Topological susceptibility in QCD at high temperature: a status report

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Gauge topology 3: from lattice to colliders
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Outline

Why studying θ dependence at high temperature?

$$\mathcal{L}_{QCD}^{\theta} = \mathcal{L}_{QCD} + \theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F^{a\,\mu\nu} F^{a\,\rho\sigma}$$

θ-dependence = dependence on θ of the vacuum energy $E(\theta)$ (at $T = 0$) or of the free energy $F(\theta, T)$

Why studying on the lattice θ-dependence at high T?

theory: to better understand some nonperturbative features of finite T strongly coupled theories (e.g. to investigate the relevance of instantons at *not so high* temperature and the range of validity of DIGA)

phenomenology: to obtain (under specific cosmological assumptions) upper bounds for the axion scale f_a

The general form of $F(\theta, T)$

$$F(\theta, T) = -\frac{1}{V_4} \log \int [\mathscr{D}A][\mathscr{D}\bar{\psi}][\mathscr{D}\psi] \exp\left(-\int_0^{1/T} \mathrm{d}t \int \mathrm{d}^3x\, \mathcal{L}_\theta^E \right)$$

Assuming analiticity at $\theta = 0$ the free energy density can be written as:

$$F(\theta, T) - F(0, T) = \frac{1}{2}\chi(T)\theta^2 \left[1 + b_2(T)\theta^2 + b_4(T)\theta^4 + \cdots \right] ,$$

and it is easy to see that

$$\chi = \frac{1}{V_4}\langle Q^2 \rangle_0 \qquad b_2 = -\frac{\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2}{12\langle Q^2\rangle_0}$$

$$b_4 = \frac{\langle Q^6\rangle_0 - 15\langle Q^2\rangle_0\langle Q^4\rangle_0 + 30\langle Q^2\rangle_0^3}{360\langle Q^2\rangle_0}$$

and so on, where $\langle \quad \rangle_0$ denotes the average at $\theta = 0$.

Dilute Instanton Gas Approximation

At very high T ($T \gg \Lambda_{QCD}$) one can show that the θ dependence is dominated by weakly interacting objects of topological charge ± 1 and the free energy is given by (Gross, Pisarski, Yaffe 1981)

$$F(\theta, T) - F(0, T) \approx \chi(T)(1 - \cos\theta)$$

so that

$$b_2 = -\frac{1}{12} \quad b_4 = \frac{1}{360} \quad b_{2n} = (-1)^n \frac{2}{(2n+2)!}$$

and the susceptibility scales with the temperature as following

$$\chi(T) \propto m^{N_f} T^{4 - \frac{11}{3}N - \frac{1}{3}N_f}$$

when N_f light flavours are present.

An useful toy model

Quantum mechanics of particle on a circumference (aka quantum rotor)

$$L[x] = \frac{1}{2}\dot{x}^2 - \theta\dot{x}$$

where $x \in [0, 1)$ with periodic b.c.

This is probably the simplest model with θ-dependence and it has been used several times in the past to discuss the peculiarities of θ-related physics in an exactly solvable model: e.g.

(Shulman PR 1968) Jackiw RMP 1980 Asorey, Esteve, Pacheco PRD 1983
Bietenholz, de Forcrand, Gerber 1509.06433 Bonati, D'Elia 1709.10034
Ramamurti, Shuryak, Zahed 1802.10509

It will be useful in the following to "visualize" the problems that are encountered in lattice simulations.

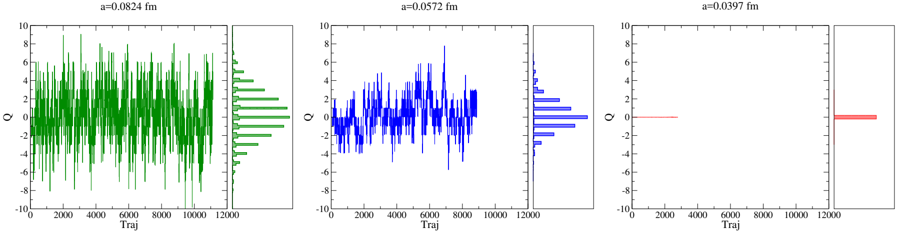
$SU(3)$ with light fermions at or close to the physical point

