The Roberge-Weiss transition

Phase structure of QCD at imaginary chemical potential and generic number of flavors.

A case study: $N_f = 8$

Michele Andreoli

Pisa Univ. & INFN

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Lattice basics

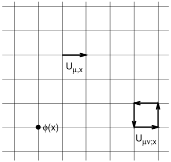
A first principle non perturbative QCD formulation

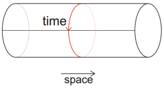
$$S[\psi,\bar\psi,U] = \underbrace{-\beta_G \sum_P \frac{1}{3}\mathrm{ReTr}[\prod_P U]}_{S_G[U]} + \underbrace{\sum_f \bar\psi_f M_f \psi_f}_{S_F[\psi,\bar\psi,U]}$$ and $$Z = \int \mathscr{D}U\mathscr{D}\bar\psi\mathscr{D}\psi e^{-S[\psi,\bar\psi,U]} \equiv \langle e^{-S}\rangle_{FG}$$

- Fields
  - $U_{x,\mu} \approx e^{igaA_\mu(x)}$, $\psi = (\psi_{x_1}, \psi_{x_2}, \ldots)$, $x \in \Lambda$
- Fermion matrix with naive μ
  - $\hat H \to \hat H - \mu\psi^\dagger\psi$
    - Dirac $M_f = (\partial_\mu - igA_\mu)\gamma_\mu + m_f - \mu_f\gamma_0$
- Chemical potential as U(1) field:
  - $\mu \sim igA_0$, therefore $U^{\pm}_{x,0} \to U^{\pm}_{x,0}e^{\pm\mu a}$,
- “Staggered” (Kogut-Susskind)
  - $(M_f)_{x,y} = am_f\delta_{x,y} + \sum_{\nu=1}^{4}\frac{\eta_{x;\nu}}{2}\left[e^{+a\mu_f\delta_{\nu,4}}U_{x;\nu}\delta_{x,y-\hat\nu} - e^{-a\mu_f\delta_{\nu,4}}U^\dagger_{x-\hat\nu;\nu}\delta_{x,y+\hat\nu}\right]$
  - skeleton $M(U,\mu) \sim U_0 e^{\mu a} + U_0^{+} e^{-\mu a}$

lattice domain

$$\Lambda = a\mathbb{Z}^4 = \{x | \frac{x_\mu}{a} \in \mathbb{Z}\}$$





$$\beta = \int_0^{N_\tau a} d\tau = aN_\tau = \frac{1}{T}$$
$$V = \int d^3x = (aN_s)^3$$
$$\beta_G = \frac{2N_c}{g^2}$$

Montecarlo

$$Z = \int \mathscr{D}U \mathscr{D}\bar{\psi}\mathscr{D}\psi e^{\frac{\beta_G}{3}\sum_P \mathrm{ReTr}[\prod_P U] - \bar{\psi}M\psi} \underset{\int \mathscr{D}\bar{\psi}\mathscr{D}\psi e^{-\bar{\psi}M\psi} = \det M}{\underbrace{\Longrightarrow}} Z = \int \mathscr{D}U e^{\frac{\beta_G}{3}\sum_P \mathrm{ReTr}[\prod_P U]} \det M[U]$$

- Probability
  - $$P[U] = \frac{e^{-S_G[U]} \cdot \det M[U,\mu]}{Z}$$
  - with $Z = \int \mathscr{D}U e^{-S_G[U]} \det M(U,\mu) = \langle \det M(U,\mu) \rangle_G$
- Tools
  - $\det M = \prod_f \det M_f^{\frac{1}{4}}(U,\mu_f)$ *(1/4 root trick)*
  - Pseudo-fermions: $\det M = \int \mathscr{D}\phi \mathscr{D}\phi^\dagger e^{-\phi^\dagger \frac{1}{M}\phi}$
  - Multi-fermions: $\det M = (\det M^{\frac{1}{n}})^n$
  - Remez algorithm: $\frac{1}{M^\alpha} = \sum_i \frac{a_i}{M+b_i}$
- RHMC (Rational Hybrid MonteCarlo)
  - generate U_i with $P(U_i) \sim e^{-S_G[U_i]} \det M[U_i]$
  - calculate $$\langle \mathscr{O} \rangle = \frac{1}{N_{conf}} \sum_{i \in conf} O[U_i]$$

