

Modern Challenges for Lattice Field Theory

KITP, March 2005

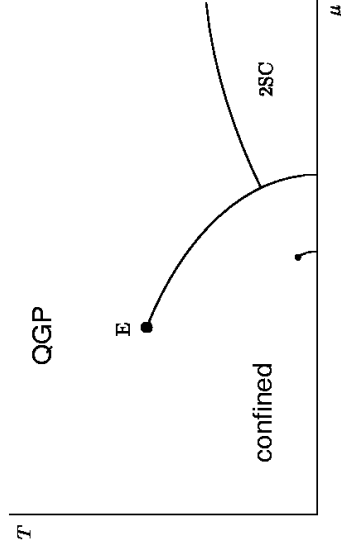
## Simulations of QCD at finite baryon density, via imaginary chemical potential

Philippe de Forcrand (ETH Zürich & CERN)

- Present: Analytic continuation, with Owe Philipsen (U. Münster)
- Future: Canonical approach, with Slavo Kratochvila (ETH)

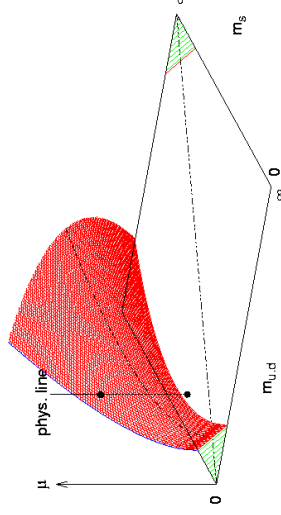
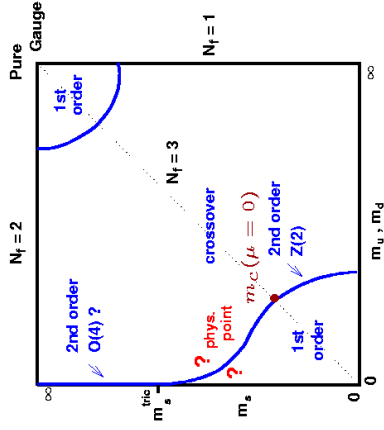
• Confinement loses meaning when matter is **heated and/or compressed**

• rich phase structure



• non-perturbative  $\rightarrow$  **lattice simulations**

### The QCD phase transition at finite $T, \mu = 0$



Finite density,  $\mu \neq 0$ :

$$D(\mu)^\dagger = \gamma_5 D(-\mu^*) \gamma_5 \Rightarrow \det(D) \notin R, \text{ unless } \mu = i\mu_I \text{ (e.g. 0)}$$

Sign problem

Circumventing the sign problem:

#### I. Multi-dimensional reweighting in $(\mu, \beta)$

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

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

#### II. Taylor expansion of I

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

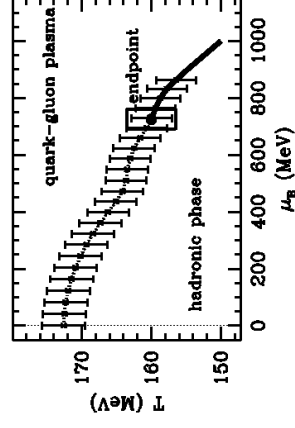
#### III. Imaginary $\mu$ + analytic continuation

fermion determinant positive  $\Rightarrow$  no sign problem

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

- vary **two** parameters  $(\mu, T) \Rightarrow$  uncorrelated results
- control over systematics

Fodor & Katz



Bielefeld/Swansea

Gavai & Gupta

de Forcrand & Philipsen

D'Elia & Lombardo; Chen & Luo; Azcoiti et al.

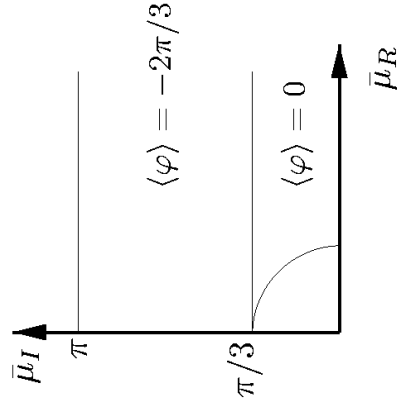
## QCD at complex $\mu$ : general properties