- Trunin, Burger, Ilgenfritz, Lombardo, Müller-Preussker
  J. Phys. Conf. Ser. **668**, 012123 (2016) [arXiv:1510.02265 [hep-lat]].
- Bonati, D'Elia, Mariti, Martinelli, Mesiti, Negro, Sanfilippo, Villadoro
  JHEP **1603**, 155 (2016) [arXiv:1512.06746 [hep-lat]].
- Petreczky, Schadler, Sharma
  Phys. Lett. B **762**, 498 (2016) [arXiv:1606.03145 [hep-lat]].
- Borsanyi, Fodor, Kampert, Katz, Kawanai, Kovacs, Mages, Pasztor, Pittler, Redondo, Ringwald, Szabo
  Nature **539**, 69 (2016) [arXiv:1606.07494 [hep-lat]].
- Burger, Ilgenfritz, Lombardo, Trunin
  arXiv:1805.06001 [hep-lat].

The problems on the lattice: freezing

As the continuum limit is approached it gets increasingly difficult to correctly sample the various topological sectors.

exponential critical slowing-down

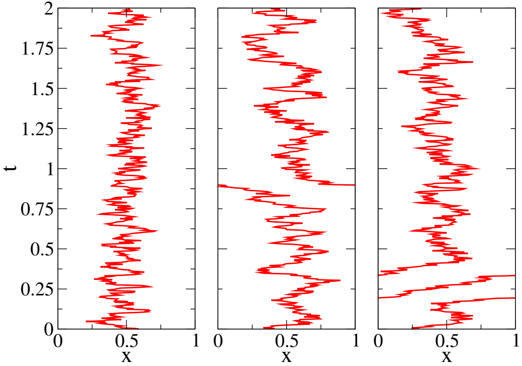


from Bonati, D'Elia, Mariti, Martinelli, Mesiti, Negro, Sanfilippo, Villadoro 1512.06746

The problems on the lattice: freezing

This is an algorithmic problem: basically all the update schemes used in lattice simulations changes the configuration in a way that becomes almost continuous when the lattice spacing gets small.

To change the topological sector we need "large" updates, that are very difficult to achieve.



Examples of configurations from the QM toy model:
(left) $Q = 0$
(center) $Q = -1$
(right) $Q = 2$

The problems on the lattice: slow convergence as $a \to 0$

- Most lattice discretizations of the fermion action introduce an explicit breaking of chiral symmetry, that is recovered only in the continuum limit.
- On the other hand topology is extremely sensitive to chiral symmetry.

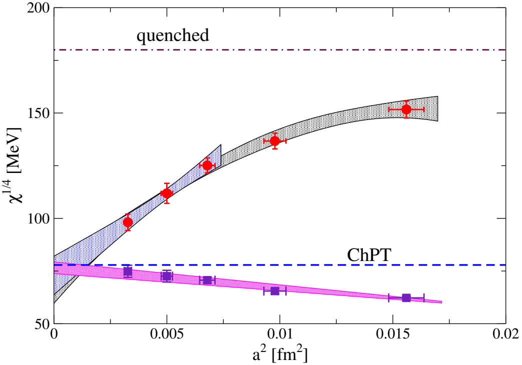
Consequence: large lattice artefacts

Possible way out

- use very fine lattice spacings. Computationally very demanding and sometimes practically impossible due to freezing.
- use a discretization that does not break chiral symmetry (overlap fermions). In simulations with overlap fermions the topological charge is frozen for all the values of the lattice spacing.
- use solid theoretical results to speed up by hand the convergence

The problems on the lattice: slow convergence as $a \to 0$

At $T = 0$ it is possible to use solid theoretical results (χPT) to speed up by hand the convergence.



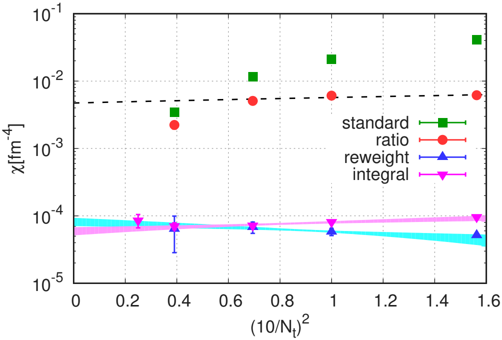
from Bonati et al. 1512.06746, see also Borsanyi et al. 1606.07494

Purple points have been corrected by using the mass of the non-Goldstone pions on the lattice to rescale the results for χ.

