Galileo Galilei Institute, Firenze apeNEXT : Computational Challenges and First Physics Results 8 February 2007

#### Topics on QCD at nonzero Temperature and Density

Maria Paola Lombardo INFN-Laboratori Nazionali di Frascati, Roma

Goal : Understanding the Theory and Phenomenology of the Phases and Phase Transitions of QCD



#### Topics and **Methods**

- High Temperature QCD at  $\mu_B = 0$ Twisted Mass Wilson,  $N_f = 2$
- QCD at nonzero baryon density
  - Thermodynamic of the hadronic phase
  - The strongly interactive Quark Gluon Plasma

Analytic Continuation from Imaginary  $\mu$ , Staggered Fermions,  $N_f = 4$ 

• Summary, Outlook

## High Temperature QCD

E.-M. Ilgenfritz, M. Mueller-Preussker, M. Petschlies, K. Jansen, M. P. Lombardo, O. Philipsen, L. Zweidlewicz

Based on

- E.-M. Ilgenfritz, M. Mller-Preussker, A. Sternbeck, K. Jansen, I. Wetzorke, M. P. Lombardo, O. Philipsen PoS.LAT2006:140
- Work in progress

# Phase transitions of two plus one flavor QCD Pisarski, Wilczek; original discussion

Basile, Pelissetto, Vicari 2005; RG analysis



	$U(1)_A$ anomaly	suppressed anomaly at $T_c$	
$\operatorname{QCD}$	$\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R \to \mathrm{SU}(N_f)_V$	$\mathrm{U}(N_f)_L \otimes \mathrm{U}(N_f)_R \to \mathrm{U}(N_f)_V$	
$N_f = 1$	crossover or first order	O(2) or first order	
$N_{f} = 2$	O(4) or first order	$\mathrm{U}(2)_L \otimes \mathrm{U}(2)_R / \mathrm{U}(2)_V$ or first order	
$N_f \ge 3$	first order	first order	

#### Phase transitions of two flavors QCD in the up=down, T plane Three possibilities

- 1. 2nd order phase transition at  $\mu = 0$
- 2. 1st order Phase Transition at  $\mu = 0$  with endpoints (three flavor like)
- 3. 1st order Phase Transition at  $\mu = 0$  without endpoint (?)



Numerical goals:

- Precision determination of  $T_c(m_{\pi})$
- Fit  $T_c(m_\pi) T_c = am_\pi^\alpha$  NB :  $\alpha = \frac{\ln \alpha}{2}$

NB : 
$$\alpha = \frac{\ln((T_c(m_\pi) - T_c)/a)}{\ln m_\pi}$$

The Universality Class of Nf=2 QCD from the Lattice: Reviews by O. Philipsen (Lat05) and U. Heller (Lat06) Staggered Fermions:

- O(2) or O(4) with Nt=8 but scaling window very narrow other behaviours cannot be ruled out (Kogut Sinclair 2004-2006)
- O(2) at strong coupling very high precision low masses Chandrasekharan Strouthos
- First order ( O(2) / O(4) ruled out) Nt=4 Pisa Group

Wilson fermions:

• Apparently compatible with O(4) scaling Nt=4- CP-Pacs 2001 : but within very large systematic errors





 $T_c$  Data Compiled by P. Petreczki, 2006 (various authors)

Free fermions rom MILC, 1996

#### Why and How Twisted Mass QCD Thermodynamics ?

Wilson fermions have several advantages over staggered fermions, but they also have a more subtle chiral behaviour, and a complicated phase structure, both at T = 0 and at finite temperature

The twisted mass approach

- prevents the occurrence of exceptional configurations and should make it relatively easy to reach mass values of the light pseudoscalar mesons close to the physical pion mass
- once the Wilson hopping parameter  $\kappa$  is set to its critical value, the twisted mass term behaves as a conventional quark mass, and, at the same time, an O(a) improvement is automatically guaranteed.

