

# Thermodynamics of QCD with two flavours from simulation at imaginary chemical potentials

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Based on arXiv:0904.1400,  
*Thermodynamics of two flavor QCD from imaginary chemical potentials*  
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# Introduction

## Aim of the work

Study of the behaviour of Hadronic Matter in QCD:

- in a system with two flavours of quark: Up e Down
- near deconfining temperature  $T_c$
- at non null particle density (two chemical potentials)

## Performed Analysis

- Reconstruction of Free Energy
- Validity of the Hadron Resonance Gas model at  $T < T_c$
- Computation of susceptibilities of baryon and isospin densities
- Analytic continuation of the average phase factor  $\langle e^{i2\theta} \rangle$

## Used tools

- Lattice formulation of QCD
- Numerical Integration (Monte Carlo)
- Analytic continuation from imaginary chemical potential

Strong interaction theory according to Standard Model

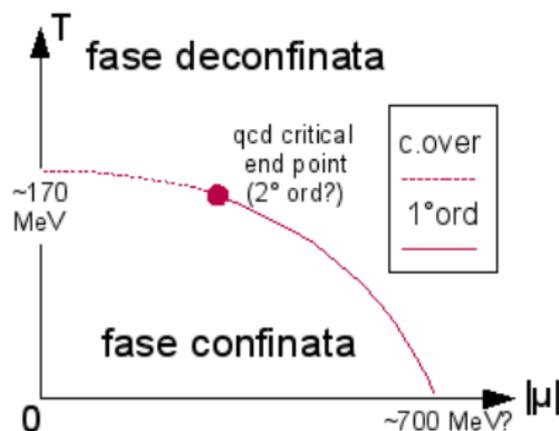
$$\mathcal{L}_E^{QCD} = \sum_{f=1}^{n_f} \bar{\psi}^f (\not{D} + m_f) \psi^f + \frac{1}{4} \sum_{a=1}^{n_c} \mathcal{F}_{\mu\nu}^a \mathcal{F}_{\mu\nu}^a$$

### Perturbative range: high energies

- asymptotic freedom
- free quarks
- deep inelastic scattering

### Non-perturbative range: low energies

- quark confinement (hadronization)
- hadron decaying



### Physic relevance

- heavy ions scattering: fluctuation of the number of produced particles
- evolution of the first universe:  $170 \text{ MeV} \sim 2 \text{ T Kelvin}$
- properties of compact astrophysics objects: white dwarves, neutron stars

# The Lattice

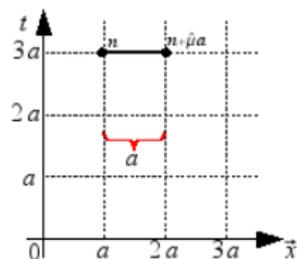
## Computation of observables through path integral

$$\langle \hat{O} \rangle_{\beta} = \frac{\int D[\psi] e^{-S_E^{\beta}[\psi]} O(x)}{\mathcal{Z}}, \quad S_E^{\beta}[\psi] = \int_0^{\beta \hbar} dt \int d^3x \mathcal{L}_E(x), \quad \beta \equiv \frac{1}{k_B T}$$

Theory diverges in Infrared and in Ultraviolet  $\rightarrow$  regularization needed

## Lattice

- Grid of step  $a$ , spatial volume  $L^3$
- Fields defined over grid points and links
- $\langle \hat{O} \rangle_{\beta}$  finite number of standard integrals



$\rightarrow$  UV and IR cut-off, possibility of numerical integration $\leftarrow$

## Problems

- Finite volume: dependence upon the size  $L$
- Continuum limit: results of the original theory only in the limit  $a \rightarrow 0$  realized in a non trivial way: renormalization