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

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

Roberge & Weiss

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



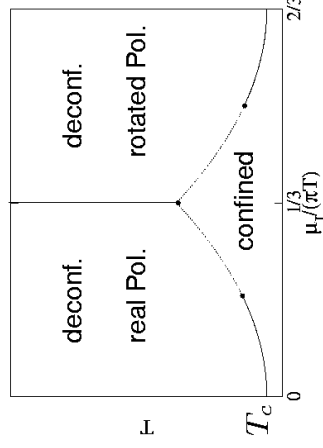
Z(3)-transitions:

$$\bar{\mu}_I^c = \frac{2\pi}{3} \left( n + \frac{1}{2} \right)$$

pert./strong coupling:

1st order for high T

crossover for low T



analytic continuation within arc,  $\mu_B \lesssim 500 \text{ MeV}$ :  $\langle \mathcal{O} \rangle = \sum_n c_n \bar{\mu}_I^{2n} \Rightarrow \mu_I \rightarrow i\mu_I$

### 1a. Analyticity of the (pseudo-) critical line in finite V

location of phase transition from maximum of susceptibilities:

$$\chi(\beta, a\mu, V) = VN_t \langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle, \quad \mathcal{O} \in \{\text{plaq}, \bar{\psi}\psi, |P(x)|\}$$

- finite volume: suscept. **always** finite and analytic
- Critical line  $\beta_c(a\mu)$  defined by peak  $\chi_{max} \equiv \chi(a\mu_c, \beta_c)$
- implicit function theorem:  $\chi(\beta, a\mu)$  analytic  $\Rightarrow \beta_c(a\mu)$  **analytic!**

$$\text{symmetries: } \Rightarrow \beta_c(a\mu) = \sum_n c_n (a\mu)^{2n}$$

### What to expect in physical units?

Natural expansion parameter is  $\frac{\mu}{\pi T}$ :

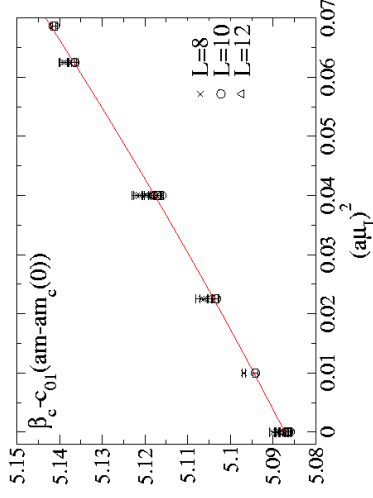
- thermal perturbation theory

- $\mu_I \rightarrow$  shift in Matsubara frequencies  $(2n+1)\pi T$

$$\Rightarrow \frac{T_c(\mu)}{T_c(\mu=0)} = 1 - \mathcal{O}(1) \left( \frac{\mu}{\pi T_c(0, m)} \right)^2 + \mathcal{O}(1) \left( \frac{\mu}{\pi T_c(0, m)} \right)^4 + \dots$$

$N_f = 3$  results, quark mass dependence

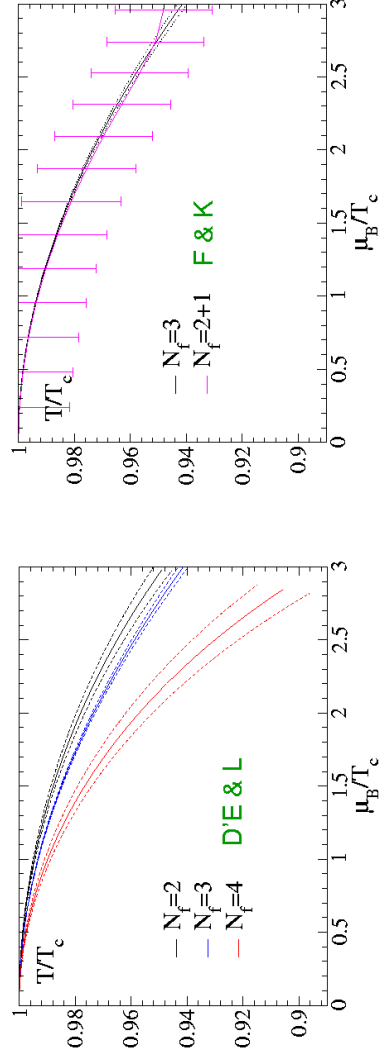
$$\beta_c(a\mu, am) = \sum_{k,l=0} c_{kl} (a\mu)^{2k} (am - am_c(0))^l$$



⇒ sensitive to  $\mu^4$ , but data very well described by  $\mu^2$  fit !