Numerical work at T=0 used in this project relies on: F. Farchioni et al., Eur. Phys. J. C 39, 421 (2005); F. Farchioni et al., PoS LAT2005, 072 (2006) K. Jansen and C. Urbach [ETM Collaboration], arXiv:hep-lat/0610015; A. Shindler, PoS LAT2005, 014 (2006); C. Urbach, K. Jansen, A. Shindler and U. Wenger, Comput. Phys. Commun. 174, 87 (2006)

#### The TM Action

• Fermion sector

$$S_q = \sum_x \left\{ \left( \overline{\chi}_x [\mu_\kappa + i\gamma_5 \tau_3 a\mu] \chi_x \right) - 0.5 \sum_{\mu=\pm 1}^{\pm 4} \left( \overline{\chi}_{x+\hat{\mu}} U_{x\mu} [r+\gamma_\mu] \chi_x \right) \right\} ,$$

 $\mu_{\kappa} \equiv am_0 + 4 = 1/2\kappa$ ,  $am_0$  the bare "untwisted" quark mass in lattice units and  $\mu$  the twisted quark mass;

• Gauge sector: Symanzik improved

$$S_g = \beta \sum_x \left( c_0 \sum_{\mu < \nu; \, \mu, \nu = 1}^4 \left\{ 1 - \frac{1}{3} \operatorname{Re} U_{x\mu\nu}^{1 \times 1} \right\} + c_1 \sum_{\mu \neq \nu; \, \mu, \nu = 1}^4 \left\{ 1 - \frac{1}{3} \operatorname{Re} U_{x\mu\nu}^{1 \times 2} \right\} \right) \,,$$

 $U_{x\mu\nu}^{1\times 2}$  is the planar rectangular (1 × 2), and we use tree-level Symanzik improved gauge action (tlSym)  $c_1 = -1/12$ .

#### The strategy and the simulations

- The simulations were performed on a  $16^3 \times 8$  and on a  $16^3 \times 10$  lattice with an improved version of the HMC algorithm and with a Symanzik tree-level improved gauge action.
- They used approximatively three months×crate of apeNEXT

#### A model for tmQCD Mike Creutz, 1996; Steve Sharpe, 2005

Effective potential for Wilson fermions

$$V(\vec{\pi}, \sigma, L) = \lambda (\sigma^2 + \vec{\pi}^2 - v^2)^2 + \alpha_0 (K^2 - K_c(\beta)^2) \sigma$$
(1)  
+ \alpha\_1 \sigma^2   
+ m\_t \pi\_3

- The first line is the standard "linear" sigma model with its O(4) chiral symmetry.
- The second line is the mass term generated by not being at the critical kappa.
- The third term is the quadratic warping : It is a chiral symmetry breaking lattice artifact (cfr. Sharpe and Singleton)
- The  $m_t$  term is the twisted mass. Without the  $\alpha_1$  term this can be rotated into the  $\alpha_0$  mass term along the curve of constant  $m_t^2 + \alpha_0^2 (K^2 K_c^2)^2$ . Only lattice artifacts make it physically significant.

- Runs at fixed  $\beta$  : mass scan
  - $-\beta = 3.75$  and  $\beta = 3.9$  in order to take advantage of the T = 0 results: we cross the critical line by varying the quark mass.
  - $-N_t$  and  $\beta$  need to satisfy:

$$T_c^{chiral} < T^{simulation} = 1/(N_t a(\beta)) < T_c^{quenched}$$

- For  $T^{simulation} > T^{quenched}_c$  the hadronic phase cannot exist, while for  $T^{simulation} < T^{chiral}_c$  the QGP cannot exist, irrespective of the mass value.
- We fixed  $N_t = 8$  by taking into account the lattice spacing from the T = 0 studies  $a(3.75) \simeq 0.12$  fm and  $a(3.9) \simeq 0.095$  fm as well as the known critical temperatures  $T_{chiral}^c = 170$  MeV  $T_{quenched}^c = 270$  MeV.
- Runs at fixed  $\mu$  :  $\beta$  scan
  - $-\mu = 0.006$  corresponding to  $m_{\pi} \simeq 380 MeV$
  - Crossing with critical line guaranteed, at some temperature and physical mass

#### **Results at** $\beta = 3.75, \ \mu = 0.005$

At  $\beta = 3.75$ , the ETMC T = 0 results show that the minimum pion mass which can be reached with our twisted mass parameter  $\mu = 0.005$  is  $m_{\pi} \simeq 400$ MeV extrapolating existing results at  $\mu = 0.005$ . F. Farchioni *et al.*, PoS LAT2005, 072 (2006)

Our first goal here is merely to check whether a thermal phase transition or a crossover can be found in the required range  $\kappa_t < \kappa_c$ .



