QCD phase diagram at small μ/T

C. Bonati
Università di Pisa & INFN, Pisa (Italy)

Work in collaboration with
M. D'Elia, M. Mariti, M. Mesiti, F. Negro, F. Sanfilippo, K. Zambello

Phase diagram of strongly interacting matter:
From Lattice QCD to Heavy-Ion Collision Experiments

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Outline

The deconfinement transition at zero baryonic density

The deconfinement/chiral symmetry restoration transition at vanishing baryon density has been extensively studied using Lattice QCD and its properties are by now well established.

It is not a "phase transition" but just a smooth analytical crossover; as a consequence all "critical properties" are observable dependent.

In the following all Lattice QCD results will be related to the chiral symmetry restoration aspects.

Critical temperature:

$T_c|_{\rm BW} = 152(5)\,{\rm MeV}$ Aoki et al. Phys. Lett. B **643**, 46 (2006)

$T_c|_{\rm hotQCD} = 154(9)\,{\rm MeV}$ Bazavov et al. Phys. Rev. D **85** 054503 (2012)

The sign problem at nonvanishing density

Lattice QCD $\sim$ statistical mechanics with energy $=$ euclidean 4d action

Fermions cannot be directly simulated but they can be integrated out:
$S_{eff}(A) = S_G(A) - \log\det[m + \not{D}(A)]$

We need $\det[m + \not{D}(A)] > 0 \ \forall A$ to use importance sampling in Lattice QCD Monte-Carlo simulations.

In all lattice discretizations a relation of the following form holds true:

$$\gamma_5 \not{D}(\mu)\gamma_5 = \not{D}(-\mu^*)^\dagger$$

If $\Re(\mu) = 0$ this relation implies that if $\lambda \in \sigma[\not{D}(A)]$ then also $\lambda^* \in \sigma[\not{D}(A)]$, so that $\det[m + \not{D}(A)] > 0$.

For real μ values $\det[\not{D}(A)] \notin \mathbb{R}^+$: sign problem.

Possible way out of the sign problem

Most used (partial) solutions:

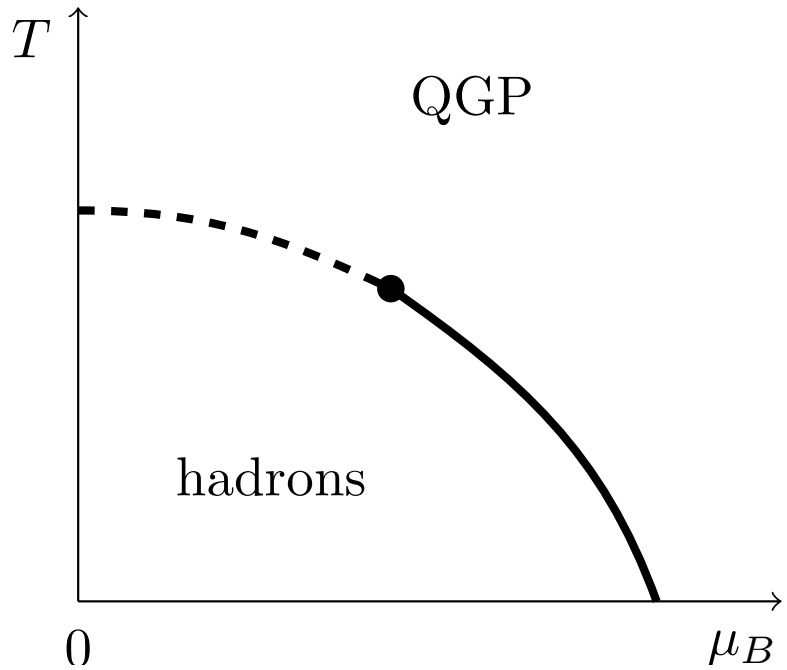
reweighting First sample the distribution at $\mu = 0$ then reweight it to $\mu \neq 0$. Problem: the overlap between the two distributions goes to zero exponentially as $V \to \infty$.

Taylor expansion Expand everything in powers of μ. The coefficients can typically be computed at $\mu = 0$. Problem: the higher the coefficient the more noisy the estimator the worse the scaling with the volume of the signal to noise ratio.

imaginary μ Perform simulation at imaginary chemical potential (where there is no sign problem) then analytically continue to real μ. Problem: systematical errors of the continuation.

Other possibilities: Lefschetz thimble, complex Langevin, canonical simulations, strong coupling methods, dual variables, density of state methods, ...

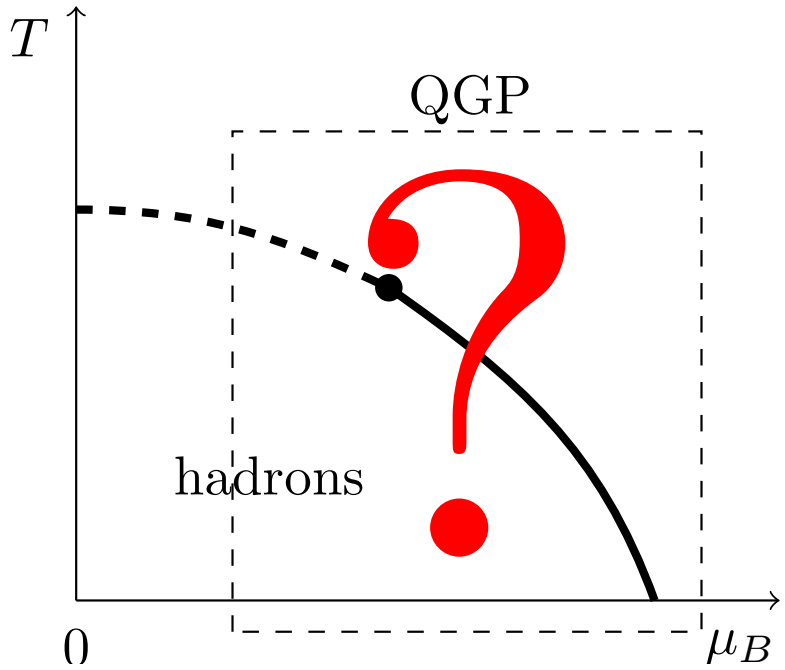
The expected phase diagram in the $T - \mu_B$ plane



Main features:

- analytic crossover for $\mu = 0$ (no known symmetries to break, it would be a real transition for massless or infinitely massive quarks)
- first order transition for $T = 0$ (simple argument based on light particles counting)
- a second order transition somewhere in the middle

The known phase diagram in the $T - \mu_B$ plane



The region that can be reliably explored by Lattice QCD is the region of "small" μ_B, where the results obtained by using different methods can be tested against each other.

A well posed problem is the determination of $T_c(\mu_B)$ in this region.

