Topological susceptibility in high temperature QCD:
a new investigation with spectral projectors and a comparison with other approaches

Based on the join work with:
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- ***Axions***
- ***LQCD & Axions***
- ***Recent results & Outlook***

Narcissus by Caravaggio

Caravaggio

Axions were originally proposed to deal with the strong CP problem

Massless QCD $$\mathcal{L}_{QCD} = \sum_{i=1}^{N_f} \bar{\psi}_a^i \not{D}_{ab} \psi_b^i - \frac{1}{4} G_{\mu\nu}^A G_A^{\mu\nu}$$

Symmetries @ the classical level

$$U(N_f)_L \times U(N_f)_R \sim SU(N_f)_L \times SU(N_f)_R \times U(1)_L \times U(1)_R$$

Non trivial vacuum (quark condensate $\langle \bar{\psi}\psi \rangle \neq 0$) breaks spontaneously non singlet chiral symmetries

$$SU(N_f)_L \times SU(N_f)_R \to SU(N_f)_V$$

$U(1)_V$ is the conserved barion number

Diagonalized mass terms

$$\mathcal{L}_m = -\sum_{i=1}^{N_f} \left(m_i \, \bar{\psi}_L^i \psi_R^i + m_i^* \, \bar{\psi}_R^i \psi_L^i \right)$$

Explicitely broken symmetries:

if the masses are different from zero $SU(N_f)_A$ is broken

$SU(N_f)_V$ is broken if the masses are not equal

ANOMALY: we have to introduce a regularization

Two examples:

a) GW fermions: the action is invariant under a global chiral transformation but the fermion measure is not invariant (Fujikawa)

b) Wilson fermions: the action is not invariant but the measure is invariant

a) GW fermions: if we rotate the quark fields by a phase

$$\psi_i \to e^{i\alpha_i}\,\psi_i \quad \bar{\psi}_i \to \bar{\psi}_i\, e^{i\alpha_i}$$

Then, because of the variation of the measure, the action is modified as $\mathcal{L}_{QCD} + \mathcal{L}_{\{m_i\}} \to$

$$\mathcal{L}_{QCD} + \mathcal{L}_{\{m_i e^{2i\alpha_i}\}} + \left(\theta + \sum_{i=1}^{N_f} 2\alpha_i\right) \frac{N_f g^2}{32\pi^2} G^A_{\mu\nu} \tilde{G}^{\mu\nu}_A$$

Indeed the functional integral depends on the invariant combination

$$det[m_f]e^{-i\theta}$$

and if we apply a rotation to make the masses real (and positive)

$$\theta \to \theta - arg[det[m_f]]$$

$$\delta \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-S} =$$

$$i \int d^4x \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \alpha(x) \left[\partial_\mu J^5_\mu(x) - 2m\bar{\psi}\gamma_5\psi(x) - \frac{N_f g^2}{32\pi^2} G^A_{\mu\nu} \tilde{G}^{\mu\nu}_A(x) \right] e^{-S}$$

From the rotation of the Action

From the rotation of the fermion measure

TOPOLOGICAL CHARGE DENSITY AND SUSCEPTIBILITY

$$Q(x) = \frac{g^2}{32\pi^2} G^A_{\mu\nu} \tilde{G}^{\mu\nu}_A(x) \qquad \int d^4x \, Q(x) = n$$

$$Q(x) = -\frac{1}{2} \mathrm{Tr}\left[\gamma_5 D(x,x)\right] \qquad \chi_t = \int d^4x \, \langle Q(x) Q(0) \rangle$$

M. Luscher, Phys. Lett. B428 (1998) 342

b) Wilson Fermions: if we rotate the quark fields by a phase

$$\psi_i \to e^{i\alpha_i}\,\psi_i \quad \bar{\psi}_i \to \bar{\psi}_i\, e^{i\alpha_i}$$

then the variation of the action is given by (Bochicchio & al.)

$$\delta S = i\alpha(x)\ \left[\partial_\mu J^5_\mu(x) - 2M\bar{\psi}\gamma_5\psi(x) + X_5(x)\right]$$

where the last term is the chiral rotation of the Wilson term:

$$\bar{X}_5(x) = \bar{Z}_5\left[X_5(x) - 2\bar{M}\bar{\psi}\gamma_5\psi - (\bar{Z}_J - 1)\partial_\mu J^5_\mu(x) + Z_{G\tilde{G}}\frac{N_f g^2}{32\pi^2}G^A_{\mu\nu}\tilde{G}^{\mu\nu}_A(x)\right]$$

where the matrix elements of the operator on the l.h.s. are of O(a) (or a^2 with improved actions and operators)

$$\bar{Z}_J\partial_\mu J^5_\mu(x) - 2\bar{m}\bar{\psi}\gamma_5\psi(x) - Z_{G\tilde{G}}\frac{N_f g^2}{32\pi^2}G^A_{\mu\nu}\tilde{G}^{\mu\nu}_A(x) + O(a) = 0$$

