degree of freedom

$$\hat{H} = 1/2\omega a^\dagger a + 1/2\omega = \omega(\hat{N} + 1/2)$$

$$\begin{aligned}\mathcal{Z} &= \text{Tre}^{-\beta(H-\mu\hat{N})} = \text{Tre}^{-\beta(\omega-\mu)\hat{N}} \\ &= \sum_0^\infty \text{Tre}^{-\beta(\omega-\mu)n} = (1 - e^{-\beta(\omega-\mu)})^{-1}\end{aligned}$$

$$N = (e^{\beta(\omega-\mu)} - 1)^{-1}$$

- 1 fermionic degree of freedom

$$\hat{H} = 1/2\omega a^\dagger a - 1/2\omega = \omega(\hat{N} - 1/2)$$

$$\begin{aligned}\mathcal{Z} &= \text{Tre}^{-\beta(H-\mu\hat{N})} = \text{Tre}^{-\beta(\omega-\mu)\hat{N}} \\ &= \sum_0^1 \text{Tre}^{-\beta(\omega-\mu)n}\end{aligned}$$

$$N = (e^{\beta(\omega-\mu)} + 1)^{-1}$$

Example I : Relativistic free fermionic gas

Non interacting particles: \mathcal{Z}

$$\mathcal{Z} = \prod \mathcal{Z}'$$

$$\ln \mathcal{Z} = d^3 x \int d^3 p (\ln(e^{-\beta(\omega - \mu)} + 1) + \ln(e^{-\beta(\omega + \mu)} + 1))$$

Note! Relativistic particles!

- Fermions (+ μ) and antifermions ($-\mu$).
- $\omega = \sqrt{(p^2 + m^2)}$.
- Relativistic chemical potential

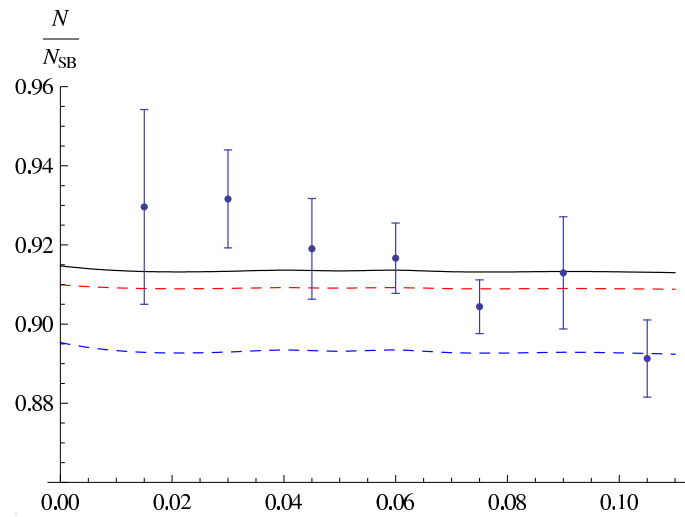
\mathcal{Z} can be exactly computed in the chiral limit $m = 0$:

$$\begin{aligned} T \ln \mathcal{Z} &= V \mu^4 / (12\pi^2) + V \mu^2 T^2 / 6 + 7V \pi^2 T^4 / 180 \\ n &= 4V \mu^3 / 12\pi^2 + 2V \mu T^2 / 6 \end{aligned}$$

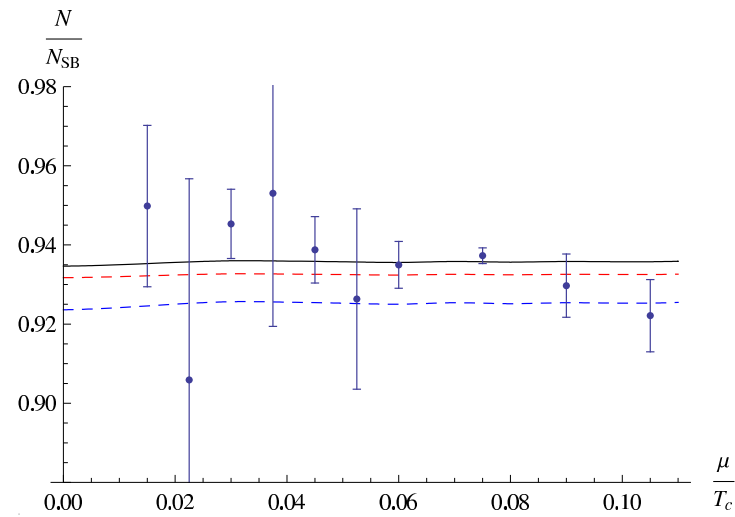
Ideally, this should be the state of the quarks at very high temperatures!

APPROACH TO FREE FIELD : ANALYTIC RESULTS VS. LATTICE DATA

Based on A. Vuorinen, 2004



$T = 1.5T_c$



$T = 3.5T_c$

D'Elia, Di Renzo, MpL, Vuorinen, in progress

More observables : Response Functions
Susceptibilities

$$\chi_{j_u, j_d}(T) = \left. \frac{\partial^{(j_u + j_d)} p(T, \mu_u, \mu_d)}{\partial \mu_u^{j_u} \partial \mu_d^{j_d}} \right|_{\mu_u = \mu_d = 0} .$$

Test for fluctuations.

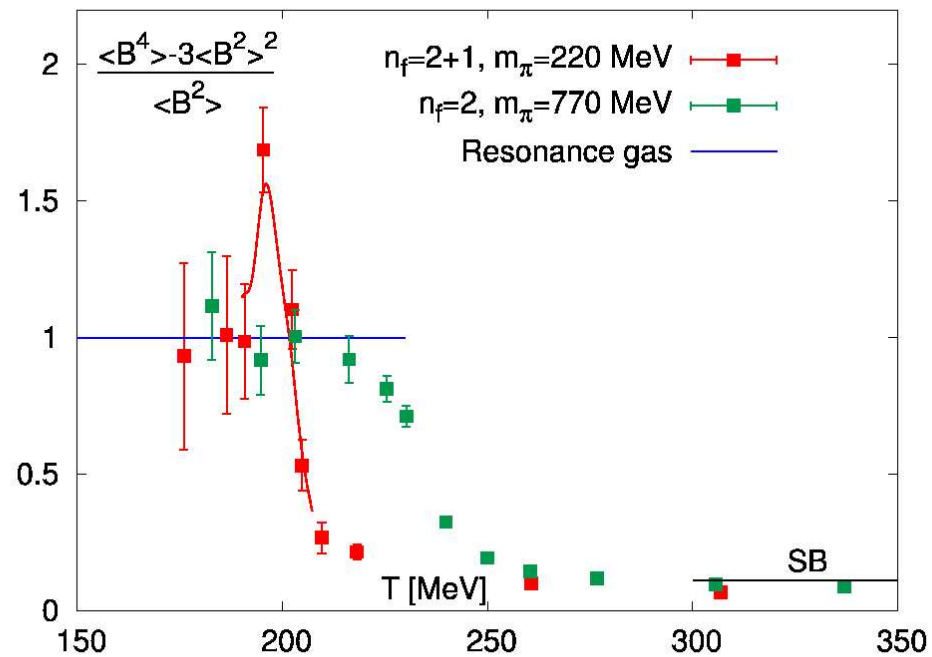
Taylor coefficients of the excess pressure:

$$\Delta p(T, \mu_u, \mu_d) \equiv p(T, \mu_u, \mu_d) - p(T, \mu_u = 0, \mu_d = 0)$$

$$\Delta p(T, \mu_u, \mu_d) = \sum_{j_u, j_d} \chi_{j_u, j_d}(T) \frac{\mu_u^{j_u}}{j_u!} \frac{\mu_d^{j_d}}{j_d!} ,$$

containing information about baryon density effects in the EoS.