In summing up:

$$Z = \langle \det M(U,\mu) \rangle_G$$

$$\begin{pmatrix} \bar{\psi}_1 & \bar{\psi}_2 & \cdots \end{pmatrix} \begin{pmatrix} M_{11} & M_{12} & \cdots \\ M_{21} & \ddots & M_{31} \\ \cdots & M_{32} & \ddots \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$$

$i,j = 1 \ldots N_\tau N_s^3$

Why complex chemical potential?

$$\boxed{Z(\mu) = \langle \det \left[U_0 e^{\mu a} + U_0^{+} e^{-\mu a} \right] \rangle_G}$$

1) $\det M(U,\mu)^\star = \det M(U,-\mu^\star)$
2) $Z(\mu) = Z(-\mu)$ if $\langle\rangle_G = \langle\rangle_{G^\star}$
3) $Z(\mu)^\star = Z(-\mu^\star)$

- Standard Montecarlo unfeasible if $\mu \in \mathscr{R}$ ("sign problem")
  - $\det M(U,\mu)$ is real only if $\mu^\star = -\mu$ (see 1)
    - Way out: Imaginary chemical potential, Taylor expansion, analytic cont., Reweighting at $\mu = 0$, etc
- Anyway, Nothing is wrong in the QCD formulation at imaginary μ:
  - after averanging on the background gauge fields,
    - $Z(\mu) = \langle \det M(U,\mu) \rangle_G$ is real (see 2,3)

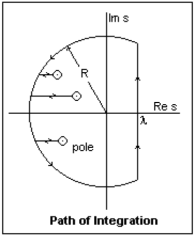
The sign problem

Complex μ: the canonical approach

$$\boxed{Z(\mu) = \langle \det\left[U_0 e^{\mu a} + U_0^{+} e^{-\mu a}\right]\rangle_G}$$ and $\det M = e^{Tr \ln M} \underbrace{\sim}_{aN_\tau = \beta} \left[\left(Tr \prod_\tau U_0^{\pm}\right) e^{\pm\beta\mu}\right]_\supset$

- Fugacity expansion (*Laurent expansion* in $\zeta = e^{\beta\mu}$)
  - $$\boxed{Z_{GC}(\mu) = \sum_{N=-\infty}^{\infty} (e^{\beta\mu})^N \cdot z_N}$$
  - $$\boxed{z_N = \oint \frac{d\zeta}{2\pi i} \frac{Z_{GC}(\zeta)}{\zeta^{N+1}}}$$ *(Cauchy's integral formula)*
- Canonical $Z_C(N) \equiv z_N$
  - $$\boxed{Z_C(N) = \oint \frac{\mathrm{d}(\beta\mu)}{2\pi i} Z_{GC}(\mu) \cdot e^{-(\beta\mu)\cdot N}}$$ *(Laplace tras.)*
- Thermodynamic definitions:
  - $Z_{GC}(\mu) = Tr[e^{-\beta(\widehat{H}_{QCD} - \mu\widehat{N})}]$ ("gran canonical")
  - $Z_C(N) = Tr[e^{-\beta\widehat{H}_{QCD}}\delta(\widehat{N} - N)]$ ("canonical")

$\beta\mu$ complex plan



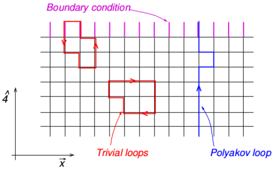
Note:

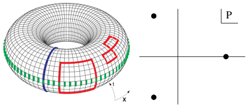
- $Z_{GC}(\mu)$ and $Z_C(N)$ share the same information (Laplace transforms)