## Discrete Grand Partition Function

$$\mathcal{Z}[T, \mu_1, \mu_2] = \int D[U] e^{-S_{E.L}^{gauge}[U]} \prod_{i=u,d} \sqrt[4]{\det M[\mu_i, U]}, \quad U_{n,v} \in SU(3)$$

$$M_{m,n}[\mu] = \delta_{m,n} \hat{m} + \frac{1}{2} \sum_v \eta_{i,v} \left[ U_{m;v} e^{a\mu\delta_{v,4}} \delta_{m,n+\hat{v}} - U_{m-\hat{v};v}^\dagger e^{-a\mu\delta_{v,4}} \delta_{m,n-\hat{v}} \right]$$

- $\mu_{u,d}$  chemical potential coupled to *Up* & *Down* quark
- Limit  $a \rightarrow 0$ : two quarks of mass  $m$ , original symmetries (?)

If  $\mu = 0$ :  $\langle n_{part} + n_{antipart} \rangle_\beta = 0$ , system at null baryon density

### Zero density

- if  $\mu = 0$ :  $\det M[\mu] > 0$
- integrand: probability distribution over field configurations
- integral: computable with Monte Carlo methods

### Non zero density: the sign problem

- if  $\mu \neq 0$ :  $\det M[\mu]$  complex
- theory well defined:  $\mathcal{Z}$  and observables still reals
- serious *numerical* problem: Monte Carlo methods not applicable

We write  $\det M = |\det M| e^{i\theta}$ . Estimator of the severity of the problem:  $\langle e^{2i\theta} \rangle$

# Investigation tools for finite density

Methods that  
uses simulations  
at  $\mu = 0$

$$\text{Taylor } \langle O \rangle_{\mu} = C_0 + C_1 \mu + C_2 \frac{\mu^2}{2!} + \dots, \quad C_i \equiv \left\langle \partial_{\mu}^{(i)} O \right\rangle_{\mu=0}$$

$$\text{Reweighting } \langle O \rangle_{\mu} = \langle O \cdot R(\mu = 0) \rangle / \langle R(\mu = 0) \rangle$$

## Imaginary chemical potential method

Observation:  $\det M[U, \mu] > 0$  if  $\mu$  purely imaginary  $\rightarrow$  Monte Carlo

- 1 Simulations at imaginary  $\mu$
  - 2 Fit data with appropriate function  $f(\mu)$
  - 3 Continuation of  $f$  to real  $\mu$
- $\mathcal{L}$  even in  $\mu$ : continuation from  $\mu^2 < 0$  to  $> 0$
  - Assumption:  $F$  analytic around  $\mu = 0$
  - Crucial point: choice of fit function

Verified where no sign problem (finite isospin,  $SU(2)$ )

## Definition of used chemical potentials

Adimensional potential:  $\theta \equiv \mu/T$

- connected with quark density:  $n_q = n_u + n_d$ :  $\theta_q \equiv \frac{\theta_u + \theta_d}{2}$  (quark potential)
- connected with isospin density:  $n_I = \frac{n_u - n_d}{2}$ :  $\theta_I \equiv \frac{\theta_u - \theta_d}{2}$  (isospin potential)

# QCD with imaginary chemical potential

$T > T_c$

- $F$  is a discontinuous function

$$F(\theta_q, \theta_l) = \sum_{i,j} c_{ij} \theta_q^{2i} \theta_l^{2j}$$

- breaking of  $Z_3$  symmetry
- unphysical transition (R.W)
- limits to analytic continuation