Susceptibilities Towards Free Field



RBC-Bielefeld Collaboration, 2008

Example II : Interacting Fermions

3 d Gross Neveu Model

$$L = \bar{\psi}(\not{\partial} + m)\psi - g^2/N_f[(\bar{\psi}\psi)^2 - (\bar{\psi}\gamma_5\psi)^2]$$

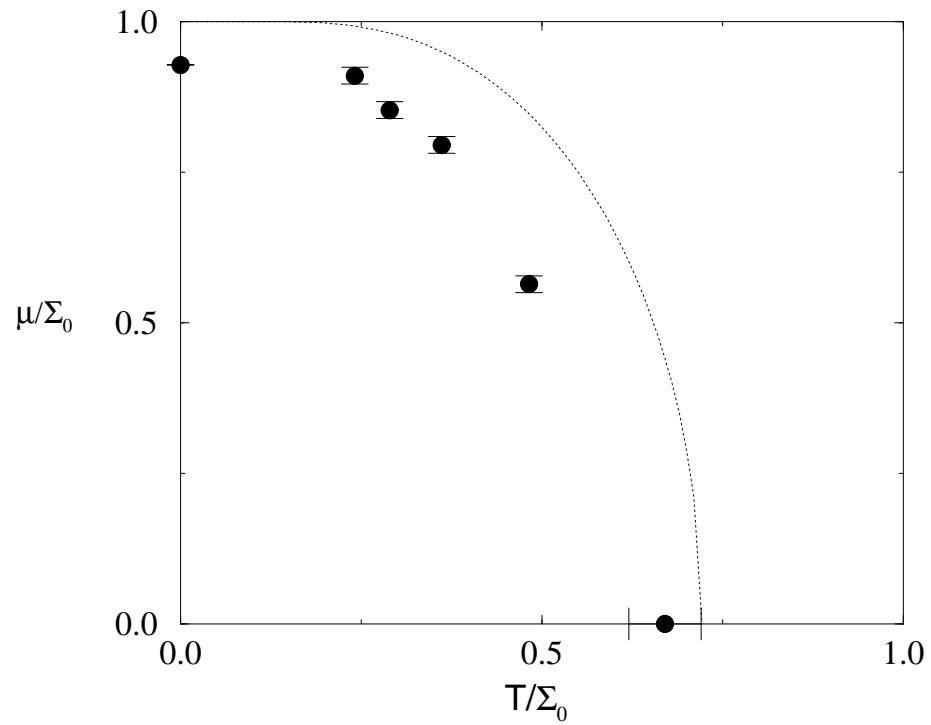
Global Chiral Invariance

$$\begin{aligned}\psi_i &\rightarrow e^{i\alpha\gamma_5}\psi_i \\ \bar{\psi}_i &\rightarrow \bar{\psi}_i e^{i\alpha\gamma_5}\end{aligned}$$

Basic Properties

- A $T = \mu = 0$ and g 'large', spontaneous symmetry breaking, Goldstone mechanism.
- Rich particle spectrum
- Amenable to a lattice study at $T, \mu \neq 0$!!!!

Phase diagram of the 3d Gross Neveu model



da S. Hands, 1998

Mean Field Solution vs Exact Lattice Results

-
- Grand Canonical Formalism at finite T , μ
 - Basic Observables : number density, susceptibilities
 - Free Fermions : Exact Solution
 - Simple model with interacting fermions : mean field solution
 - Phase Diagram at nonzero T and μ of a purely fermionic model
 - Simple calculations : can reproduce limiting behaviour and give generic information; in general inaccurate

Lattice QCD
=
*first principles calculations from the
QCD Lagrangian*

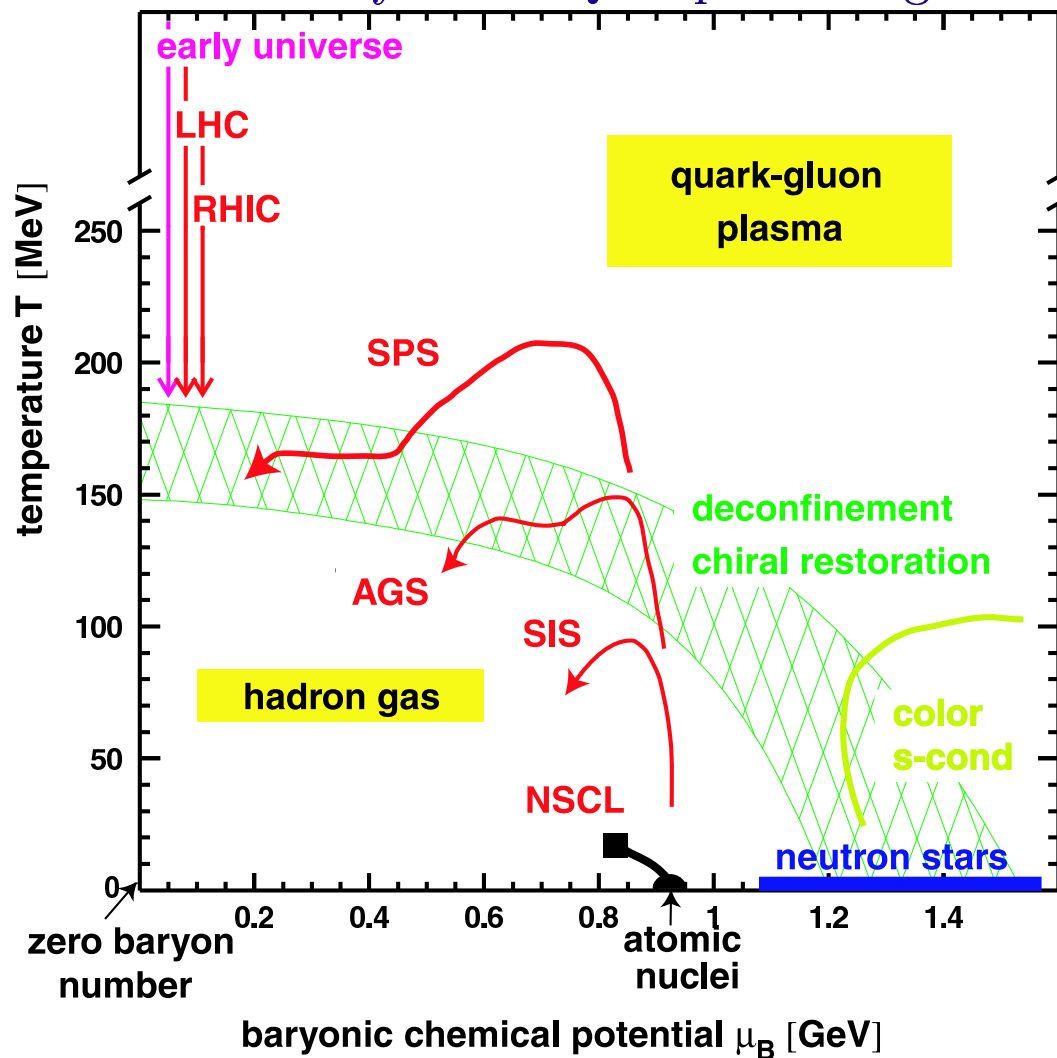
$$\mathcal{L} = \mathcal{L}_{YM} + \bar{\psi}(i\gamma_{\mu}D_{\mu} + m + \mu\gamma_0)\psi$$