• Conjugate Gradient (CG) Iterations superimposed with  $\frac{\partial \langle P \rangle}{\partial \kappa}$  (magnified) as a function of  $\kappa$  at fixed  $\beta = 3.75$  and  $\mu = 0.005$ 



• The results indicate a thermal transition or crossover at  $\kappa_t = 0.165(1)$ .

$$\kappa_t < \kappa_c(T=0) = 0.1669$$

**Results at**  $\beta$  = 3.9,  $\mu$  = 0.005

The minimum pion mass at T = 0 for our  $\mu = 0.005$ , inferred from these results, is about 350 MeV.



• A direct comparison between the results at the two  $\beta$  values : the number of Conjugate Gradient iterations



• The plaquette  $\langle P \rangle$ . We performed local fits to a straight line  $\langle P \rangle = a + b\kappa$  within subsequent intervals of width  $\Delta \kappa = 0.002$ , and we show the tangent in the inflection point.



• The parameters b are used as estimators of the derivative of the Plaquette w.r.t. to  $\kappa$ .



These results indicate a phase transition or crossover around  $\kappa = 0.1597$ located according to the maximal slope  $b_{max}$ .



#### **Polyakov loop distributions**



The steepest slope of the plaquette and of the Polyakov loop, as well as the broadening of the probability distributions suggest a crossover or phase transition at  $\kappa_t$ :

$$\kappa_t(eta=3.9,\mu=0.005)=0.1597(5)$$

and, as it was also observed at  $\beta = 3.75$ ,

$$\kappa_t < \kappa_c(T=0) = 0.16085$$
.

#### Maximal Twist at Finite Temperature

Study of the transition with varying  $m_{quark}$  at  $k = k_c$ 

$$m_{quark} = \sqrt{(\mu^2 + (0.5(1/k - 1/k_c))^2))}$$

T=0 Maximal Twist K. Jansen and C. Urbach [ETM Collaboration], arXiv:hep-lat/0610015;



β	$L^3 \times T$	$a\mu_{ m min}$	$\kappa_{ m crit}(a\mu_{ m min})$	$r_0/a(a\mu_{ m min})$
3.9	$24^3 \times 48$	0.004	0.160856	5.184(41)
4.05	$32^3 \times 64$	0.003	0.15701	6.525(101)



#### Fixed $\mu = 0.006$ scan at Maximal Twist



Red points :  $K_c$  Blu line : Pade' interpolation



## **Summary of the numerical results**

- We have studied QCD with two flavors of dynamical Wilson fermions including a twisted mass term on a  $16^3 \times 8$  lattice at two values of the temperature:  $\beta = 3.75$  corresponding to  $T \simeq 205$  MeV and  $\beta = 3.9$  corresponding to  $T \simeq 259$  MeV.
- In either cases we have simulated O(10) values of bare quark masses, by varying the hopping parameter  $\kappa$  at constant  $\mu = 0.005$ . We have observed a behavior consistent with a crossover at a critical value of  $\kappa_t$ , which is less than the critical  $\kappa$  at T = 0. This behavior is similar to that observed with ordinary Wilson fermions
- We have scanned the phase diagram at **maximal twist** at  $\beta = 3.9$ ,  $N_t = 8$ , confirming the location of the smooth crossover observed at a fixed  $\mu$
- We have scanned the phase diagram at maximal twist  $k_c = k_c(\beta)$  and a fixed  $\mu = 0.005$ , observing the transition at  $\beta \simeq 3.95$
- The simple picture based on chiral symmetry is verified : the improvement effects of the twisted mass are not visible within our errors