Z_3 center symmetry

$$Z = \int \mathscr{D}U \underbrace{e^{\frac{\beta_G}{3}\sum_P \mathrm{ReTr}[\prod_P U]}}_{e^{-S_G} = gauge} \cdot \underbrace{\left(Tr\prod_\tau U_0^\pm\right) e^{\pm\beta\mu}}_{\det M = fermions}$$

- Center symmetry $U_0 \to \xi U_0$
  - $\boxed{\det = 1} \Longrightarrow \boxed{\xi^{N_c} = 1}$, i.e
    $\xi_k = e^{k\frac{2\pi i}{3}} = \{1, \frac{2\pi}{3}i, \frac{4\pi}{3}i\} \in Z_3$
- The "gauge part" is invariant
  - $\mathrm{Tr}[\prod_P U] \to \mathrm{Tr}[\prod_P U]$, $\mathscr{D}U \to \mathscr{D}U$
- The "fermion part" explicitly breaks
  - $P \sim Tr[\prod_\tau U_0]$ *(Polyakov loop)*
    - so $P \to \xi P$
- Order parameter
  - $\boxed{\langle P \rangle \neq 0 \Longrightarrow Z_3 \quad \text{broken}}$





Polyakov loop $P \sim Tr\prod U_0$

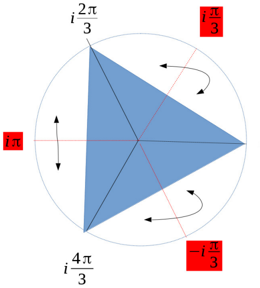
Note:

1. *In the SU(3) pure gauge, $\langle P \rangle \neq 0$ at high temperature, signalling the spontaneous symmetry breakdown of the Z_3 symmetry*

RW: the symmetry

$$\boxed{\det M = e^{Tr \ln M} \sim \left[Tr\left(\prod_{\tau} U_0 e^{+\beta\mu}\right) + h.c. \right]_{\supset}} \quad \text{and} \quad \boxed{Z = \langle \det M(U,\mu) \rangle_G}$$

- The Roberge-Weiss symmetry
  - if $U_0 \to e^{i\frac{2\pi}{3}k} U_0$ and $\beta\mu \to \beta\mu - i\frac{2\pi}{3}k$
    - $\boxed{Z(\beta\mu) = Z(\beta\mu - i\frac{2\pi}{3}k)}$
- Charge symmetry $\mu \to -\mu$
  - $Z(\mu) = Z(-\mu)$ is even
    - $\theta' = -\theta + k\frac{2\pi}{3} \implies \frac{\theta'+\theta}{2} = k\frac{\pi}{3}$.
    - Parity+Rotation=Reflection about $\theta = k\frac{\pi}{3}$
- If $P_{i\pi}(U) = P_{i\pi}(U^{\star})$
  - RW $\sim$ charge symmetry



$\beta\mu$ complex plane

Z_3 : effect on the spectrum

$$Z_{GC}(\mu) = \sum_{N=-\infty}^{\infty} (e^{\beta\mu})^N \cdot z_N$$

- Fact: if Z_3 is exact:
  - Under $\xi \in Z_3$, $z_N = \xi^N z_N$ so symmetry implies $z_N = 0$ if $N \; mod \; 3 \neq 0$
- At low temperature:
  1. Z_3 is exact,
  2. μ periodicity is "smoothly" realized
     - only $z_0, z_{\pm 3}, z_{\pm 6}, z_{\pm 9}, \ldots$ survives
     - mesons and baryons ($\Longrightarrow$*confinement*)
- At high temperature:
  1. Z_3 spontaneously broken,
  2. μ periodicity is realized in non-analytic way
     - every allowed: $z_0, z_{\pm 1}, z_{\pm 2}, z_{\pm 3} \ldots$
     - + free quarks and antiquarks ($\Longrightarrow$*deconfinement*)

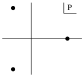
Conclusions:

- Writing $N = 3b + q$, with $q = N \; mod \; 3$, if Z_3 is exact, only the terms with $q = 0$ survives in the fugacity expansion $Z_{GC}(\mu) = \sum_b z_{3b} \cdot (e^{3\mu\beta})^b$. *b is the baryonic number B; $3\mu = \mu_B$ the baryonic chemical potential*