A vast phase space to be explored:

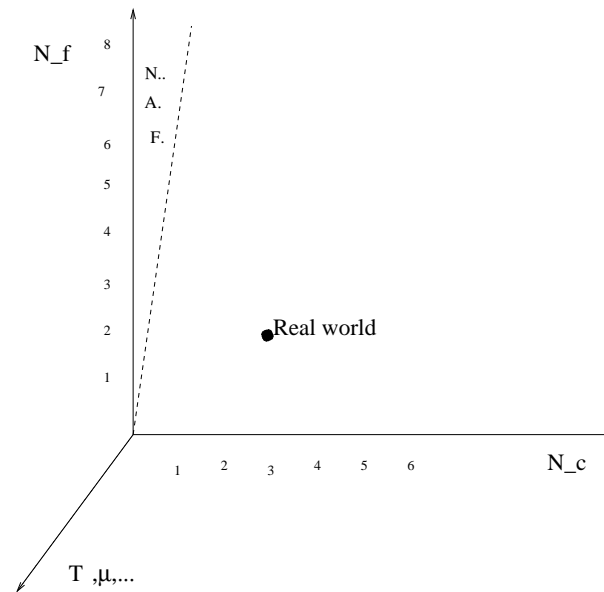
*Real baryon chemical potential, temperature, isospin chemical potential.
And also: Imaginary chemical potential, number of color and number of flavor, bare
masses*

to address phenomenological issues as well as to study more theoretical questions

Phenomenological challenges:
 ab initio study of the QCD phase diagram



Theoretical questions can (or, rather, should ?) be addressed in a larger phase space:



-
- *High T*
 - Chiral symmetry pattern : order disorder, light baryons
 - Deconfinement/screening: string breaking via recombination with light pairs
 - Instanton molecules
 - *High μ*
 - Chiral symmetry pattern : instability at the Fermi surface
 - Deconfinement/screening : string breaking via recombination with real particles
 - Instanton chains

Differences at high T and high μ in the *gauge dynamics* provide further motivation to study nonzero μ on a lattice.

Lattice QCD at Finite Temperature and Density

Lecture I

I Formulation

II Computational Schemes

II.1 Effective Fermionic Models - Analytic approaches

II.2 Effective Gluonic Models - Numerical approaches

III QCD at Finite Baryon Density: Methods

III.1 Derivatives

III.2 Reweighting

III.3 Expanded Reweighting

III.4 Imaginary Chemical Potential

IV Results - Discussion : Tomorrow's lecture

I Formulation

Grand Canonical Formalism and Path Integral

★ Chemical Potential for Conserved Charge \hat{N}

$$\begin{aligned}\hat{\rho} &= e^{-(H - \mu \hat{N})/T} \\ \mathcal{Z} &= \text{Tr} \hat{\rho} = \int d\phi d\psi e^{-S(\phi, \psi)}\end{aligned}\tag{1}$$

★ Temperature: Reciprocal of **Imaginary** Time

$$S(\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$

with boundary conditions for fermions and bosons

$$\begin{aligned}\phi(t=0, \vec{x}) &= \phi(t=1/T, \vec{x}) \\ \psi(t=0, \vec{x}) &= -\psi(t=1/T, \vec{x})\end{aligned}$$

★ \mathcal{Z} = partition function of a statistical system in $d+1$ dimension, where T is the reciprocal of the imaginary time.

★ Thermodynamics and spectrum properties are treated on the same footing.

Lattice QCD at $T, \mu \neq 0$

★ **Temperature:** as in the continuum $T = 1/N_t * a$

★ **Density**

In the continuum: $L(\mu) = L_0 + \mu J_0$ $J_0 = \bar{\psi} \gamma_0 \psi \rightarrow N - \bar{N} = \int J_0$

On the lattice:

$$L(\mu) = \bar{\psi}_x \gamma_0 e^{\mu a} \psi_{x+\hat{0}} - \bar{\psi}_{x+\hat{0}} \gamma_0 e^{-\mu a} \psi_x$$

$$J_0 = -\partial_\mu L = \bar{\psi}_x \gamma_0 e^{\mu a} \psi_{x+\hat{0}} + \bar{\psi}_{x+\hat{0}} \gamma_0 e^{-\mu a} \psi_x$$

Time Forward propagation enhanced by $e^{\mu a}$

Time Backward propagation discouraged by $e^{-\mu a}$

Particles-antiparticles asymmetry!

More on The Lattice (digression)

Path integral is regulated on a four dimensional lattice

- Gauge fields: link variables $U_\mu(x)$ for parallel transport of field \mathcal{A} from x to $x + \hat{\mu}a$

$$x \xrightarrow{U_\mu(x)} x + \hat{\mu}a$$

$$U_{x,\mu} = \text{P exp} \left(ig \int_x^{x+\hat{\mu}a} dx^\mu A_\mu(x) \right)$$

- Gauge invariants and Yang Mill Action:

$$\begin{aligned} W_{n,\mu\nu}^{(1,1)} &= 1 - \frac{1}{3} \text{Re} \left[\text{Tr} \left(\text{square} \right) \right]_{n,\mu\nu} \\ &= \text{Re Tr } U_{n,\mu} U_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu}^\dagger U_{n,\nu}^\dagger \\ &= \frac{g^2 a^4}{2} F_{\mu\nu}^a F_{\mu\nu}^a + \mathcal{O}(a^6) \end{aligned}$$

- Lattice Yang Mill Action

$$\beta S_G = \beta \sum_{\substack{n \\ 0 \leq \mu < \nu \leq 3}} W_{n,\mu\nu}^{(1,1)} \rightarrow \int d^4x \mathcal{L}_{YM} + \mathcal{O}(a^2)$$

$$\beta = 6/g(a)^2.$$

- Lattice fermions

Simply:

$$\psi(x) \rightarrow \psi(n) !$$

$$\partial_\mu \psi_f(x) = (\psi(n + \hat{\mu}) - \psi(n - \hat{\mu}))/2a,$$

[doubling problem and chiral symmetry: staggered fermions, Wilson fermions, chiral fermions]

$\mu \bar{\psi} \gamma_0 \psi$ on the lattice

Naive discretisation:

$$\begin{aligned} \phi_{LATT}(n_1, n_2, n_3, n_4) &= \phi(n_1 a, n_2 a, n_3 a, n_4 a) \\ \Delta_\mu \phi_{LATT}(n_1, n_2, n_3, n_4) &= \\ (\phi(n_1 a, (n_\mu + 1)a, n_3 a, n_4 a) &- \phi(n_1 a, (n_\mu - 1)a, n_3 a, n_4 a))/2a \end{aligned}$$

Problems with free fermions: the internal energy ϵ diverges in the continuum limit $a \rightarrow 0$

$$L = \bar{\psi}_x \gamma_\mu \psi_{x+\hat{\mu}a} + m \bar{\psi}_x \psi_x + \mu \bar{\psi}_x \gamma_0 \psi_x$$

$$\epsilon \propto \frac{\mu^2}{a^2} \rightarrow_{a \rightarrow 0} \infty$$

Elegant solution : μ is an external field in the 0th direction

$$\bar{\psi} \gamma_\mu A_\mu \psi \leftrightarrow i \mu \bar{\psi} \gamma_0 \psi$$

- External fields live on lattice link. (cfr. electrodynamics: $A \rightarrow \theta = e^{(iA)}$)
- $L(\mu) = \bar{\psi}_x \gamma_0 e^{\mu a} \psi_{x+\hat{0}} - \bar{\psi}_{x+\hat{0}} \gamma_0 e^{-\mu a} \psi_x$

- *Simple interpretation*

- *Time Forward propagation enhanced by $e^{\mu a}$*

- *Time Backward propagation discouraged by $e^{-\mu a}$*

Particles-antiparticle asymmetry!

