

Exploring the QCD phase diagram with the DOS method

Christian Schmidt



Introduction / Motivation

1) Formulation of the method

the idea of the DOS method, simulations with constrained plaquette,
generating configurations with measure $|\det M|$

2) The phase diagram from the plaquette

simulation details, determination of the scale,
the plaquette and its susceptibility, ...

... a triple point in the phase diagram ?

3) The quark number density

... a dense quark matter phase ?

Final Remarks

Exploring the QCD phase diagram with the DOS method

Christian Schmidt



... work in collaboration with

Zoltan Fodor
University of Wuppertal

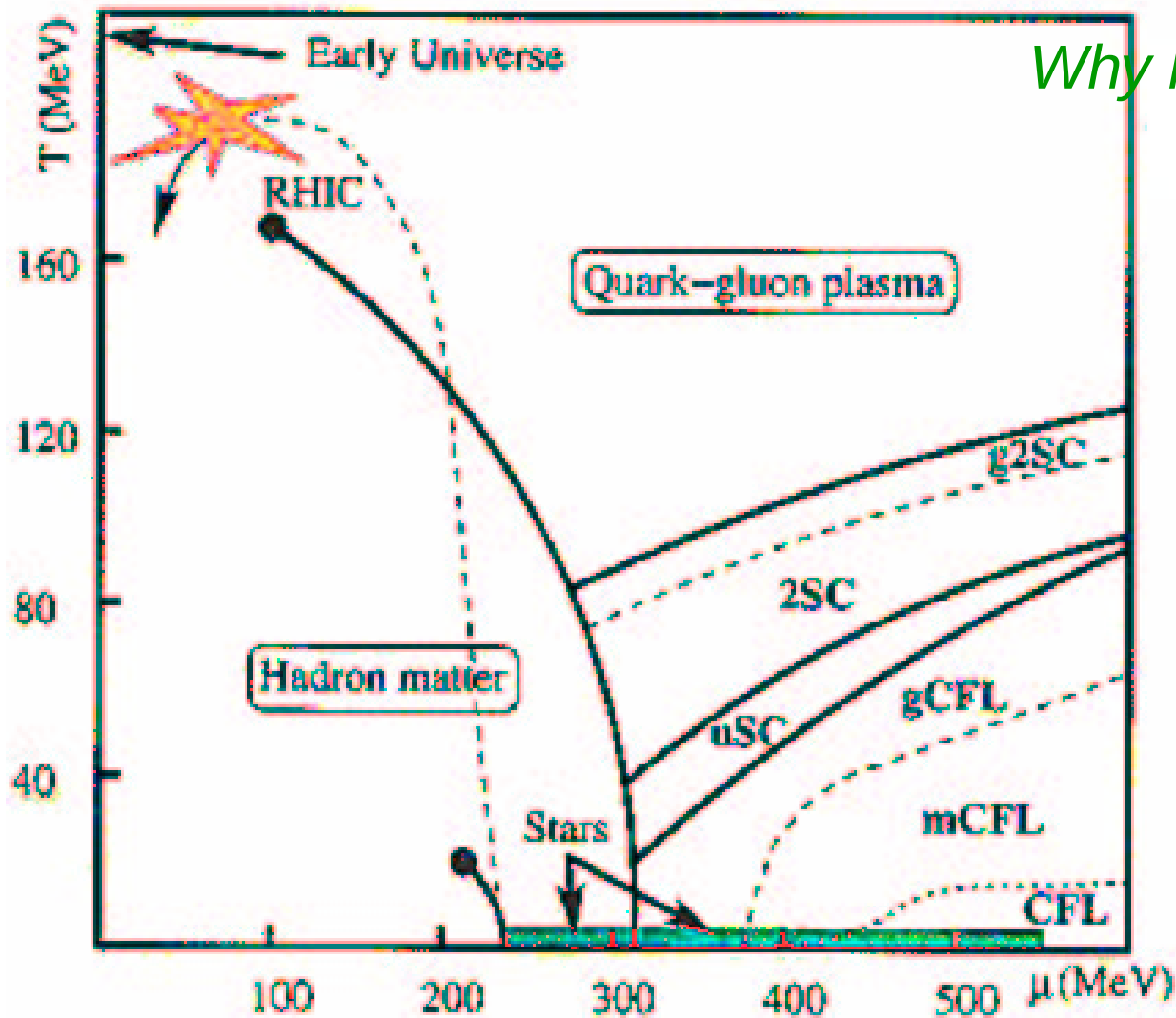
Sandor Katz
University of Budapest

Motivation

The phase diagram of hot and dens matter

Ruster, Shovkov, Rischke, Nucl. Phys. A743 (2004), 127

Why lattice calculations ?



Motivation

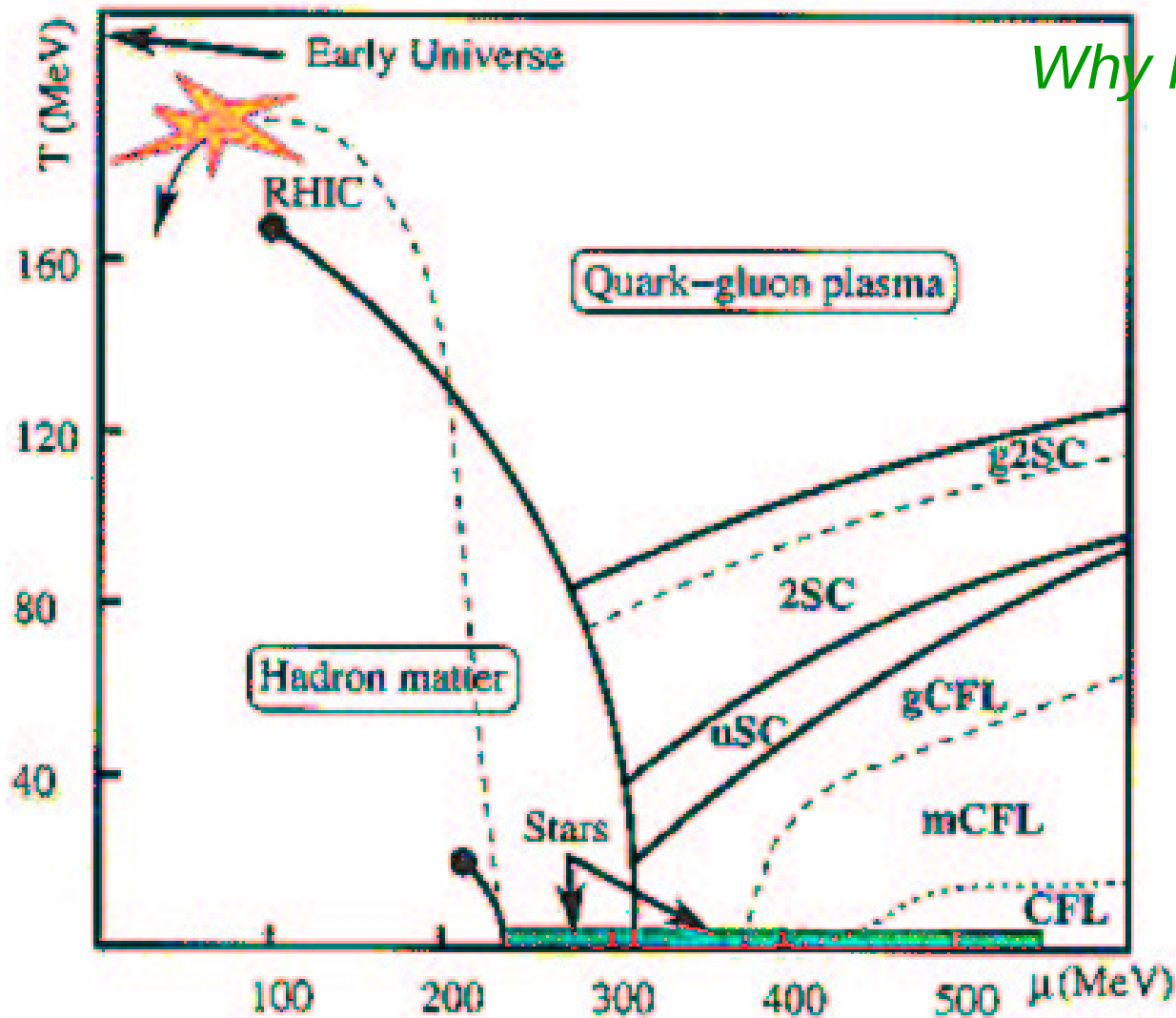
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Why lattice calculations ?