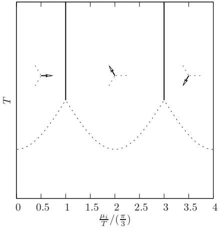
RW: phase transition

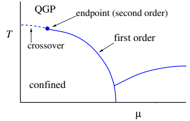
Hint, maximize: $\boxed{\det M \sim Re(P \cdot e^{\beta\mu})}$ $\sim$ Ising $\vec{s} \cdot \vec{H}$

- At high T
  - $\mu = 0$
    - the quark determinant favors the configurations with $\boxed{\arg P \approx 0}$.
  - $\mu\beta = \pm i2\pi/3$
    - $P \sim (e^{\beta\mu})^\star = e^{-\beta\mu} \Longrightarrow \boxed{\arg P \sim -\{\frac{2\pi}{3}, \frac{4\pi}{3}\}}$
  - P changes abruptly if $\mu\beta \in \{i\pi, -i\pi/3, i\pi/3\}$,
- At low T
  - At low temperatures the transition is smooth and we have a crossover (dashed lines)
- Order parameter: $\boxed{|Im(P)|}$
  - symmetric phase $= 0$
  - broken phase $\neq 0$



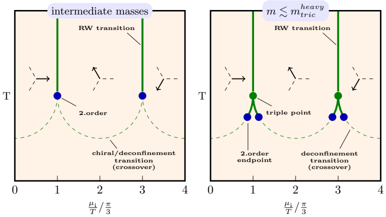
P orientation

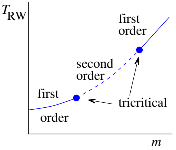


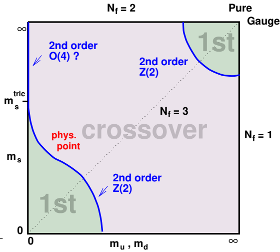


$$\frac{T(\mu)}{T_c} \approx 1 - b\mu^2 + c\mu^4 \ldots .$$

The aim of this work







- Numerical simulations have shown that Roberge-Weiss transition is first order for large masses (*quenched limit*), second order for intermediate masses, and again first order when masses are small (*chiral limit*).
  - The nature of the endpoints is not-trivial and depends on N_f and fermion mass
  - Detailed studies exist only for the cases $N_f = 2$ and $N_f = 2{+}1$
  - The Gell-mann-Low RG function $\beta(g)$, on which important QCD properties - as the *asymptotic freedom* - are based, depends crucially on the number of flavors N_f. In particular, for N_f larger then $33/2$, the confinement property could change and the phase transition could become weaker or disappear too.

Aim:

- To extend the simulations to other combinations of masses and flavors, in order to confirm that as a general behavior

Simulation setup

Conf:

N_f	am_q	N_τ	N_s	$\frac{\mu}{T}$	samples	therm.	jackknife	betastep
8	0.2	4	12,16,20	$i\pi$	15000	1000	300	0.001

- Order parameter
  - $|Im(P)|$
- Imaginary chemical potential:
  - $\boxed{\beta\mu = i\pi}$
- Temperature tuned with the inverse gauge coupling $\beta_G = \frac{6}{g^2}$
  - $(4.940, 4.960, 4.980, 4.985, 4.990, 5.000, 5.020)$

