Lattice QCD simulations with external backgrounds

Massimo D'Elia

University of Pisa & INFN

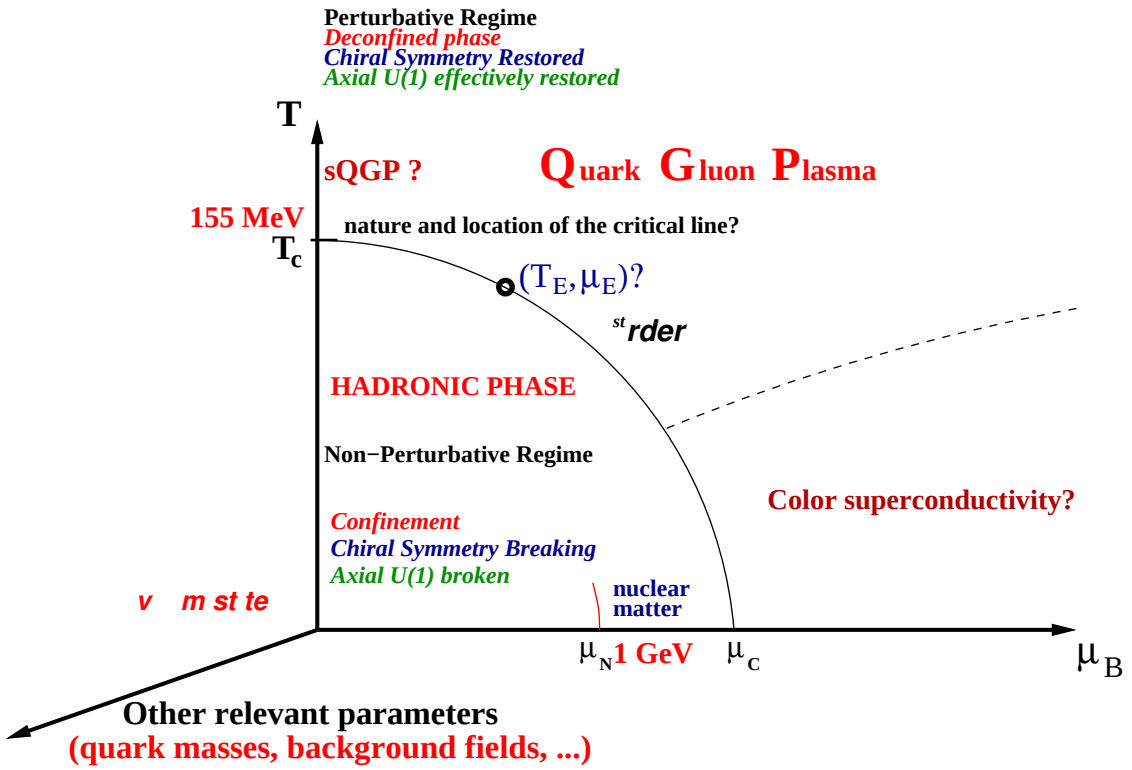
Mini-Workshop on Lattice and Functional Techniques for Exploration of Phase Structure and Trasport Properties in Quantum Chromodynamics - Dubna, July 10 - 14, 2017

OUTLINE (I + II)

- **Lattice QCD in magnetic background fields:**
  - $\surd$ **General properties**
  - $\surd$ **$Q\bar{Q}$ interactions in a strong magnetic background**
  - $\surd$ **Effects on color flux tubes**
  - **– New phases for compactified $SU(N)$ gauge theories in a magnetic background**

- **Lattice QCD with imaginary chemical potentials:**
  - **– General properties and the curvature of the pseudocritical line**
  - **– Generalized susceptibities from imaginary chemical potentials**
  - **– Discussion on the possible location of the critical point**

The QCD phase diagram: not just temperature ...



What we would like to know:

- Location and nature of deconfinement/chiral symmetry restoration as a function of other external parameters (μ_B, external fields, ...)
- Properties of the various phases of strongly interacting matter
- Critical endpoint at finite μ_B?

Problems in lattice QCD at $\mu_B \neq 0$

$$Z(\mu_B, T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}} - \mu_B N_B}{T}}\right) = \int \mathcal{D}U e^{-S_G[U]} \det M[U, \mu_B]$$

$\det M[\mu_B]$ **complex** $\Longrightarrow$ **Monte Carlo simulations are not feasibile.**

By now, we can rely on a few approximate methods, viable only for small μ_B/T, like

- **Taylor expansion of physical quantities around $\mu = 0$**

  Bielefeld-Swansea collaboration 2002; R. Gavai, S. Gupta 2003

- **Reweighting (complex phase moved from the measure to observables)**

  Barbour et al. 1998; Z. Fodor and S, Katz, 2002

- **Simulations at imaginary chemical potentials (plus analytic continuation)**

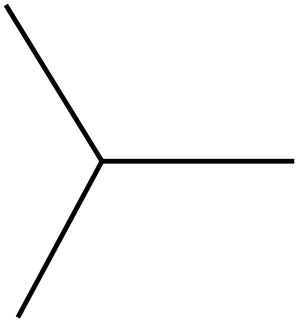
  Alford, Kapustin, Wilczek, 1999; Lombardo, 2000; de Forcrand, Philipsen, 2002; MD, Lombardo 2003.

Others are being developed but still not fully operative (Langevin simulations, density of states, Lefschetz thimble, rewriting the partition function in terms of dual variables, ...)

In alternative: canonical approach (see talks by Atsushi, Vitaliy)

I will discuss some results from simulations at imaginary μ

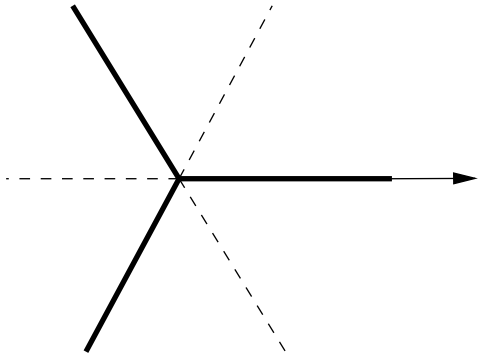
Let us remember the interesting things happening in the T imaginary chemical potential plane, in connection with the realization of center symmetry. Imaginary $\mu = i\mu_I$ rotates fermion temporal b.c. by μ_I/T



Pure gauge theory

Exact Z_3 center symmetry

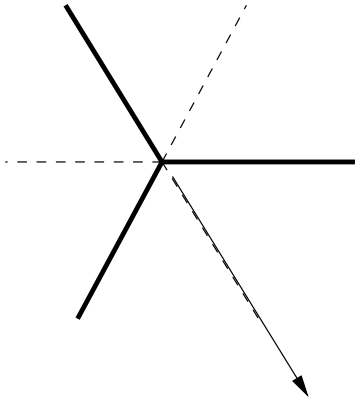
Spontaneously broken at $T > T_c$



Full QCD, $\mu = 0$

Determinant couples to holonomy

Its trace is always real



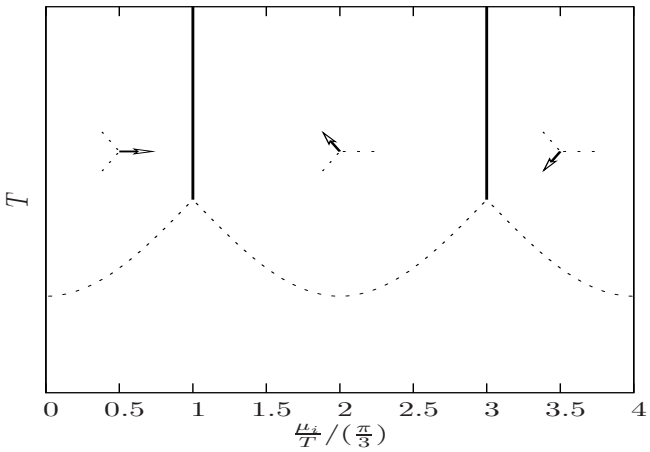
Full QCD, $\theta_I \equiv \mu_I/T \neq 0$

Determinant couples to holonomy * $e^{i\theta_I}$

Minimum for the holonomy rotates with θ_I

At high T, the absolute minimum is decided by $\theta_I \implies$ appearance of Roberge-Weiss transitions as a function of θ_I (one every $2\pi/N_c$ interval)

This is true only for degenerate quark chemical potentials, otherwise competing influences, first RW can move farther or disappear



Continuation to real μ is conceivable for quantities with an expected analytic behavior around $\mu = 0$

An example is the dependence of T_c on μ_B:

$$\frac{T(\mu_B)}{T_c} \simeq 1 - \kappa \left(\frac{\mu_B}{T(\mu_B)} \right)^2 = 1 - 9\kappa \left(\frac{\mu}{T(\mu)} \right)^2$$

μ is the quark chemical potential, κ is the curvature of the pseudo-critical line at $\mu_B = 0$ and can be obtained either by Taylor expansion technique or by numerical simulations at imaginary μ_B, assuming analyticity around $\mu_B = 0$:

$$\frac{T(\mu_I)}{T_c} \simeq 1 + 9\kappa \left(\frac{\mu_I}{T(\mu_I)} \right)^2$$

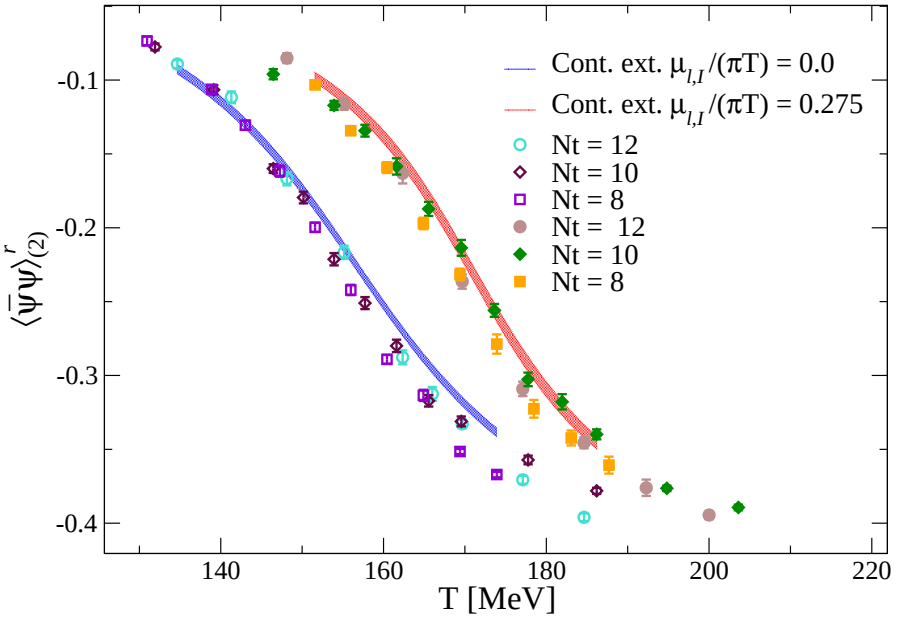
In the imaginary chemical potential approach, T_c is computed as a function of μ_I from various quantities