— quantitative approach to

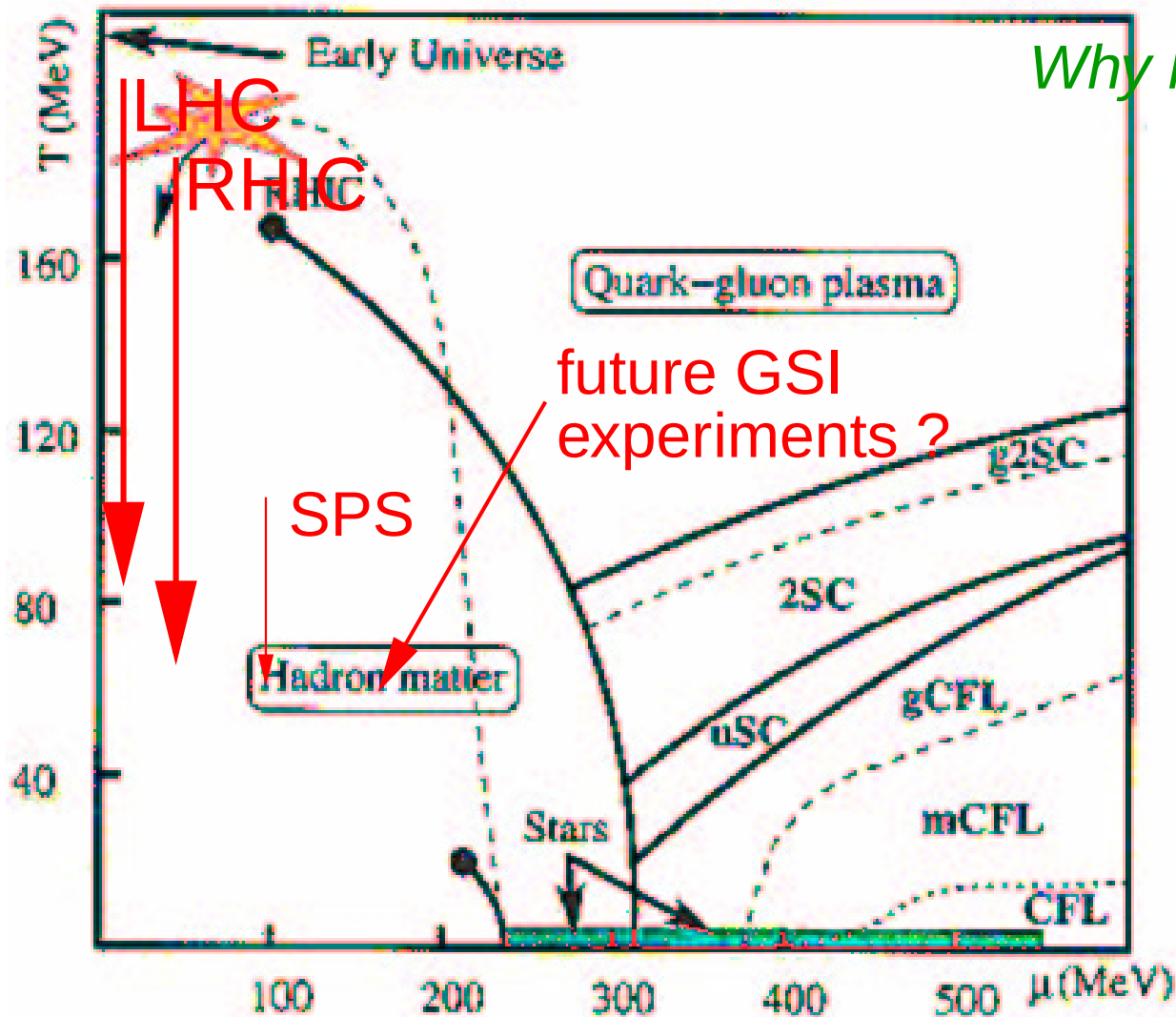
QCD at $T \approx T_c$



Motivation

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Why lattice calculations ?

— quantitative approach to
QCD at $T \approx T_c$

important for

● Heavy Ion
Collisions

“fire ball”

$\approx 10^{-22}$ s

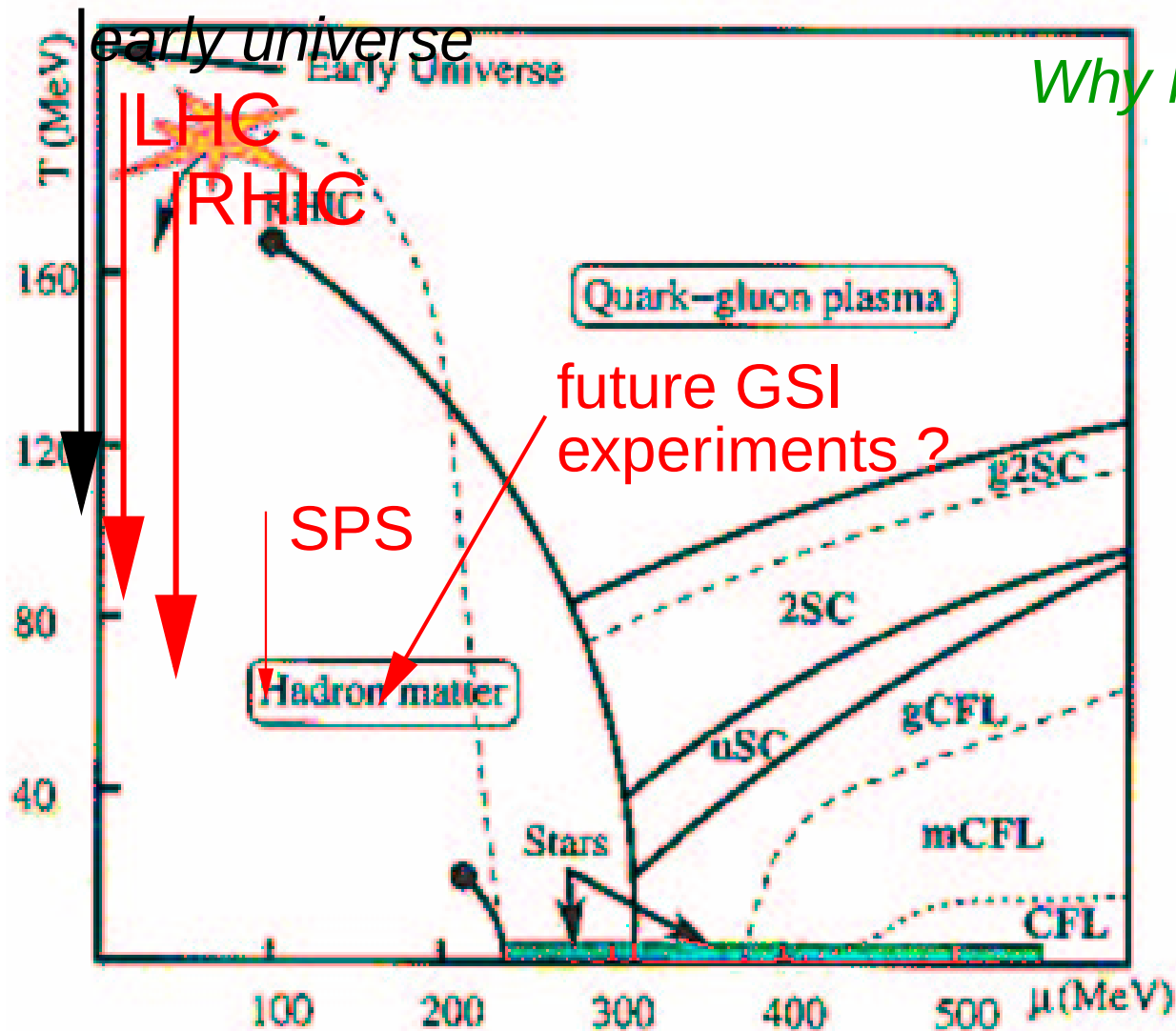
→ *thermal
equilibrium only
for the strong
processes*

→ $\mu_s = 0$

Motivation

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Why lattice calculations ?

— quantitative approach to

QCD at $T \approx T_c$

important for

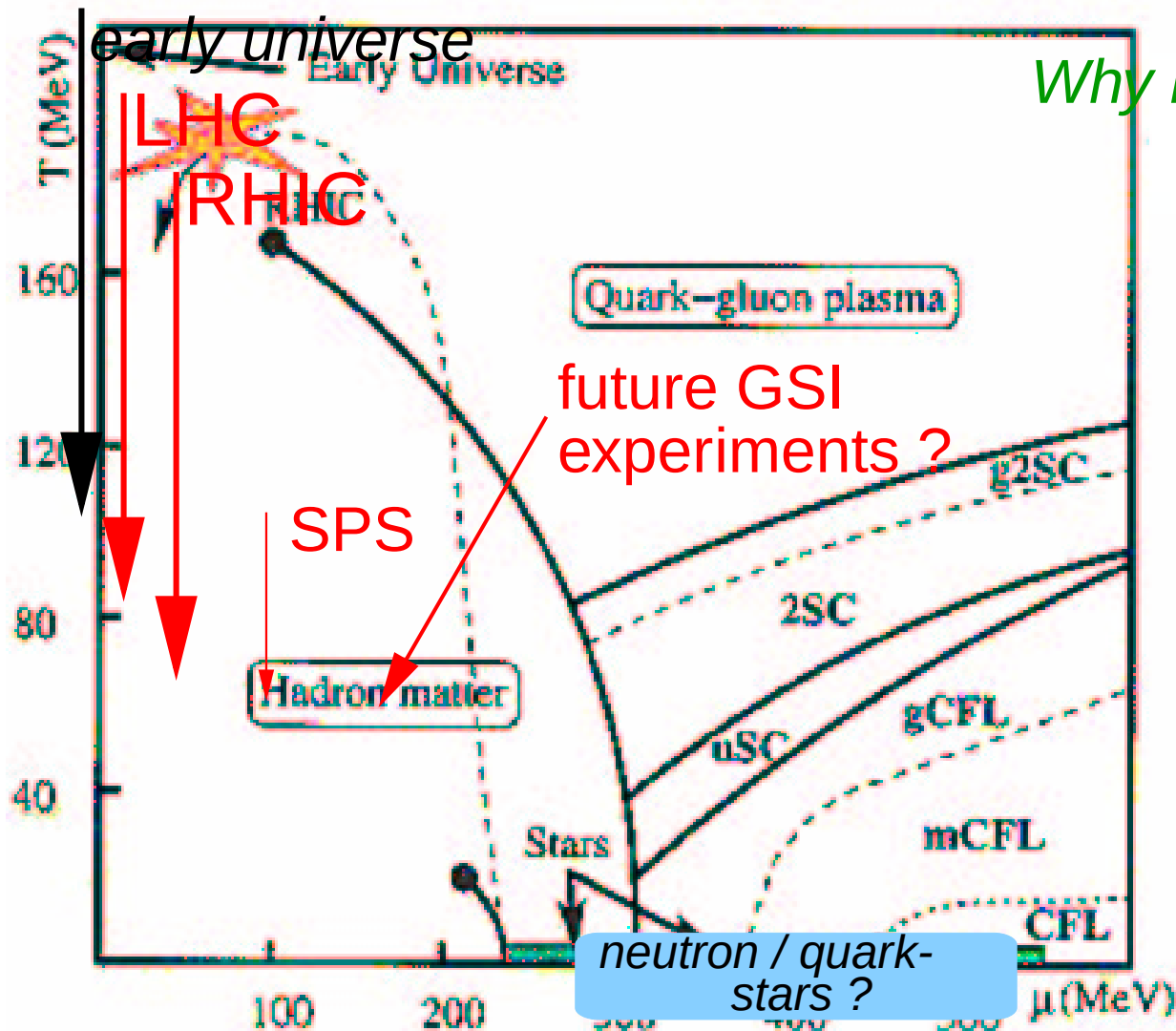
- Heavy Ion Collisions
- Cosmology

QCD phase-transition in the early universe
 $\approx 10^{-4}$ s
after the big bang
→ *inhomogeneities of the universe ?*

Motivation

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Why lattice calculations ?