The problems on the lattice: slow convergence as $a \to 0$

At $T \neq 0$ proposal by Borsanyi et al. 1606.07494: eigenvalue reweighting.
For staggered fermions the additional weight factor of each configuration should be

$$w[U] = \prod_f \prod_{\substack{would\ be\\ zero\ modes}} \left(\frac{m_f}{i\lambda_n[U] + m_f} \right)^{N_f/4}$$



This procedure strongly reduces both χ and its $a-$dependence.
How significant is the possibility of misidentification of the would be zero modes? (e.g. in case $I\bar{I}$ are present)

The problems on the lattice: finite volume effect

As T gets large we have $\chi(T) \to 0$ and the typical amount of topological fluctuation in a system of volume V_4, $\langle Q^2 \rangle = V_4 \chi(T)$, goes to zero.

The probability $P(Q)$ of observing a configuration with charge Q gets strongly peaked at $Q = 0$ and the sampling becomes very difficult.

This is *not* an algorithmic problem

although from the practical point of view it looks like freezing.

For the quantum rotor it can be seen (using Poisson s.f.) that

$$P(Q) = \frac{\exp(-TQ^2/2)}{\sum_{\mathcal{Q}\in\mathbb{Z}} \exp(-T\mathcal{Q}^2/2)}$$

and $P(1)/P(0) = \exp(-T/2)$: exponentially large (in T) statistics are needed to estimate $\chi(T)$.

The problems on the lattice: finite volume effect

Proposal by Borsanyi et al. 1606.07494: $\sim$ thermodynamic integration.

For $\chi V_4 \ll 1$ one can use ($\beta =$ lattice coupling, not $1/T$)

$$\chi(T) \simeq \frac{1}{V_4}\frac{Z_{-1}+Z_1}{Z_0} = \frac{2}{V_4}\left(\int_{\beta_0}^{\beta}\frac{\mathrm{d}}{\mathrm{d}\bar{\beta}}\frac{Z_1}{Z_0}\mathrm{d}\bar{\beta} + \frac{Z_1(\beta_0)}{Z_0(\beta_0)}\right) \simeq$$

$$\simeq \frac{2}{V_4}\left(\chi(T_0) + \int_{\beta_0}^{\beta}\left(\langle S\rangle_{\bar{\beta},1} - \langle S\rangle_{\bar{\beta},0}\right)\mathrm{d}\bar{\beta}\right)$$

where $\langle\quad\rangle_{\bar{\beta},Q} =$ average computed at fixed topological sector Q.

Two possible objections:

- interaction between instantons is neglected from the beginning
- for expectation values to be computed in a stochastically exact way we need ergodicity

A new approach to the finite volume effect

Multicanonical algorithm (Berg, Neuhaus 9202004) to overcome the "low probability" regions problem: sample a non-physical distribution and reweight the results.

S is the original action, $S' = S - V$ is the modified action

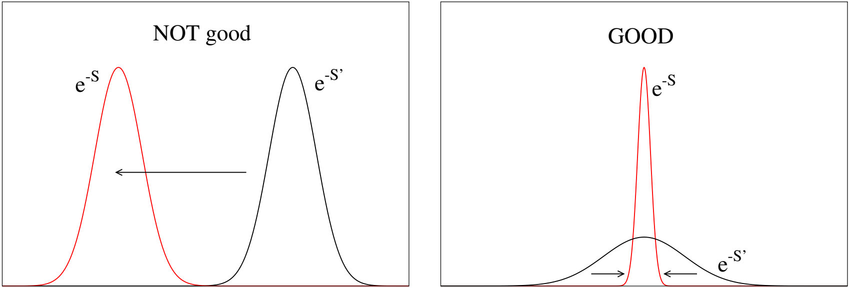
$$\langle \mathcal{O} \rangle_S = \frac{\int \mathcal{O}(x) e^{-S(x)} \mathscr{D}x}{\int e^{-S(x)} \mathscr{D}x} = \frac{\langle \mathcal{O} e^{-V} \rangle_{S'}}{\langle e^{-V} \rangle_{S'}}$$

If the sampling of e^{-S} is "difficult" and the sampling of $e^{-S'}$ is "easy", it is more efficient to use the r.h.s. than the l.h.s.

The algorithm is stochastically exact irrespectively of the specific form of the potential V, however a wise choice is needed to make it efficient.

A possible pitfall

A common pitfall when using reweighting is to extend it beyond its range of applicability, by trying to connect almost orthogonal distributions.