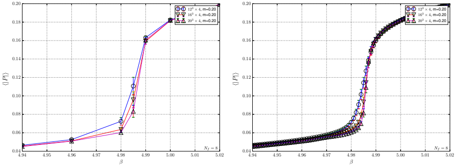
SW+HW

- Zephiro cluster (9 GPU) at INFN Pisa
- C++ CUDA RHMC

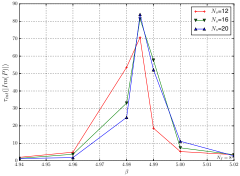
Numerical tools

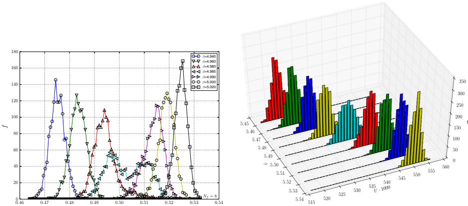
- Multi-histogram re-weighting
  - $\langle O \rangle = \frac{\sum w \cdot O}{\sum w} = \frac{\sum r \frac{w}{r} \cdot O}{\sum r \frac{w}{r}} = \frac{\langle \frac{w}{r} \cdot O \rangle_r}{\langle \frac{w}{r} \rangle_r}$
  - The method is successful, as long there is a good overlapping between the plaquette energy histograms, and especially in the critical region
- Jackknife resampling
  - accounting correlations
  - variance error estimates
  - $\tau_{int} = \frac{1}{2} + \sum_{n=0}^{\infty} c(n \cdot \Delta\tau)$
  - $N_{eff} \approx \frac{N}{2\tau_{int}}$ (slowing down)

reweighting example



τ_{int}

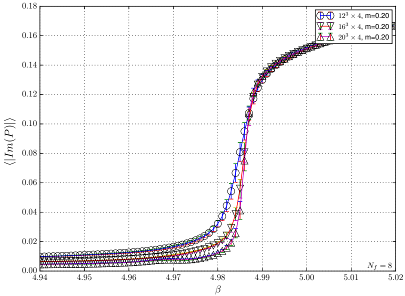


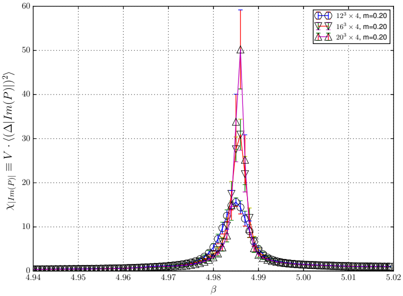


plaquette histogram

Order parameter: Polyakov loop

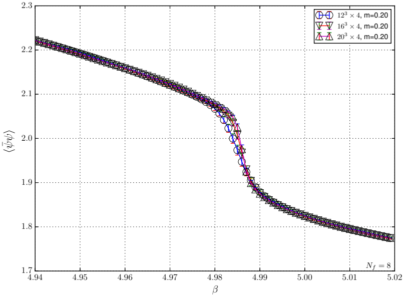
- Polyakov loop
  - $$P = \frac{1}{V}\sum_{\mathbf{x}} \frac{1}{N_c} Tr_c \prod_{\tau=0}^{N_\tau - 1} U_0(\tau, \mathbf{x})$$
    - Low T: $\langle ImP \rangle = 0$ (Z_3 *restored*)
    - High T: $\langle ImP \rangle \neq 0$ (Z_3 *broken*)
- Polyakov loop susceptibilty
  - $$\chi = V\langle(\delta|Im(P)|)^2\rangle$$
    - χ at crititical point $\Longrightarrow$ peak

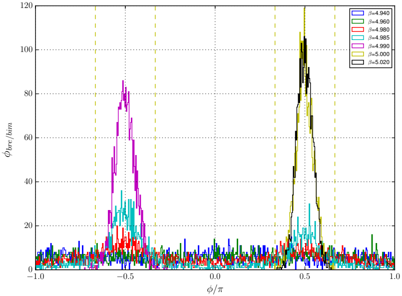




Fermionic measures

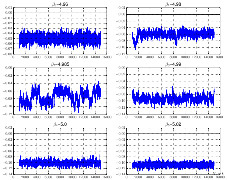
- Chiral condensate (*left plot*)
  - $\langle\overline{\Psi}\Psi\rangle = -\frac{\partial \ln Z_{GC}}{\partial m} = -\frac{N_f}{N_\tau N_s^3}\langle Tr[\frac{1}{M}]\rangle_G$
    - high T $\Longrightarrow$ chiral sym. restored
- Quark number (*right plot*)
  - $Z(\beta\mu)$ is even $\Longrightarrow \langle N\rangle(\beta\mu)$ is odd
  - $\langle N\rangle = \frac{\partial \ln Z_{GC}(\beta\mu)}{\partial\beta\mu} = a(\beta\mu) + b(\beta\mu)^3 + \ldots$
    - $\langle N\rangle \sim \beta\mu$ purely imaginary