— quantitative approach to
QCD at $T \approx T_c$

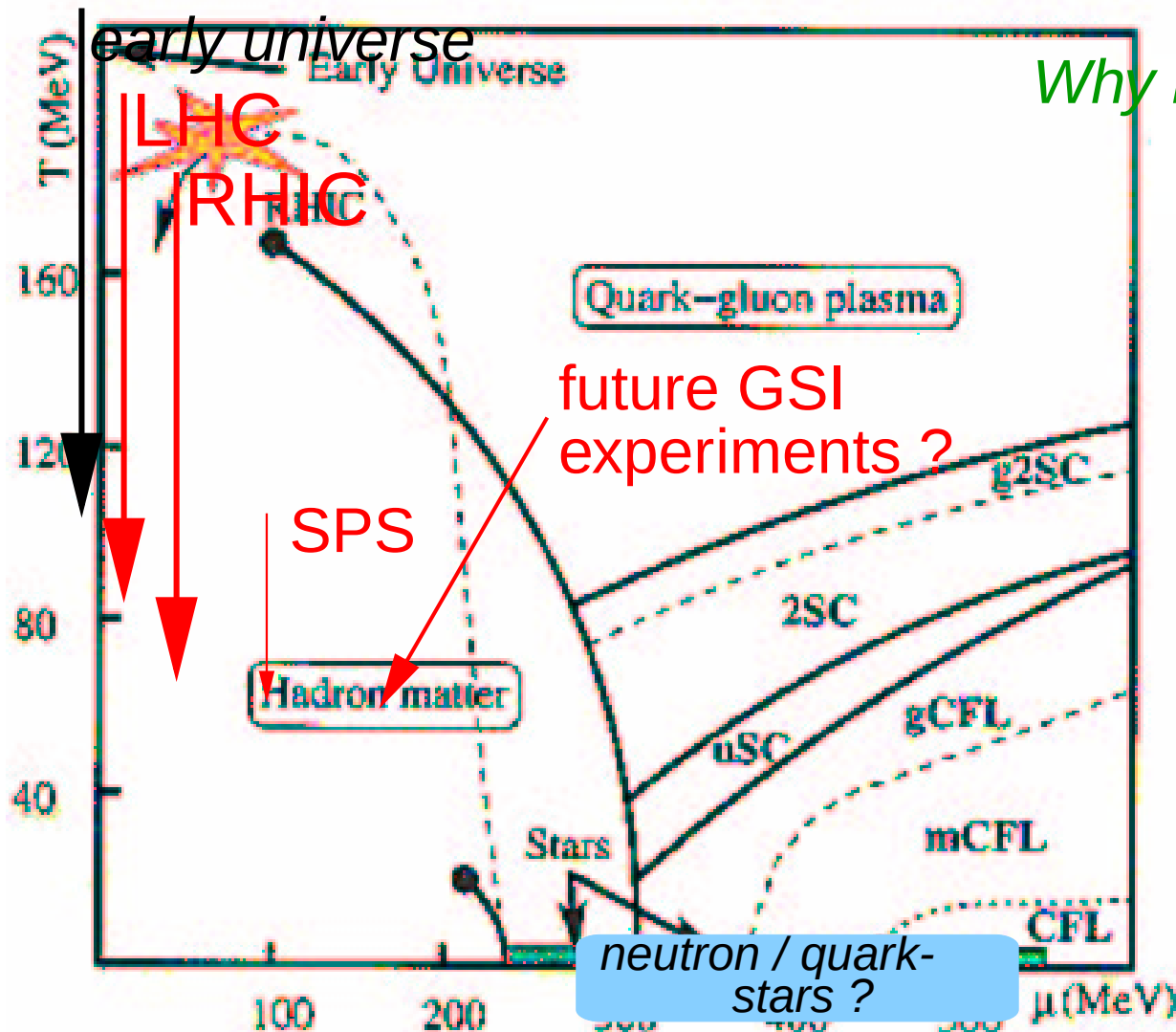
important for

- Heavy Ion Collisions
- Cosmology
- Astrophysics

Motivation

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Why lattice calculations ?

— quantitative approach to
QCD at $T \approx T_c$

important for

- Heavy Ion Collisions
- Cosmology
- Astrophysics

Lattice results:

$$T_c \simeq 170 \text{ MeV}$$

$$\epsilon_c \simeq 0.7 \text{ GeV/fm}^3$$

(Karsch, Laermann, Peikert)

1) The Formulation of the DOS Method

► general idea: reordering of the partition function

constrained partition function or density of states:

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

Operator ϕ
constrained to
value x

grand canonical expectation values:

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

weights $g(U)$ and $f(U)$ have to fulfill
 $g(U)f(U) = \det M(U) \exp\{S_G(U)\}$

possible operators ϕ :

- $\phi = P$ (Plaquette), Bhanot, Bitar, Salvador, (1987); Karliner, Sharpe, Chang, (1988); Azcoiti, di Carlo, Grillo, (1990); Luo, (2001); Takaishi (2004)
- $\phi = \theta$ (complex phase), Gocksch, (1988)
- $\phi = n_q$ (quark number density), Ambjorn, Anagnostopoulos, Nishimura, Verbaarschot, (2002)

1) The Formulation of the DOS Method

► our setup

constrained Operator:

$$\Phi = P \equiv \sum_y \sum_{1 \leq \mu < \nu \leq 4} \left[\text{Tr} P_{\mu\nu}(y) + \text{Tr} P_{\mu\nu}^\dagger(y) \right]$$

→ gluon action (S_G) also constrained

weight functions:

$$g(U) = |\det M(U)| \exp\{S_G(U)\} \quad f(U) = \exp\{i\theta\}$$

→ phase quenched simulations
→ simulations at finite isospin chemical potential

in practice:

$$\rho(x) \equiv Z_P(x) \approx \int \mathcal{D}U \, g(U) \exp \left\{ -\frac{1}{2} \gamma (x - P)^2 \right\}$$

→ delta function is replaced by a sharply peaked Gaussian potential

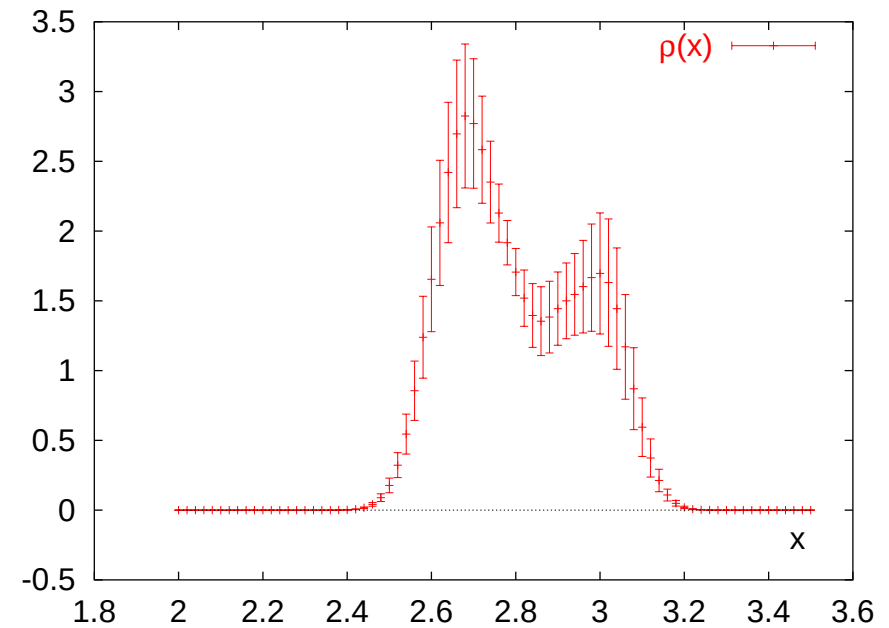
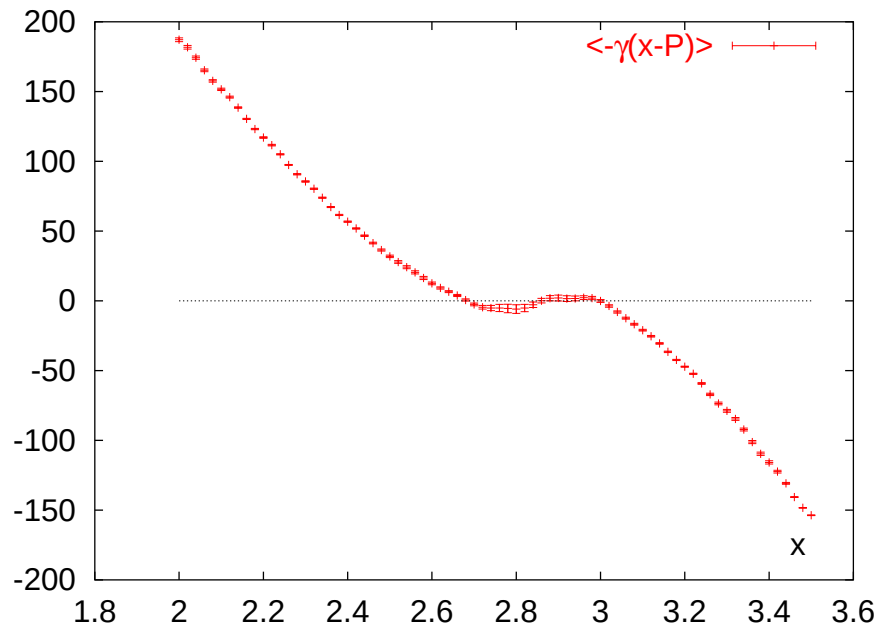
1) The Formulation of the DOS Method