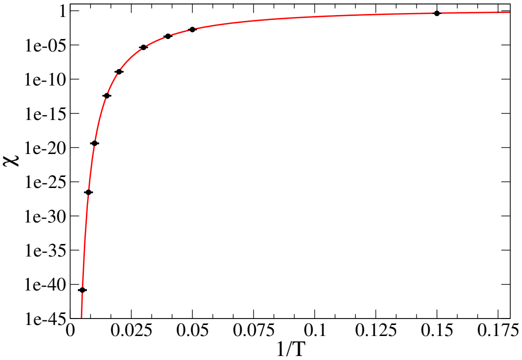


Whenever the state $Q = 0$ is "macroscopically populated" in the distribution $e^{-S'}$ the reweighting is solid.

A simple example of application

For the case of the quantum rotor we know the exact form of $P(Q)$ and we can select V in such a way as to have flat $P'(Q)$ in a given range $[-Q_{max}, Q_{max}]$:

$$V(Q) = \begin{cases} -TQ^2/2 & |Q| \leq Q_{max} \\ -TQ_{max}^2/2 & |Q| > Q_{max} \end{cases}$$



from

Bonati, D'Elia 1709.10034

The QCD case

In the QCD case one can think of proceeding analogously to the quantum rotor case, by adding a potential $V(Q)$ to the action.

Technical difficulty: the simulation algorithm used in QCD (Hybrid Monte Carlo) requires $V(Q)$ to be a differentiable function of the gauge field.

Lattice technicality that solves the difficulty: most of the discretizations of the topological charge used on the lattice are not integer at $a \neq 0$.

Using smoothing techniques (cooling, smearing, ...) one can built discretizations of Q that are more and more peaked at integer values.

Stout smearing has the advantage of being a differentiable smoothing, so we can use $V(Q_L)$, where Q_L is the discretized topological charge defined after some stout smearing steps.

How to choose an appropriate discretization of Q

Q_L has to be the discretized Q defined after some stout smearing steps.

How many steps?

Just a few steps. The distribution of Q_L has almost no peak on integer values (good for HMC) and Q_L has negligible overlap with the "true" integer valued topological charge (bad for the sampling)

A lot of steps. The distribution of Q_L is strongly peaked on integer values (bad for HMC) and Q_L has high overlap with the "true" integer valued topological charge (good for the sampling)

In practice it was found that $10 \div 20$ smearing steps (depending on the lattice spacing) are a good compromise.

The potential V

The form of the potential V is not critical for the exactness of the method (but remember the pitfall) but it is important for the practical effectiveness of the approach.

We tested several possibilities (on $[-Q_{max}, Q_{max}]$ and extended to constant outside this interval):

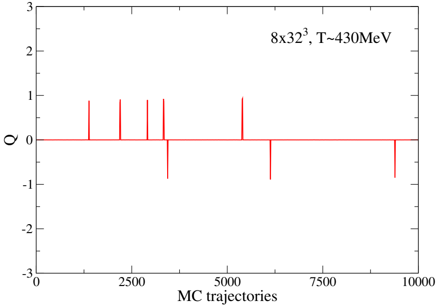
$V(Q) = bQ^2$: most natural choice at $T = 0$ but at high T it tends to oversample the large $|Q|$ region (pitfall danger)

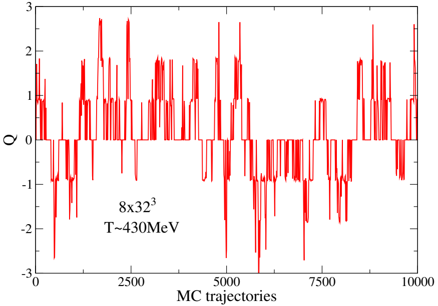
$V(Q) = b|Q|$: DIGA inspired choice, problems at $Q = 0$ likely due to the non-differentiability

$V(Q) = \sqrt{b^2 Q^2 + \epsilon}$: it seems DIGA for large $|Q|$ and it does not oversample this region, no problems at $Q = 0$. It works

An example of application of the method

QCD with $N_f = 2+1$ flavours at physical masses, $Q_{max} = 3$ $b = 6$, $\epsilon = 2$