General parametrization of $T_c(\mu_B)$

Since $Z(\mu_B) = Z(-\mu_B)$, in general $T_c(\mu_B)$ is an even function of μ_B. For small μ_B we thus expect

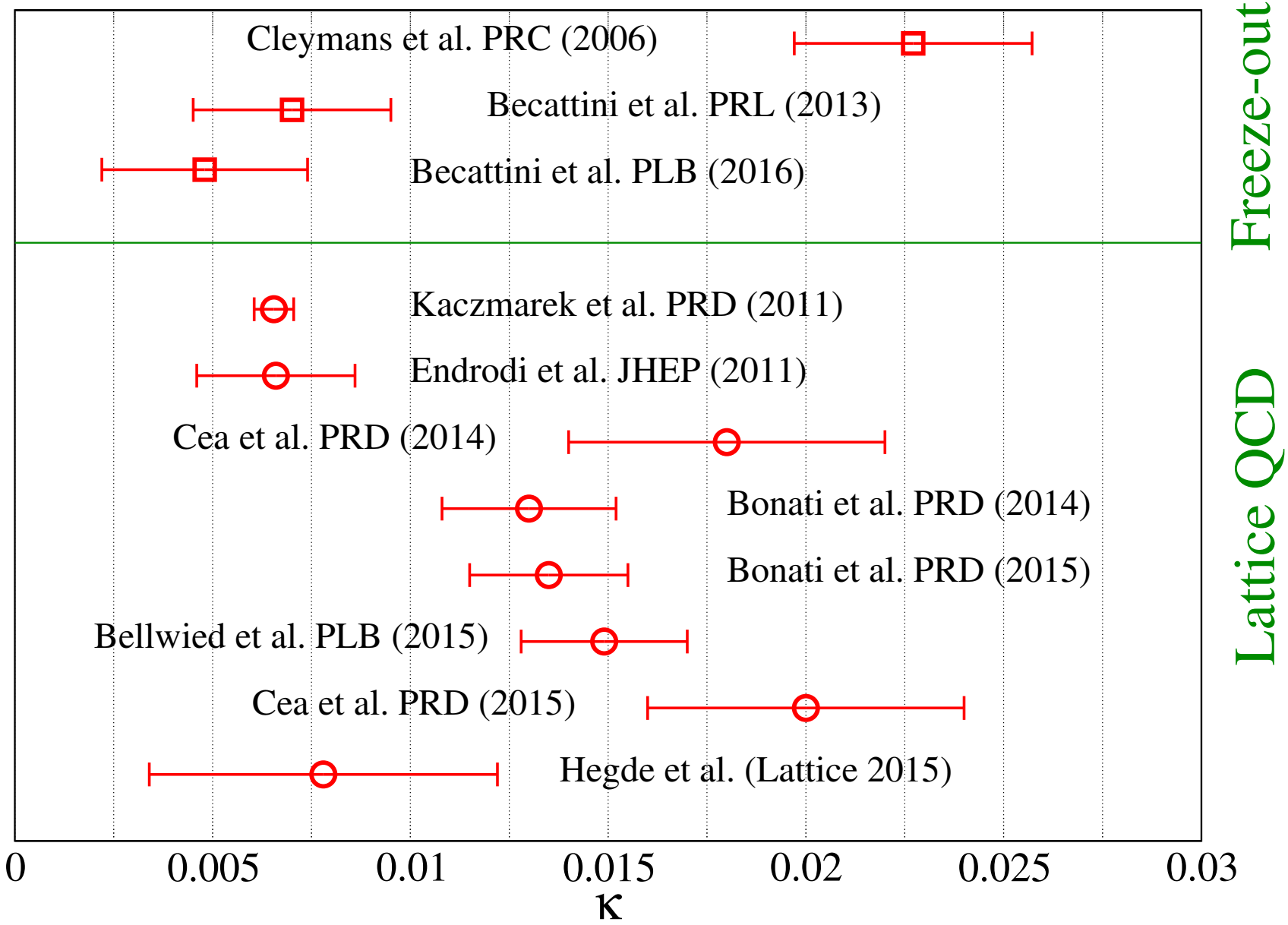
$$T_c(\mu_B) = T_c(0)\left(1 - \kappa\left(\frac{\mu_B}{T_c(0)}\right)^2 + c\left(\frac{\mu_B}{T_c(0)}\right)^4 + \cdots\right) =$$

$$= T_c(0)\left(1 - \kappa\left(\frac{\mu_B}{T_c(\mu_B)}\right)^2 + c'\left(\frac{\mu_B}{T_c(\mu_B)}\right)^4 + \cdots\right)$$

κ is the curvature of the critical line in the $T - \mu_B$ plane at $\mu_B = 0$ and it is an equilibrium property of QCD.

The precise relation between κ and the curvature κ_f of the freeze-out line is nontrivial from the theoretical point of view. On the other hand it seems reasonable that $\kappa \approx \kappa_f$.

Various determinations of κ/κ_f



A reminder on the quark chemical potentials

The relations between the conserved charges and the quark numbers are

$$B = (N_u + N_d + N_s)/3$$
$$Q = (2N_u - N_d - N_s)/3$$
$$S = -N_s$$

The quark chemical potentials are defined in such way that

$$B\mu_B + Q\mu_Q + S\mu_S = N_u\mu_u + N_d\mu_d + N_s\mu_s$$

thus

$$\mu_u = \mu_B/3 + 2\mu_Q/3$$
$$\mu_d = \mu_B/3 - \mu_Q/3$$
$$\mu_s = \mu_B/3 - \mu_Q/3 - \mu_S$$

Typical setups and strangeness neutrality

In (almost) all simulations $\mu_Q \equiv 0$ and one of the two following extreme cases is used:

$$1) \quad \mu_u = \mu_d = \mu_B/3; \quad \mu_s = 0$$
$$2) \quad \mu_u = \mu_d = \mu_B/3; \quad \mu_s = \mu_B/3$$

that correspond to

$$1) \quad \mu_S = \mu_B/3$$
$$2) \quad \mu_S = 0$$

If we want to impose strangeness neutrality ($\langle N_s \rangle = 0$) we need

$$0 = \frac{\partial \log Z(\mu_B, \mu_S)}{\partial \mu_S} \simeq \left.\frac{\partial \log Z}{\partial \mu_S \partial \mu_S}\right|_{\mu=0} \mu_S + \left.\frac{\partial \log Z}{\partial \mu_S \partial \mu_B}\right|_{\mu=0} \mu_B + \cdots$$

from which we get a relation between μ_B and μ_S.

Strangeness neutrality and Q/B ratio

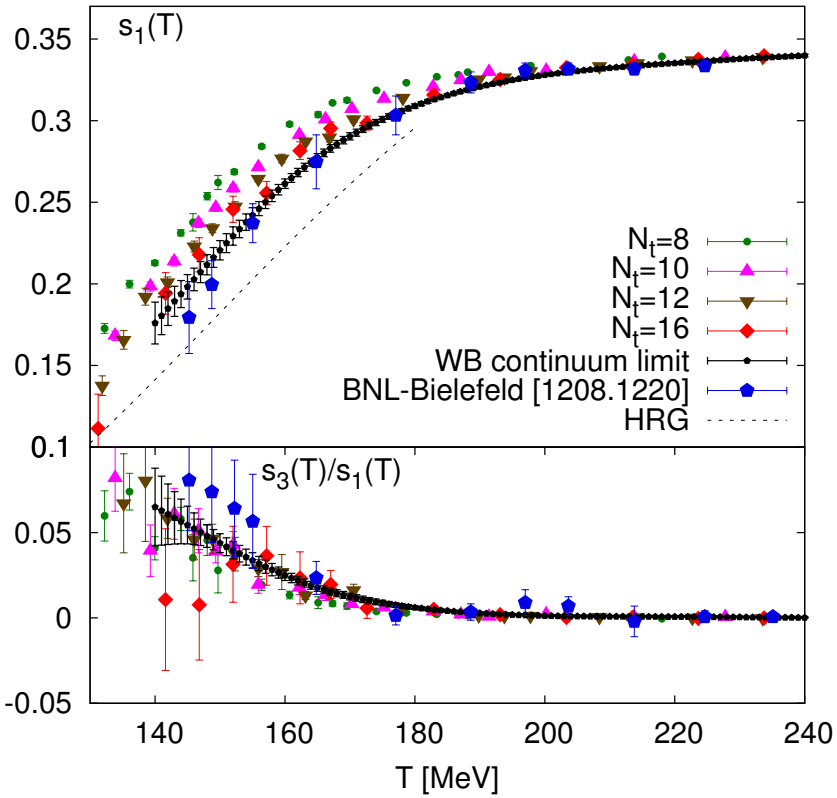
Explicitly one can write

$$\frac{\mu_S}{T} = s_1(T)\frac{\mu_B}{T} + s_3(T)\left(\frac{\mu_B}{T}\right)^3 + \cdots$$