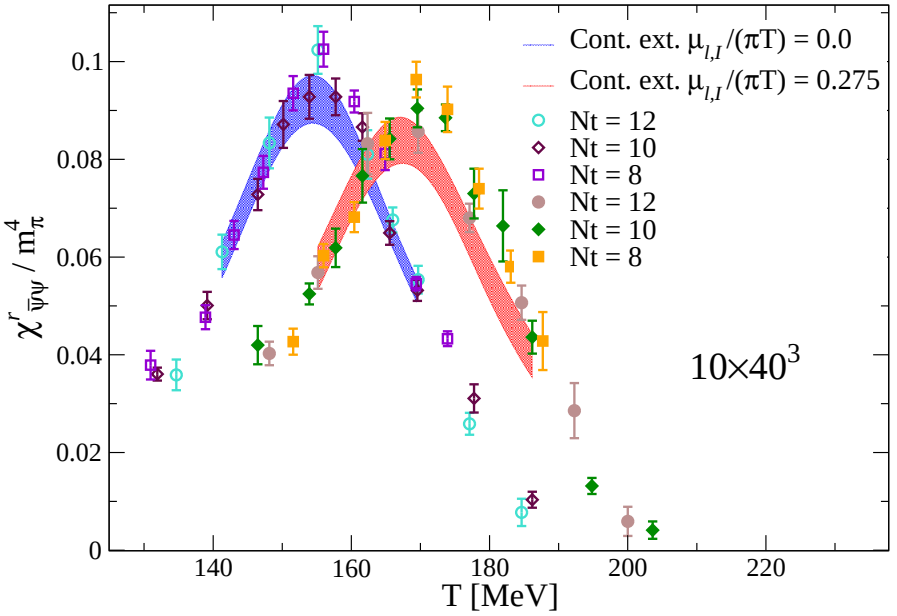
We (Bonati et al., arXiv:1507.03571) consider in particular the chiral condensate and its susceptibility as probes for the location of the pseudo-critical temperature:

$$\langle \bar{\psi}\psi_f \rangle = \frac{T}{V}\frac{\partial \log Z}{\partial m_f} \qquad \chi^f_{\bar{\psi}\psi} = \frac{\partial \langle \bar{\psi}\psi_f \rangle}{\partial m_f} = \chi^{disc}_{\bar{\psi}\psi} + \chi^{conn}_{\bar{\psi}\psi}$$

$$\chi^{disc}_{\bar{\psi}\psi} \equiv \frac{T}{V}\left(\frac{N_f}{4}\right)^2 \left[\langle (\mathrm{tr} M_f^{-1})^2 \rangle - \langle \mathrm{tr} M_f^{-1} \rangle^2\right] \qquad \chi^{conn}_{\bar{\psi}\psi} \equiv -\frac{T}{V}\frac{N_f}{4}\langle \mathrm{tr} M_f^{-2} \rangle \, .$$

which are then properly renormalized by subtracting $T = 0$ expectations values.





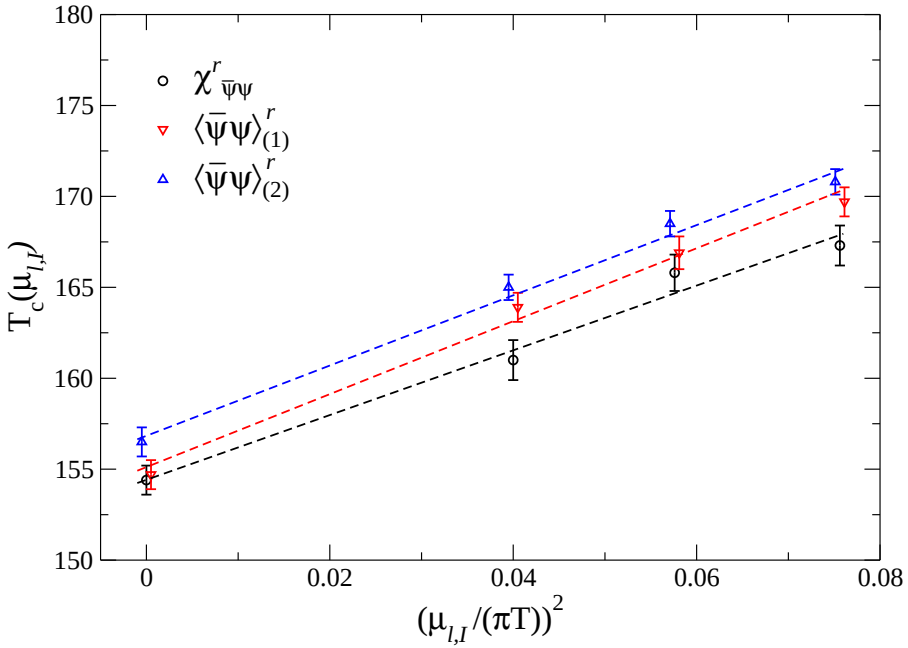
chiral condensate **chiral susceptibility**

Localizing the pseudocritical temperature for various imaginary chemical potentials from various observables (continuum extrapolation)

(results from Bonati et al., arXiv:1507.03571)

then, assuming analyticity, κ is extracted by fitting a linear dependence in μ_I^2 for small μ_I.

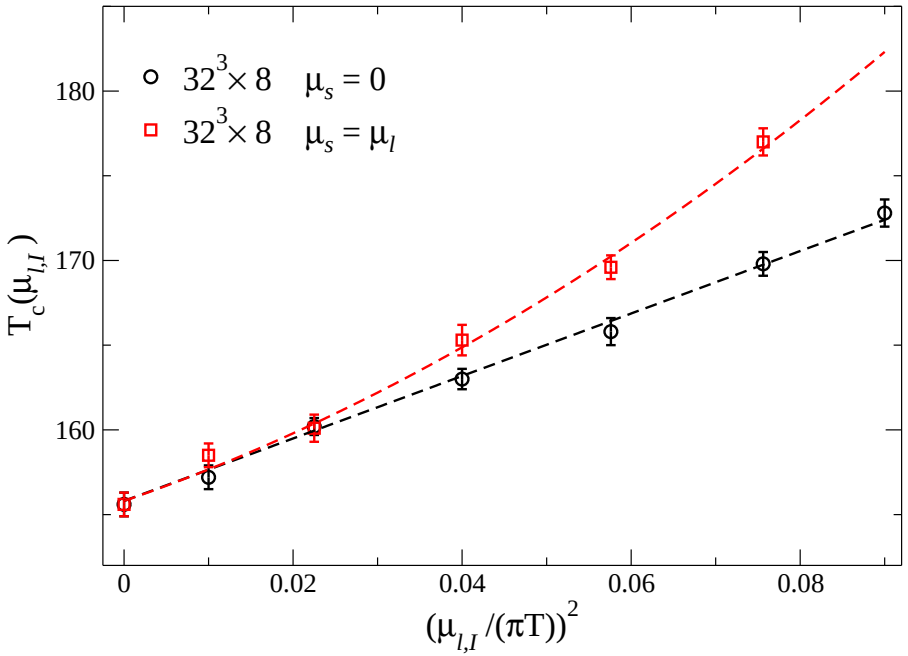
T_c location depends on the observable, slope in μ_I^2 is much less sensitive



Results obtained for $\mu_u = \mu_d = \mu_l;\ \ \mu_s = 0$

Comparison with $m_{u_s} = \mu_u = \mu_d = \mu_l$ shows deviations, but limited to higher order terms in μ^2, curvature is unaffected

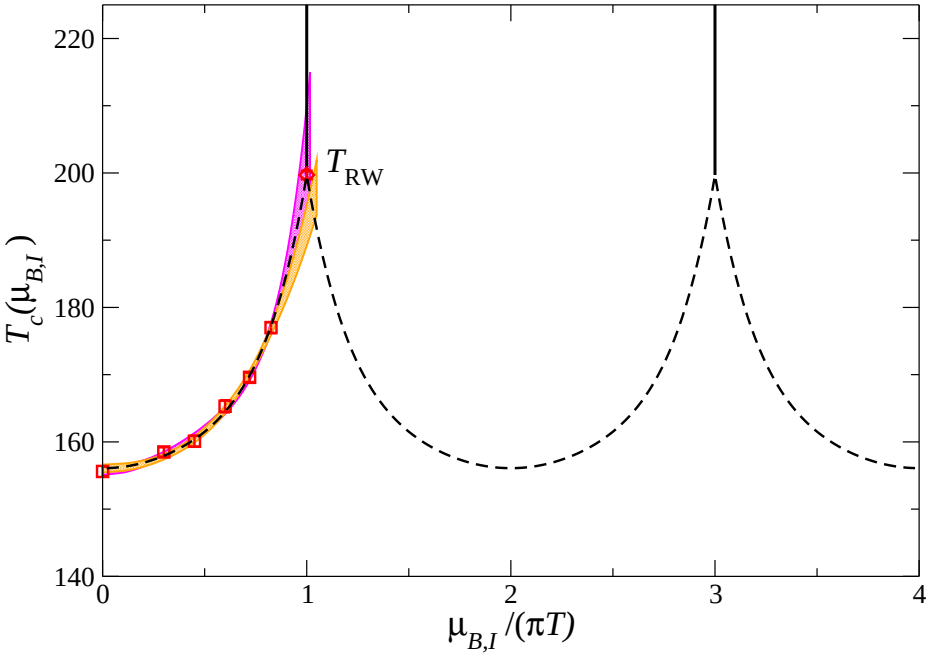
Experimental conditions: $\mu_s \sim 0.25\mu_l$ (to ensure strangeness neutrality)



Non-linear terms for $\mu_s = \mu_l$ likely due to the nearby presence of the Roberge-Weiss endpoint.