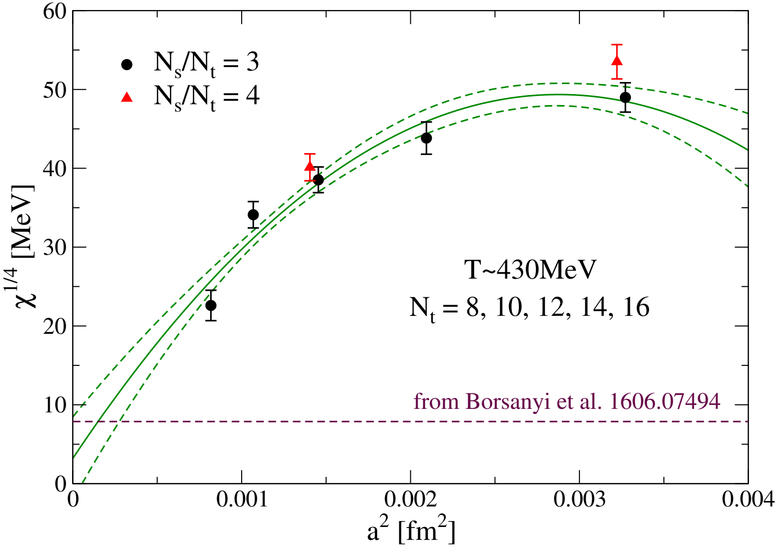




$$a^4\chi = (4.1 \pm 1.6) \times 10^{-8} \qquad a^4\chi = (6.1 \pm 1.1) \times 10^{-8}$$

The error computation is much more solid (no more rare events) and taking into account the computational overhead of the method ($\lesssim 50\%$), we have a $\simeq 45\%$ improvement in efficiency.

Preliminary continuum limit



Discussion and possible improvements

- for larger T the method becomes much more convenient since $\chi \to 0$, moreover for higher T the overhead also gets smaller
- still room for further coding improvements to reduce the overhead
- possibility of improving the choice of the potential V
  - use of the systematic iterative procedure described by Berg, Neuhaus 9202004
  - use out-of-equilibrium methods like metadynamics (Laio, Parrinello 0208352, Laio, Martinelli, Sanfilippo 1508.07270)
- possibility of reducing also the freezing problem using the same algorithm with a proper choice of the potential

Conclusions

- Lattice investigations of topology in QCD at high T continue to be very challenging
- Notwithstanding these difficulties LQCD simulations remain the fundamental tool to investigate these topics at moderately high T and huge improvements have been obtained in recent years (and maybe something new is behind the corner)
- A short term important goal is to perform accurate and unbiased studies to investigate the possible sources of systematics that are present in the different approaches, to be sure that we are not missing something important.

Thank you for your attention!

Backup slides with something more

Possible solutions of the strong CP problem

1. At least a massless quark ($m_u = 0$).
2. Assume a CP invariant lagrangian for the standard model and explain CP violation by CP SSB.
3. "Dynamical" θ angle.

Realization of mechanism 3: add to SM a pseudoscalar field a with coupling $\frac{a}{f_a} F\tilde{F}$ and only derivative interactions. Since the free energy has a minimum at $\theta = 0$, a will acquire a VEV such that $\theta + \frac{\langle a \rangle}{f_a} = 0$.

Goldstone bosons have only derivatives coupling, so the simplest possibility is to think of a as the GB of some $U(1)$ axial symmetry (Peccei-Quinn symmetry). The effective low-energy lagrangian is thus

$$\mathcal{L} = \mathcal{L}_{QCD} + \frac{1}{2}\partial_\mu a \partial^\mu a + \left(\theta + \frac{a(x)}{f_a}\right) q(x) + \frac{1}{f_a}\left(\substack{\text{model dependent}\\ \text{terms}}\right)$$

Axions as dark matter

Cosmological sources of axions: 1) thermal production 2) decay of topological objects 3) misalignment mechanism