► expectation values

density of states:

$$\frac{d}{dx} \ln \rho(x) = \langle -\gamma(x - P) \rangle_x$$

→ using the integral method to obtain $\ln \rho(x)$



integrate and exponentiate

1) The Formulation of the DOS Method

► expectation values

plaquette and its susceptibility:

$$\langle P \rangle = \int dx \, x \rho(x) \langle \cos(\theta) \rangle_x$$

$$\langle P^2 \rangle = \int dx \, x^2 \rho(x) \langle \cos(\theta) \rangle_x$$

→ calculate $\langle \cos(\theta) \rangle_x$ by measuring all eigenvalues of the reduced fermion matrix ($6L_s^3 \times 6L_s^3$, μ -dependence shifted to first and last time slice)

Fodor and Katz (2002)

→ perform two numerical integrations to get $\langle P \rangle$ and $\langle P^2 \rangle$

→ susceptibility is given by
 $\chi_P = \langle P^2 \rangle - \langle P \rangle^2$

1) The Formulation of the DOS Method

► simulations with constrained plaquette

molecular dynamical Hamiltonian:

$$\mathcal{H} = -\frac{1}{2} \sum_{y,\mu} \text{Tr} H_{\mu}^2(y) - S_G - S_F - \frac{1}{2} \gamma (x - P)^2$$

→ use the hybrid-R algorithm

Gottlieb, Liu, Toussaint, Renken, Sugar, (1987)

→ introduce the additional potential into the molecular dynamical Hamiltonian

gauge force:

$$i\dot{H}_{\mu}(y) = \left[\frac{\beta}{3} U_{\mu}(y) T_{\mu}(y) \left(1 + \frac{\gamma(x - P)}{\beta} \right) \right]_{\text{TA}}$$

→ only a factor of $(1 + \gamma(x - P)/\beta)$ difference

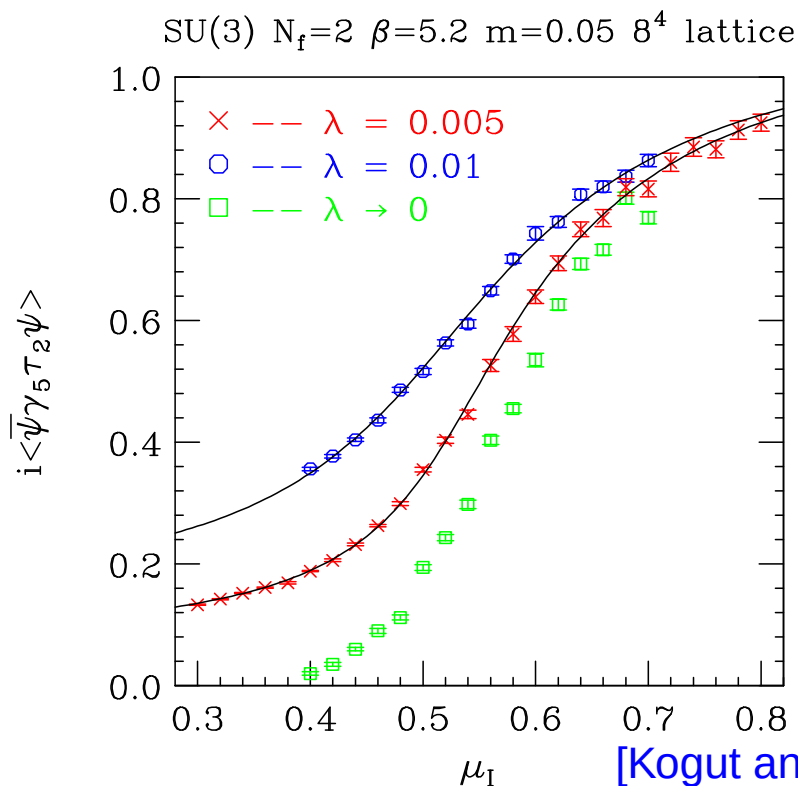
→ measurement of the plaquette in each molecular dynamical step necessary

1) The Formulation of the DOS Method

► generating configurations with measure $|\det M(\mu)|$

fermion matrix:

$$M = \begin{pmatrix} M_{KS}(\mu) & \lambda\epsilon \\ -\lambda\epsilon & M_{KS}(-\mu) \end{pmatrix}$$



- a 8 flavor theory with a small iso-spin symmetry breaking term $\propto \lambda$
Kogut and Sinclair, (2002)
- procedure in complete analogy to the even/odd ordering
- use the square root trick to reduce from 8 to 4 flavors
- extrapolation $\lambda \rightarrow 0$ necessary
- λ -dependence may only be strong for $\mu_I > m_\pi$

1) The Formulation of the DOS Method

► combining the DOS method with multi-parameter reweighting

reweighting procedure:

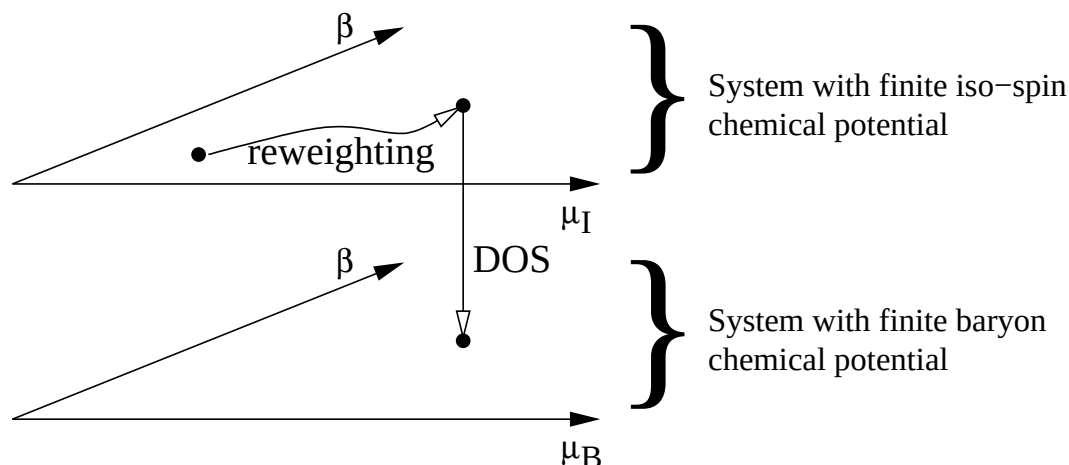
$$\langle Of(U) \rangle_x(\mu, \beta) = \langle Of(U)R(\mu, \mu_0, \beta, \beta_0) \rangle_x / \langle R(\mu, \mu_0, \beta, \beta_0) \rangle_x$$

$$\langle f(U) \rangle_x(\mu, \beta) = \langle f(U)R(\mu, \mu_0, \beta, \beta_0) \rangle_x / \langle R(\mu, \mu_0, \beta, \beta_0) \rangle_x$$

$$\frac{d}{dx} \ln \rho(x, \mu, \beta) = \langle (x - P)R(\mu, \mu_0, \beta, \beta_0) \rangle_x$$

reweighting operator:

$$R(\mu, \mu_0, \beta, \beta_0) = g(\mu, \beta) / g(\mu_0, \beta_0) = \frac{|\det(\mu)|}{|\det(\mu_0)|} \exp\{\Delta S_G\}$$



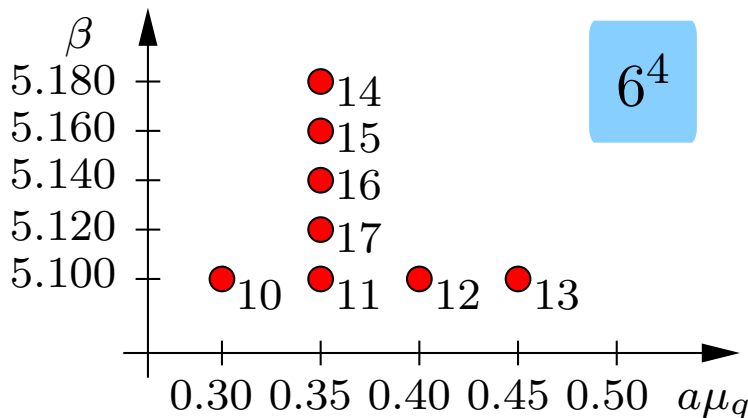
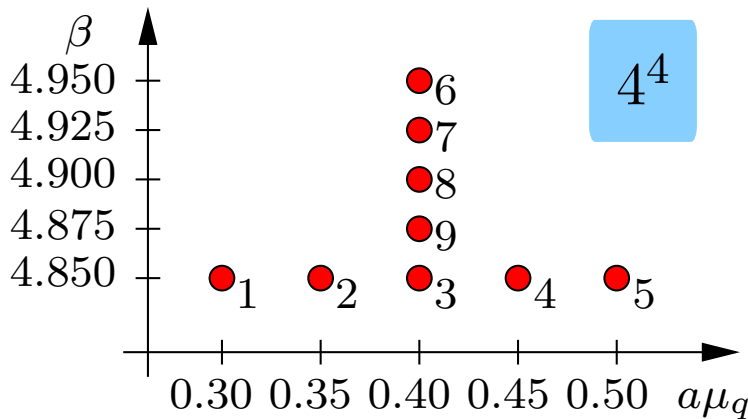
→ reweight all terms separate, before integrating over x