T_{RW} quite large at the physical point, $T_{RW}/T_c = 1.34(7)$

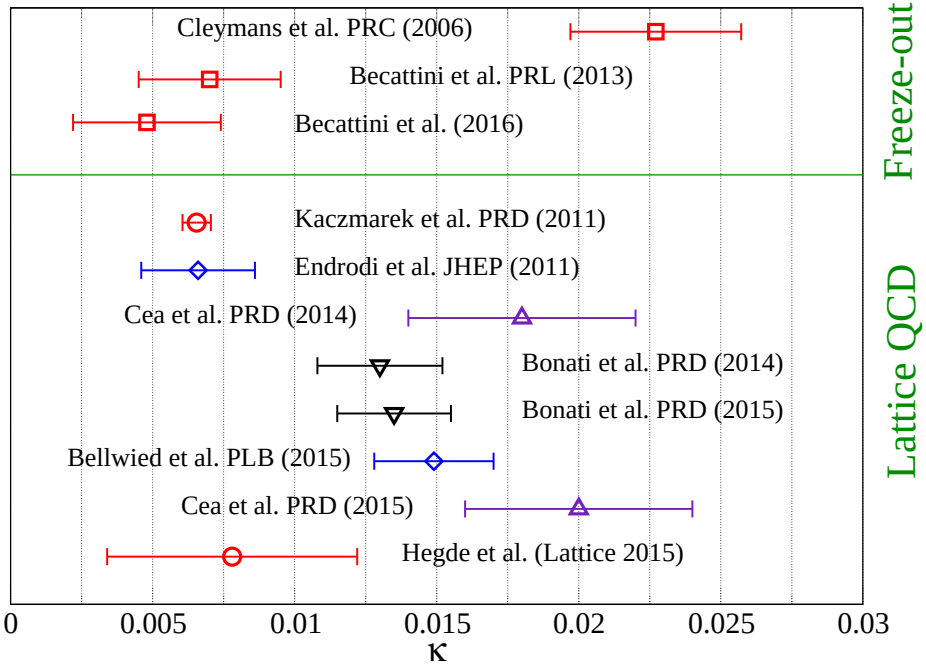
(Bonati, MD, Mariti, Mesiti, Negro, Sanfilippo, arXiv:1602.01426)



The curvature of the pseudo-critical line: various lattice determinations and comparison with freeze-out

Convergence of most recent results indicates good control over possible systematic effects.

Slight tension between Taylor expansion and analytic continuation is being clarified



Analytic continuation reveals a powerful tool also for the determination of generalized susceptibilities:

$$F(T,V,\mu_u,\mu_d,\mu_s) = F(T,V,0) + VT^4 \sum_{i+j+k=even} \frac{\chi_{ijk}(T)}{i!j!k!} \hat{\mu}_u^{(i)} \hat{\mu}_d^{(j)} \hat{\mu}_s^{(k)}$$

where V is the spatial volume, $\hat{\mu}_q \equiv \mu_q/T$ and odd monomials are zero due to the symmetry under charge conjugation of the theory at zero chemical potentials. The coefficients

$$\chi_{ijk}(T) = \frac{1}{VT^4} \frac{\partial^{(i+j+k)} F(T,\mu)}{\partial\hat{\mu}_u^{(i)} \partial\hat{\mu}_d^{(j)} \partial\hat{\mu}_s^{(k)}} \Bigg|_{\mu_u=\mu_d=\mu_s=0}$$

where μ_i are quark number chemical potentials. They can be linked to fluctuations of conserved charges through the relations

$$\begin{aligned} \mu_u &= \mu_B/3 + 2\mu_Q/3 \\ \mu_d &= \mu_B/3 - \mu_Q/3 \\ \mu_s &= \mu_B/3 - \mu_Q/3 - \mu_S \,. \end{aligned}$$

Usually quite difficult to go to high orders: subtraction of many terms in the computation, large fluctuations in higher order correlations

Possible idea to improve

Determines the generalized susceptibilities up to a given order $i+j+k$ as a function of the imaginary chemical potentials

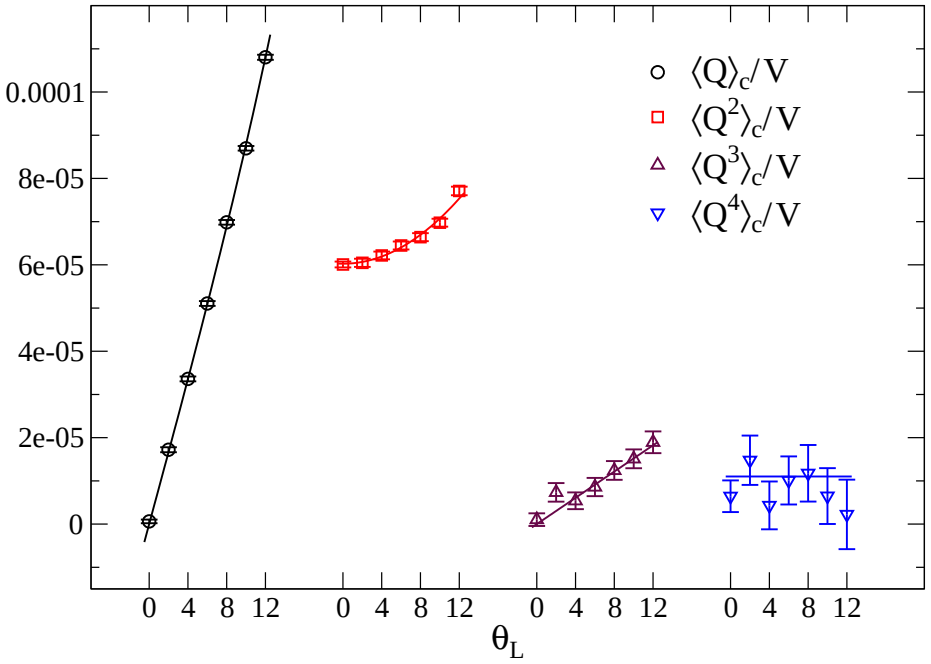
$$\chi_{ijk}(\mu_u,\mu_d,\mu_s) = \sum_{\substack{l=i\\m=j\\n=k}}^{\infty} \frac{\chi_{lmn}(0,0,0)\,\hat{\mu}_u^{l-i}\hat{\mu}_d^{m-j}\hat{\mu}_s^{n-k}}{(l-i)!(m-j)!(n-k)!}$$

From a global fit of their dependence on μ_u, μ_d, μ_s, one extracts the higher order susceptibilities.

The idea is not new (MD, Lombardo, 2002; MD, Sanfilippo, 2009, de Forcrand, Takahashi, 2009; Bellwied et al., 2016; see also talk by Vitaliy)

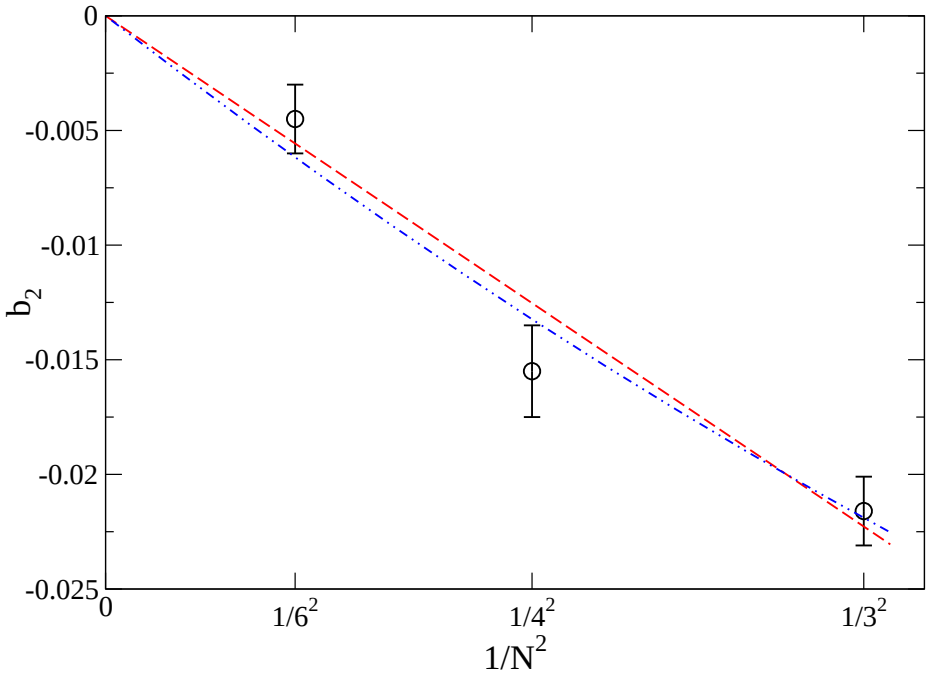
Major bonus wrt determination at $\mu = 0$: one determines directly the response to an external source instead than a fluctuation, signal-to-noise improves dramatically.

The same idea applies to the study of θ dependence: the dependence of lower order cumulants on imaginary θ allows a determination of larger order cumulants



This has recently allowed to check the predicted large N behavior of the fourth order cumulant in pure gauge $SU(N)$:

$$b_2 \propto 1/N^2$$



A priori a very difficult task! A vanishing signal drowning in a Gaussian sea

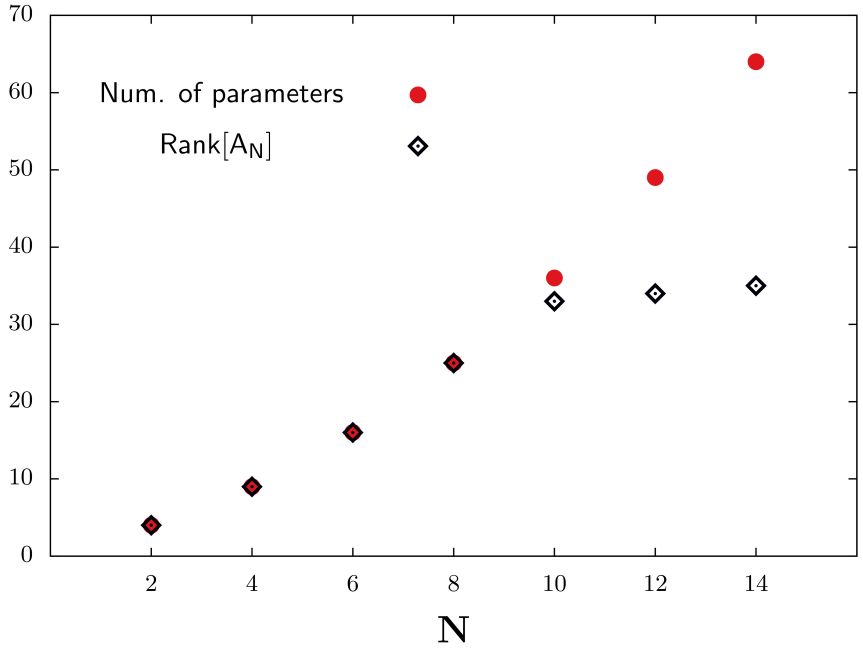
(Bonati, MD, Scapellato, arXiv:1512.01544; Bonati, MD, Rossi, Vicari, arXiv:1607.06360)