- $\lim_{a \rightarrow 0} J_0 = -\partial_\mu L = \bar{\psi}_x \gamma_0 e^{\mu a} \psi_{x+\hat{0}} + \bar{\psi}_{x+\hat{0}} \gamma_0 e^{-\mu a} \psi_x = \mu \bar{\psi} \gamma_0 \psi$

Via an unitary transformation for the field

$$L(\mu) = L(0)$$

+ boundary conditions

Explicit dependence on fugacity

Lattice QCD Thermodynamics at a Glance

$$\begin{aligned}\mathcal{L}_{QCD} &= 6/g^2 \text{Tr} U_{n,\mu} U_{n+\hat{\mu},\nu} U_{n+\hat{\nu},\mu}^\dagger U_{n,\nu}^\dagger \\ &+ \sum_{i=1}^3 (\bar{\psi}_x \gamma_i U_i(x) \psi_{x+\hat{i}} - \bar{\psi}_{x+\hat{i}} \gamma_i U_i^\dagger(x) \psi_x) \\ &+ \bar{\psi}_x \gamma_0 e^\mu U_0(x) \psi_{x+\hat{0}} - \bar{\psi}_{x+\hat{0}} \gamma_0 e^{-\mu} U_0^\dagger(x) \psi_x \\ &+ m \bar{\psi} \psi\end{aligned}$$

Imaginary time

and

Inverse
Temperature

d-dimensional space

II Computational Schemes

$$\mathcal{Z} = \int d\phi d\psi e^{-S(\phi, \psi)}; (\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$
$$\mathcal{L}_{QCD} = \mathcal{L}_{YM} + \bar{\psi}(i\gamma_\mu D_\mu + m)\psi + \mu \bar{\psi} \gamma_0 \psi$$

Two options:

1. Integrate out gluons first:

$$\mathcal{Z}(T, \mu, \bar{\psi}, \psi, U) \simeq \mathcal{Z}(T, \mu, \bar{\psi}, \psi) \rightarrow$$

effective *approximate* fermion models

2. Integrate out fermions *exactly* as S is bilinear in $\psi, \bar{\psi}$
 $S = S_{YM}(U) + \bar{\psi} M(U) \psi$

$$\mathcal{Z}(T, \mu, U) = \int dU e^{-(S_{YM}(U) - \log(\det M))}$$

$$\mathcal{Z}(T, \mu, U) = \int dU e^{-(S_{YM}(U) - \log(\det M))}$$

starting point for numerical calculations

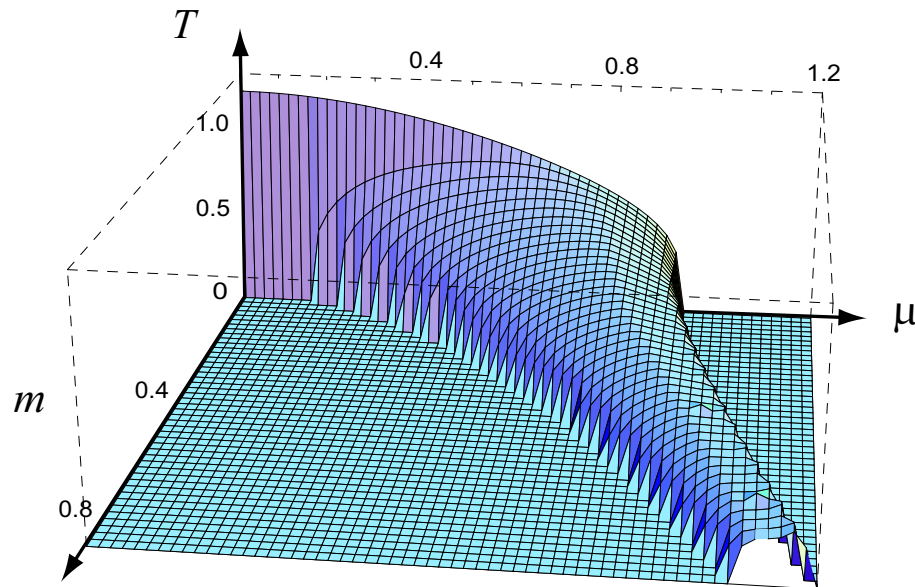
II. 1 Effective Fermionic Models on the Lattice

Lattice Strong Coupling Calculations:

Starting point : Yang Mill Action decouples

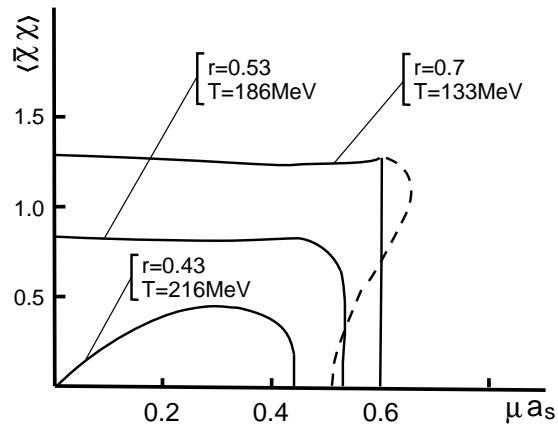
at $g = \infty \rightarrow \int dU$ exact

Work on two color QCD by Y. Nishida, K. Fukushima, and T. Hatsuda



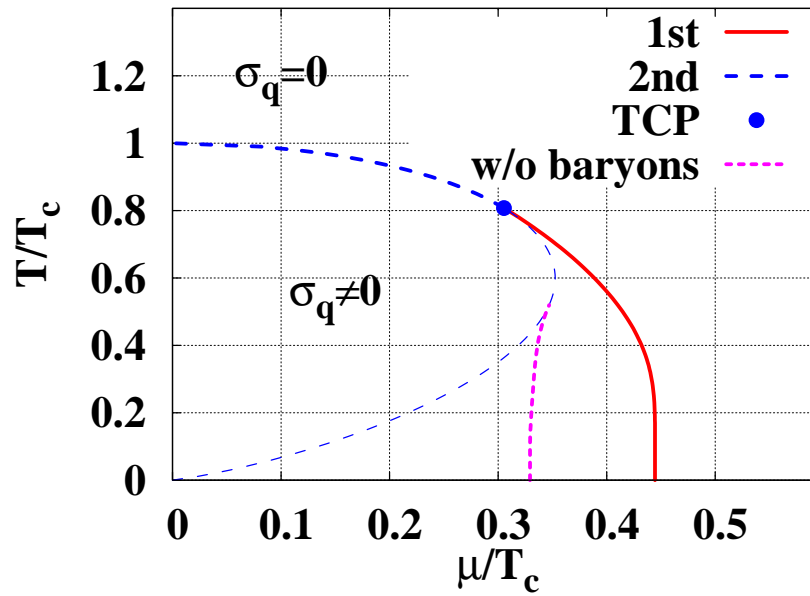
Initial studies by F. Karsch, U. Wolff, and others.