$T < T_c$

- $F$  is a smooth function of  $\theta_q, \theta_l$

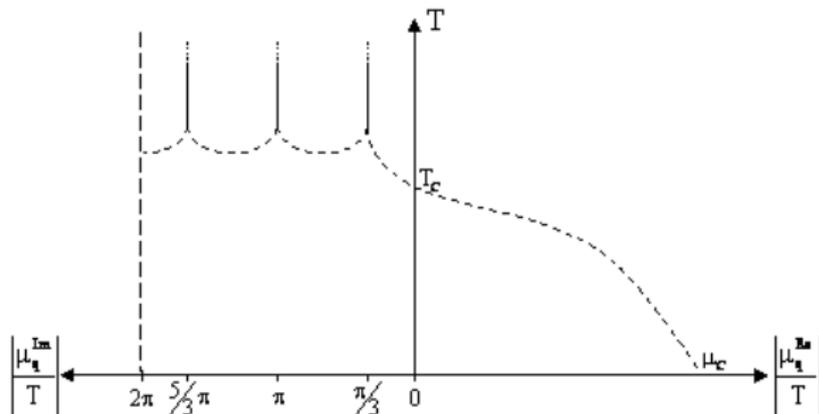
$$F(\theta_q, \theta_l) = V \sum_{h,l} W_{h,l} \cos(3h\theta_q) \cos(2l\theta_l)$$

- $h, l$  integer of the same parity
- constraints to  $W_{h,l}$  from effective models
- information from whole imaginary plane

$Z_3$  symmetry

$$F(\theta_q + \frac{2\pi}{3}) = F(\theta_q)$$

(Roberge & Weiss)



## Aim of the work

We want to **reconstruct** the expression of  $F(T, \theta_l, \theta_q)$

- If we knew the value of derivative of  $F$  with respect to  $\theta_{l,q}$  (isospin and quark densities) we could integrate it numerically and obtain the value of  $F$
- As we have a finite amount of *sample* of  $n_q, n_l$  we will perform a fit
- We need to make an ansatz over the functional expression of  $F$
- Below  $T_c$ : we suppose Hadron Resonance Gas model describe the system
- Interesting check the *HRG* model

Having obtained the expression of  $F$  it is easy to calculate other quantity

- We will calculate generalized susceptibilities
- We will evaluate the average phase factor  $\langle e^{2i\theta} \rangle$

# Hadron Resonance Gas Model

## Effective description of matter below $T_c$

- Hadronic matter: relativistic non interacting gas containing all existing hadron particles
- By imposing correct statistical  $\rightarrow$  simple expression for  $\mathcal{Z}$
- Good agreement with Heavy Ions Scattering Experiments

## Model previsions

Each family with baryon number  $B$  and isospin  $I$  gives an additive contribution to  $F$ :

$$F(T, \theta_q, \theta_I) = \sum_{fam} W_{B,I}(T) \cosh(3B\theta_q) \sum_{I_3 \geq 0} \cosh(2I_3\theta_I)$$

$W_{B,I}(T) = \frac{2VT^3}{\pi^2} \left(\frac{m}{T}\right)^2 g K_2\left(\frac{m}{T}\right)$ ,  $m$  mass of particle,  $g$  degeneration of  $\{B, I\}$  family

- Continuable to imaginary  $\theta$ :  $\cosh \rightarrow \cos$
- By deriving with respect to  $\theta_q$  or  $\theta_I$ , quark density  $n_q$  and isospin density  $n_I$  is obtained

# Technical Details

## Studied theory

- 2 degenerate quark (Up, Down)
- Standard staggered action
- 2 chemical potentials  $\mu_u, \mu_d$
- Pion Mass:  $m_\pi \simeq 280 \text{ MeV}$

## Numerical Setup

- Lattice spacing:  $a \simeq 0.3 \text{ fm}$
- Lattice size:  $16^3 \times 4 \simeq (5 \text{ fm})^3 \times 1.2 \text{ fm}$
- Setup taken from Gupta e Gavai '05  
N.B:  $T_c \simeq 170 \text{ MeV}$
- 5 temperatures, many points on  $\mu_l, \mu_q$  plane

## Statistics

$T/T_c$	$n_{\text{points}}$	$n_{\text{conf}}^{\text{average}}$
0.9	95	2300
0.951	95	2400
1	95	3500
1.048	24	3100
1.25	77	2300

- Value of chemical potentials  $\theta_q$  and  $\theta_l$  ranging from 0 to  $\pi$
- More points near the origin and along the  $\theta_l = 0$  axis

# Check of HRG model

Below  $T_c$  it is trivial that  $F$  can be decomposed in a sum of sinusoidal functions

## Non trivial checks of the model

- 1  $F$  contains only terms corresponding to known hadrons:

$$(B, l) = (0, 0), (0, 1), (1, 1/2), (1, 3/2)$$

→ good fit with the only coefficients:

$$W_{0,0}, W_{0,1}, W_{1,1/2}, W_{1,3/2} \neq 0$$

- 2 Comparison between  $W_{B,l}$  fitted and predicted from physical hadrons spectrum.