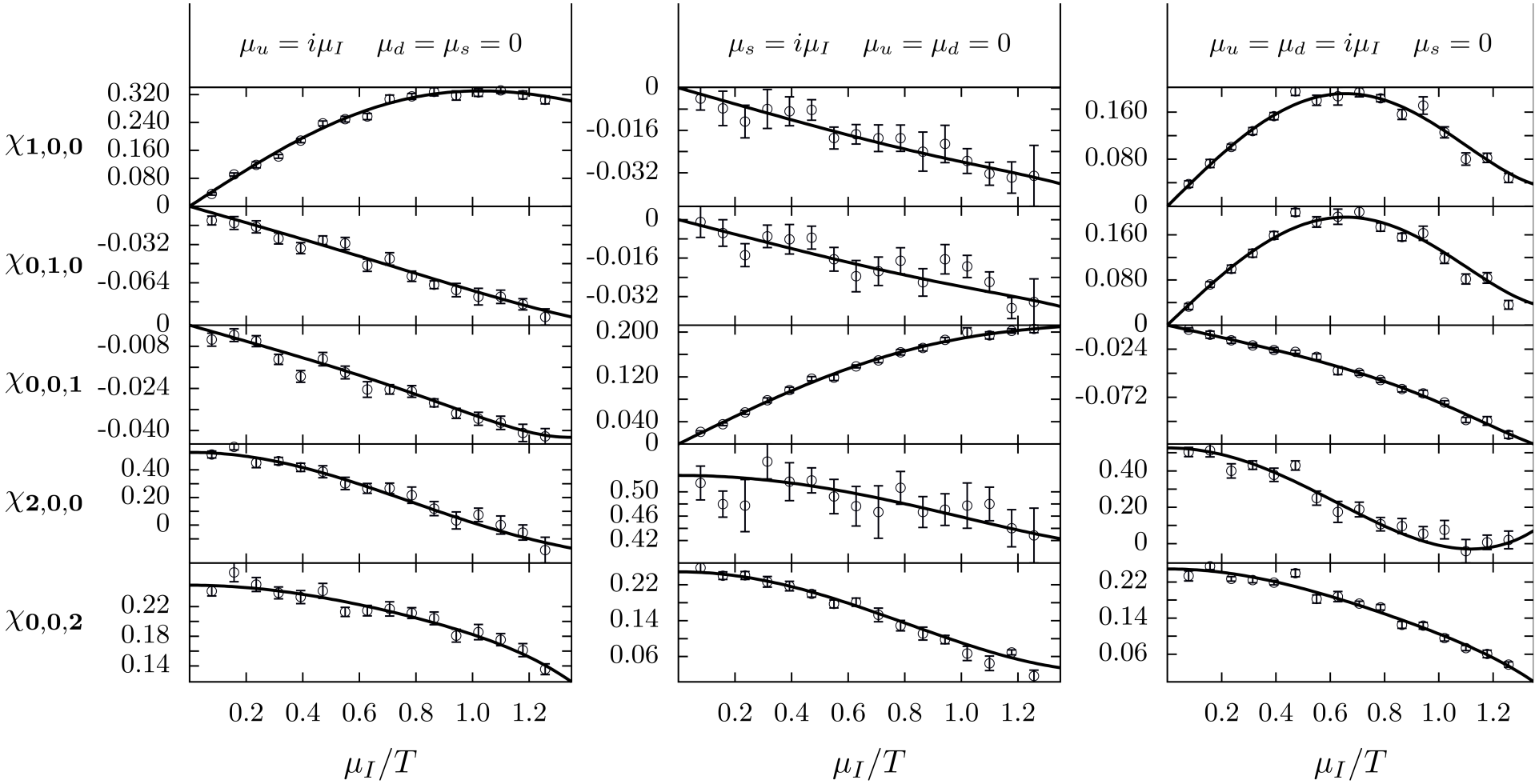
We have tried to apply this idea to $N_f = 2{+}1$ QCD, with the idea of a full determination of all susceptibilities up to a given order (Gagliardi, M., Sanfilippo, 1611.08285, physical point)

We have 3 different flavors, do we need $O(10) \times O(10) \times O(10) \sim O(10^3)$ different simulations?

If we need susceptibilities up to a given order, just points on a few lines suffice. With 6 lines ($6 \times O(10)$ simulations) we can determine everything up to order 8).

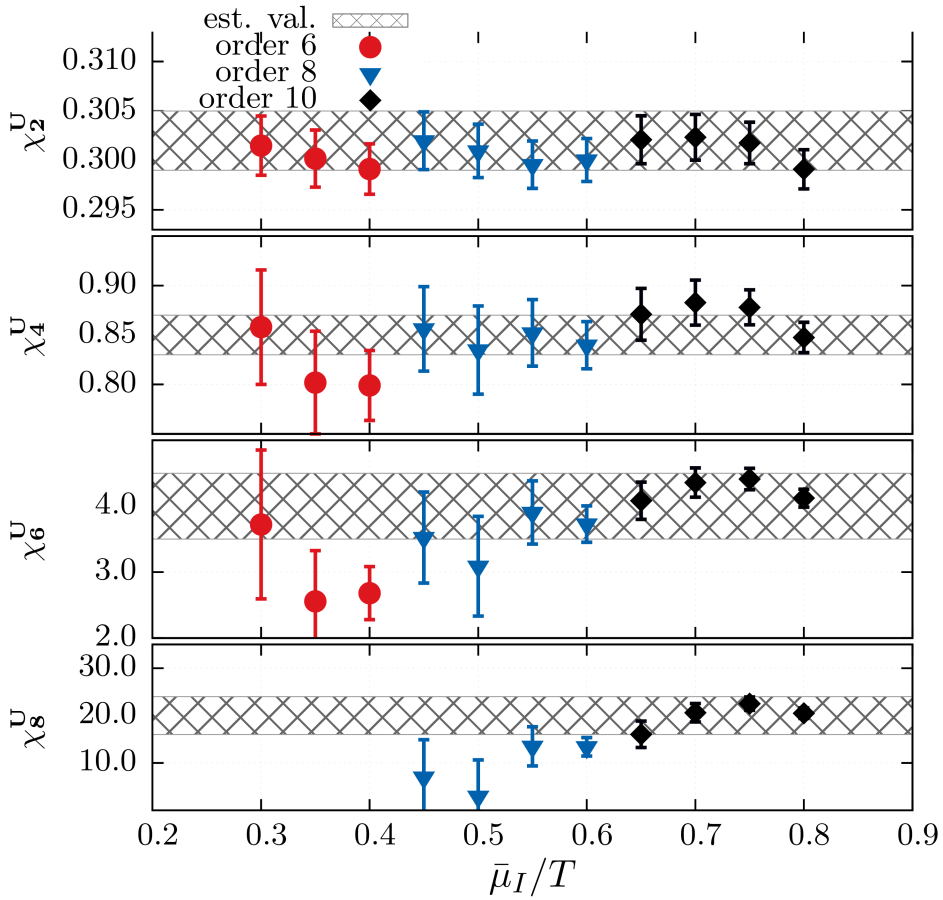
$$
\begin{aligned}
(\mu_u,\ \mu_d,\ \mu_s) &= (i\mu_I,\ \ 0,\ \ 0) \\
(\mu_u,\ \mu_d,\ \mu_s) &= (\ 0,\ \ 0,\ i\mu_I) \\
(\mu_u,\ \mu_d,\ \mu_s) &= (i\mu_I,\ \ i\mu_I,\ \ 0) \\
(\mu_u,\ \mu_d,\ \mu_s) &= (i\mu_I, -i\mu_I,\ \ 0) \\
(\mu_u,\ \mu_d,\ \mu_s) &= (i\mu_I,\ \ i\mu_I,\ \ i\mu_I) \\
(\mu_u,\ \mu_d,\ \mu_s) &= (i\mu_I, -i\mu_I,\ \ i\mu_I)
\end{aligned}
$$





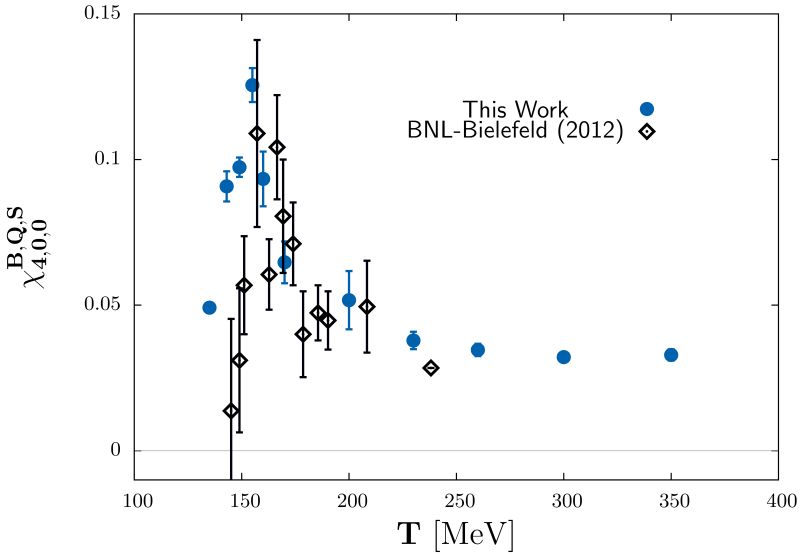
Gagliardi, M., Sanfilippo, 1611.08285, physical point of $N_f = 2 + 1$ QCD, only $N_t = 8$ by now

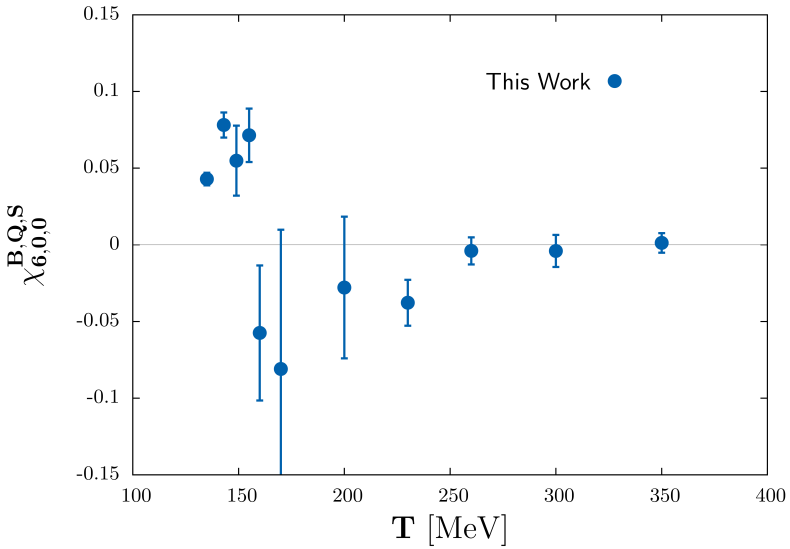
Optimal choice seems a direct determination and fit of all cumulants up to order 2



There is of course a drawback to pay: the fit involves arbitrariness in the fitting polynomial and in the fitted range.