The θ term and the strong CP problem

- Because of the anomaly QCD depends, in general, on a parameter θ
- A priori θ can have any value; physics invariant for $\theta \to \theta + 2\pi$
- This parameter gives rise to CP (P) violation
- Neutron EDM $\leq 2.9\ 10^{-26}$ e . cm implies $\theta \leq 10^{-9} - 10^{-10}$

Several possibilities among which:

-The mass of one quark is equal to zero

-Peccei-Quinn symmetry and the axion (Weinberg-Wilczek); see also M. A. Shifman, A. I. Vainshtein and V. I. Zakharov; A. R. Zhitnitsky, M. Dine, W. Fischler and M. Srednicki, …. etc.

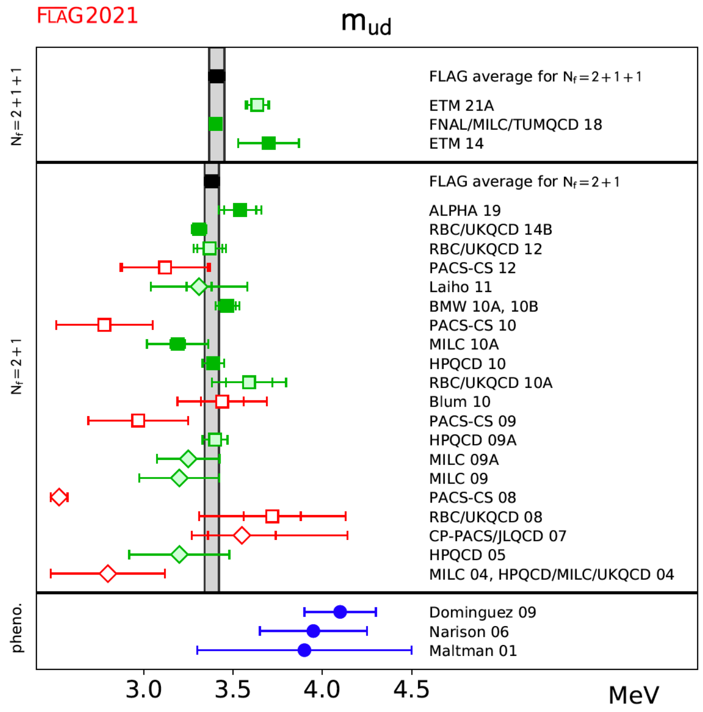


Figure 2: Mean mass of the two lightest quarks, $m_{ud} = \frac{1}{2}(m_u + m_d)$. The bottom panel shows results based on sum rules [205, 208, 210] (for more details see Fig. 1).

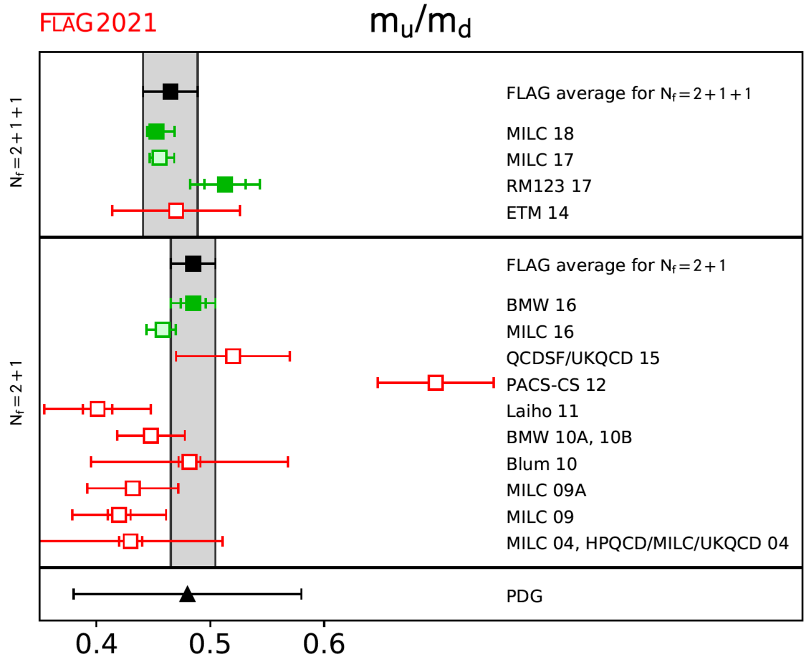


Figure 4: Lattice results and FLAG averages at $N_f = 2+1$ and $2+1+1$ for the up-down-quark masses ratio m_u/m_d, together with the current PDG estimate.