Work from the 80's on three color :
B. Petersson and collaborators, P. Damgaard, F. Karsch and many others.



$$\mathcal{L} = G \frac{1}{8N_c^2} [(\bar{\psi}\tau^-\psi)^2 + (\bar{\psi}\tau^-\gamma_5\psi)^2]$$

CSC/CFL Phase from Strong Coupling?



The phase diagram of QCD at strong coupling *Kawamoto et al, 2005*.

$$\mathcal{Z}(T, \mu, U) = \int dU e^{-(S_{YM}(U) - \log(\det M))}$$

$$M^\dagger(\mu_B) = -M(-\mu_B)$$

$\det M > 0 \rightarrow$ *Importance Sampling*

- $\mu = 0 \rightarrow \det M$ is *real*
Particles-antiparticles *symmetry*
- *Imaginary* $\mu \neq 0 \rightarrow \det M$ is *real*
(Real) Particles-antiparticles *symmetry*
- *Real* $\mu \neq 0$ *Particles-antiparticles* *asymmetry*
 $\rightarrow \det M$ is *complex in QCD*
- QCD with a real baryon chemical potential:
 use information from the accessible region

$$\text{Re}\mu = 0, \text{Im}\mu \neq 0$$

III QCD AT FINITE BARYON DENSITY-METHODS

QCD and a Complex μ_B

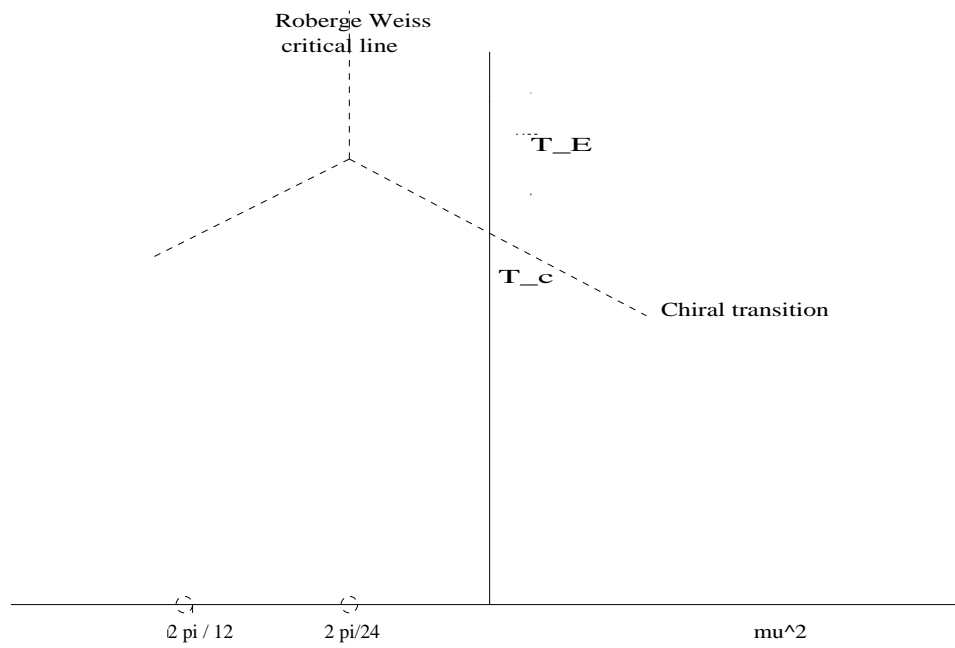
A map: complex $\mu \rightarrow$ complex μ^2 .

$\mathcal{Z}(\mu^2)$ is real valued for real μ^2

Analogy with statistical models in external fields

*The Phase Diagram in the T, μ_B^2 Plane Region accessible to simulations:
 μ^2 real ≤ 0 .*

- $\mu = 0$ Derivatives, Reweighting, Expanded reweighting
- $\mu^2 \leq 0$ Imaginary chemical potential



The Roberge and Weiss analysis

$$\mathcal{Z}(\nu) = \text{Tr} e^{-\beta H + i\beta\nu N} = e^{-\beta H + i\theta N}$$

1. $\mathcal{Z}(\theta)$ has a periodicity 2π anyway.
2. If only color singlet are allowed, then $N = 0 \text{ mod } (N_c)$ and periodicity becomes $2\pi/N_c$

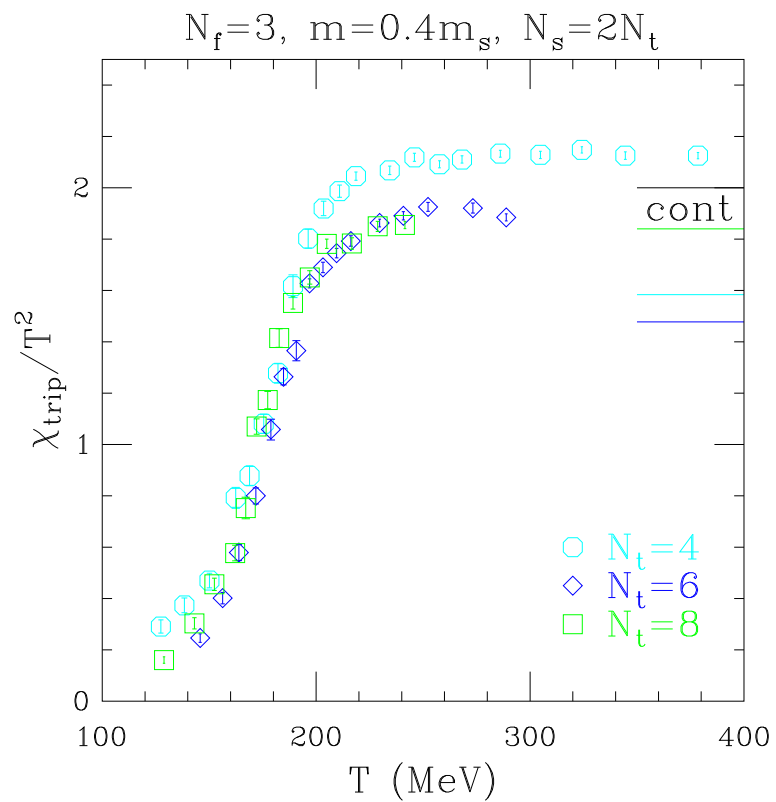
However (Roberge Weiss (1986))