#### Results in physical units so far



## **QCD at nonzero baryon density:** The hadron gas and the strongly interactive QGP

M. D'Elia , F. Di Renzo, M. P. Lombardo



Picture by Stephen Bass, QM2006 Based on

- M. P. Lombardo arXiv:hep-lat/0612017; PoS LAT2005 (2006) 168; Prog.Theor.Phys.Suppl.153:26-39,2004
- M. D'Elia, M.P. Lombardo Phys. Rev. D 70 (2004) 074509; Phys. Rev. D 67 (2003) 014505
- M. D'Elia , F. Di Renzo, M. P. Lombardo AIP Conf. Proc. 806 (2006) 245
- M. D'Elia , F. Di Renzo, M. P. Lombardo : Work in Progress

### **Properties of the sQGP:**

and details of the phase diagram depend on the details of the interaction



...also the high T region is getting complicated...

# Importance Sampling and The Positivity Issue $\mathcal{Z}(T,\mu,U) = \int dU e^{-(S_{YM}(U) - \log(\det M))}$

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

 $\mu = 0 \rightarrow \det M$  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

$$Re\mu = 0, Im\mu \neq 0$$



The Phase Diagram in the T,  $\mu_B^2$  Plane (sketchy) Region accessible to simulations:  $\mu^2$  real  $\leq 0$ .

#### **Region accessible to simulations:** $\mu^2$ real $\leq 0$ . : Methods

Multiparameter Reweighting  $(\mu = 0)$ :Fodor, Katz, Csikor, Egri, Szabo, TothDerivatives  $(\mu = 0)$ :Gupta, Gavai and collaborators; MILC; QCD-TaroExpanded Reweighting  $(\mu = 0)$ Bielefeld-Swansea

Analyitic continuation from Imaginary µ Strong Coupling QCD MpL Dim. Reduced QCD Laine, Hart, Philipsen QCD de Forcrand, Philipsen,Kratochvila D'Elia, MpL, Di Renzo Azcoiti, Di Carlo, Galante, Laliena, Staggered Luo et al. Wilson <u>Models</u> Giudice, Papa; de Forcrand, Kim.... Needs well controlled series expansion and/or reliable parametrizations. Tools for analytic continuation from imaginary chemical potential: \* Taylor Series (best at high T)

$$O(\mu_I) = \sum_k a_k \mu_I^k \to O(\mu) = \sum_k (i)^k a_k \mu^k$$

MpL, Hart, Laine, Philipsen, de Forcrand and Philipsen, D'Elia and MpL, Azcoiti et al, Luo, Papa and Giudice, ..

**\* Fourier Analysis** (best in the hadronic phase)

$$O(\mu_I) = \sum_k a_k exp(ki\mu_I)O(\mu) = \sum_k a_k exp(k\mu)$$

D'Elia and MpL, de Forcrand and Kratovchila

**\* Pade' Approximants** (best in the sQGP region)

MpL; Cea, Cosmai, D'Elia, Papa

First Physics Applications : Baker, Gammel et al. (1961)



#### The Hadron Gas and the Fourier Analysis

The *Hadron Resonance Gas* model might provide a description of QCD thermodynamics in the confined, hadronic phase of QCD (Karsch, Redlich, Tawfik,...)

$$\frac{P(T,\mu) - P(T,0)}{T^4} \simeq F(T)(\cosh(\frac{\mu_B}{T} - 1)$$
$$F(T) \simeq \int dm \rho(m)(\frac{m}{T})^2 K_2(\frac{m}{T})$$

A simple approach to the HRG is offered by the imaginary chemical potential.  $_{(D'Elia,MpL, 2002, 2004)}$ 

Observables are periodic and continuous for imaginary chemical potential. (Roberge, Weiss, 1986)

$$O_e = ae_F + \sum be_F cos(N_c N_t \mu)$$

$$O_o = ao_F + \sum bo_F sin(N_c N_t \mu)$$

When HRG holds true, one term in the Fourier series should suffice.  $sinh(x) \rightarrow sin(x)$ 

$$n(\mu) = \frac{\partial P(\mu)}{\partial \mu} = Ksin(N_c N_t \mu)$$

The Taylor approach requires an infinite number of terms while the Fourier analysis needs only one.