$$\begin{aligned} \frac{T_c(\mu, m)}{T_c(\mu = 0, m_c(0))} &= 1 + 1.937(17) \frac{m - m_c(0)}{\pi T_c} \\ &\quad + 0.602(9) \left( \frac{\mu}{\pi T_c(0, m)} \right)^2 + 0.23(9) \left( \frac{\mu}{\pi T_c(0, m)} \right)^4 \end{aligned}$$

$N_f$ -dependence



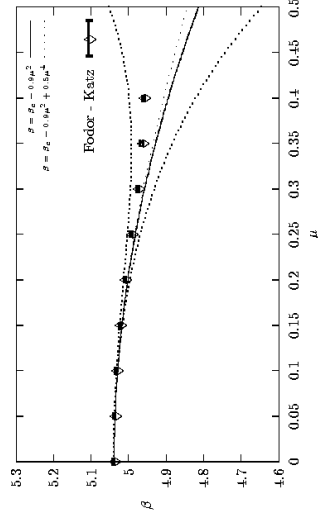
- curvature  $\propto N_f$  when  $N_c \rightarrow \infty$  Toublan
- $N_f = 2 + 1$  same as  $N_f = 3$  as long as  $m_s \ll \pi T$

**Comparison:**

$$N_f = 4$$

imag.  $\mu$  vs. reweighting

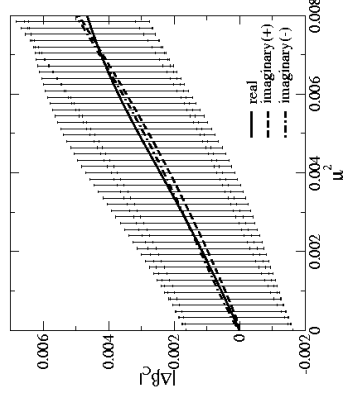
D'Elia, Lombardo



**Comparison:**

real  $\mu$  vs. imag.  $\mu$   
to leading order

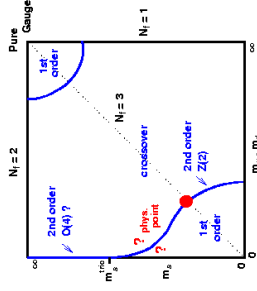
Bielefeld/Swansea



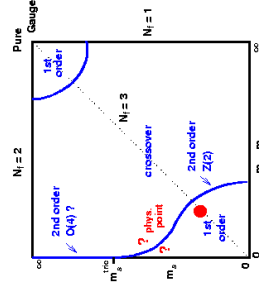
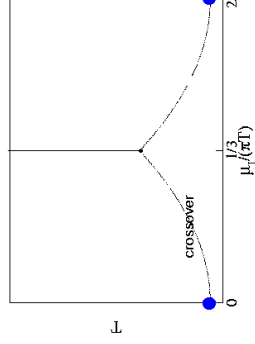
**Comparison:**

analyt. continuation ok in SU(2) Giudice, Papa

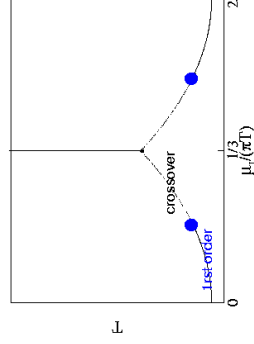
**Ib. Critical endpoint  $(\mu, m_c(\mu))$ ): numerical strategy**



$$m = m_c(0)$$



$$m < m_c(0)$$



**Expect:**

$$\frac{m_c(\mu)}{m_c(\mu=0)} = 1 + c_1 \left(\frac{\mu}{\pi T}\right)^2 + \dots$$

$m = 0 \Rightarrow$  true chiral phase transition  $\Rightarrow c_1 \leq 9$

**Detecting criticality:**

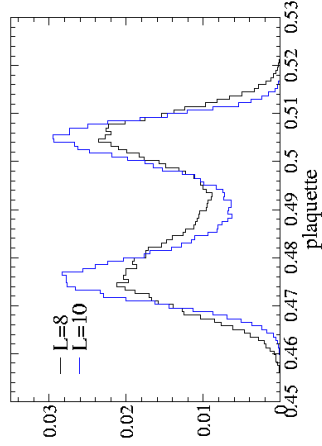
$$\text{Binder cumulant } B_4 \equiv \frac{\langle (\delta\bar{\psi}\psi)^4 \rangle}{\langle (\delta\bar{\psi}\psi)^2 \rangle^2}$$