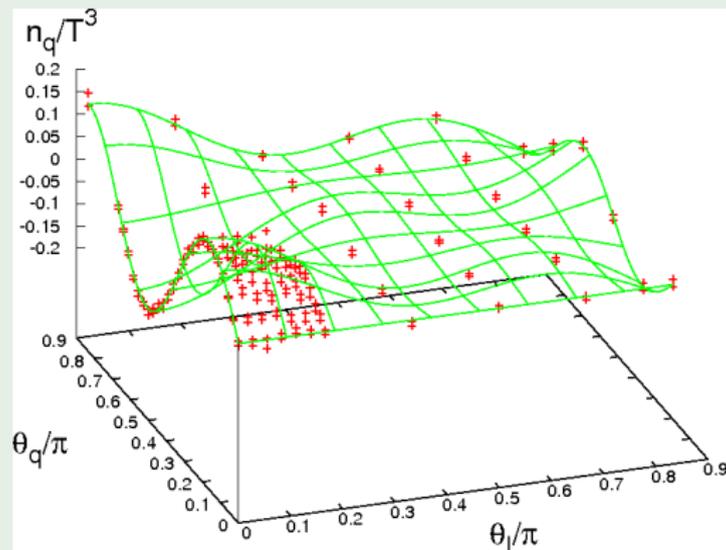
Problems:

- easily affected by lattice artefacts  $a \neq 0$
- non physical mass spectrum:  $m_\pi^{\text{simulate}} \neq m_\pi^{\text{physical}}$

$$T = 0.9 T_C$$

Fit of  $W_{B,I}$  coefficients of  $F$  from HRG model with only pions, nucleons and delta

Fit of Baryon density at  $T = 0.9 T_C$



- $\chi^2/d.o.f = 206/186 \simeq 1.1 \rightarrow$  good agreement between model and data
- slight indication of successive terms ( $B = 2$ )

$$T = 0.95 T_c, T = T_c$$

### At $T = 0.95 T_c$

At this temperature HRG model starts to breakdown

- fit with the only  $\pi, n, \Delta$  gives  $\chi^2/d.o.f = 281/186 \simeq 1.5$
- better fit by including  $B > 1$  term (lower  $\chi^2$ )
- effect of the order of % but well visible

### At $T = T_c$

At this temperature HRG does not work at all!

- fit with the only  $\pi, n, \Delta$  gives  $\chi^2/d.o.f = 808/186 \simeq 4.3$
- many terms with  $B > 1$  needed to get reasonable fit
- formation of larger and larger cluster of quarks

Comparable results obtained by Fourier Decomposition of  $n_q$  and  $n_l$

# Comparison with real data

$W_{B,I}$  calculated from physical hadrons masses

$T/T_C$	$W_{0,1}^{phys}$	$W_{0,1}^{latt}$	$W_{1,\frac{1}{2}}^{phys}$	$W_{1,\frac{1}{2}}^{latt}$	$W_{1,\frac{3}{2}}^{phys}$	$W_{1,\frac{3}{2}}^{latt}$
0.9	0.457	0.216	0.0307	0.0115	0.0126	0.0198
0.95	0.498	0.258	0.0428	0.0218	0.0189	0.0296
1	0.545	0.326	0.0576	0.0340	0.027	0.040