N_f	m_u	m_d	m_u/m_d	R	Q
2+1+1	2.14(8)	4.70(5)	0.465(24)	35.9(1.7)	22.5(0.5)
2+1	2.27(9)	4.67(9)	0.485(19)	38.1(1.5)	23.3(0.5)

Table 11: Our estimates for the masses of the two lightest quarks and related, strong isospin-breaking ratios. Again, the masses refer to the $\overline{\text{MS}}$ scheme at running scale $\mu = 2\,\text{GeV}$. Mass values are given in MeV.

The common lore

1) Implement a continuum $U(1)_{PQ}$ global chiral symmetry by adding extra particles (scalars, fermions);

2) The symmetry is spontaneously broken and this gives rise to a Goldstone boson, **the axion;**

3) Since the quark masses are different from zero the pseudo-Goldstone boson has a non zero mass which depends on the quark masses.

At low energy, neglecting heavy degrees of freedom, the effective action is given by

$$\mathcal{L} = \mathcal{L}_{SM} + \frac{1}{2}\partial_\mu\phi\partial^\mu\phi + \mathcal{L}_{int}\left[\bar{\psi}, \psi, \partial_\mu\phi\right] + \left(\theta + \frac{\phi}{f_\phi}\right)\frac{g^2}{32\pi^2}G^A_{\mu\nu}\tilde{G}^{\mu\nu}_A(x)$$

where f_ϕ depends on the particular model.

This action, if not for the anomaly, is invariant under the non linear $U(1)_{PQ}$ transformation $\phi \to \phi + \alpha f_\phi$.

Let us define an effective axion action

$$e^{-S_{\mathit{eff}}(\partial_\mu\phi,\phi)} = \int \mathcal{D}\left[\psi, \bar{\psi}, G^A_\mu \dots\right] e^{-S\left(\psi,\bar{\psi},G^A_\mu,\dots,\partial_\mu\phi,\phi\right)}$$

Minimizing the Axion Potential

$$e^{-S_{\mathit{eff}}(\partial_\mu\phi,\phi)} = \int \mathcal{D}\left[\psi,\bar{\psi},G_\mu^A\ldots\right] e^{-S\left(\psi,\bar{\psi},G_\mu^A,\ldots,\partial_\mu\phi,\phi\right)}$$

The minimum of the effective potential

$$\frac{\partial V_{\mathit{eff}}}{\partial\phi} = -\frac{1}{f_\phi}\,\frac{g^2}{32\pi^2}\langle G_{\mu\nu}^A \tilde{G}_A^{\mu\nu}(x)\rangle = 0$$

corresponds to $\varphi/f_\phi = -\vartheta$ and solve the strong CP problem; from the second derivative of the effective potential we may compute the axion mass

$$m_\phi^2 = \frac{1}{f_\phi^2}\chi_t = \frac{1}{f_\phi^2}\int d^4x\,\langle Q(x)Q(0)\rangle$$

ZERO TEMPERARTURE AND CHIRAL EXPANSION

2 flavours: the relevant (naïve) Ward identity

$$\chi_t = \frac{1}{4}\langle 0|m_u\bar{u}u + m_d\bar{d}d|0\rangle -$$
$$\frac{1}{4}\int d^4x\,\langle 0|T\left[\left(m_u\bar{u}\gamma_5 u + m_d\bar{d}\gamma_5 d\right)[x]\left(m_u\bar{u}\gamma_5 u + m_d\bar{d}\gamma_5 d\right)[0]\right]|0$$

Expanding at small quark masses and saturating the T-product with Goldstone boson intermediate states we get

$$\chi_t = -\frac{1}{4}f_\pi^2 m_\pi^2 \frac{4m_u m_d}{(m_u+m_d)^2}$$

M. A. Shifman, A. I. Vainshtein and V. I. Zakharov ; W. A. Bardeen and S.-H.H. Tye

The result depends on the number of flavours. For example if we add the strange quark and make an expansion at small quark masses we get