## HRG accurate up to $T \simeq .985T_c$ : Fits



<u>HRG accurate up to  $T \simeq .985T_c$ : Direct check</u> in an 'effective mass analysis' style:

$$Mismatch = n(\mu)/sin(N_c N_t \mu) - k$$

k = 0.0039(2) T = 0.95 $T_c$ ; k = 0.0062 (4) T = 0.985 T<br/>c $T_c$ 



D'Elia, MpL, 2004

#### Thermodynamics of the Hot Phase:

Monitoring the approach to a free gas of quarks and gluons





#### Corrections to Free Field

A. Vuorinen 2004:

$$P(T,\mu) = \frac{\pi^2}{45} T^4 \left( 8 + 7N_c \frac{n_f}{4} \right) + \frac{n_f}{2} \mu^2 T^2 + \frac{n_f}{4\pi^2} \mu^4 + \dots$$

Alternatively (Rafelski, Letessier 2003)

$$P(T,\mu) = f(\mu) \left(\frac{\pi^2}{45} T^4 \left(8 + 7N_c \frac{n_f}{4}\right) + \frac{n_f}{2} \mu^2 T^2 + \frac{n_f}{4\pi^2} \mu^4\right)$$

Trivial possibility:  $f(\mu)$  is a <u>constant</u>.

Possible interpretation: a free field with an effective number of flavors  $N_{eff}$  different from  $N_f$ 

$$P(T,\mu) - P(T,0) = (N_{eff}/n_f)(\frac{n_f}{2}\mu^2 T^2 + \frac{n_f}{4\pi^2}\mu^4) = (\frac{N_{eff}}{2}\mu^2 T^2 + \frac{N_{eff}}{4\pi^2}\mu^4)$$

#### Nearly Free Field for $T > 1.5T_c$

 $f(\mu) = (N_{eff}/N_f)$  estimated on the lattice appear to be a constant for  $T \ge 1.5T_c \ne 1$  i.e.  $N_{eff} \ne N_f$ 





 $T_c < T < 1.5T_c$ : a Strongly Coupled Quark Gluon Plasma?

 $\hat{\mathbb{T}}$ 

0.1

 $\hat{\Box}$ 

0.12

 $\langle \hat{\mathbf{I}} \rangle$ 

0.16

0.14

 $$\mu I$$  Francesco Di Renzo, Massimo D'Elia, MpL, hep-lat/0511029, and in progress

0.08

0.06

0.75

0.7

0

0.02

0.04

#### Thermodynamics of the Hot Phase close to $T_c$ :

At large T the QGP is a gas of nearly free quarks, it is strongly interacting in the regime  $T = (1 - 3) T_c$ . As both heavy ion experiments and lattice simulations are now showing, in this region the QGP displays rather strong interactions between the constituents: hence not only deconfined quarks, also bound states, colored bound states, etc. etc. : example :  $qq\bar{q}\bar{q} \rightarrow qq + \bar{q}\bar{q}$ (Shuryak, Zahed, 2004, 2005, 2006)

Contribution of the bound states to thermodynamical quantities?

Parameterizations for masses of the bound states

 $M_{\pi} \approx 10 T_c \left(1 - \exp(-3(T - T_c)/T_c)\right) ,$ 

which is set to vanish at  $T = T_c$ .

 $M_{\rm colored} \approx 11.5 T_c \left( (T/3T_c)^{0.5} + 0.1T_c/(T-T_c) \right)$ which decouples at  $T = T_c$ .

#### The QGP pressure

In analogy with the "resonance gas" at  $T < T_c$ , the contributions of all bound states for  $T > T_c$  can be simply added to the statistical sum, as independent particles.

Reduction factor:

$$R(T) = \frac{1}{1 + \exp[C(T - T_{z.b.})]}$$

which reduces the contribution at the zero binding point  $T_{z.b.}$  by 1/2 and eliminates it at higher T. Shuryak and Zahed use a parameter  $C = 2/T_c$ .