Systematic effects must be carefully checked

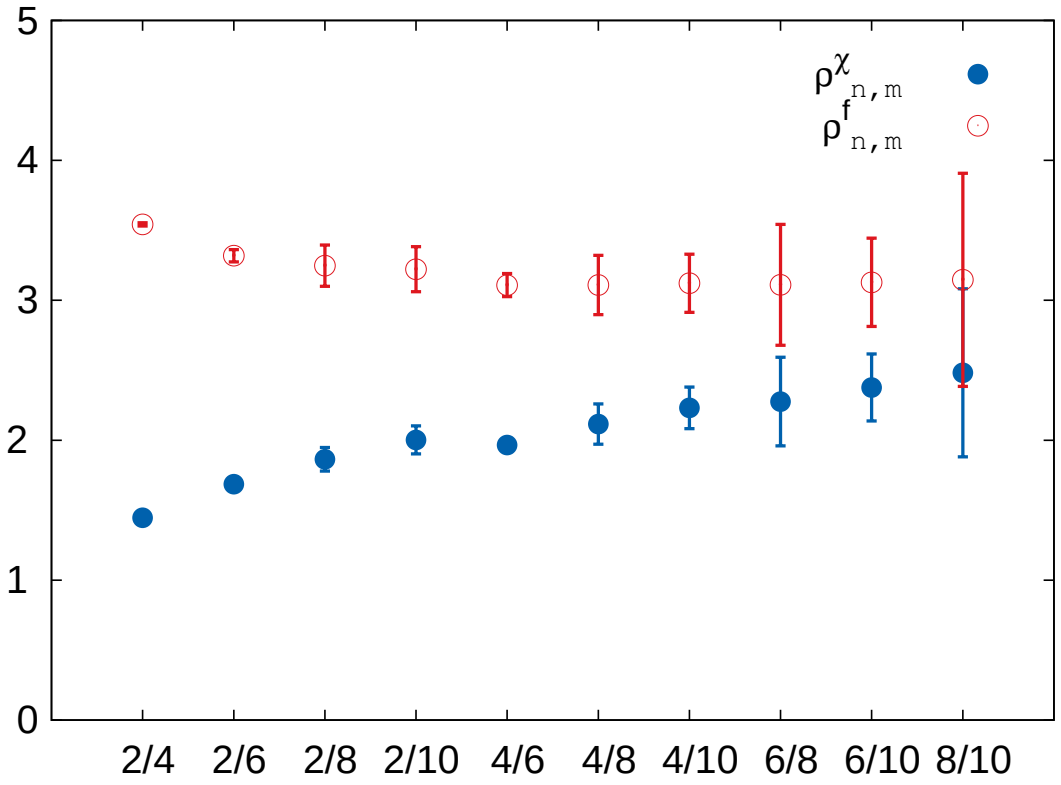




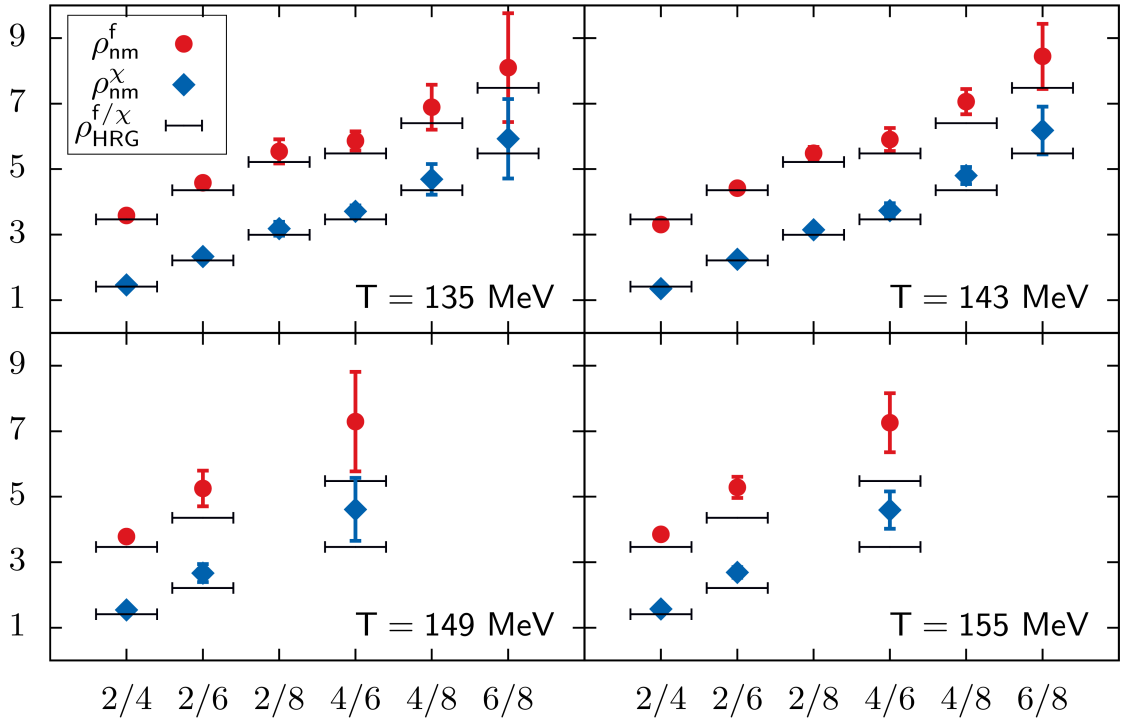
from them we can reconstruct the free energy dependence and extract estimates of the radius of convergence of the various terms

$$\mathcal{F}(T,\mu_B) = \mathcal{F}(T,0) + VT^4 \sum_n \frac{\chi^B_{2n}}{(2n)!} \left(\mu_B/T\right)^{2n}$$

$$\rho^f_{n,m} = \left(\frac{\chi^B_n/n!}{\chi^B_m/m!}\right)^{\frac{1}{(m-n)}} \qquad \rho^\chi_{n,m} = \left(\frac{\chi^B_n/(n-2)!}{\chi^B_m/(m-2)!}\right)^{\frac{1}{(m-n)}}$$

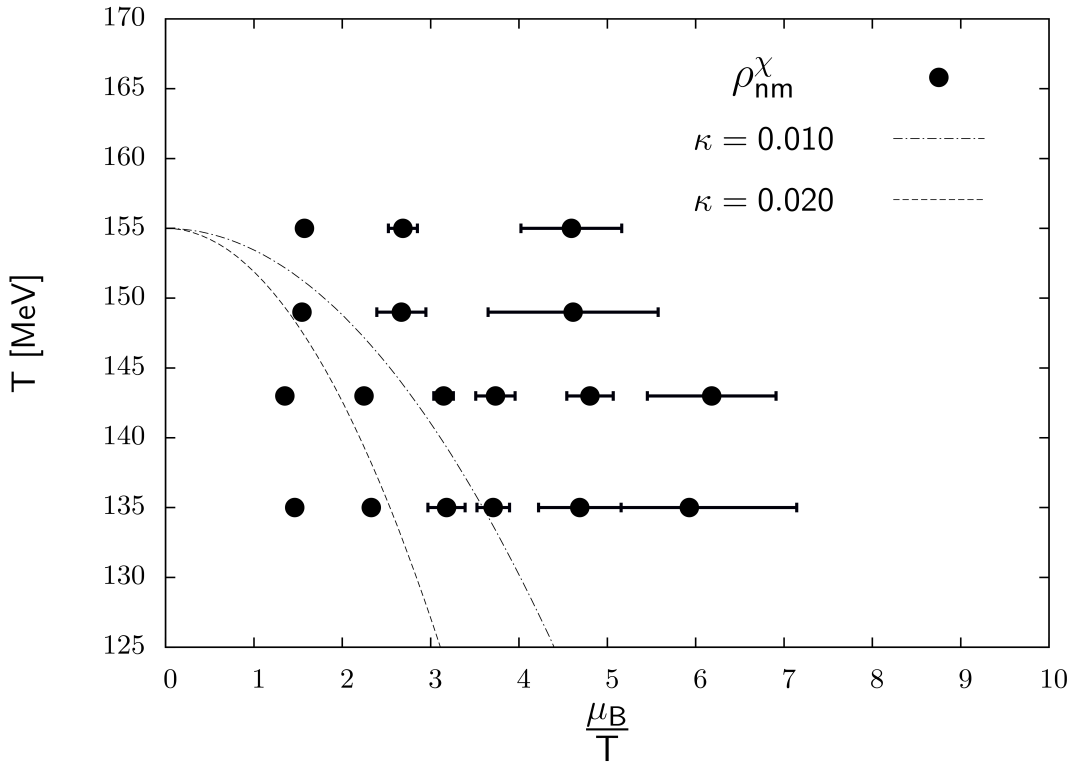


Such a game works well when applied to synthetic functions, e.g. $F = (\mu_B - 2.5)^{0.5}$ **in the figure**



"no-convergence" for the radius of convergence in QCD with $N_f = 2 + 1$ flavors

Data are compared to predictions of the same quantities from the Hadron Resonance Gas model



in particular, the possible critical point seems confined well beyond the pseudo-critical line ...

similar results obtained by A. Bazavov et al., 1701.04325

CONCLUSIONS (maybe)

- **We have good control over the small $\mu_B/$ properties of the QCD phase diagram. Simulations at imaginary μ are a valuable tool to achieve that.**

- **Large μ_B properties, including the possible location/existence of the critical endpoint, are still affected by large systematic uncertainties**

- **At this point, assuming I still have 3 minutes, let me go back to a purely theoretical *divertissement* with magnetic fields, otherwise I stop here.**

Non-Abelian gauge theories with compactified directions in magnetic backgrouds

QUESTION

what happens if we compactify one dimension in the presence of an electromagnetic background $F_{\mu\nu}$?