- Correct order of magnitude
- Physical values greater than lattice ones

## Possible explanations

- quark heavier than “real”  
→  $m_{hadr}$  greater than reals
- continuum limit still far  
→  $m_{\pi}a \simeq 0.5$
- simplified theory  
(2 quark, no electroweak)
- partial knowledge of resonances
- failure of *HRG* model

## Generalized susceptibilities

Successive derivatives of the free energy:

$$\hat{\chi}_{n_1, n_2}(\mu_1, \mu_2, T) \equiv - \left( \frac{\partial}{\partial \theta_q} \right)^{n_1} \left( \frac{\partial}{\partial \theta_l} \right)^{n_2} \frac{F}{V}(T, \theta_q, \theta_l)$$

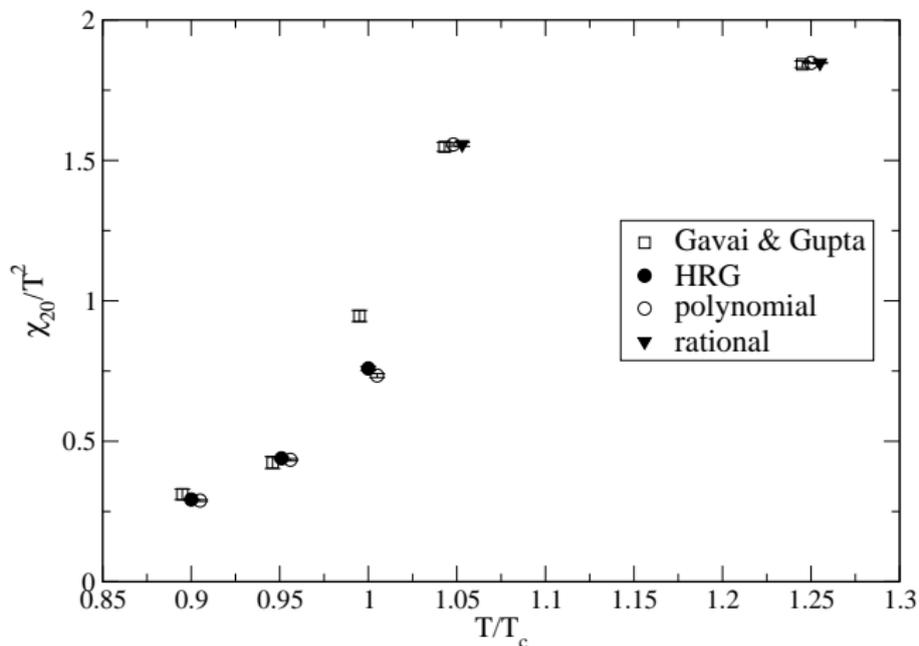
- Relevant in heavy ions scattering experiments
- Calculator at null density with Taylor expansion method (Gupta e Gavai '05)
- Important check of imaginary potential method