**Resulting Pressure** 

## A direct attempt at confronting this prediction on the lattice Ejiri, F. Karsch and K. Redlich

Colored States contribution to the pressure is given by:

$$\frac{P}{T^4} = \frac{1}{2} \left( F_q(T) + R_2(T, 2) F_{qg}(T) \right) \left( \cosh(\mu_u/T) + \cosh(\mu_d/T) \right) + \frac{1}{3} R_C(T, 1.4) F_{qq}(T) (\cosh(2\mu_u/T) + \cosh(2\mu_d/T) + \cosh((\mu_u + \mu_d)/T)) ,$$
(2)

As in the hadronic phase, the ratio of quartic and quadratic cumulants of the Pressure reflects the relevant degrees of freedom that carry the quark number, isospin or charge, respectively. Going imaginary:

$$\frac{P}{T^4} = \frac{1}{2} \left( F_q(T) + R_2(T, 2) F_{qg}(T) \right) \left( \cos(\mu_u/T) + \cos(\mu_d/T) \right) + \frac{1}{3} R_C(T, 1.4) F_{qq}(T) (\cos(2\mu_u/T) + \cos(2\mu_d/T) + \cos((\mu_u + \mu_d)/T)) ,$$
(3)

#### sQGP from an imaginary $\mu$ analysis

Search for colored states in  $n(i \mu)$  by use of a simple trigonometric parametrization (Fourier)

 $n(i\mu, T) = A_q(T)sin(\mu/T) + B_{qq}(T)sin(2\mu/T) + C_{qqq}(3\mu/T)$ 





Search for colored states in Polyakov( $i \mu$ ) by use of a simple trigonometric parametrization (Fourier)

A(T), B(T), C(T) might change sensibly with the chemical potential since the masses themselves will depend on  $\mu$ : We certainly need to take into account the  $\mu$  dependence here:

$$M_{\text{colored}} \approx 11.5 T_c \left( (T/3T_c)^{0.5} + 0.1T_c/(T - T_c) \right)$$

#### A power law fit (Pade' of log )

 $Pol(\mu_I) \propto (\mu_I^{c\,2} - \mu_I^2)^{(\beta)}$ 



(Im mu) The data in the candidate region for a strongly coupled QCD are very well accounted for by a conventional critical behaviour: interplay by the nonperturbative features of the plasma and the continuation of the critical line at negative  $\mu^2$ 





$$n(\mu_I) \propto \mu_I (\mu_I^{c\,2} - \mu_I^2)^{(\gamma)}$$
$$\chi_q = (\mu_c^2 - \mu^2)^{-\alpha}; \alpha = 1 - \gamma$$
FIT I:  $\gamma = 0.23(3)\alpha = 0.77(3)$ FIT II:  $\gamma = 0.18(2)\alpha = 0.82(2)$ 

Consistent with a crossover from mean field to CEP

# Quark Number Susceptibility at a CEP (see Hatta Ikeda for a discussion in QCD)



FIT with open  $\mu_c : \alpha = 0.66(16)$ FIT with constrained  $\mu_c : \alpha = 0.44(22)$ 

### Analytic continuation of $n(\mu_I)$



 $n(\mu) = K(\mu(\mu_I^{c\,2} + \mu^2)^{(\gamma)})$ 

 $\gamma\simeq.2$ Stephan-Boltzmann Law:  $\rightarrow\gamma=1$ 

## Summary

#### • Tool I : Twisted Mass Thermodynamics

At the very beginning, looks promising, however usefulness of the maximal twist still to be fully understood.

- Tool II Analytic continuation from imaginary chemical potential Well understood and controlled tool for QCD at high temperature and moderately high densities.
  - Taylor Expansion : cfr. Bielefeld-Swansea Group.
  - Fourier Analysis : especially useful for Hadron Phase.
  - Pade' approximants : justifies continuation beyond radius of convergence of Taylor; mathematical basis for power law fits in the sQGP region.

#### • Results

Several results from imaginary chemical potential on the critical line, the hadron phase and the strongly interactive QGP. Particularly useful for confronting with analytic calculations and phenomenological models. However, our results so far are restricted to four flavor QCD.

- Outlook
  - Near future : tuning two flavor twisted mass QCD. Rather expensive since meaningful setup requires  $N_t > 8$ . Computing  $T_c$  and establish universality class.
  - Next : two plus one plus one flavor? introducing chemical potential? ..?