The question can be easily answered when the compactified direction is spatial and the background is magnetic, since Monte-Carlo simulations are perfectly feasible in this case

M. D. and M. Mariti, Phys. Rev. Lett. 118, no. 17, 172001 (2017) [arXiv:1612.07752 [hep-lat]].

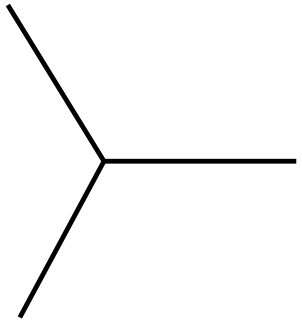
In brief:

- the electromagnetic field couples to the holonomy in the compactified direction (like an imaginary chemical potential does)

- center symmetry is explicitly broken by the presence of dynamical fermions, however the selected center sector, because of the coupling to the e.m. field, becomes space dependent

- For small compactifications, due to the perturbative holonomy potential, local minima develop in each center sector, so that changing center sector gives rise to interfaces, which cost energy.
  Hence, a complicated pattern of phase transitions can arise at which interfaces are created or destroyed, depending on the balance between compactification radius and background field strength.

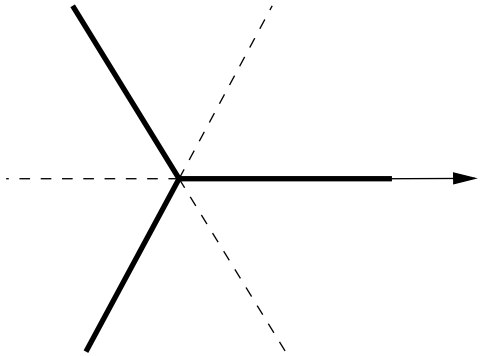
Let us remember the interesting things happening in the T imaginary chemical potential plane, in connection with the realization of center symmetry. Imaginary $\mu = i\mu_I$ rotates fermion temporal b.c. by μ_I/T



Pure gauge theory

Exact Z_3 center symmetry

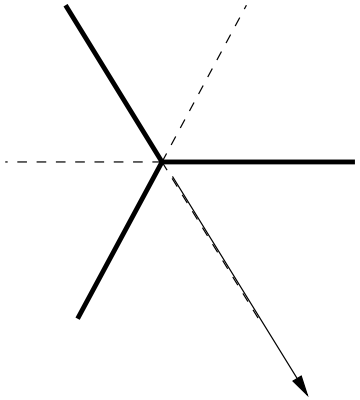
Spontaneously broken at $T > T_c$



Full QCD, $\mu = 0$

Determinant couples to holonomy

Its trace is always real

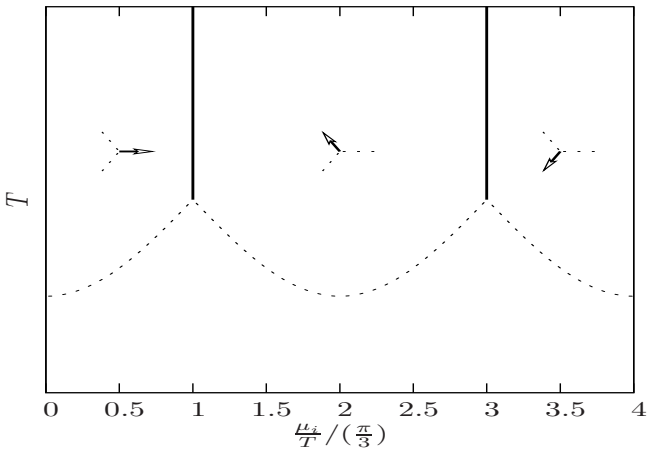


Full QCD, $\theta_I \equiv \mu_I/T \neq 0$

Determinant couples to holonomy * $e^{i\theta_I}$

Minimum for the holonomy rotates with θ_I

In the high T region, the absolute minimum (i.e. the preferred center sector) is decided by θ_I. That leads to the appearance of Roberge-Weiss transitions as a function of θ_I (one every $2\pi/N_c$ interval)



A general $U(1)$ background field, coupled to the electric charge of quark, will do a similar thing. The covariant derivative is modified as follows

$$D_\nu = \partial_\nu + i\, g A^a_\nu T^a + i\, q a_\nu \tag{1}$$

where T^a are the $SU(3)$ generators and q is the coupling to the external $U(1)$ field a_μ. For simplicity we consider quarks degenerate in mass and electric charge.

If a dimension is compactified, the coupling of dynamical fermions to the holonomy involves the external field directly, i.e. the coupling is to

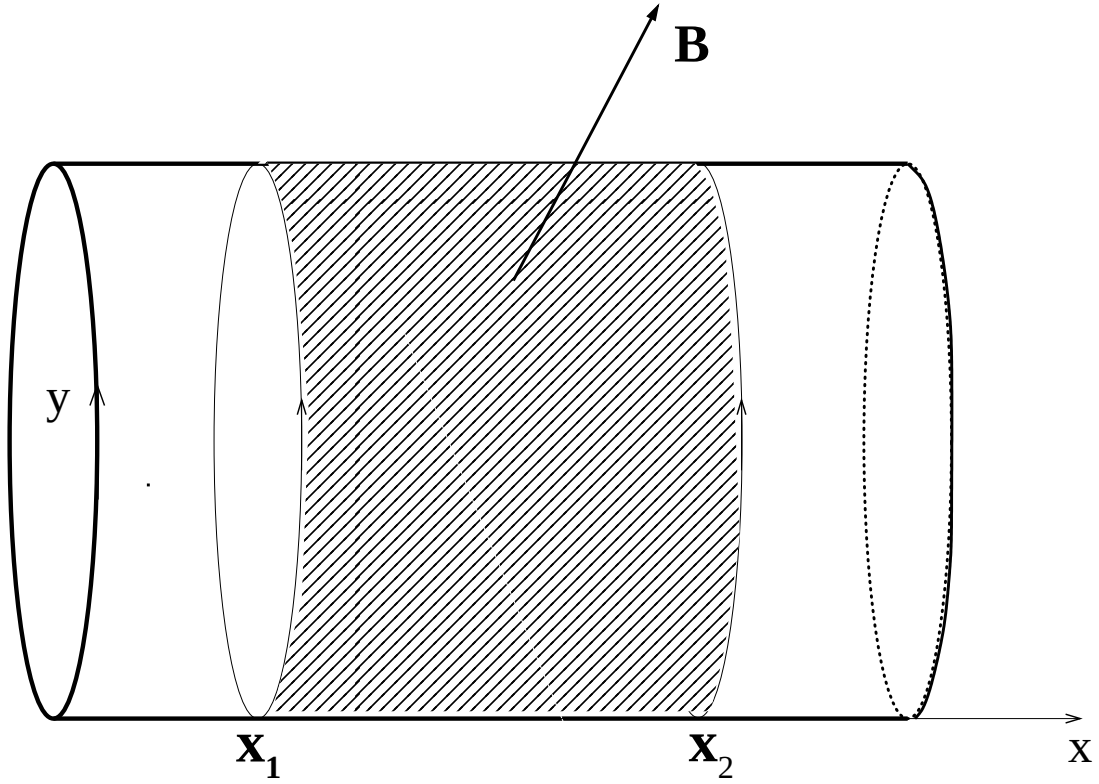
$$\mathrm{Tr}\exp\left(\int dx_\mu i(gA_\mu + qa_\mu)\right) = Le^{i\phi(\vec{x})}\,.$$

where $\phi(\vec{x})$ is a phase factor which, contrary to the case of an imaginary chemical potential, can depend on the coordinates $\vec{x}$ orthogonal to the compactified direction

That will give rise to a coupling to holonomy which changes from point to point, that will give rise to different orientations of the holonomy and to the rise of an interesting phenomenology.

The specific example we will consider:

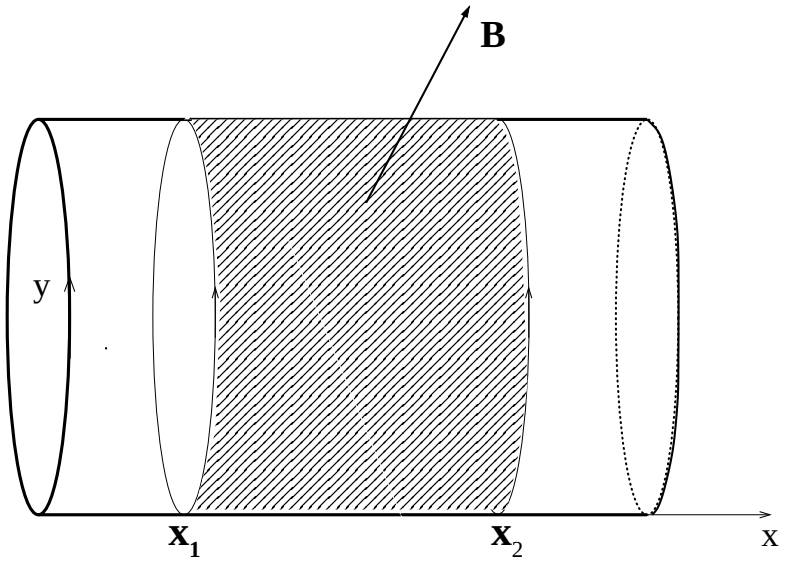
A cilinder with a magnetic background orthogonal to its surface



one can view this as a spatial compactified dimension with a magnetic field. However, because of the spatially varying boundary conditions, thermal or non-thermal is completely irrelevant, so a thermal gauge theory with an imaginary electric field is perfectly equivalent.

The value of a single phase factor is not relevant and depends on the $U(1)$ gauge choice.

However phase differences are meaningful and gauge invariant



$$e^{i(\phi(\mathbf{x_2})-\phi(\mathbf{x_1}))} = \exp\left(iq\int dy(a_y(\mathbf{x_2},y)-a_y(\mathbf{x_2},y))\right) = e^{iq\Phi_\mathbf{B}}$$

where $\Phi_\mathbf{B}$ is the total magnetic field flux going through the shadowed surface.

The value of such a flux is, for any given distribution of magnetic field, a property of the points $\mathbf{x_1}$ and $\mathbf{x_2}$ only (also in higher dimensions)

Therefore, we expect that $N_c q\Phi_B/(2\pi)$ different center sectors should be explored.

For small compactification, when the holonomy develops local minima, that would imply the formation of $N_c q\Phi_B/(2\pi)$ center interfaces between $\vec{x}_1$ and $\vec{x}_2$.

Does the "lattice" of center domains and interfaces really form?

Interfaces have an energy cost, could it be more convenient to stay (locally) in the wrong sector without forming any interface?