**3d Ising universality :**  $B_4(m_c, \mu_c) \rightarrow 1.604$ ,  $V \rightarrow \infty$

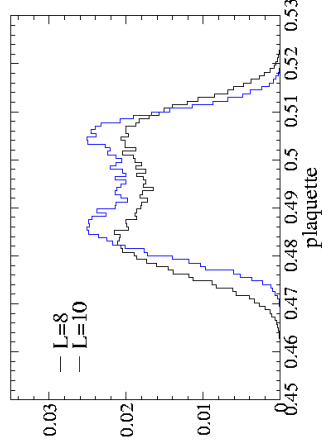
$(B_4 = 1 \text{ (first-order), } 3 \text{ (crossover) for } V = \infty)$

need **VERY LONG** MC runs for sufficient tunneling statistics

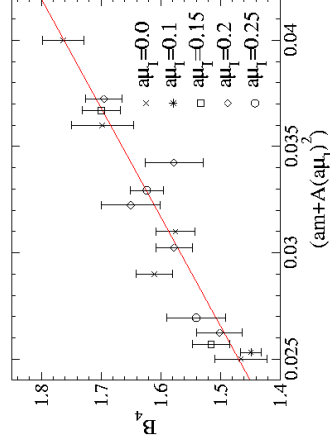
first-order



crossover



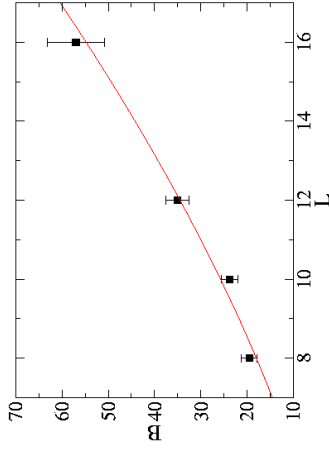
**Taylor series**  $B_4(am, a\mu) = 1.604 + B(am - am_c(0) + A(a\mu)^2) + \dots$



$\Rightarrow \frac{m_c(\mu)}{m_c(\mu=0)} = 1 + 0.84(36) \left(\frac{\mu}{\pi T}\right)^2 + \dots$  **high quark mass sensitivity of  $\mu_c$ !**

$m_c(0)$  in agreement with **Bielefeld, Columbia**;  $c_1(\text{Bielefeld, impr.}) \sim 600(300)$  ?

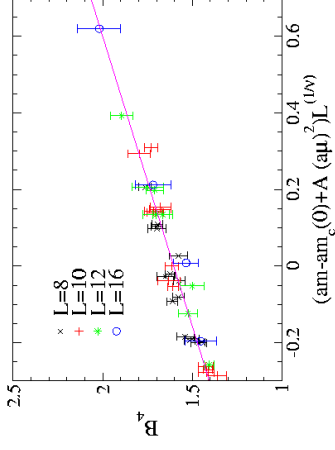
**Finite size scaling**



FSS:

$$\nu = 0.62(3)$$

$$\nu(Ising) = 0.63$$



**Can one expect the critical point to be at “small”  $\mu$ ?**

If  $\mu_c \lesssim 120$  MeV (F & K), then

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

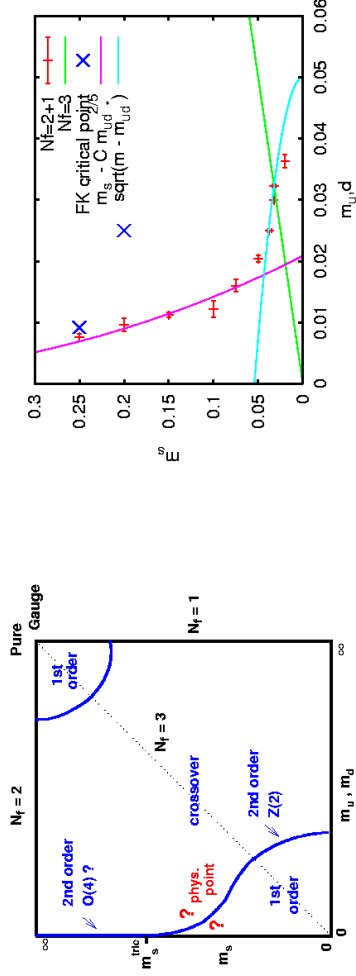
**fine tuning of quark masses!**

**Outlook:**  $N_f = 2 + 1$

Two-step procedure:

**I.**  $(m_s, m_{u,d})$  phase-diagram at  $\mu = 0 \Rightarrow m_s^c(m_{u,d})$

Phase diag. 4d:  $(T, \mu, m_{u,d}, m_s)$



$\Rightarrow$  strong non-linearities, **no linear extrapolations from  $N_f = 3$ !**

$\Rightarrow$  new **Fodor & Katz** qualitatively consistent with our results  $(m_{u,d}/m_{u,d}^c \sim 1.1)$

$\Rightarrow$  consistent with  $O(4)$ , **tri-critical point**,  $m_s^{\text{tric}}/T \sim 2.8$

**II.** repeat calculation for  $\mu \neq 0$

## II. Canonical ensemble

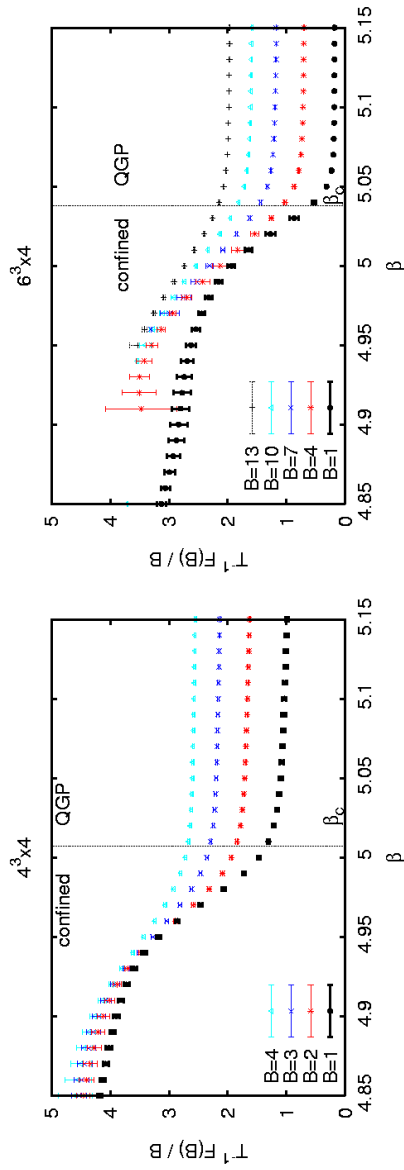
with Slavo Kratochvila (hep-lat/0409072)

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

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

- Sample  $Z_{MC}(\mu = i\mu_{MC})$
- $\Rightarrow \frac{Z_C(B)}{Z_{MC}(i\mu_{MC})} = \left\langle \frac{1}{\det(i\mu_{MC})} \int d\mu_I \exp(i3B\frac{\mu_I}{T}) \det(i\mu_I) \right\rangle$
- 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!**
- **Overlap**: combine several  $(\mu_{MC}, \beta)$  ensembles with Ferrenberg-Swendsen
- **Here**: KS fermions,  $N_f = 4$ ,  $am = 0.05$ ,  $a \sim 0.3$  fm (P.T. first order  $\forall \mu$ )

## Free energy versus temperature



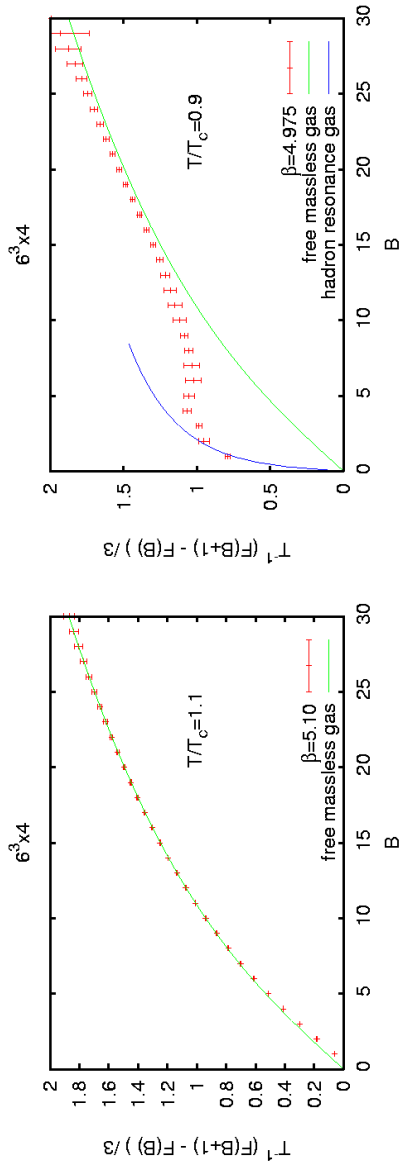


### Chemical potential versus density

Do NOT use fugacity expansion  $Z_{GC}(\mu) = \sum_B \exp(3B \frac{\mu}{T}) Z_C(B)$