At $T \approx T_c$ we have $\mu_S \simeq \mu_B/4$ and thus $\mu_s \simeq \mu_B/12 = \mu_u/4$.

In a similar way μ_Q can be fixed by imposing $\langle N_Q \rangle = r\langle N_B \rangle$, where $r = Z/A \simeq 0.4$, obtaining:

$$\frac{\mu_Q}{T} = q_1(T)\frac{\mu_B}{T} + q_3(T)\left(\frac{\mu_B}{T}\right)^3 + \cdots$$



Bazavov et al. PRL (2012)

Borsányi et al. PRL (2013)

Taylor method 1

Kaczmarek et al. PRD (2011), Hegde et al. (Lattice 2015)

If the transiton with $m_\ell \equiv m_u = m_d = 0$ is second order, since the baryon number does not break chiral symmetry, for $m_\ell \approx 0$ we can define the scaling variables

$$t \simeq \frac{1}{t_0}\left(\frac{T - T_c(0)}{T_c(0)} + \kappa\left(\frac{\mu_B}{T_c(0)}\right)^2\right) \qquad h \simeq \frac{1}{h_0}\frac{m_\ell}{m_s}$$

and thermodynamical observables have the scaling form $\phi = \phi(t, h)$, thus

$$\kappa = T_c(0)\left.\frac{\partial\phi/\partial\mu_B^2}{\partial\phi/\partial T}\right|_{\substack{\mu_B=0 \\ T=T_c}} = \frac{t_0}{\partial_t\phi|_{\substack{\mu_B=0 \\ t=0}}}\left.\frac{\partial\phi}{\partial(\mu_B/T)^2}\right|_{\substack{\mu_B=0 \\ t=0}}$$

For $\partial_t\phi$ the scaling function of the $O(4)$ model was used.

κ defined in this way is the curvature in the chiral limit $m_\ell = 0$.

Taylor method 2

Endrodi et al. JHEP (2011)

Take your favorite observable $\phi(T, \mu_B)$ that is monotone at $\mu_B = 0$ and let ϕ_0 be its value at the $\mu_B = 0$ transition. Then define $T_c(\mu_B)$ by the equation $\phi(T_c(\mu_B), \mu_B) \equiv \phi_0$. Then

$$\kappa \equiv -T_c(0) \left. \frac{\mathrm{d}T_c(\mu_B)}{\mathrm{d}\mu_B^2} \right|_{\mu_B=0} = T_c(0) \left. \frac{\partial\phi/\partial\mu_B^2}{\partial\phi/\partial T} \right|_{\substack{\mu_B=0 \\ T=T_c}}$$

Problem: why should it work? Partial solution: when the method by Kaczmarek et al. works, the method by Endrodi et. al also works (and it had to give the same answer, compare equations).

In order to gain statistics an extension of the method to $T \neq T_c$ of κ was used in this work.

Imaginary chemical potential method

Cea et al PRD 2014-2015, Bonati et al. PRD 2014-2015, Bellwied et al. PLB 2015

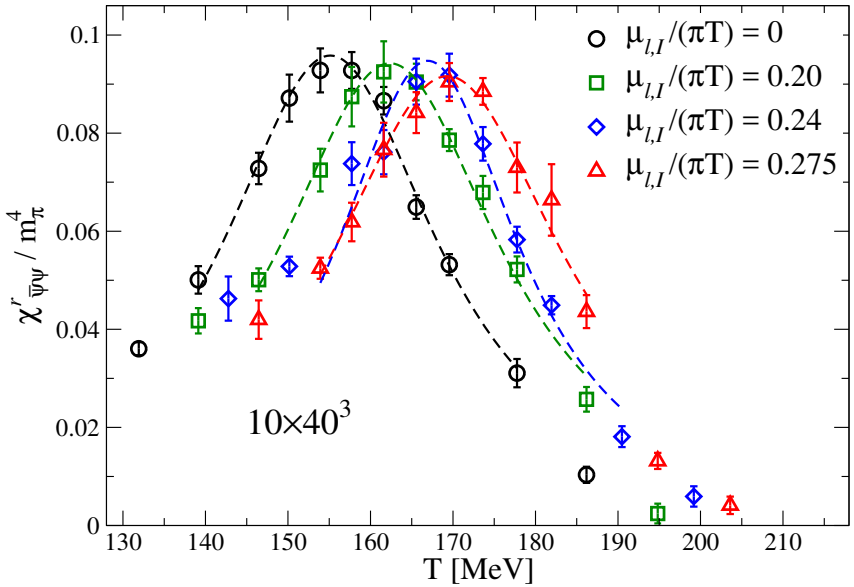
Advantage of using imaginary chemical potential: for each value of μ_B we can perform a scan in T and look for the transition using standard procedures (look for χ maxima or $\bar{\psi}\psi$ inflection points).

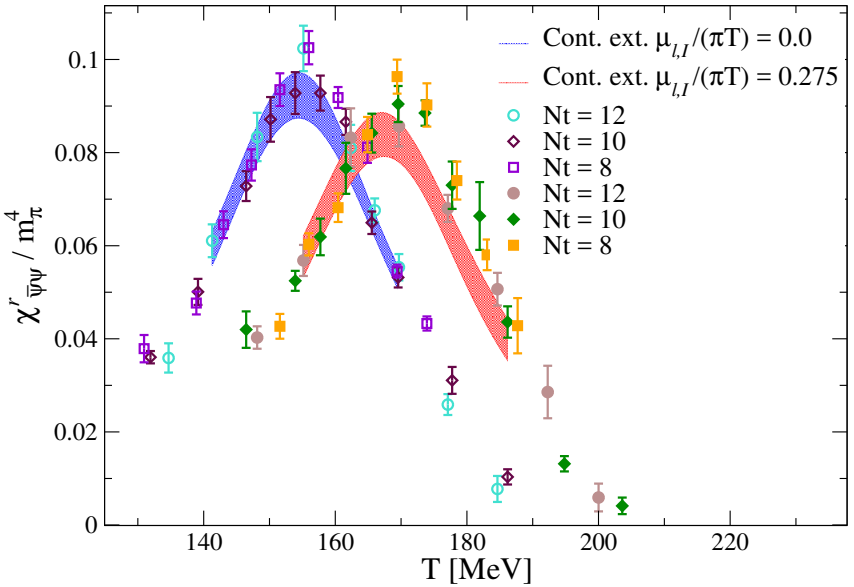
Two different procedures for the continuum limit