2) The Phase Diagram from the Plaquette

► simulation details

simulation parameters:

$N_f = 4,$ $am = 0.05$
(Kogut-Susskind fermions)



statistics: $\sim 0.2TFlop$ years

No.	P	ΔP	λ	#
1	2.26-3.59	0.01	0.01-0.02	$3 \cdot 44 \cdot 4000$
2	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
3	2.26-3.59	0.01	0.01, 0.02	$2 \cdot 44 \cdot 4000$
4	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
5	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
6	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
7	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
8	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
9	2.26-3.59	0.01	0.01	$1 \cdot 44 \cdot 4000$
10	2.78-2.98	0.01	0.01	$1 \cdot 16 \cdot 5715$
11	2.75-2.94	0.01	0.01	$1 \cdot 16 \cdot 8987$
12	2.72-2.91	0.01	0.01	$1 \cdot 16 \cdot 6800$
13	2.70-2.89	0.01	0.01	$1 \cdot 16 \cdot 2303$
14	2.70-3.23	0.01	0.01	$1 \cdot 44 \cdot 3995$
15	2.70-3.17	0.01	0.01	$1 \cdot 32 \cdot 4393$
16	2.70-3.13	0.01	0.01	$1 \cdot 32 \cdot 5915$
17	2.70-3.05	0.01	0.01	$1 \cdot 32 \cdot 6960$

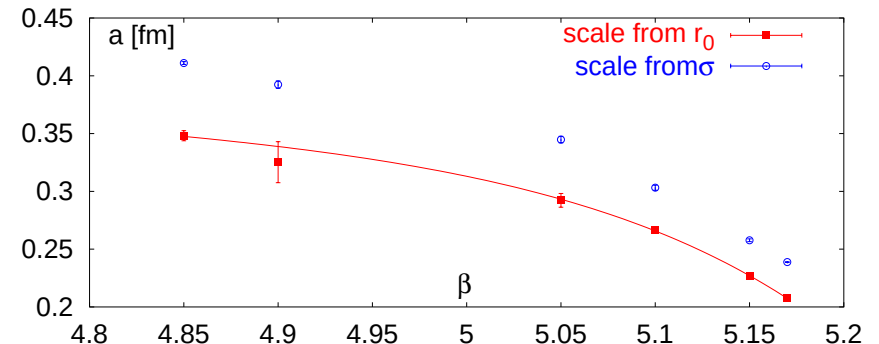
2) The Phase Diagram from the Plaquette

► simulation details

scale calculations:

$N_f = 4, \quad am = 0.05$
(Kogut-Susskind fermions)

Lattice: $10^3 \times 20$



→ calculate the heavy quark potential from Wilson loops

→ compute the Sommer radius and string tension from the potential, interpolate in β

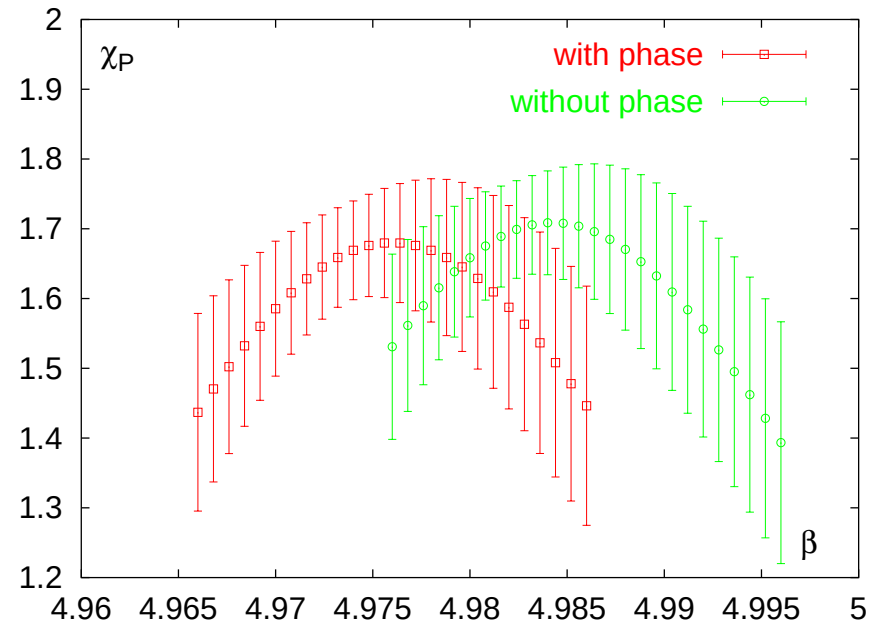
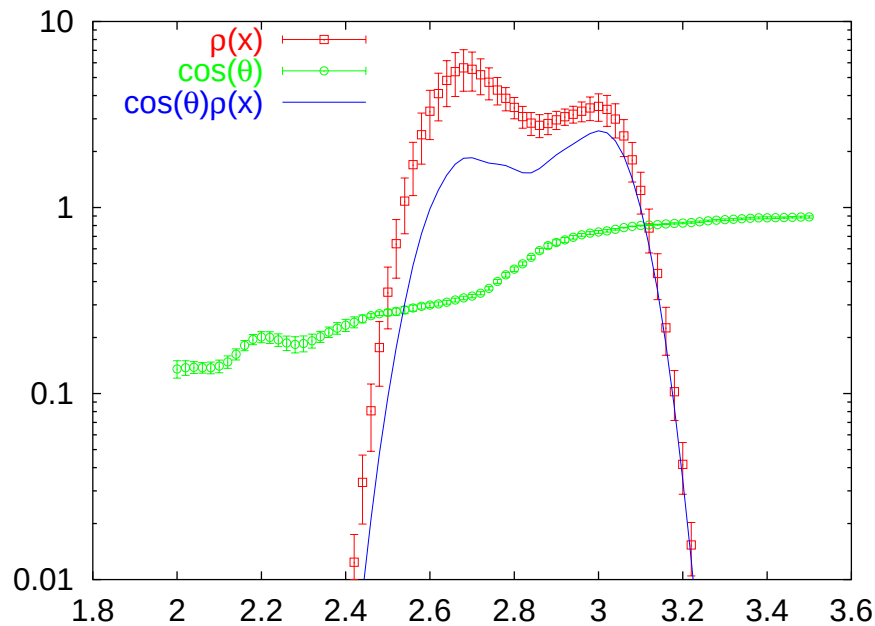
hadron masses:

β	r_0/a	$a^2\sigma$	am_π	am_N
4.85	1.436(18)	0.818(5)	0.5413(1)	2.40(4)
4.90	1.537(84)	0.745(12)	0.5447(1)	2.26(3)
4.95			0.5486(2)	2.36(3)
5.00			0.5542(3)	2.29(4)
5.05	1.711(35)	0.576(9)	0.5613(2)	2.21(2)
5.10	1.876(16)	0.445(7)	0.5715(3)	2.17(1)
5.15	2.208(17)	0.321(3)	0.5892(2)	2.03(1)
5.17	2.411(4)	0.276(1)	0.5982(1)	1.93(1)

2) The Phase Diagram from the Plaquette

► the critical temperature vs. the phase factor

$$m = 0.05, \mu = 0.3, \lambda = 0.02, \quad 4^4$$



→ low temperature phase stronger suppressed than high temperature phase

→ shift of β_c (and thus also T_c) to lower values: $T_c(\mu_S) < T_c(\mu_V)$,

with $\mu_S \equiv \mu_u = \mu_d$ and $\mu_V \equiv \mu_u = -\mu_d$

2) The Phase Diagram from the Plaquette

► the critical temperature vs. the phase factor

$\mu \equiv \mu_u = \mu_d, \mu_s = 0$						
m	N_s	from peak in χ_L		from peak in $\chi_{\bar{\psi}\psi}$		fit-range
		$d\beta_{pc}/d\mu^2$	$\beta_{pc}(0)$	$d\beta_{pc}/d\mu^2$	$\beta_{pc}(0)$	$[\mu_{min}^2, \mu_{max}^2]$
0.005	16	-0.907(648)	3.2661(12)	-1.037(620)	3.2658(11)	[0,0.0006]
	12	-1.003(538)	3.2653(11)	-1.362(689)	3.2649(8)	[0,0.002]
0.1	16	-0.257(64)	3.4792(26)	-0.281(55)	3.4795(23)	[0,0.0006]
$\mu \equiv \mu_I$						
m	N_s	from peak in χ_L		from peak in $\chi_{\bar{\psi}\psi}$		fit-range
		$d\beta_{pc}/d\mu^2$	$\beta_{pc}(0)$	$d\beta_{pc}/d\mu^2$	$\beta_{pc}(0)$	$[\mu_{min}^2, \mu_{max}^2]$
0.005	16	-0.406(68)	3.2661(12)	-0.381(60)	3.2658(11)	[0,0.0006]
	12	-0.399(99)	3.2653(11)	-0.397(70)	3.2649(8)	[0,0.002]
0.1	16	-0.265(93)	3.4791(26)	-0.319(55)	3.4796(24)	[0,0.0006]