## How to calculate them

By deriving the expression of  $F$  obtained appropriate for that  $T$

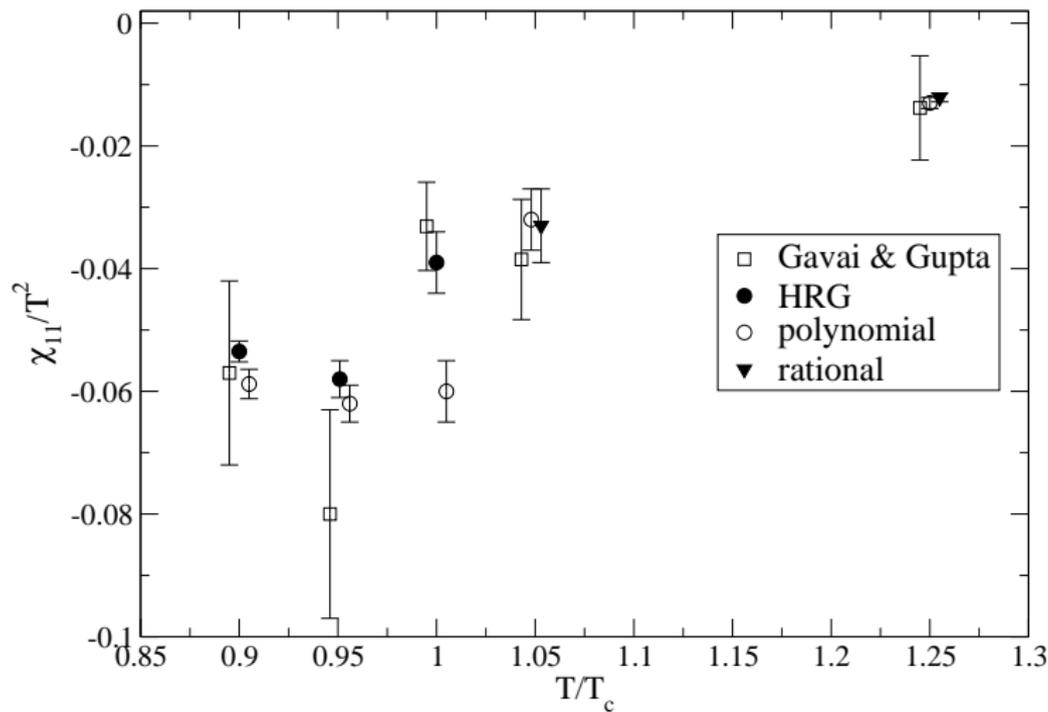
- Low  $T$ : from *HRG* model fit
- High  $T$ : from polynomial or ratio of polynomial fit