Idea of the misalignment mechanism: the EoM of the axion is

$$\ddot{a}(t) + 3H(t)\dot{a}(t) + m_a^2(T)a(t) = 0$$

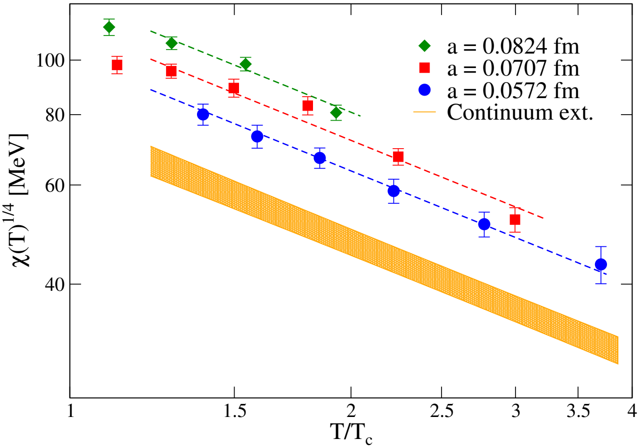
at $T \gg \Lambda_{QCD}$ the second term dominates and we have $a(t) \sim \mathrm{const}$ (assuming $\dot{a} \ll H$ initially); when $m_a \sim H$ the field start oscillating arount the minimum. When $m_a \gg H$ a WKB-like approx. can be used

$$a(t) \sim A(t) \cos \int^t m_a(\tilde{t}) \mathrm{d}\tilde{t}; \qquad \frac{\mathrm{d}}{\mathrm{d}t}(m_a A^2) = -3H(t)(m_a A^2)$$

and thus the number of axions in the comoving frame $N_a = m_a A^2 / R^3$ is conserved.

Overclosure bound: axion density $\leq$ dark matter density

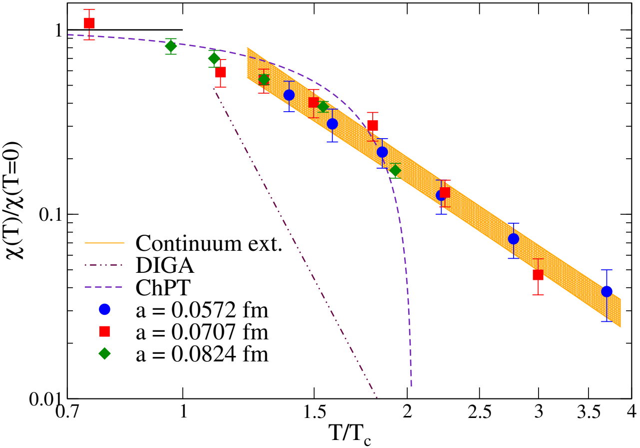
Results from 1512.06746 (Bonati et al.)



fit with $\chi(T)^{1/4} = A_0(1 + A_1 a^2)(T/T_c)^{A_2}$

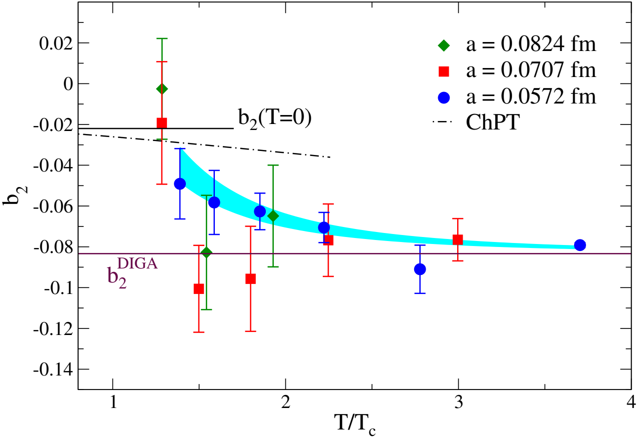
strong lattice artefacts and $4A_2 \simeq -3$.

Results from 1512.06746 (Bonati et al.)



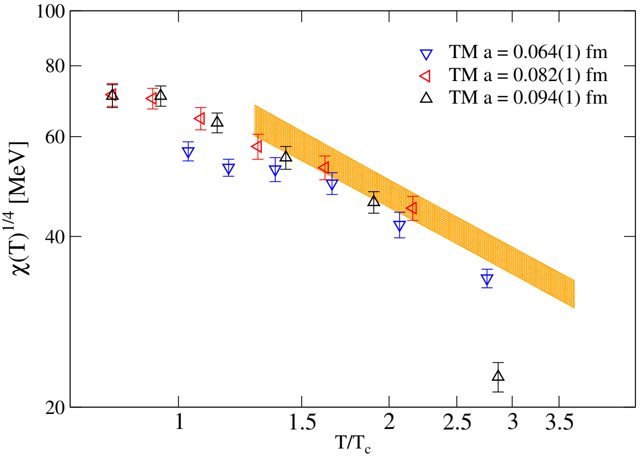
All the (visible) lattice artefacts disappears in the ratio, still $\chi(T) \sim T^{-3}$

Results from 1512.06746 (Bonati et al.)