This is an issue of energy balance. We will make an estimate of such energy balance under some simplified assumption:

- **The magnetic background is uniform and constant**
- **The compactification radius is so small that perturbative estimates for the interface tension (or for the false vacuum energy) hold true**

Uniform background field and exact center-translational symmetry

When the background field is uniform, center symmetry, which is explicitly broken by the presence of dynamical fermions, is recovered in a different form:

One can rotate temporal boundary conditions for gauge fields by $-2\pi/N_c$, and perform at the same time a translation along x by $2\pi/(qBL_cN_c)$, where L_c is the size of the compactified direction the theory will be mapped onto itself

This discrete symmetry can be:

1. **Realized exactly:**

   After each translation by $2\pi/(qBL_cN_c)$ the holonomy rotates by $-2\pi/N_c$, with more or less sharp interfaces (more and more sharp as L_c decreases)

2. **Spontaneously broken:**

   The holonomy fails to rotate as you translate, because interfaces cost too much and it is more convenient to stay in the false vacuum somewhere.

ENERGY BALANCE - I

We need to compute the balance between

- **the energy spent in creating center interfaces**
  this is a function of the interface tension and of the density of interfaces, which depends on the magnetic field strength
- **the energy spent in keeping the holonomy in a locally wrong vacuum**
  This is a function of the holonomy effective potential.

Let $L \equiv x_2 - x_1$. We consider two extreme situations:

- **All center domains are actually formed: the number of interfaces, N_{int}, is given by all the different center sectors spanned by the local phase between x_1 and x_2:**

$$N_{int} = q\Phi_B/(2\pi/N_c) = qBLL_cN_c/2\pi \,, \tag{2}$$

- **the holonomy stays in the same center sector everywhere, no interface is formed**
  one must keep the holonomy in the wrong center sector for a fraction $(N_c-1)/N_c$ of the region between x_1 and x_2.

ENERGY BALANCE - II

In the limit of asymptotically small L_c, we can recover perturbative results obtained in thermal field theory, where $L_c = 1/T$

- **The interface tension (energy per unit interface area) is proportional to $L_c^{-3}\ \log(1/L_c)$**
- **The energy density to keep the holonomy in the wrong vacuum is prop. to L_c^{-4}.**

Apart from a common factor related to the integration in the non-compactified directions

- **the energy spent to create all possible interfaces between x_1 and x_2 is prop. to**

$$qBLL_c^{-2}\log(1/L_c)$$

- **the energy spent to maintain the holonomy in the same center sector, without creating any interface, is proportional to**

$$LL_c^{-4}$$

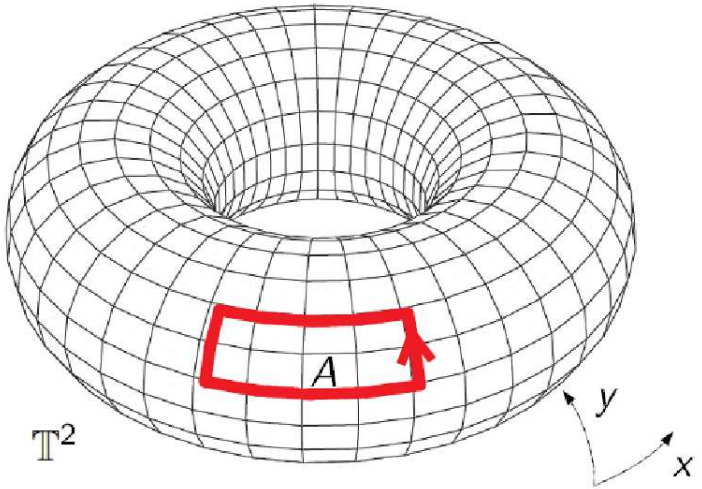
The first situation is surely favored, at fixed magnetic field, for small enough L_c and, at fixed L_c, for small enough B.

Increasing L_c or B can make instead the second situation more favorable.

Some numerical tests from lattice simulations

We have performed lattice simulations with rooted staggered fermions

- **2 flavors, degenerate both in mass and charge, pion mass quite large (800 MeV)**
- **magnetic field along $\hat{z}$, y is the short compactified direction, x is compactified as well, but of length $L_x = L \gg L_c$**
- **Since we are on a torus, magnetic field (actually, magnetic flux) is quantized.**
- **We will consider simulations at fixed B and see what happens when decreasing L_c, or at fixed L_c and see what happens when changing B**

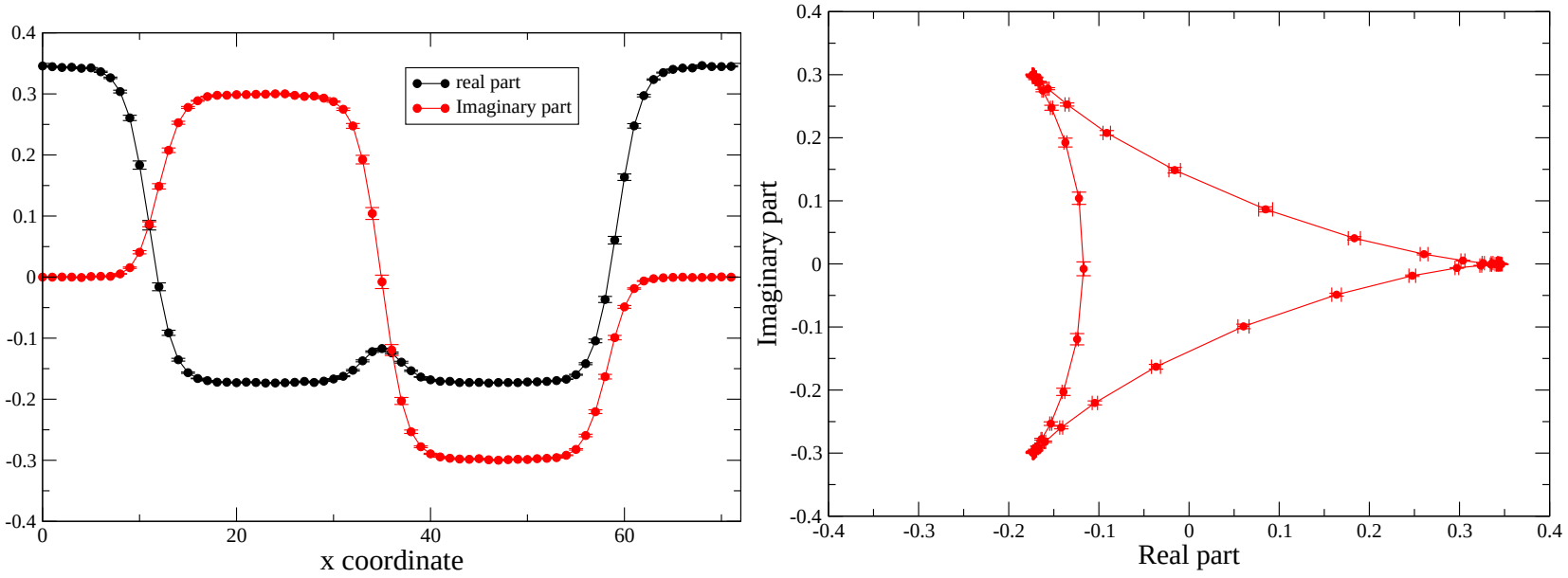


Simulations are done at fixed bare parameters ($\beta = 6.2$, $am = 0.01$)

$L_z = L_t = 24$ **for all simulations**

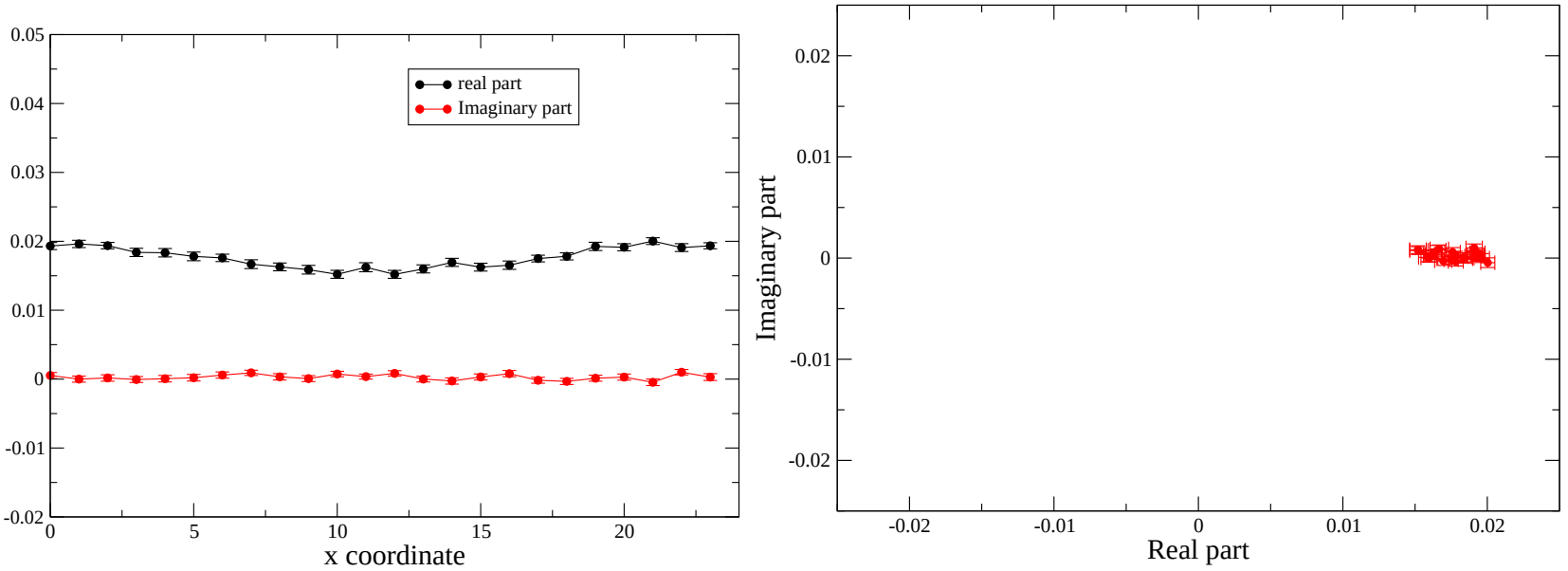
L_y **is the compactified direction** L_c

L_x **is changed so as to tune** $qB = 2\pi b/(L_x L_y a^2)$ **where** b **is an integer.**



We start by showing the behavior of the local values taken by the holonomy (at fixed x **coordinate) for the case:** $b = 1$, $L_c = 4$, $L_x = 72$