$\mathcal{Z}(\theta)$ has always period $2\pi/N_c$

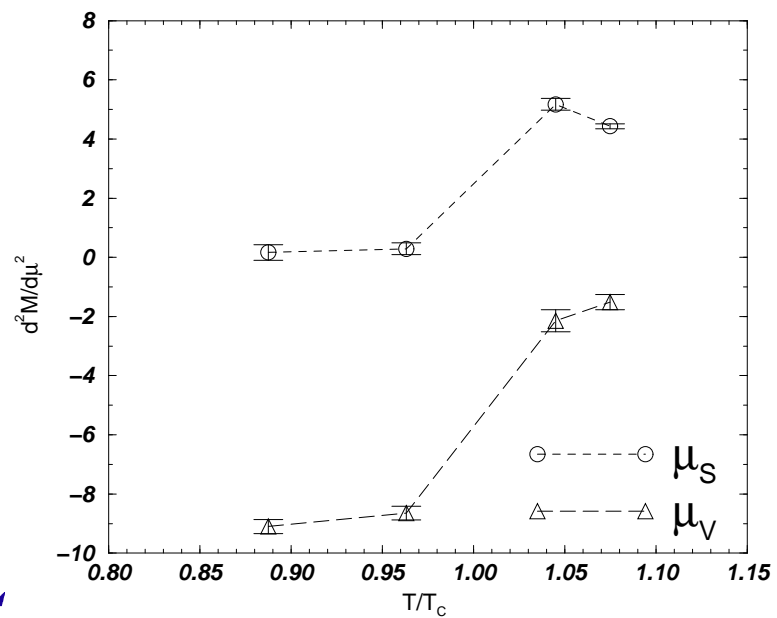
The imaginary chemical potential changes the preferred vacuum for the Polyakov loop from $\phi_P = 0$ to one of its Z_3 images

The strong coupling analysis shows that periodicity is smooth at low temperature, and p.t. theory suggests that it is sharp at high T

III.1 Derivatives at $\mu = 0.0$



MILC



QCD-

TARO

III.2 Reweighting from $\mu = 0$

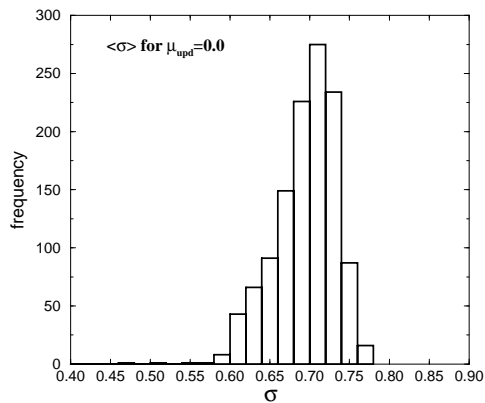
Ian Barbour's proposal, *or*
The Glasgow method:

$Z(\mu)$ can be computed using simulations at $\mu = 0$:

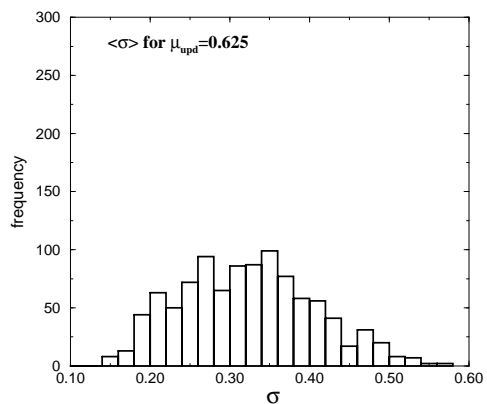
$$Z = \left\langle \frac{|M(\mu)|}{|M(\mu = 0)|} \right\rangle_{\mu=0}$$
$$Z = \frac{\int [dU][dU^\dagger] |M(\mu)| e^{-S_g[U, U^\dagger]}}{\int [dU][dU^\dagger] |M(\mu = 0)| e^{-S_g[U, U^\dagger]}}$$

Needs overlap between
simulation ensemble at $\mu = 0$
target ensemble at $\mu \neq 0$

At $T = 0$ the Glasgow procedure fails because of a poor overlap.



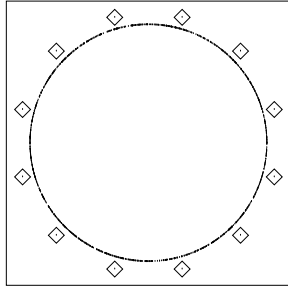
Broken phase



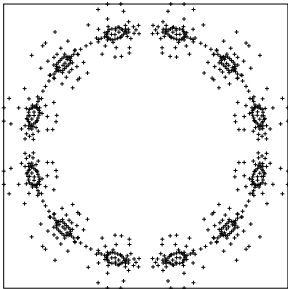
Symm. Phase

Distributions of the $\langle \sigma \rangle = \langle \bar{\psi} \psi \rangle$ fields

Example of successful reweighting at $\mu \neq 0$: no conceptual problems
1-dim SU(3) can be exactly solved (Bilic, Demeterfi, 1988)

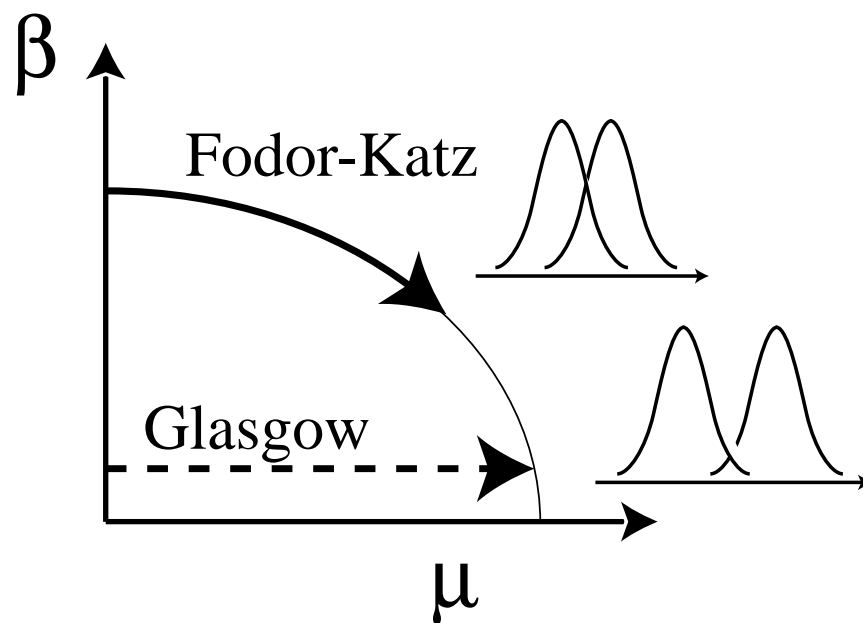


Exact Z 's zeros in the Imaginary, Real μ plane
(diamonds) and the cloud of zeros obtained from reweighting with a very
poor statistics



Z 's zeros from an high statistics reweighting : OK

Z.Fodor and F.Katz's proposal :
Multiparameter reweighting *use fluctuations around T_c to explore the critical region*



Picture taken from
S. Muroya, A. Nakamura, C. Nonaka and T. Takaishi

III.3 Taylor Expanded Reweighting

Bielefeld-Swansea

Taylor expansion of the reweighting factor as a power series in $\lambda = \mu/T$, and similarly for any operator.

Computationally convenient: simplifies calculation of determinant.