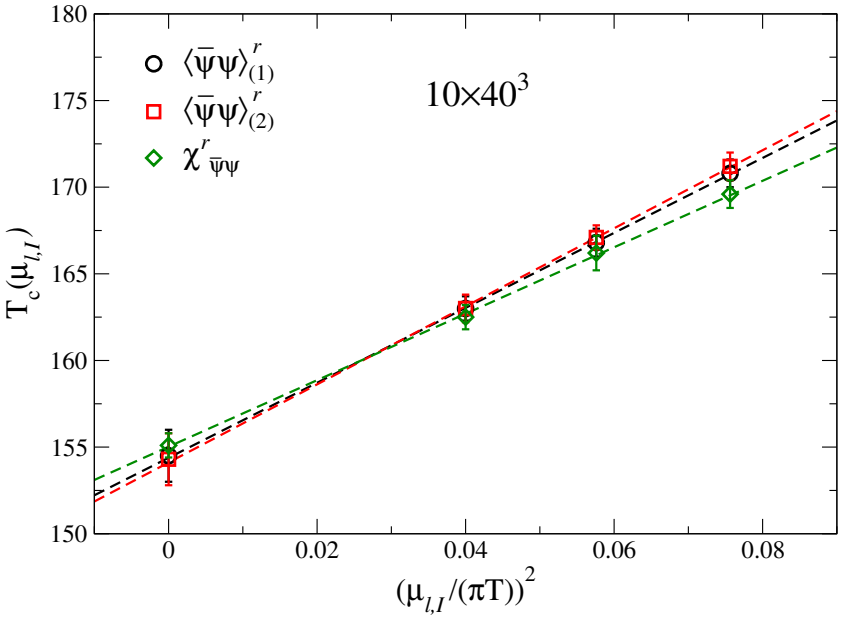
1. fix lattice spacing a
2. for each μ^I compute $T_c(\mu^I, a)$
3. compute the curvature at fixed a: κ_a
4. try several a values and extrapolate κ_a to continuum

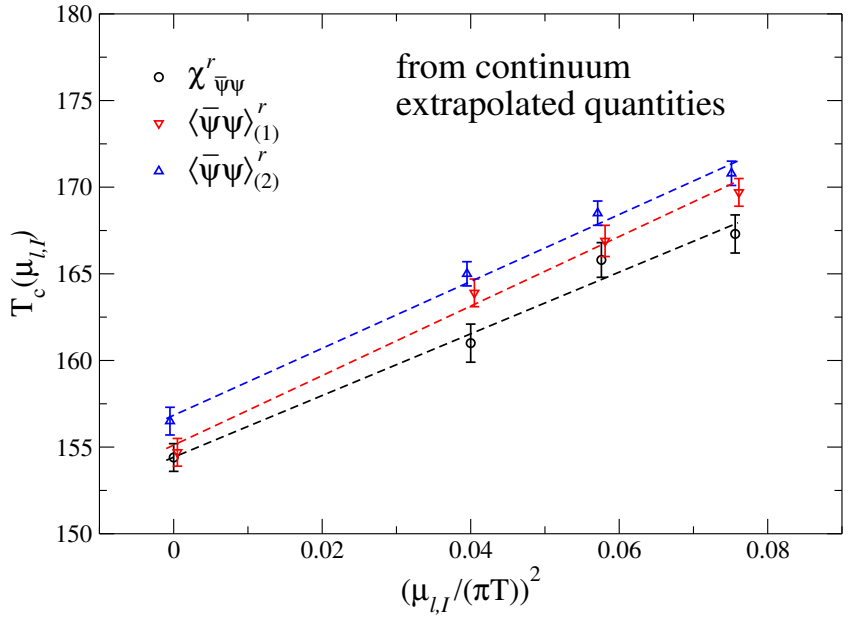
1. fix lattice spacing a
2. for each μ^I compute $\bar{\psi}\psi^r(\mu^I, a)$ and $\chi^r_{\bar{\psi}\psi}(\mu^I, a)$
3. try several a values and extrapolate $\bar{\psi}\psi^r(\mu^I, a)$ and $\chi^r_{\bar{\psi}\psi}(\mu^I, a)$ to continuum
4. find $T_c(\mu^I, a = 0)$ using the results of the previous point
5. compute κ

The two ways to the continuum limit









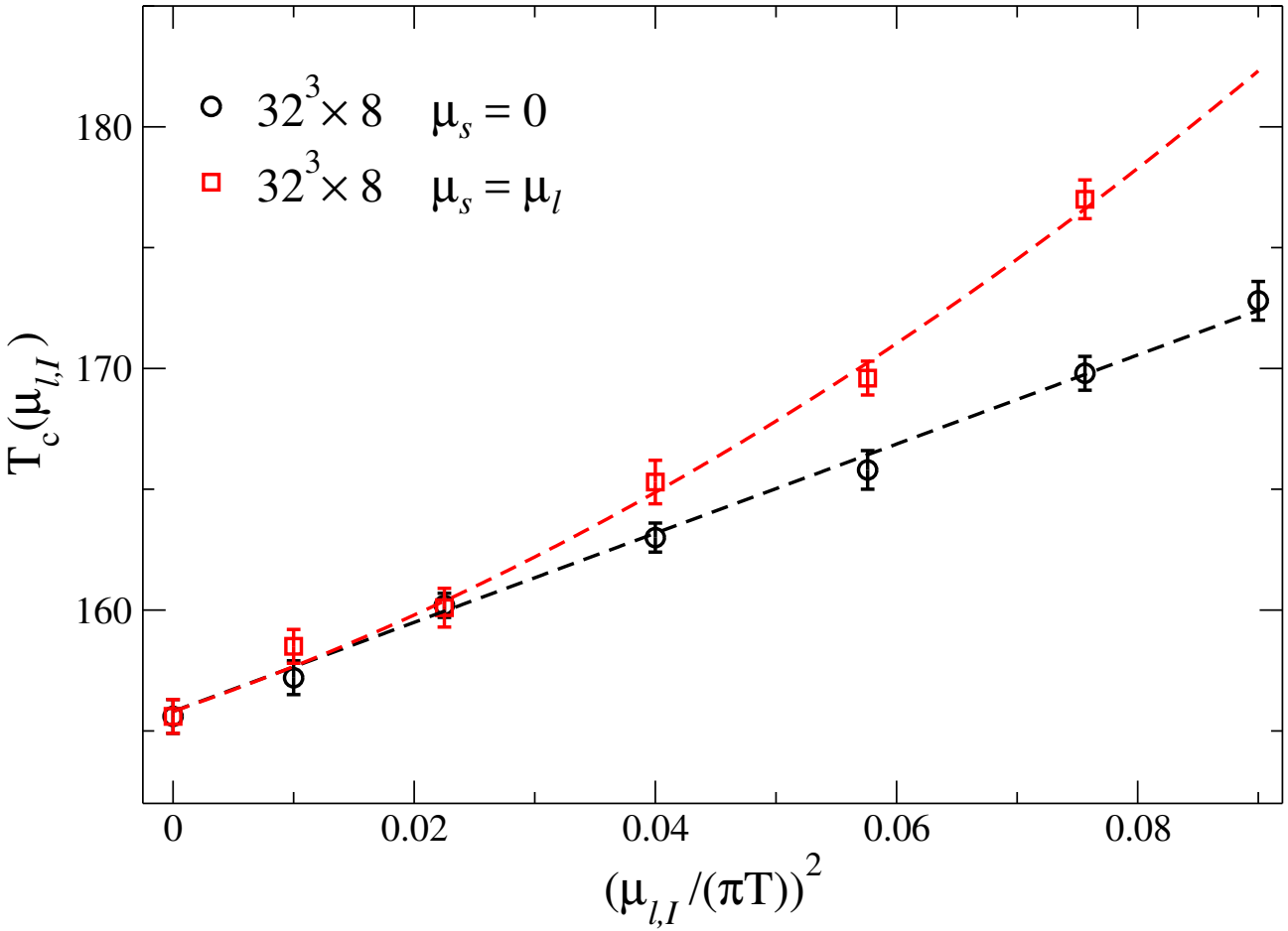
Imaginary chemical potential: systematics checklist