Bielefeld-Swansea

→ qualitative agreement with Bielefeld-Swansea results of $d\beta_{pc}/d\mu^2$

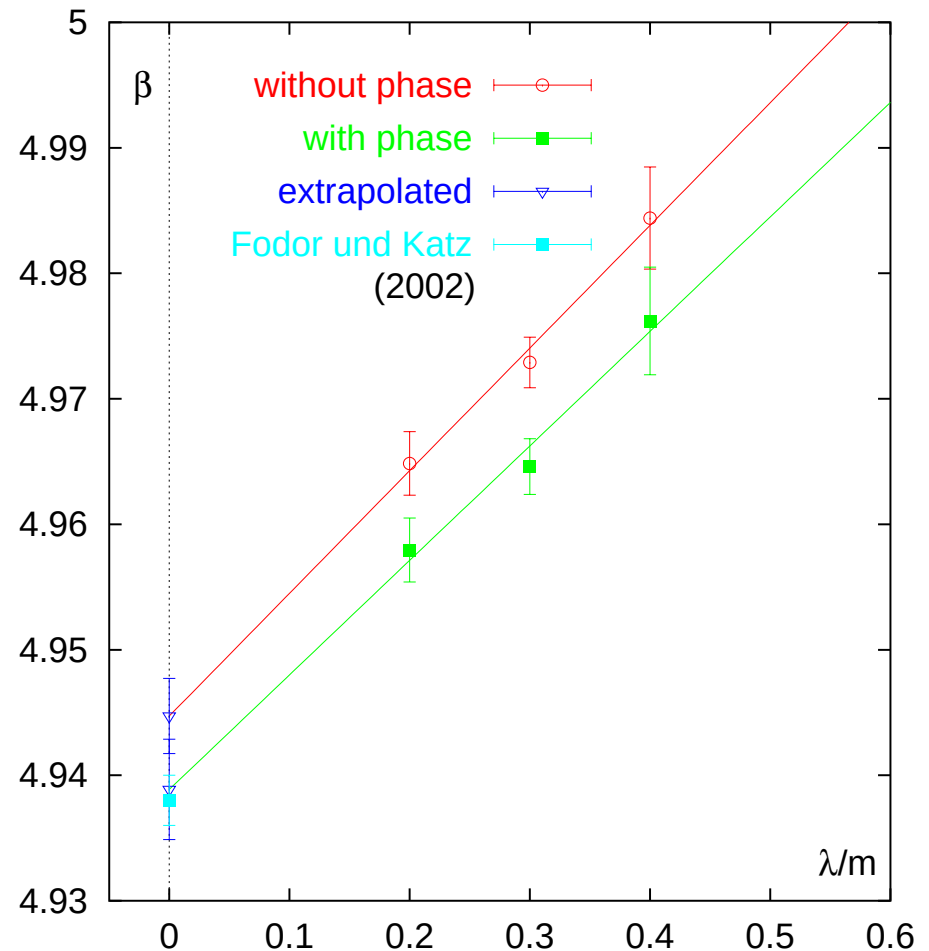
2) The Phase Diagram from the Plaquette

► the critical temperature vs. the phase factor

$m = 0.05, \mu = 0.3, \lambda \rightarrow 0, \quad 4^4$

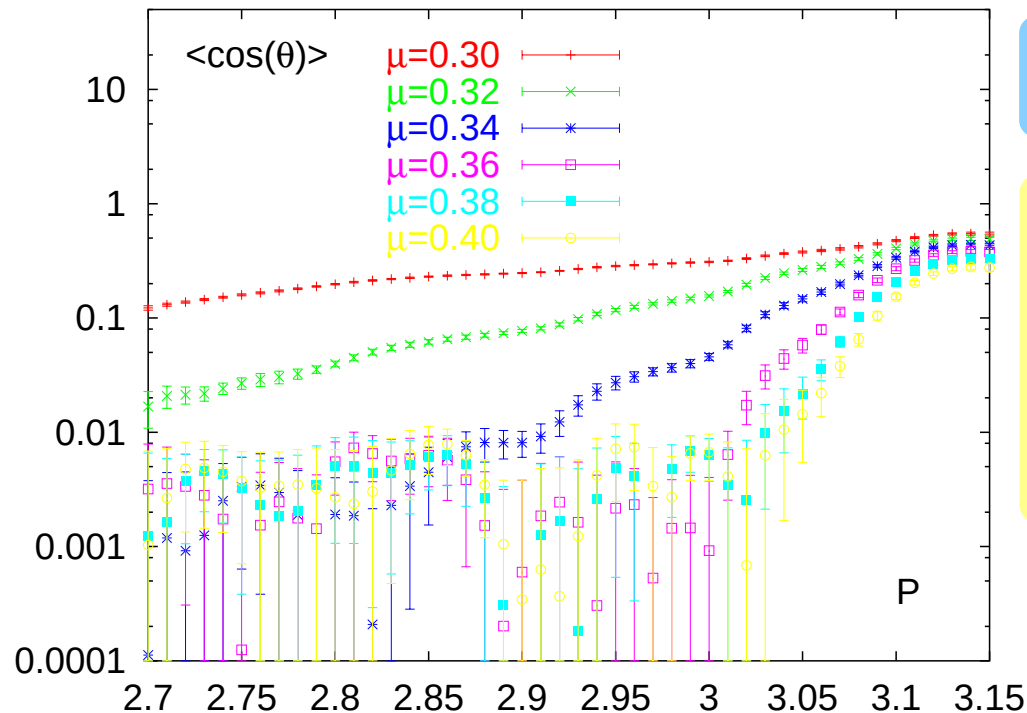
- strong λ -dependence
- extrapolated value is in good agreement with earlier results Fodor and Katz (2002)

from now on we only
show results for
 $\lambda = 0.01$ ($\lambda/m = 0.2$)!



2) The Phase Diagram from the Plaquette

► how severe is the sign problem ?



$$6^4, \beta = 5.1$$

$$\rightarrow \langle \cos(\theta) \rangle_P \lesssim 0.01$$

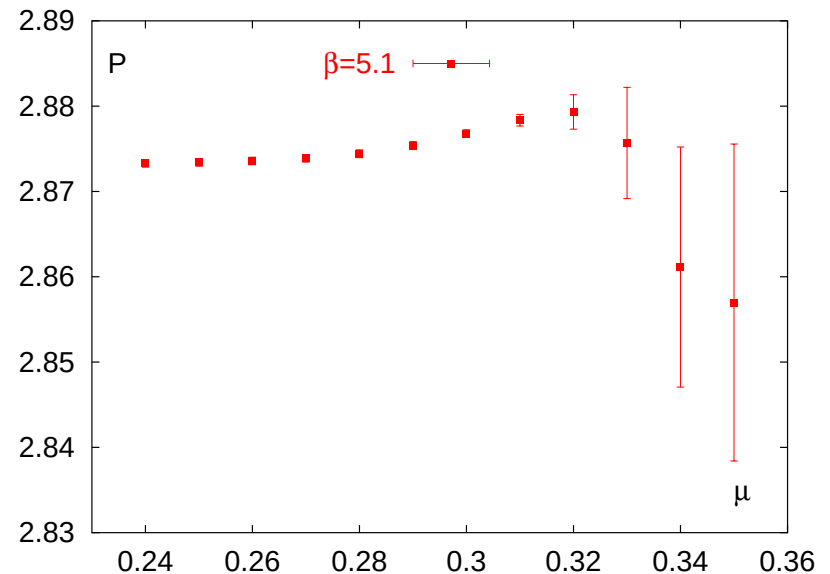
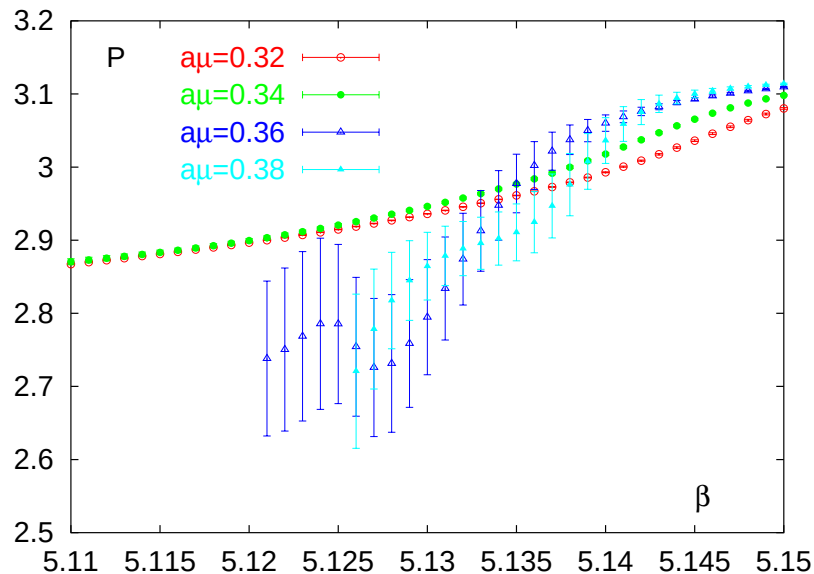
→ non zero only for a few plaquette values ($P \sim 2.85$)