Expectation values are then given by

$$\langle \mathcal{O} \rangle_{(\beta, \mu)} = \frac{\langle (\mathcal{O}_0 + \mathcal{O}_1 \lambda + \mathcal{O}_2 \lambda^2 + \dots) \exp(\mathcal{R}_1 \lambda + \mathcal{R}_2 \lambda^2 + \dots - \Delta S_g) \rangle_{\lambda=0, \beta_0}}{\langle \exp(\mathcal{R}_1 \lambda + \mathcal{R}_2 \lambda^2 + \dots - \Delta S_g) \rangle_{\lambda=0, \beta_0}}.$$

Bridge between Canonical and Grand Canonical ensembles

A. Hasenfratz, D. Toussaint, M. Alford, A. Kapustin, F. Wilczek, ...

$$Z(\mu) = \sum Z(\mathcal{N}) e^{\beta \mu B^N}$$

$$Z(i\nu) = \text{Tr} e^{-\beta(H - i\nu B^N)}$$

$$Z(\mathcal{N}) = \frac{\beta}{2\pi} \int_0^{2\pi/\beta} d\nu Z(i\nu) e^{-i\beta\nu N}$$

Idea: $\mu = 0$ fluctuations allow the exploration of $N_b \neq 0$ hence tell us about $\mu \neq 0$

Note: same argument suggests Glasgow reweighting might work

Practical Strategy:

$Z(\mu, T)$ must be

1. *analytic*

2. *non trivial*

Rule of thumb:

$$\chi(T, \mu) = \partial \rho(\mu, T) / \partial \mu = \partial^2 \log Z(\mu, T) / \partial \mu^2 > 0$$

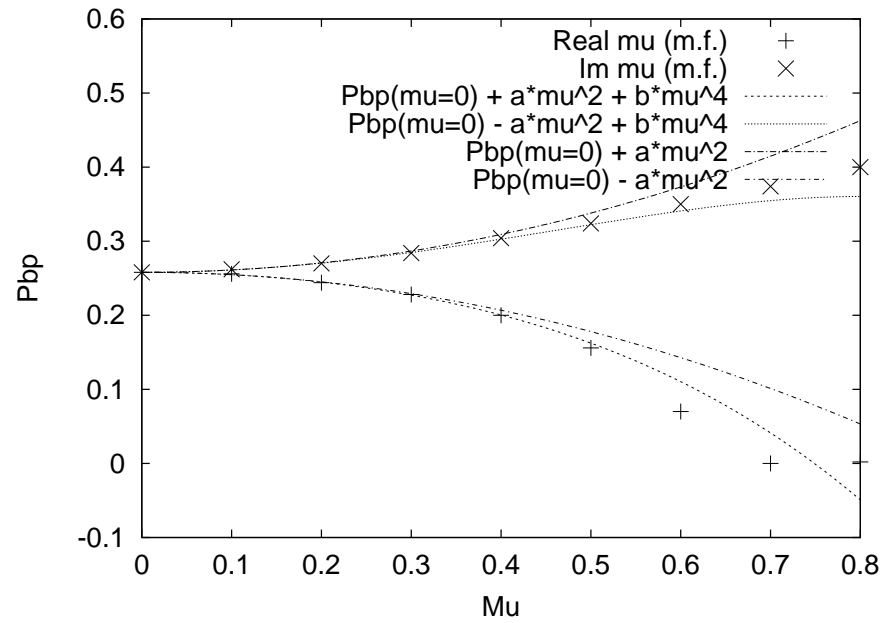
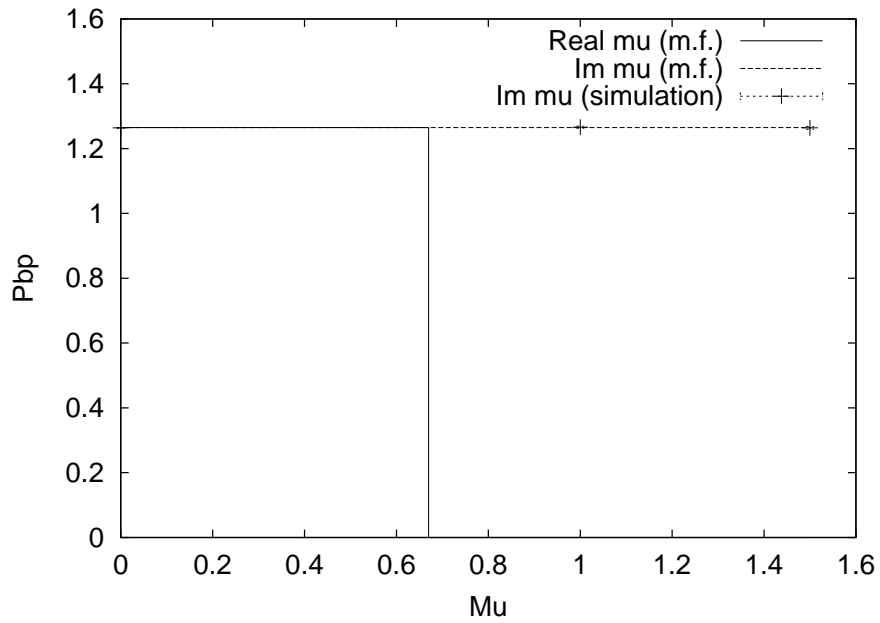
μ Imm.: Lessons from $g = \infty$

$$S_{QCD} = S_{YM} + S_F \rightarrow g \rightarrow \infty = S_F$$

$$\mathcal{Z} = \left(\int V_{eff}(\langle \bar{\psi}\psi \rangle) d\langle \bar{\psi}\psi \rangle \right)^{V_s}$$

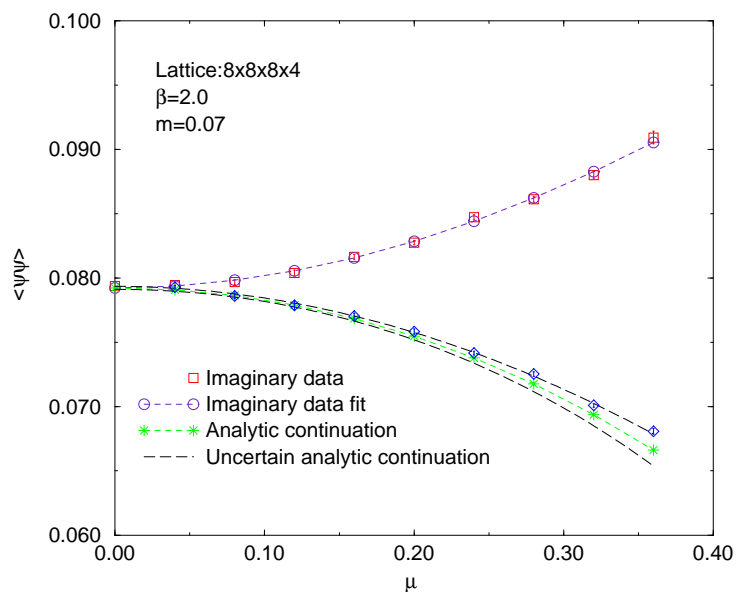
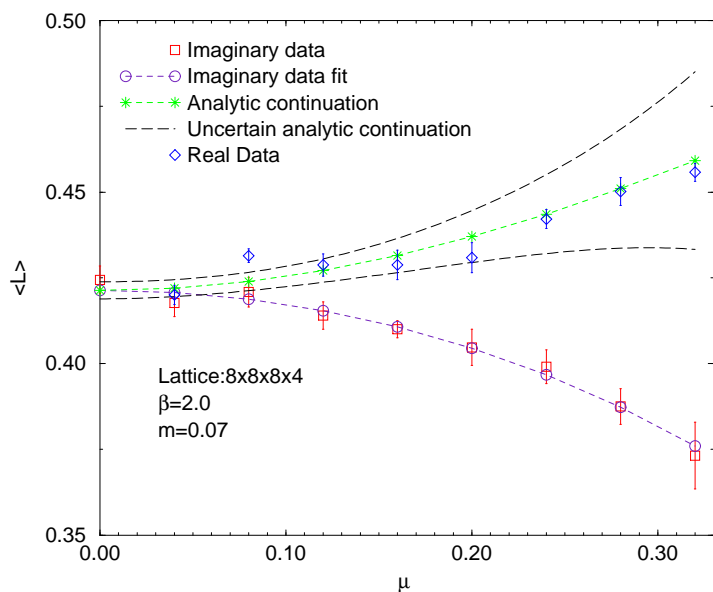
$$V_{eff}(\langle \bar{\psi}\psi \rangle, \mu) = 2\cosh(rN_t N_c \mu) + \sinh[(N_t + 1)N_c \langle \bar{\psi}\psi \rangle] / \sinh(N_t \langle \bar{\psi}\psi \rangle)$$