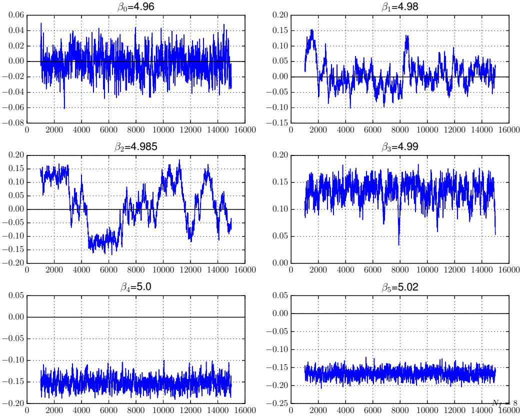




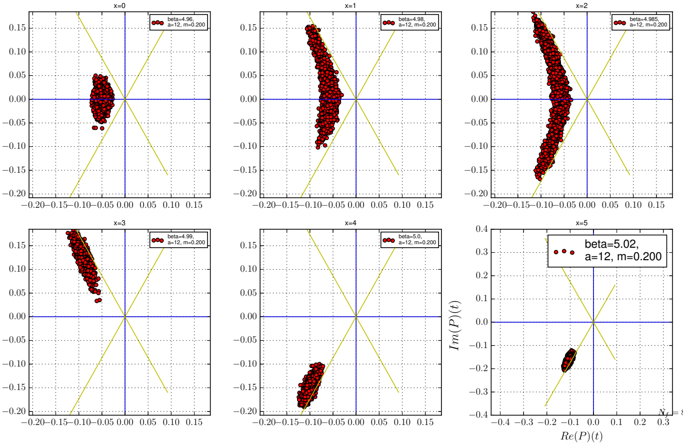
Time series

Time series for $Im(P)$ and $Re(P)$ (Polyakov loop)

- imaginary chemical potential: $\boxed{\beta\mu = i\pi}$
- metastabilities clearly detectable $\beta_G \sim 4.98 - 4.99$
- below the transition point $\langle Im(P) \rangle = 0$; above it, P select two opposite directions in the complex plane.
- Left: $Re(P)$; Right: $Im(P)$
- 