→ advantage of DOS method against the grand canonical ensemble

2) The Phase Diagram from the Plaquette

► the plaquette for $a\mu > 0.3$

6^4



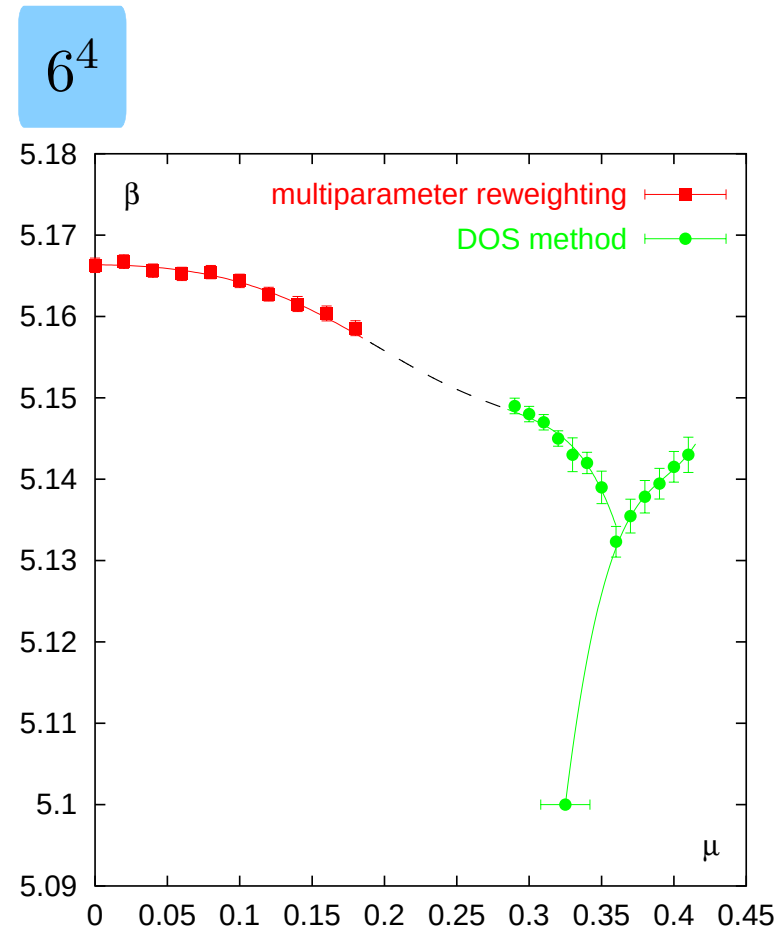
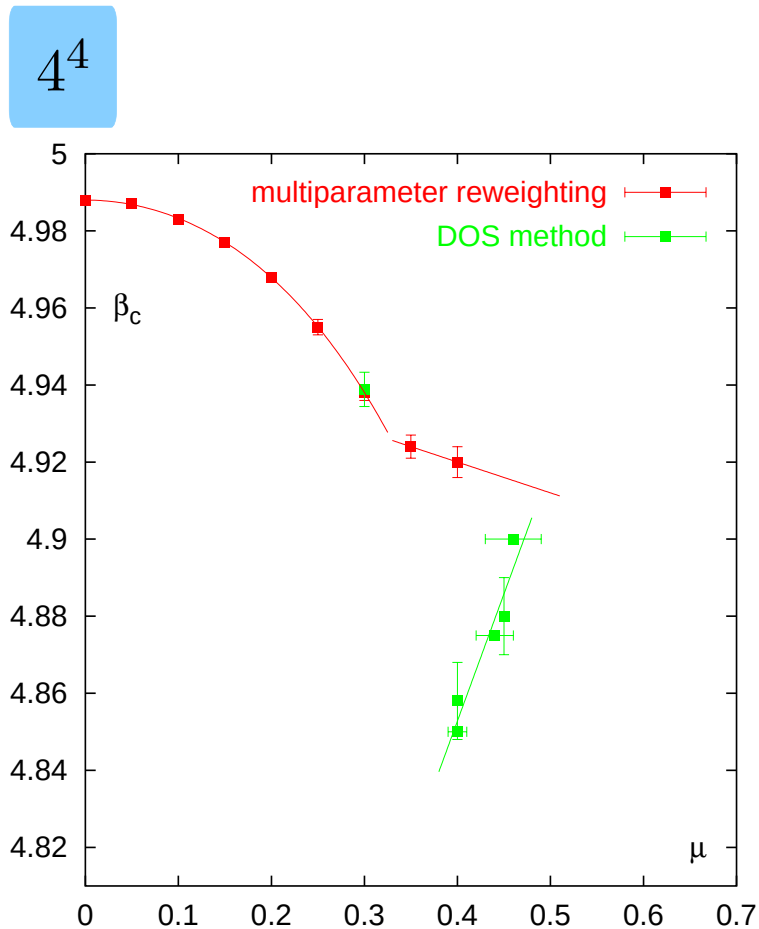
→ the critical coupling β_c increases for $a\mu \gtrsim (0.32 - 0.34)$

→ the plaquette decreases for $a\mu \gtrsim (0.32 - 0.34)$

→ a dense matter phase?

2) The Phase Diagram from the Plaquette

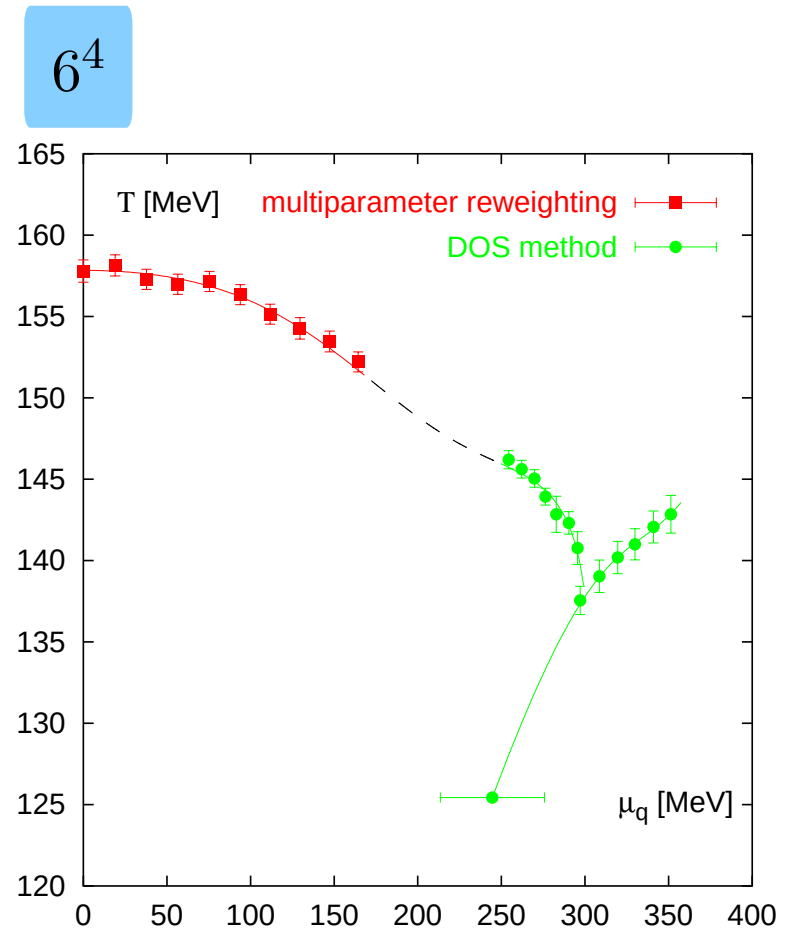
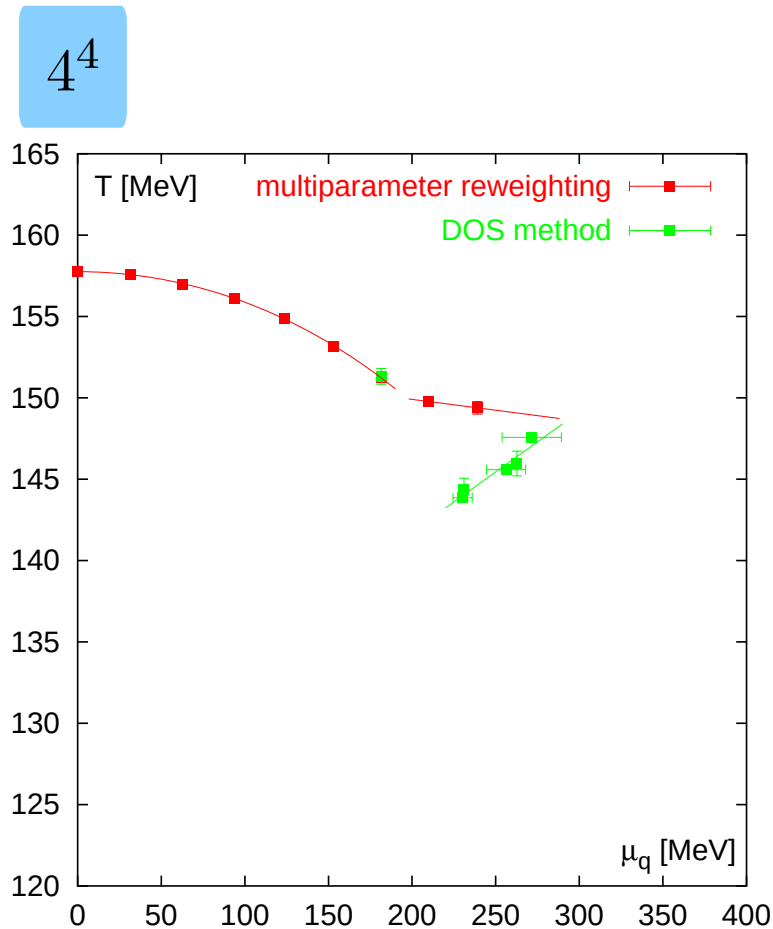
► phase diagram in lattice units



- tripel points between the hadronic phase, the QGP and a third phase
- lines are only ment to guide the eyes