$$V_{eff}(\langle \bar{\psi}\psi \rangle, i\mu) = 2\cos(rN_t N_c \mu) + \sinh[(N_t + 1)N_c \langle \bar{\psi}\psi \rangle] / \sinh(N_t \langle \bar{\psi}\psi \rangle)$$



$\langle \bar{\psi}\psi \rangle$ as a function of real and imaginary μ , for $T \simeq 0$ and $T \simeq T_c$

Two color QCD as a testbed for Imaginary μ_B



P. Giudice, Tesi di Laurea in Fisica, Universita della Calabria; Advisor A. Papa

courtesy of the Author

Gross Neveu Model

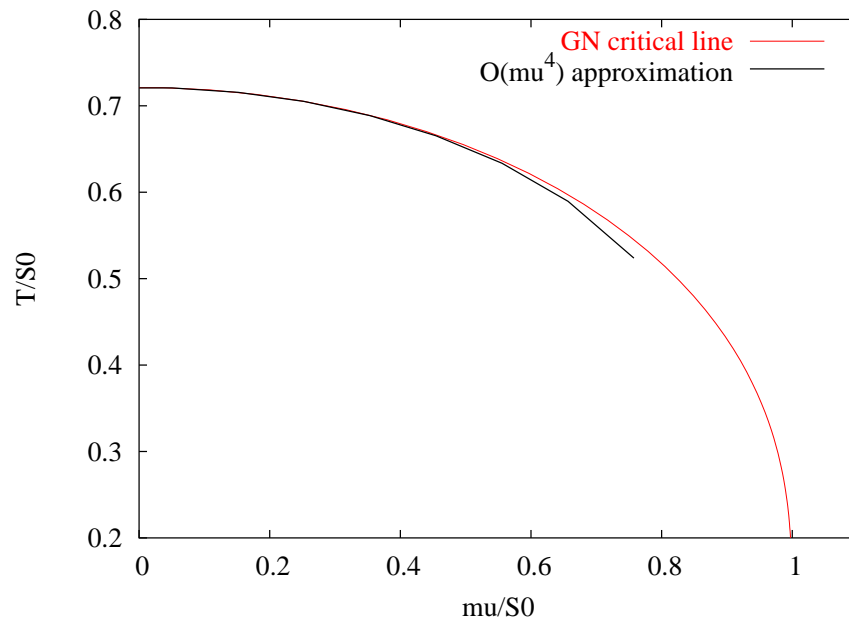
The critical line:

$$1 - \mu/\Sigma_0 = 2T/\Sigma_0 \ln(1 + e^{-\mu/T})$$

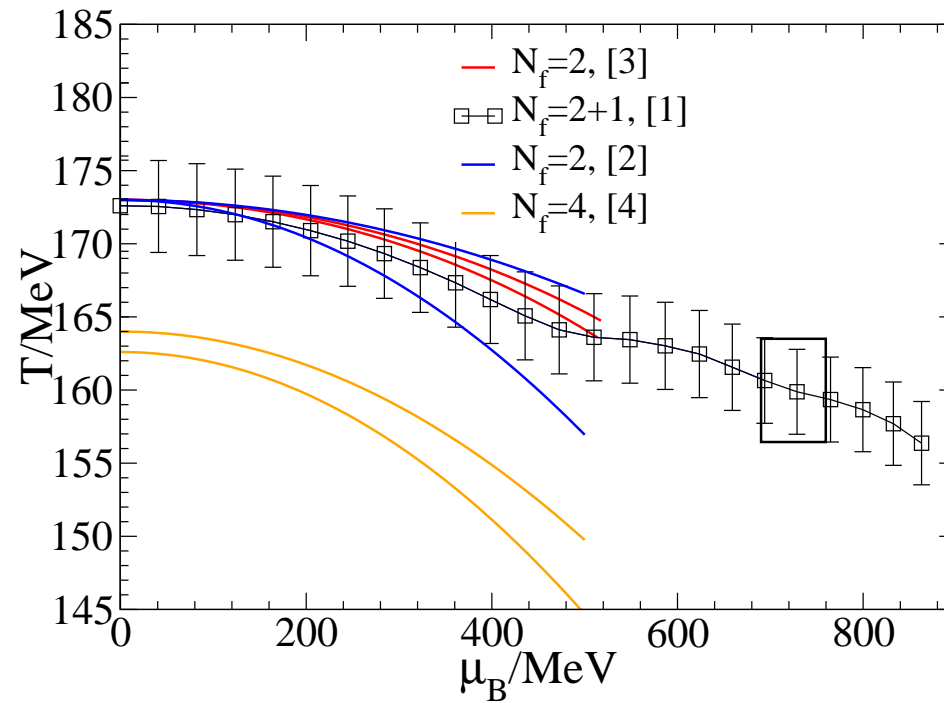
Reduces to:

$$T(T - T_c) + \mu^2/(8\ln 2) = 0$$

Second order approximation good up to $\mu \simeq T_c$



From O. Philipsen and E. Laermann
Ann. Rev. Nucl. Part. Phys. 2003



1. Fodor Z and Katz SD, *JHEP* 0203:014 (2002).
2. Allton CR et al., *Phys. Rev. D* 66:074507 (2002).
3. de Forcrand P and Philipsen O, *Nucl. Phys. B* 642:290 (2002).
4. D'Elia M and Lombardo MP, *Phys. Rev. D* 1:074507 (2003).

Lattice QCD at Finite Temperature and Density

Lecture I

I Formulation

II Computational Schemes

II.1 Effective Fermionic Models - Analytic approaches

II.2 Effective Gluonic Models - Numerical approaches

III QCD at Finite Baryon Density: Methods

III.1 Derivatives

III.2 Reweighting

III.3 Expanded Reweighting

III.4 Imaginary Chemical Potential

IV Results - Discussion : Tomorrow's lecture