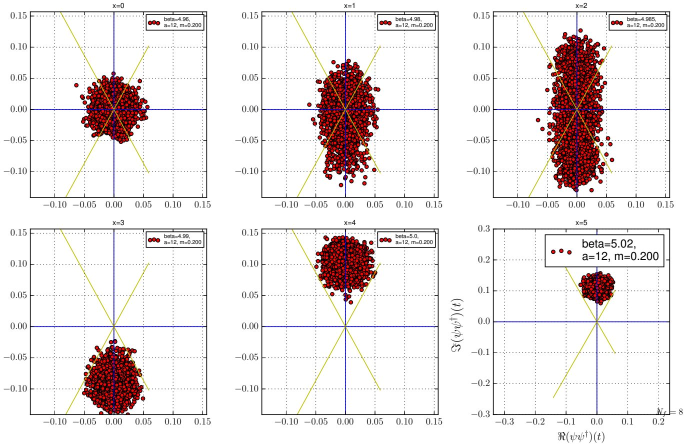


Scatter plots: Polyakov loop, $P = (P_x, P_y)$



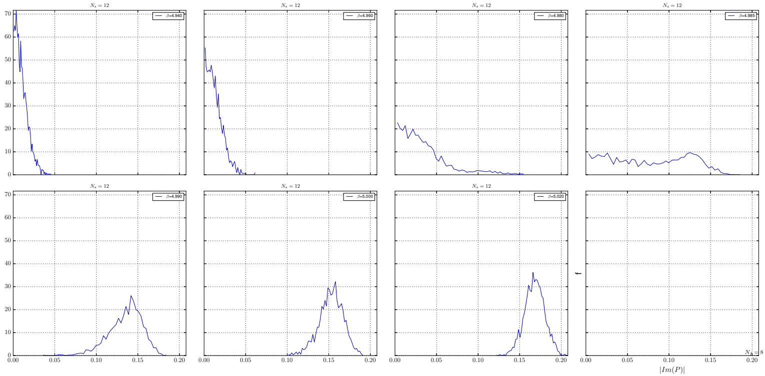
The Polyakov loop P distribution in the complex plane, at imaginary chemical potential. At low temperatures, $\langle Im(P) \rangle = 0$. At high temperature, P aligns with a direction $e^{i2\pi k/3}$, where $k \bmod 3 \neq 0$

Scatter plots: quark Number, $N = (N_x, N_y)$



Quark number $N = \psi^\star \psi$
distribution in the complex plane, at imaginary chemical potential.
$\langle N \rangle \sim \beta\mu$ *is purely imaginary.*

Distribution probability, $|Im(P)|$



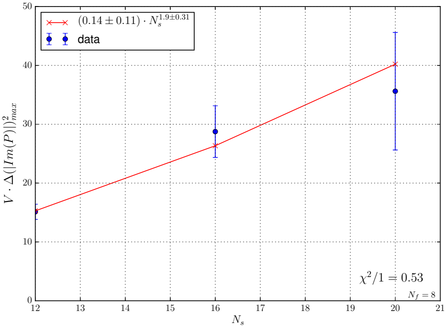
$|Im(P)|$

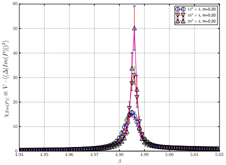
histogram distribution of the absolute value of the imaginary part of the Polyakov, $N_s = 12$

The figure shows a typical histogram of the distribution probability $P(|Im(P)|)$ across a second-order transition (from left to right and top to bottom). The top left graph corresponds to the *ordered phase*, with a single peak at $|Im(P)| = 0$. As the value of T is increased, this peak moves toward to $||Im(P)|| \neq 0$ and no other peak arises.

Finite Size Scaling (FSS)

- Scaling laws:
  - $\chi \sim t^{-\gamma}$ and $\xi \sim t^{-\nu}$, $t = (T - T_c)/T_c$
    - $\chi \sim \xi^{\gamma/\nu}$
  - at the pseudo critital point: $\xi_{peak} \sim N_s$
    - so $\boxed{\chi_{peak} \sim N_s^{\gamma/\nu}}$
  - least-square fit $\chi = a \cdot N_s^b$, to find $\boxed{b = \gamma/\nu}$.

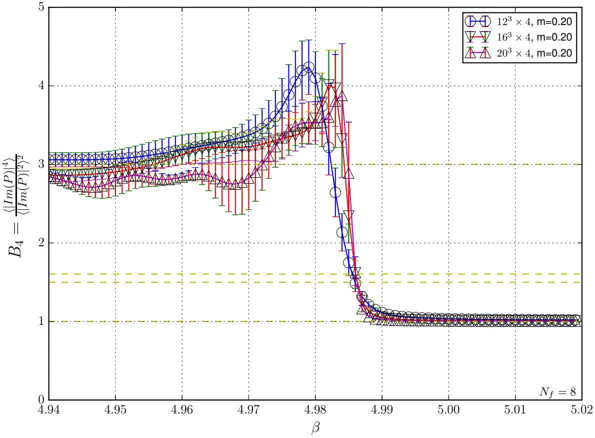




Result: $\gamma/\nu = 1.9 \pm 0.3$, compatible with $\gamma/\nu = 1.964$, corresponding to the 3D Ising universal class (a second order transition)