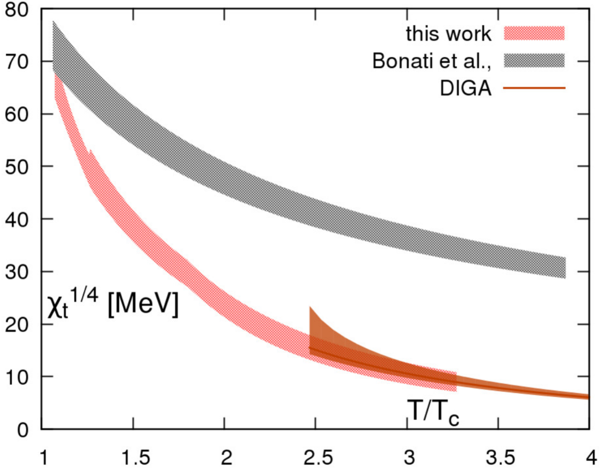
Convergence to the asymptotic value slower than in pure gauge theory, convergence from above.

Results from 1512.06746 (Bonati et al.)



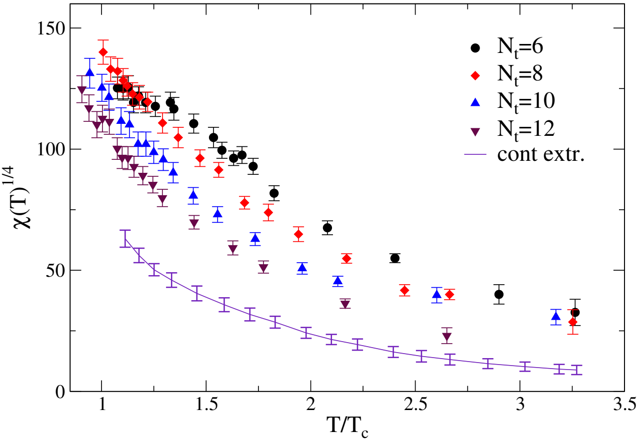
Comparison with the result by Trunin et al.,
$\chi(T)$ rescaled by $m_q^2 \sim m_\pi^4$.

Results from 1606.03145 (Petreczky et al.)



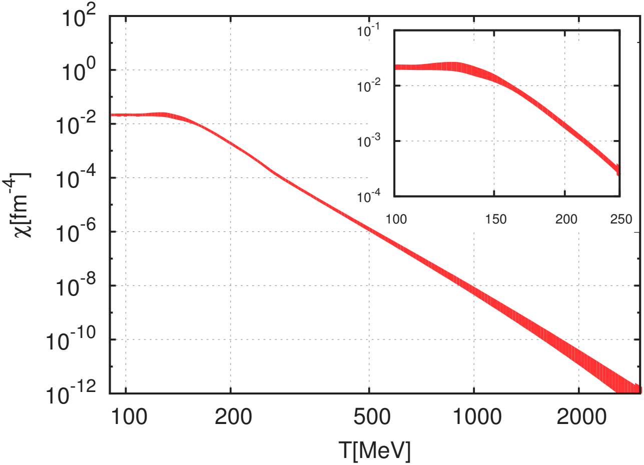
Result close to the DIGA value.

Results from 1606.03145 (Petreczky et al.)



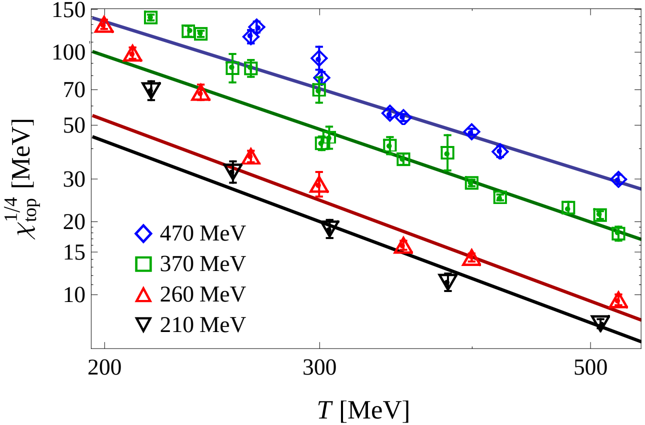
But again large lattice artefacts.

Results from 1606.07494 (Borsanyi et al.)



Result compatible with DIGA

Results from 1805.06001 (Burger et al.)



Results from 1805.06001 (Burger et al.)