- finite volume: aspect ratio 4 was shown to be enough for finite volume effects to be smaller than statistical errors.
- continuum limit: the two different ways of extracting the continuum limit gave compatible results (the small discrepancies has been used as an estimate of the systematics)
- observable dependence: to locate the transition we used both the inflection point of $\bar{\psi}\psi$ (renormalized in two different ways) and the maximum of χ. Different results were compatible with each other and the (small) differences were used as systematics.
- we also tried to use the approach of Taylor 2, i.e. to define $T_c(\mu_B)$ by $\phi(T_c(\mu_B), \mu_B)) = \phi(T_c(0), 0))$ (with $\phi = \langle\bar{\psi}\psi\rangle^r_{(1),(2)}$), obtaining reasonably consistent results.

Other systematics studied (next slides)

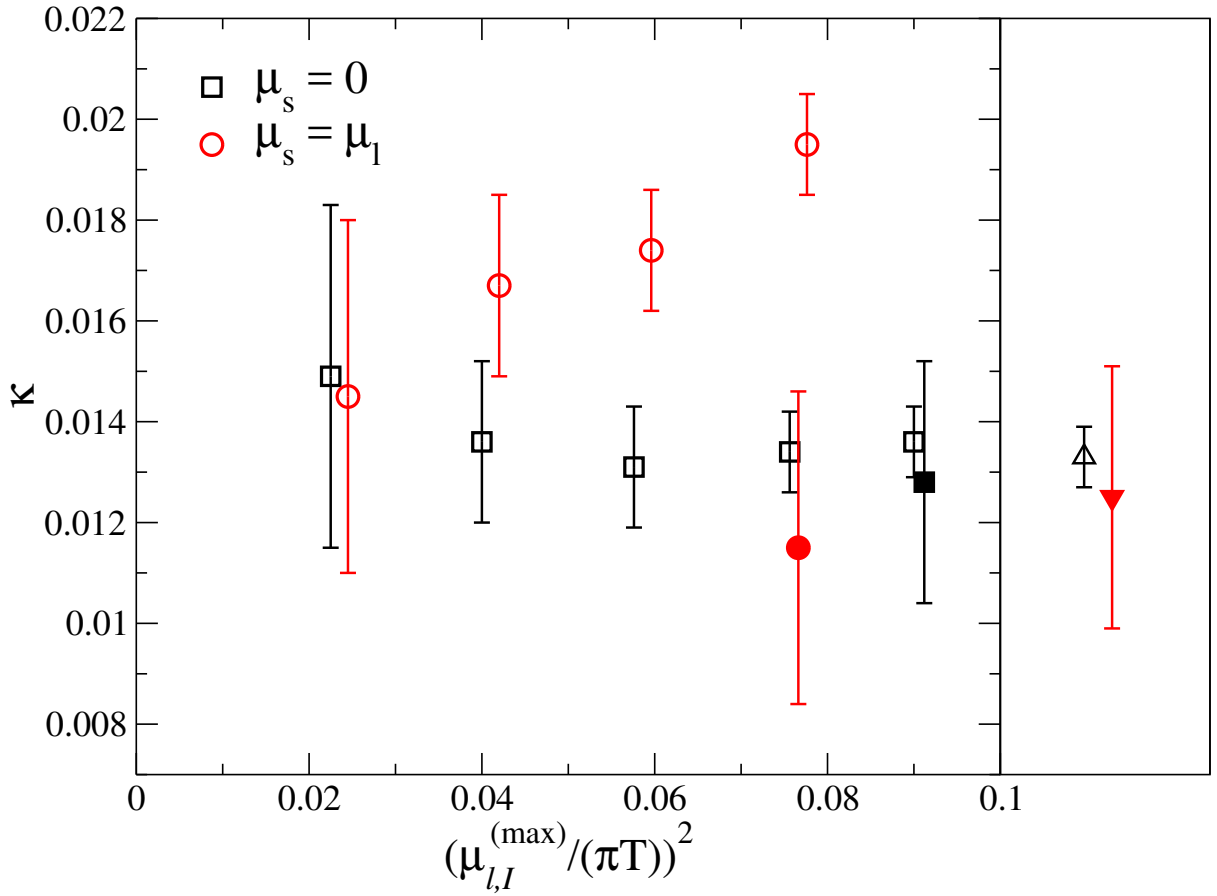
- dependence on the specific chemical potential setup adopted
- dependence on the fit ranges in μ_B adopted (i.e. possibility of contamination from higher order terms)