Binder cumulant B_4

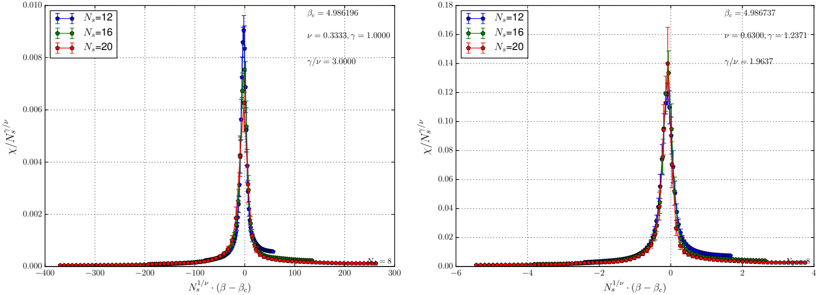
- $B_4 = \frac{\langle \delta x^4 \rangle}{(\langle \delta x^2 \rangle)^2}$ with $x = |Im(P)|$
  - $B_4 = 3$ single gaussian (*symmetric phase*)
  - $B_4 = 1$ double gaussian (*crossover*)



The B_4, at various N_s, should cross at the pseudo-critical point

Collapse plot ($|Im(P)|$)

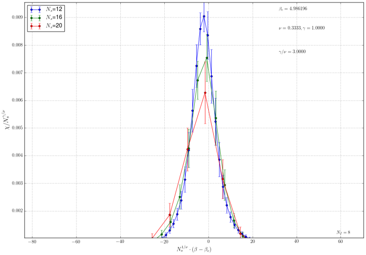
- $\boxed{\chi \sim N_s^{\gamma/\nu} f((\beta - \beta_{RW}) \cdot N_s^{1/\nu})}$ with $f(x)$ universal function
  - on the left (1th order: $\gamma = 1, \nu = 1/3$)
  - on the right (2th order 3D Ising: $\gamma = 1.2372, \nu = 0.63$)

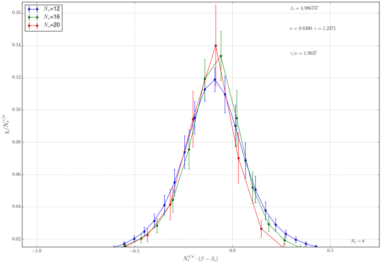


Better overlapping for 2th order, $\beta_{RW} = 4.986$

Collapse plot: zoom

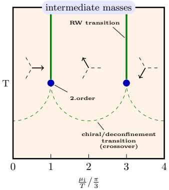
- zoom
  - on the left (1th order: $\gamma = 1, \nu = 1/3$)
  - on the right (2th order 3D Ising: $\gamma = 1.2372, \nu = 0.63$)

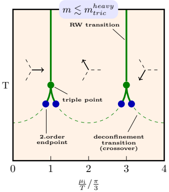


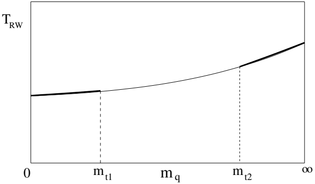


Better overlapping for 2th order, $\beta_{RW} = 4.986$

Conclusions and outlook







- We have presented the case $N_f = 8$ with $am_q = 0.2$ and imaginary chemical potential $\mu = i\pi T$ (Roberge-Weiss line)
- The result show that, for $am_q = 0.2$, the endpoint for $N_f = 8$ and $N_f = 4$ is still 2th order, so $m_{t1} < m_q < m_{t2}$

NF	m	β_{RW}	order
4	m=0.09	5.175	1th
4	m=0.20	5.310	2th
4	m=0.50	5.497	2th
8	m=0.20	4.987	2th

Next:

- To complete the case $N_f = 8$ for other masses, with a new estimate for $m_1(N_f)$ and $m_2(N_f)$.
- To explore higher values for N_f (for example: the region $N_f > 33/2$)

Thank You for the attention!

References

Tantau, Till et al.:
The beamer class. http://mirrors.ctan.org/macros/latex/contrib/beamer/doc/beameruserguide.pdf.

data

NF	m	range β	β_{RW}	order	O
2	m=0.025		5.338	1th	D
2	m=0.075		5.394	2th	D
4	m=0.090	5.14-5.22	5.175	1th	M
4	m=0.200	5,28-5.35	5.310	2th	M
4	m=0.500	5.46-5.54	5.497	2th	M
8	m=0.200	4.94-5.02	4.987	2th	M