# Susceptibility $\chi_{20}$

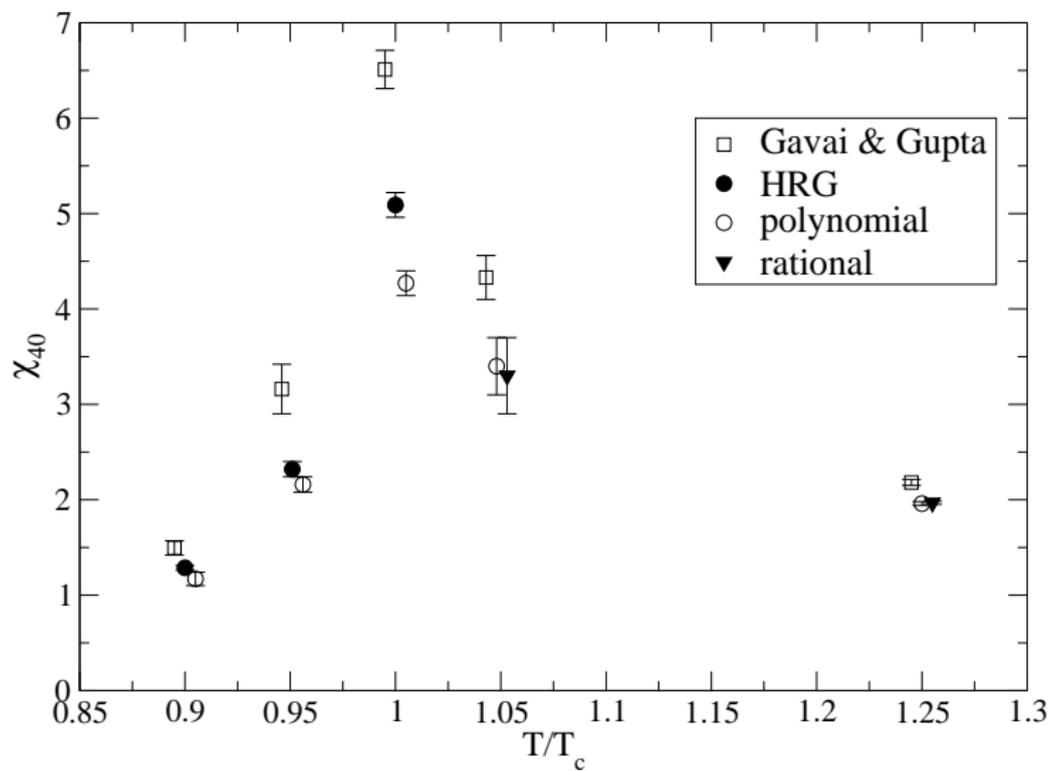


- Good agreement between polinomyal and *HRG* fit (stability of the fit)
- Good agreement with Taylor expansion data
- Problems around  $T_C$ : imaginary  $\mu$  method less sensitive to criticality

# Susceptibility $\chi_{11}$



# Susceptibility $\chi_{40}$



# Analytic continuation of average phase factor

## Regarding the sign problem

We wrote:  $\det M[U, \mu] = |\det M[U, \mu]| e^{i\theta}$

- The value of  $\langle e^{i\theta/2} \rangle_\mu$  is an estimator of the severity of the sign problem: the lower the average value, the stronger the problem.
- It is interesting to analyze it, as the extent of affidability of other method of extrapolating at real  $\mu$  relies on the estimate of this value.

Having obtained  $F$  it is easy to reconstruct the value of the average phase factor:

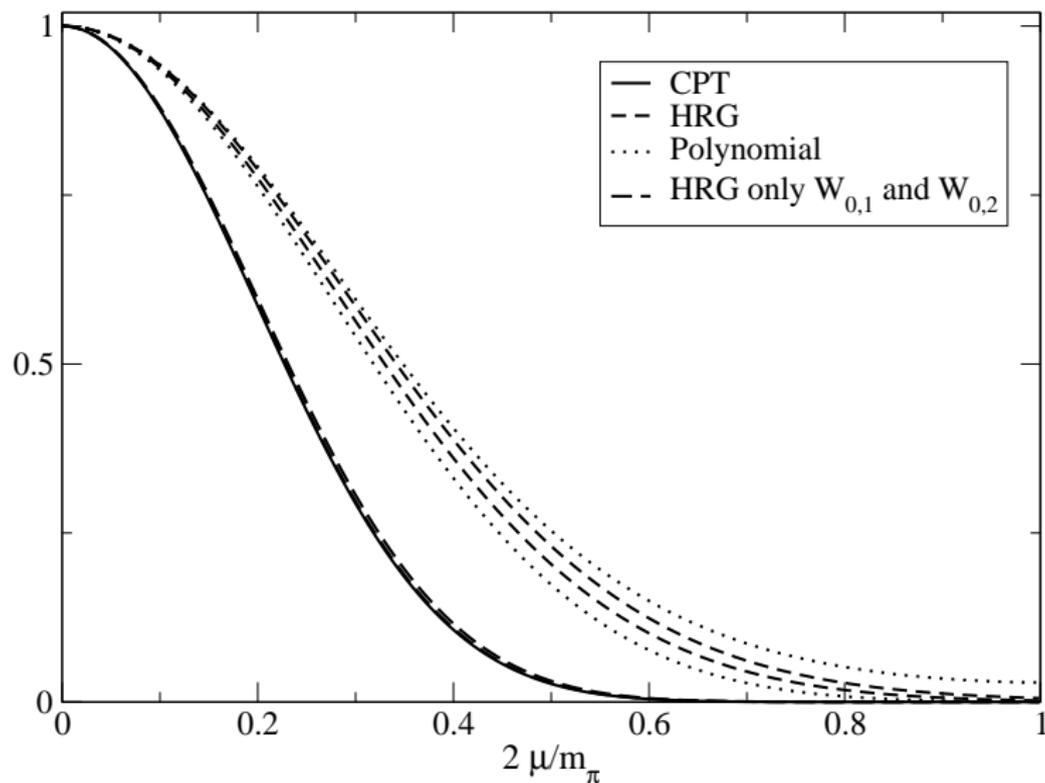
$$\langle e^{i\theta/2} \rangle_\mu = \frac{\mathcal{Z}(\mu_q = \mu, \mu_l = 0)}{\mathcal{Z}(\mu_q = 0, \mu_l = \mu)}$$