μ-systematics



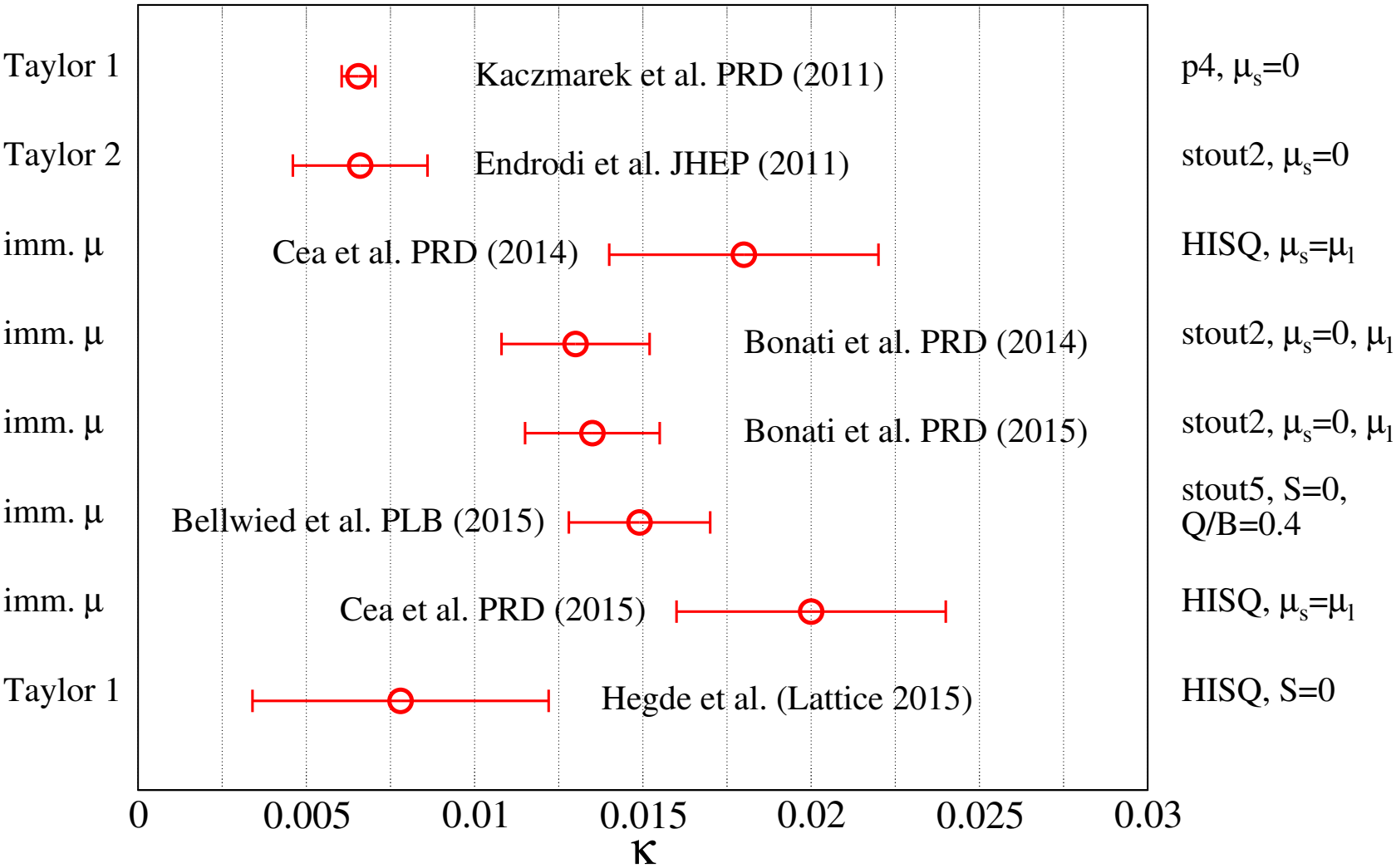
Possible explanation for the different behaviours: the different location of the Roberge Weiss transition.

μ-systematics



Empty symbols: purely quadratic fit. Filled symbols: also quartic correction. Right panel: combined fit (i.e. fixing a common value for $T_c(0)$) to both data sets when a quartic correction is used for the $\mu_s = \mu_l$ data. The empty (filled) triangle corresponds to $\mu_s = 0$ ($\mu_s = \mu_l$).

κ from LQCD summary



New Taylor expansion determination

- Use Taylor 2 (= Taylor 1)

$$\kappa_I = T_c(0) \left. \frac{\partial\phi/\partial\mu_B^2}{\partial\phi/\partial T} \right|_{\substack{\mu_B=0 \\ T=T_c}}$$

  without extending to $T \neq T_c(0)$ as done in Endrodi et al. JHEP (2011).

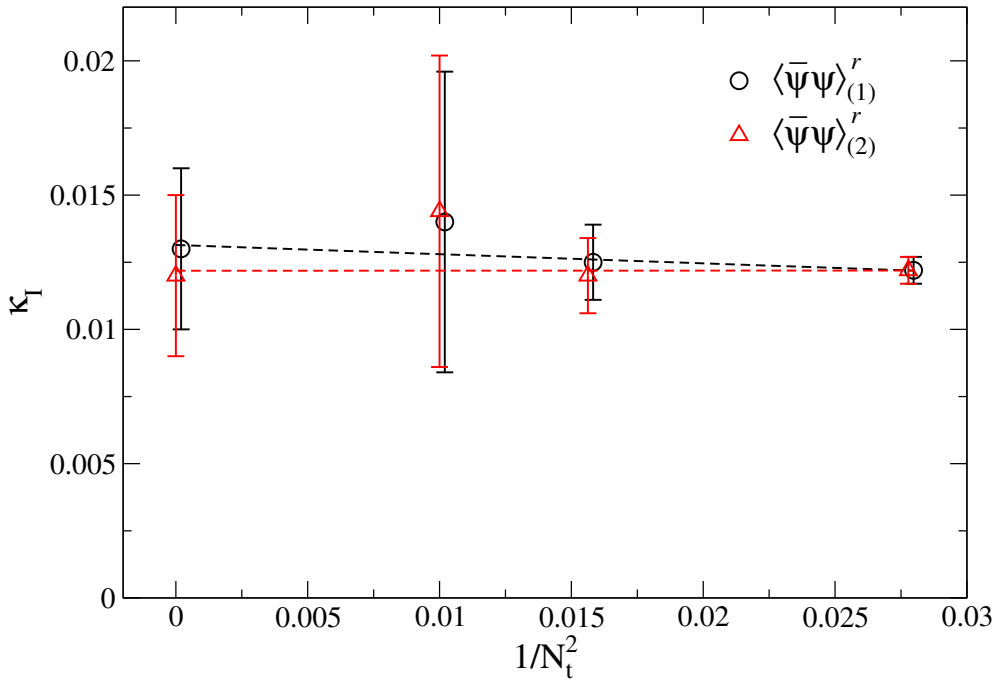
- Taylor 3: define the transition point $T_c(\mu_B)$ as the inflection point of $\phi(T, \mu_B)$ at fixed μ_B. By developing in $T - T_c(0)$ and μ_B one obtains

$$\kappa_{II} = T_c(0) \left. \frac{\frac{\partial^2}{\partial T^2}\frac{\partial}{\partial \mu^2}\phi(T,\mu_B)}{\frac{\partial^3}{\partial T^3}\phi(T,\mu_B)} \right|_{\substack{\mu_B=0 \\ T=T_c}}$$