Saddle point approximation:

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

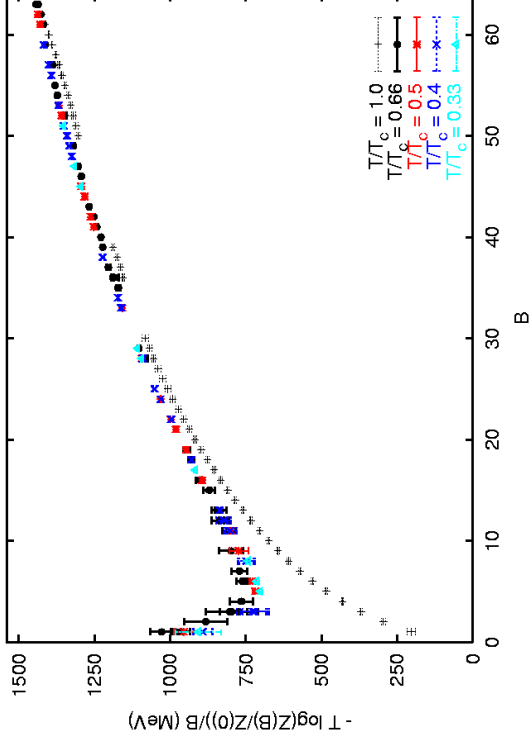


QGP

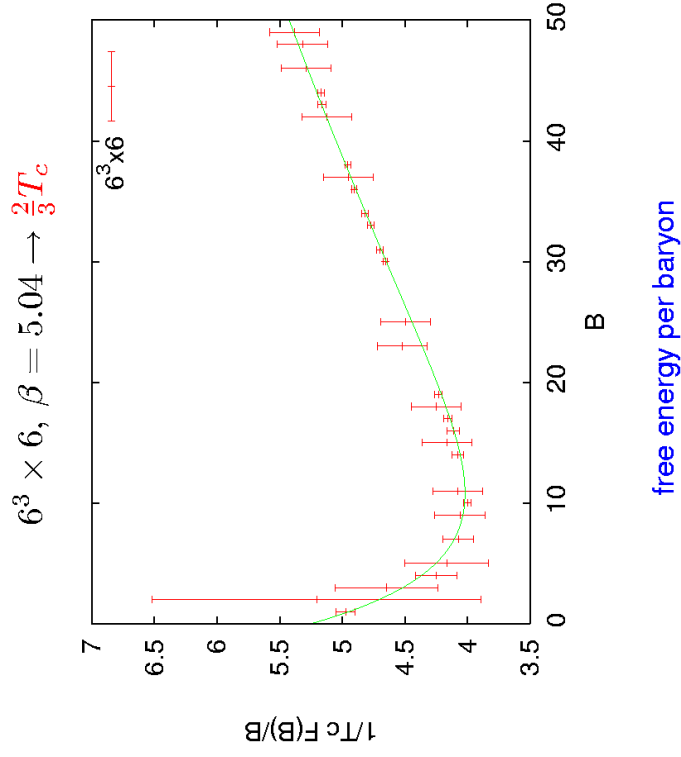
phase coexistence

Lower temperatures  $\rightarrow \frac{1}{3}T_c$  nuclear attraction

$4^3 \times 4, 6, 8, 10, 12, \beta = 5.04$



free energy per baryon



### Conclusions

- Imaginary chemical potential: no sign pb., uncorrelated results  $(\mu_I, \beta)$
- Transition line accessible to simulations for  $\mu_q/T \lesssim 1$ 
  - consistent among all approaches!
  - very flat  $\approx \mu^2$ , small quark mass dependence
  - precision calculation?
- Critical endpoint  $(T_E, \mu_E)$  still exploratory (esp.  $a \rightarrow 0$ )
- Critical endpoint extremely quark mass sensitive
  - $\Rightarrow \mu_c \lesssim 400$  MeV requires nature to fine tune  $m_q$ 's
- Canonical approach promising: low  $T$ , nuclear physics