## At $T < T_c$

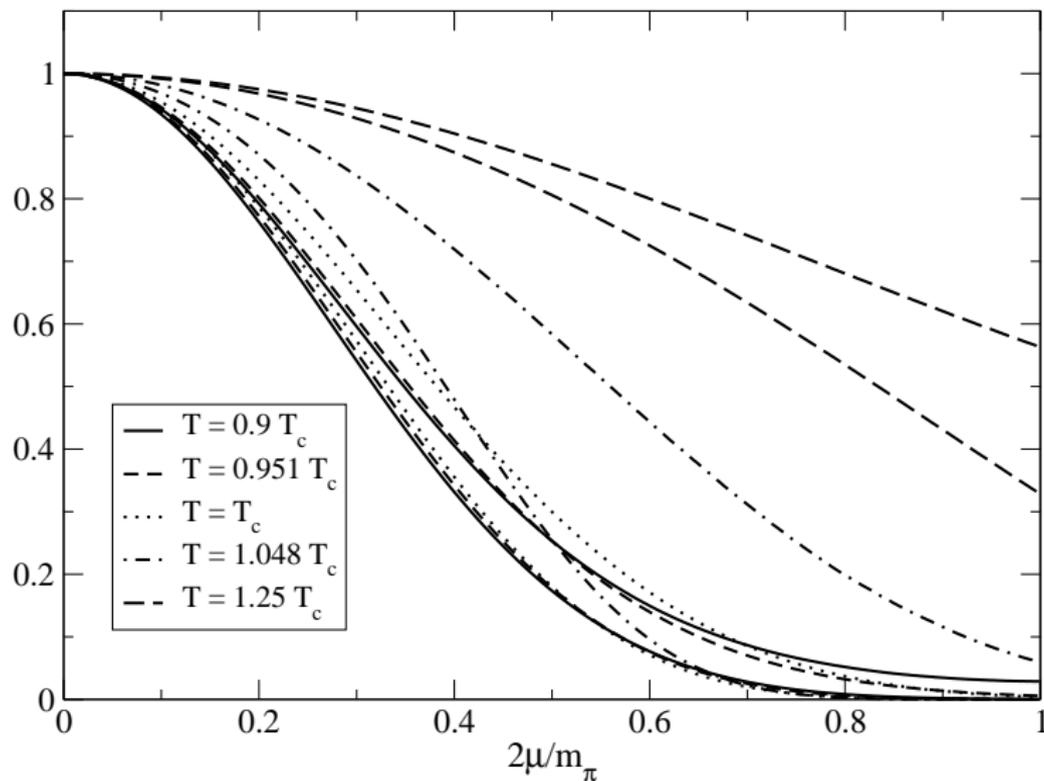
In the framework of *HRG* model:

- each hadron channel contribute separately to che average phase factor
- contributes from states with  $B \neq 0$  tend to make the sign problem less severe

# Average phase factor at $T = 0.9 T_c$



# Average phase factor at various temperature



## Performed works

Reconstruction of  $F(\mu_l, \mu_q)$   
→ two different chemical potentials

*HRG model check*

Clear violations starting at  $T = 0.95 T_C$

*Computation of generalized susceptibilities*

- Efficient method far from  $T_C$
- Problems near  $T_C$

*Continuation of  $\langle e^{i\theta/2} \rangle$*

Analysys of the amount of the sign problem

## Future perspective

*HRG model*

- Check on larger/thicker lattice
- Extrapolate to physical mass
- Test with improved actions
- Interpret violations

*Computation of susceptibilities*

Use a mix of Reweighting and Imaginary chemical potential in order to improve the estimates around  $T_C$

Coming soon: almost accepted on **Phys. Rev D**