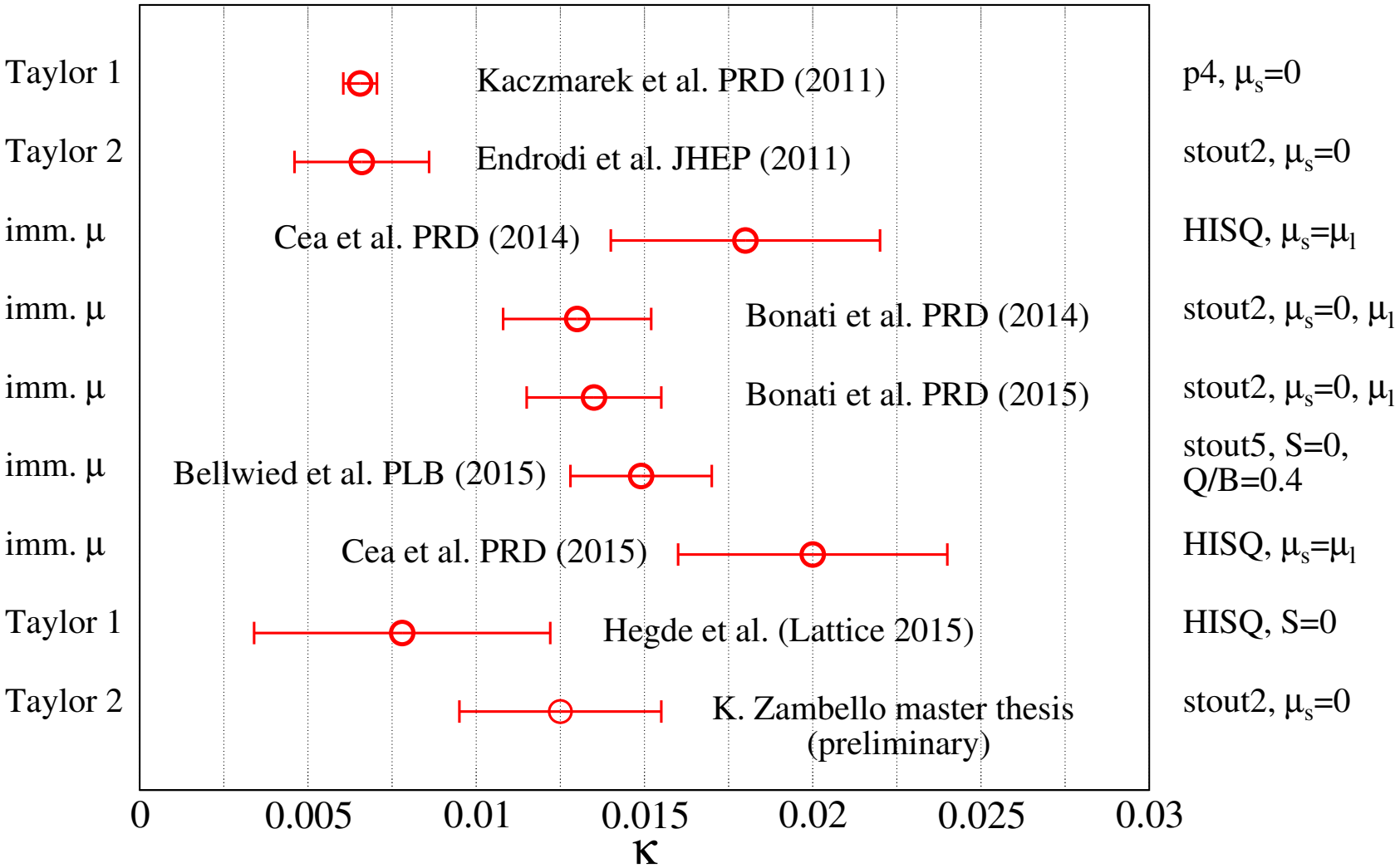
The Taylor 3 method is theoretically more solid than the other, but requires much higher statistics.

Numerical results (work in progress)

	$\langle\bar{\psi}\psi\rangle^r_{(1)}$		$\langle\bar{\psi}\psi\rangle^r_{(2)}$	
N_t	κ_I	κ_{II}	κ_I	κ_{II}
6	0.0122(5)	0.013(4)	0.0122(5)	0.013(4)
8	0.0125(14)	0.014(10)	0.0120(14)	0.013(9)
10	0.0140(56)		0.0144(58)	
∞	0.013(3)		0.012(3)	



κ from LQCD updated with work in progress



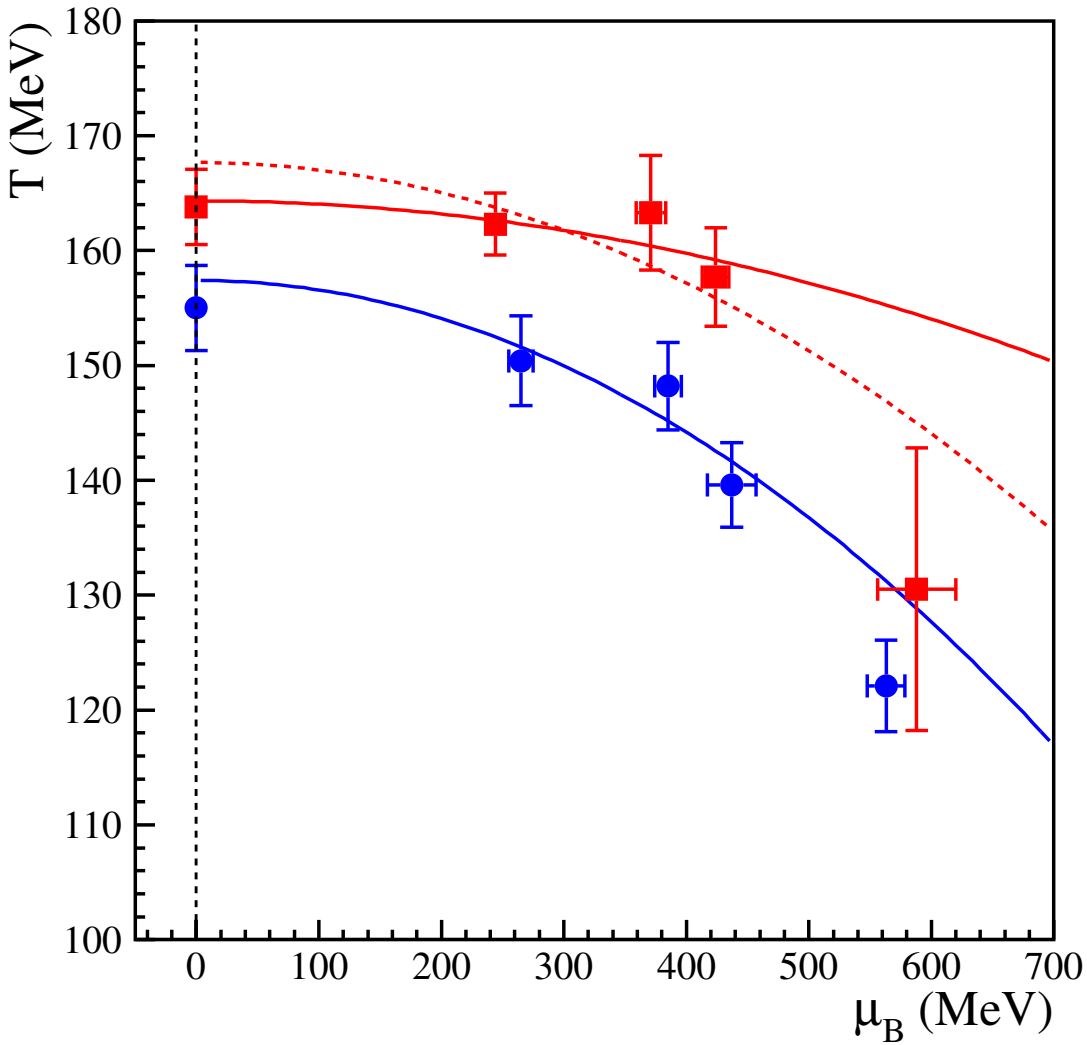
Conclusions

- The QCD phase diagram can be reliably studied for small μ_B using first principle lattice computations.
- In the past years consensus was reached on the value of $T_c(\mu_B = 0) \simeq 150\,\mathrm{MeV}$ for the (pseudo)critical temperature obtained from chiral observables.
- Results obtained in the last couple of years are converging on the value $0.1 \lesssim \kappa \lesssim 0.175$ for the curvature of the (pseudo)critical line obtained from chiral observables.
- The residual tension between the results obtained with the Taylor expansion method and the analytic continuation method is being investigated and it is likely due to an underestimation of the systematics in the first works.

Thank you for your attention!