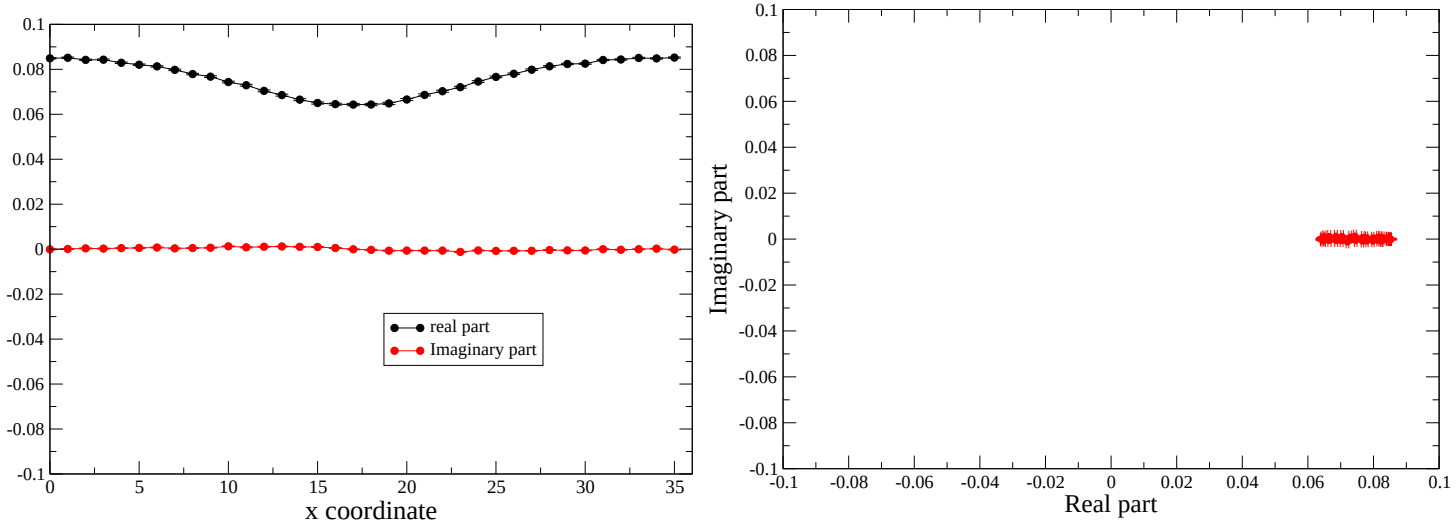
For the same values, at $B = 0$ **the system is in the deconfined phase, with a non-zero, real holonomy. At** $B \neq 0$ **the formation of center domains and center interfaces is clearly visible**



Next we enlarging L_c at fixed B:

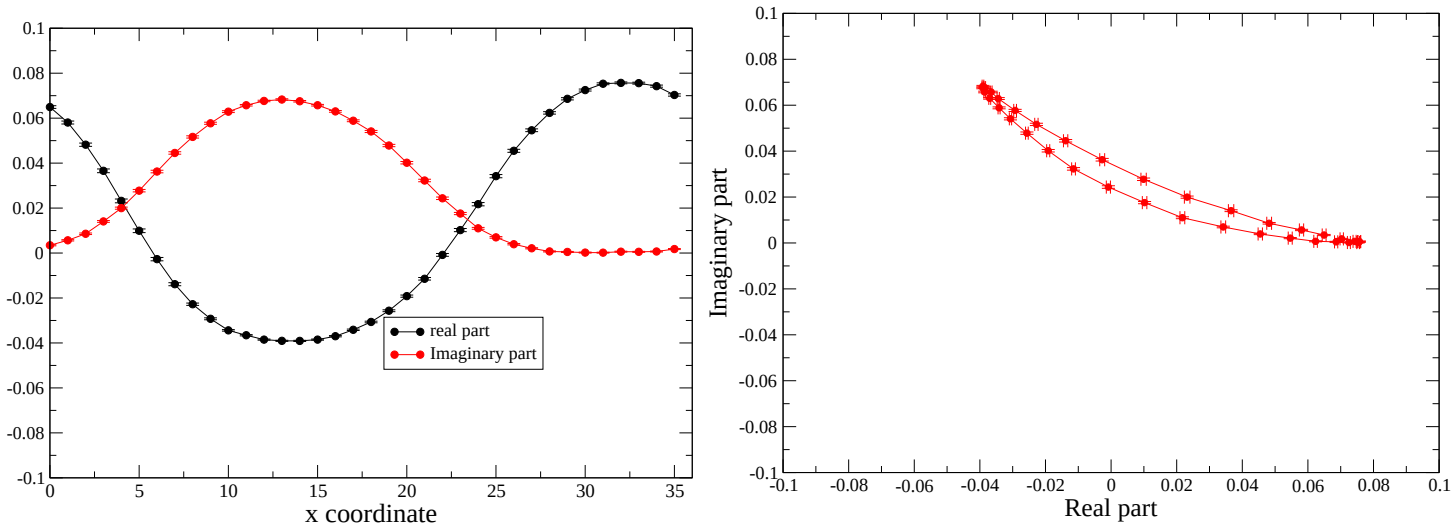
$b = 1$, $L_c = 12$, $L_x = 24$

The system is found in a different phase, the center-translational symmetry is broken spontaneously, a given center sector is selected throughout the lattice



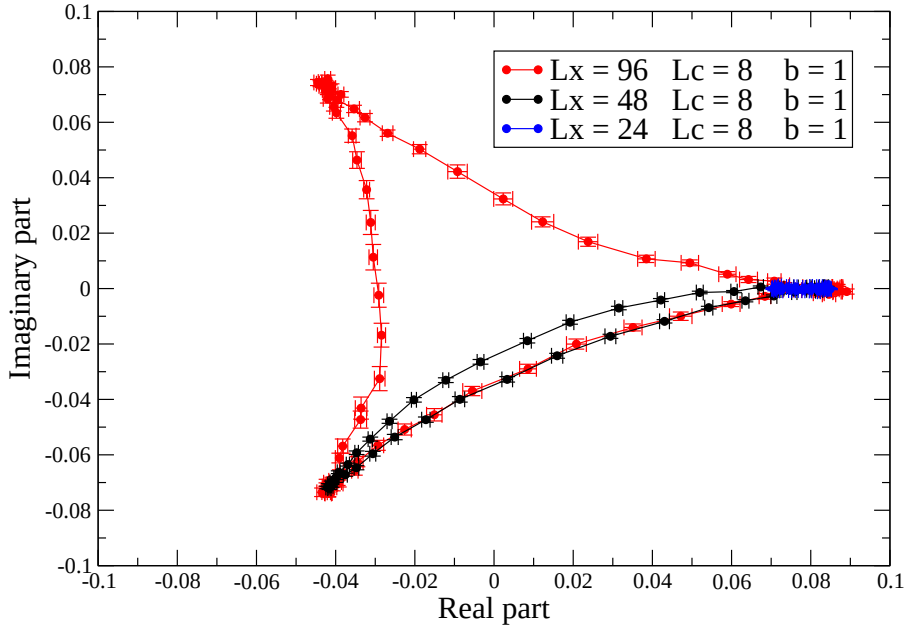
We can even have different phases: $b = 1$, $L_c = 8$, $L_x = 36$

Metastability between two different phases in which the symmetry breaks in two different ways cold start (above) and hot start (below) where one interface forms.



A similar pattern of phase transitions is observed if we change the magnetic field at fixed compactification radius, remember:

$$qB = \frac{2\pi b}{(L_x L_c a^2)}$$



We start with a center-translation symmetric system

(three center domains and three interfaces)

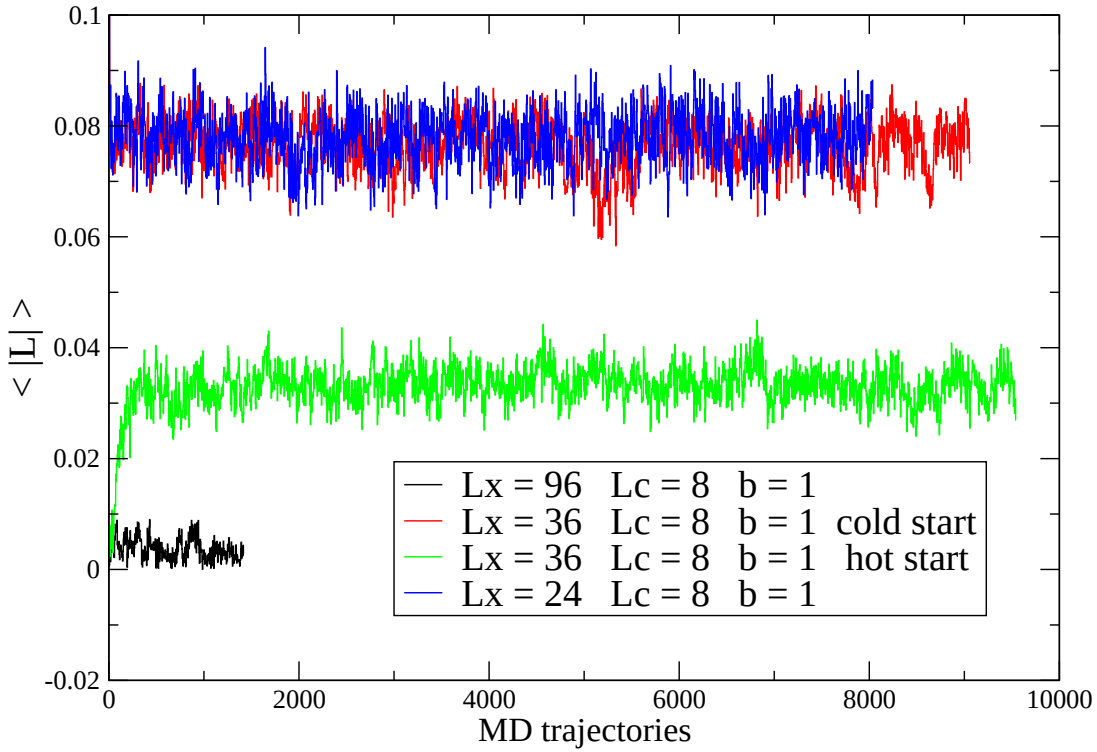
then, as we increase B we go through a phase with just two center domains

(banana phase)

and finally to a phase with a single center sector.

Going from one phase to the other takes place through first order phase transitions at which interfaces are destroyed or created.

This is clearly visible from time histories of the global Polyakov loop (averaged over whole space) which shows strong metastabilities



Is this interesting phenomenology relevant to any context?

- **Beyond the standard model theories with compactified extradimensions and cosmological magnetic backgrounds?**

- **Synthetic condensed matter systems with emergent non-Abelian symmetries and compactifed dimensions?**