2) The Phase Diagram from the Plaquette

► phase diagram in physical units

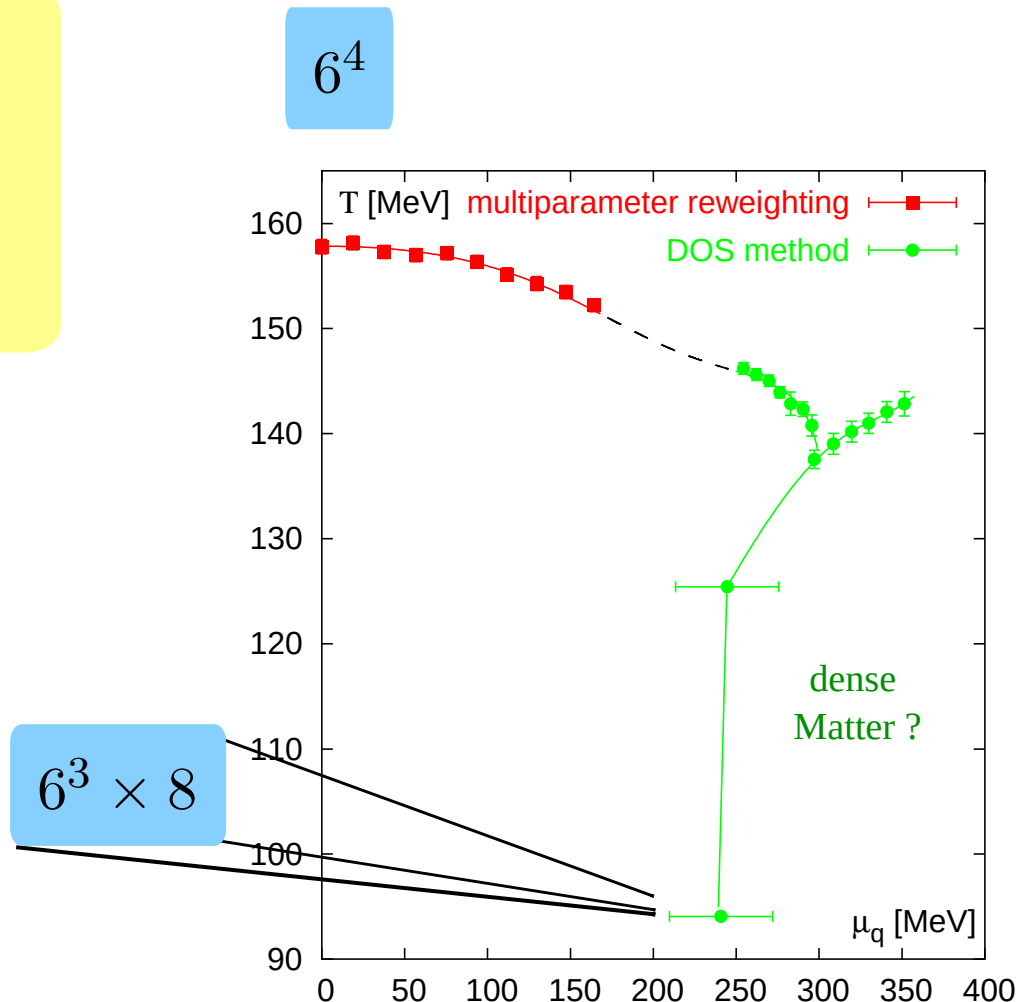


- triple point around $\mu_q \approx 300$ MeV, T_{triple} decreases from (4^4 to 6^4)
- remember m_q/T const., not m_q , not V not a !

2) The Phase Diagram from the Plaquette

► phase diagram in physical units

→ no change in μ_c
when going from
 6^4 to $6^3 \times 8$
($\beta = 5.1$, const.)



2) The Phase Diagram from the Plaquette

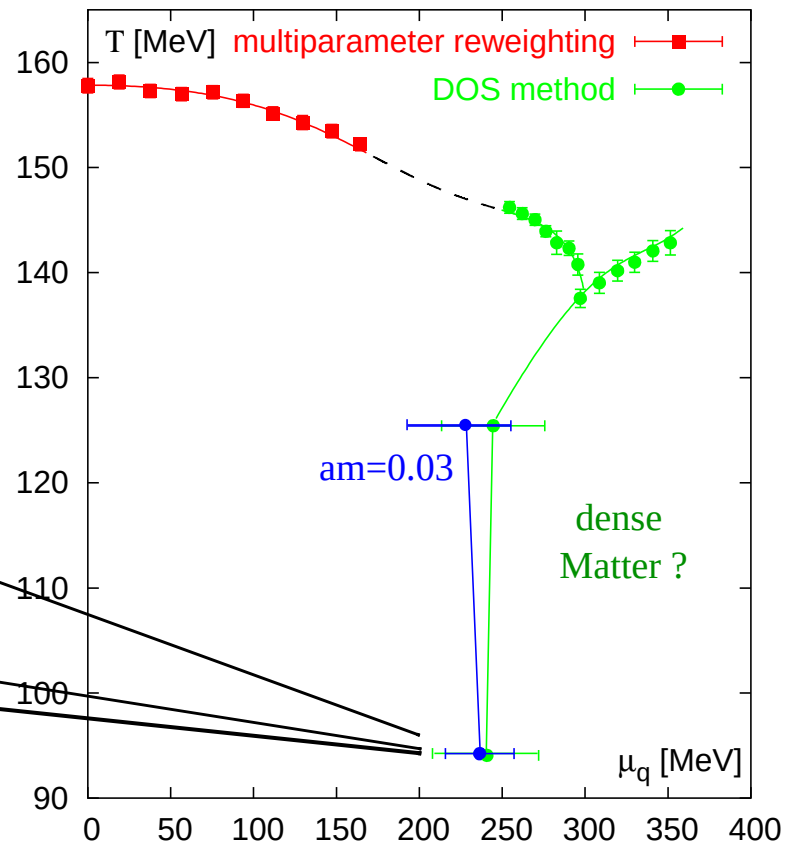
► phase diagram in physical units

→ no change in μ_c , when
going from 6^4 to $6^3 \times 8$
($\beta = 5.1$, const.)

→ **no** mass dependence in μ_c
when going from
 $am = 0.05$ to $am = 0.03$
(the transition is **not** driven by a
pion condensate)

6^4

$6^3 \times 8$



3) The quark number density

► how dens is the new phase ?

expectaion values:

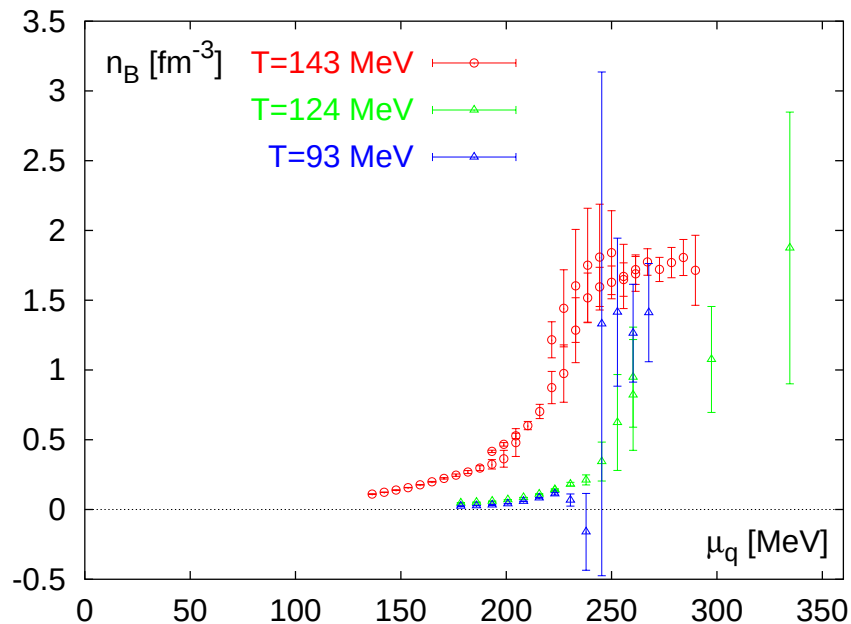
$$\begin{aligned}\left\langle \frac{d \ln \det M}{d(a\mu)} \right\rangle &= \int dx \left\langle \frac{d \ln \det M}{d(a\mu)} \cos(\theta) \right\rangle_x \rho(x) \\ \left\langle \left(\frac{d \ln \det M}{d(a\mu)} \right)^2 \right\rangle &= \int dx \left\langle \left(\frac{d \ln \det M}{d(a\mu)} \right)^2 \cos(\theta) \right\rangle_x \rho(x) \\ \left\langle \frac{d^2 \ln \det M}{d(a\mu)^2} \right\rangle &= \int dx \left\langle \frac{d^2 \ln \det M}{d(a\mu)^2} \cos(\theta) \right\rangle_x \rho(x)\end{aligned}$$

thermodynamic observables:

$$\begin{aligned}n_q &= \frac{1}{a^3 N_s^3 N_t} \left\langle \frac{d \ln \det M}{d(a\mu)} \right\rangle \\ \chi_q &= \frac{1}{a^2 N_s^3 N_t} \left\{ \left\langle \frac{d^2 \ln \det M}{d(a\mu)^2} + \left(\frac{d \ln \det M}{d(a\mu)} \right)^2 \right\rangle - \left\langle \frac{d \ln \det M}{d(a\mu)} \right\rangle^2 \right\}\end{aligned}$$

3) The quark number density

► how dens is the new phase ?



→ leading order cut-off effect has been reduced by multiplying the data with the factor $c = SB/SB(N_t)$

→ transition occurs at

$$n_B \approx (2 - 3) \times n_N$$

→ above the transition the density reaches values of

$$n_B \approx (10 - 15) \times n_N$$

→ transition becomes stronger for decreasing temperature ($T \rightarrow 0$)

→ recently it was also argued by

Alexandru, Faber, Horvath and Liu, (2004)

that density can be larger than $10 n_N$ above the transition

Final remarks

GOOD NEWS:

- The DOS method works and yields results in very good agreement with the multi-parameter reweighting technique.
- On small lattices ($4^4, 6^4$) the sign problem may be moderate enough to allow calculations around the onset of matter ($\mu_q \approx 300$ MeV)
- We have hints for a triple-point in the phase diagram at around $\mu_q \approx 300$ MeV and $T_{\text{triple}} \lesssim 135$ MeV

BAD NEWS:

- Our setup of the DOS method is very expensive, many simulation points in the space of (β, μ, x, λ) are required (integration over x , extrapolation of $\lambda \rightarrow 0$).

REMEMBER:

- calculations have performed on tiny lattices, far away from the continuum and with four degenerate flavors of staggered quarks ($m_\pi \approx 400 - 500$ MeV).