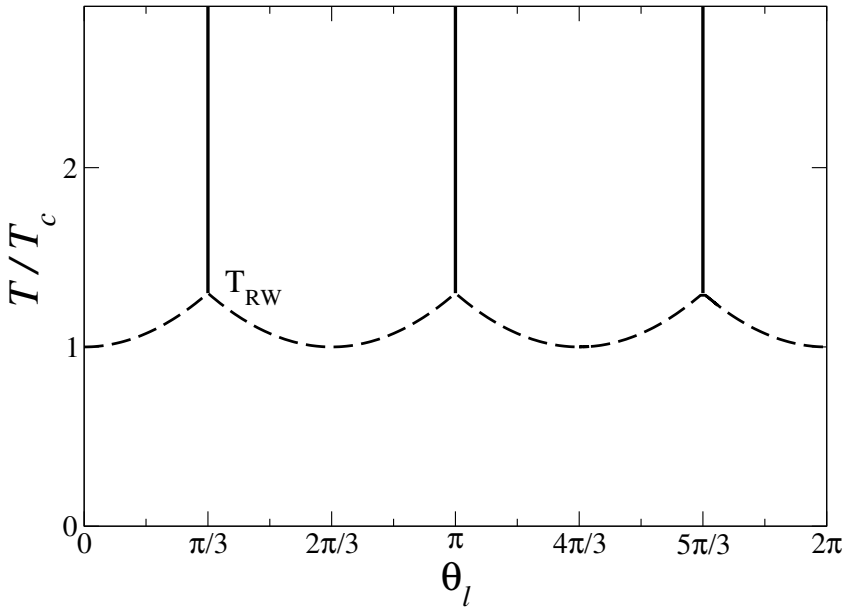
Backup slides with something more

"Real" fit range problem

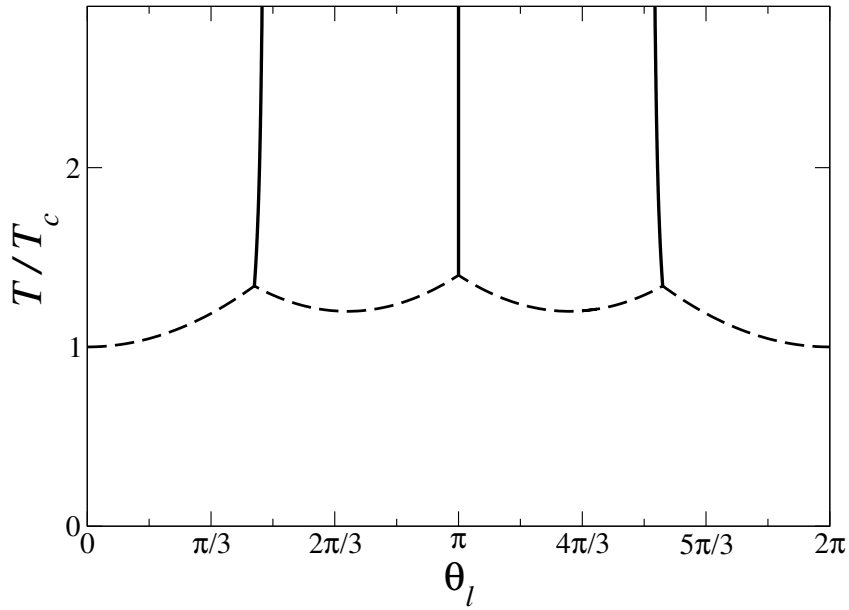


from Becattini et al. PLB 2016

Phase diagram at imaginary chemical potential



$\mu_s = \mu_\ell$, $\theta_\ell = \mu_\ell^I / T$



$\mu_s = 0$, $\theta_\ell = \mu_\ell^I / T$

Lattice technicalities (1)

Kaczmarek et al. PRD (2011)

$N_f = 2+1$ p4 staggered action, $N_t = 4, 8$,
$\mu_u = \mu_d = \mu_B/3$ and $\mu_s = 0$.

Endrodi et al. JHEP (2011)

$N_f = 2+1$ stout fermions, $N_t = 6, 8, 10$,
$\mu_u = \mu_d = \mu_B/3$ and $\mu_s = 0$.

Cea et al. PRD (2014-2015)

$N_f = 2+1$ HISQ, $N_t = 6, 8, 10, 12$,
$\mu_u^I = \mu_d^I = \mu_s^I$, $\mu_B^I \lesssim 380\,\mathrm{MeV}$.

Lattice technicalities (2)

Bonati et al. PRD (2014-2015)

$N_f = 2+1$ stout fermions, $N_t = 6, 8, 10, 12$,
$\mu_u^I = \mu_d^I = \mu_B^I/3$, $\mu_s^I = 0$
$\mu_u^I = \mu_d^I = \mu_s^I = \mu_B^I/3$
$\mu_B^I \lesssim 400\,\mathrm{MeV}$

Bellwied et al. PLB (2015)

$N_f = 2+1+1$ stout fermions, $N_t = 10, 12, 16$,
$\mu_Q = 0$ and strangeness neutrality,
some tests with $Q/B = 0.4$,
$\mu_B^I \lesssim 300\,\mathrm{MeV}$.

Hegde et al. (Lattice 2015)

$N_f = 2+1$ HISQ action, $N_t = 6$,
$\mu_\ell \equiv \mu_u = \mu_d$ and μ_s.

Lattice technicalities (3)

Renormalized chiral condensate:

- Cheng et al. PRD (2008)

$$\langle\bar{\psi}\psi\rangle^r_{(1)}(a,T) = \frac{\langle\bar{\psi}\psi\rangle_\ell(a,T) - \frac{2m_\ell}{m_s}\langle\bar{\psi}\psi\rangle_\ell(a,T)}{\langle\bar{\psi}\psi\rangle_\ell(a,T=0) - \frac{2m_\ell}{m_s}\langle\bar{\psi}\psi\rangle_\ell(a,T=0)}$$

- Endrodi et al. JHEP (2011)

$$\langle\bar{\psi}\psi\rangle^r_{(2)}(a,T) = \frac{m_\ell}{m_\pi^4}\Big(\langle\bar{\psi}\psi\rangle_\ell(a,T) - \langle\bar{\psi}\psi\rangle_\ell(a,T=0)\Big)$$

Renormalized chiral susceptibility

- Aoki et al. JHEP (2009)

$$\chi_{\bar{\psi}\psi}(a,T) = m_\ell^2\Big(\chi_{\bar{\psi}\psi}(a,T) - \chi_{\bar{\psi}\psi}(a,T=0)\Big)$$

Taylor 3 method

We use

$$\phi(T,\mu) \simeq \phi(T,0) + \mu^2 \left.\frac{\partial\phi(T,\mu)}{\partial\mu^2}\right|_{\mu=0} \equiv A(T) + \mu^2 B(T)$$

and we search for the inflection point temperature $\frac{\partial^2}{\partial T^2}\phi(T,\mu) = 0$:

$$0 = A''(T) + \mu^2 B''(T) \simeq A''(T_c(0)) + A'''(T_c(0))\big(T - T_c(0)\big) + \\ + \mu^2\Big(B''(T_c(0)) + B'''(T_c)\big(T - T_c(0)\big)\Big) .$$

Solving the equation and using $A''(T_c(0)) = 0$ one finds for $T_c(\mu)$ up to $\mathcal{O}(\mu^2)$ the expression

$$T_c(\mu) \simeq T_c(0) - \mu^2 \frac{B''(T_c(0))}{A'''(T_c(0))}$$

CEP hints from $\mu_B^2 < 0$? No!