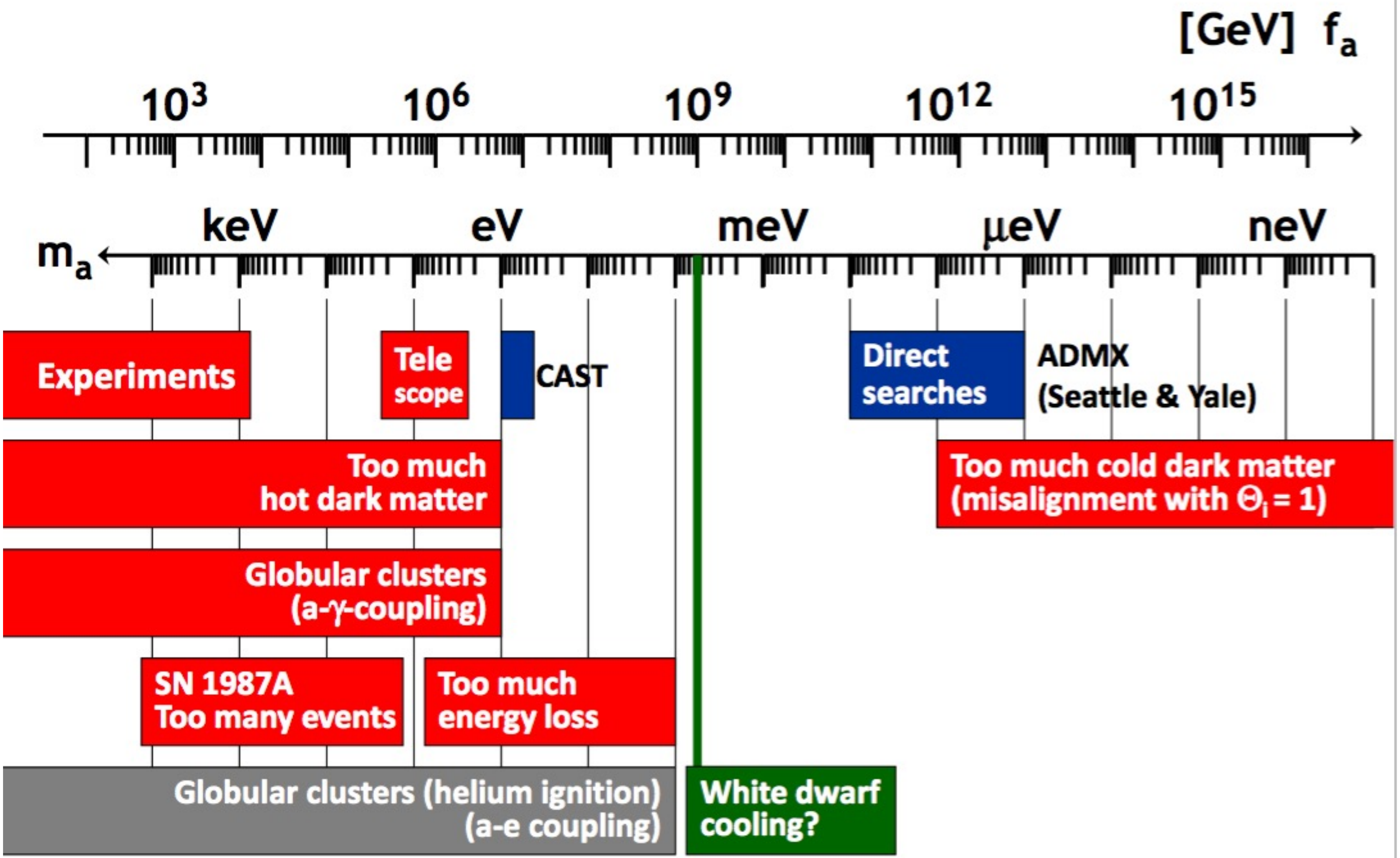
$$\chi_t = -\frac{3}{4} f_\pi^2 \left(m_\pi^2 + m_\eta^2\right) \frac{m_u m_d m_s}{(m_u + m_d + m_s)(m_u m_d + m_d m_s + m_u m_s)}$$

The topological susceptibility, and consequently the mass of the axion, vanishes whenever the mass of a quark is equal to zero. AT ZERO TEMPERATURE WE DO NOT NEED THE LATTICE !

Similar results can be obtained in chiral perturbation theory, where the NLO corrections were recently computed and it was possible to extract the axion mass, self coupling and its full potential at the percent level

P. Di Vecchia and G. Veneziano, Giovanni Grilli di Cortona, Edward Hardy, Javier Pardo Vega, Giovanni Villadoro 1511.02867

Axion Bounds and Searches



Kim-Shifman-Vainshtein-Zakharov (KSVZ) and Dine-Fischler-Srednicki-Zhitnitsky (DFSZ)

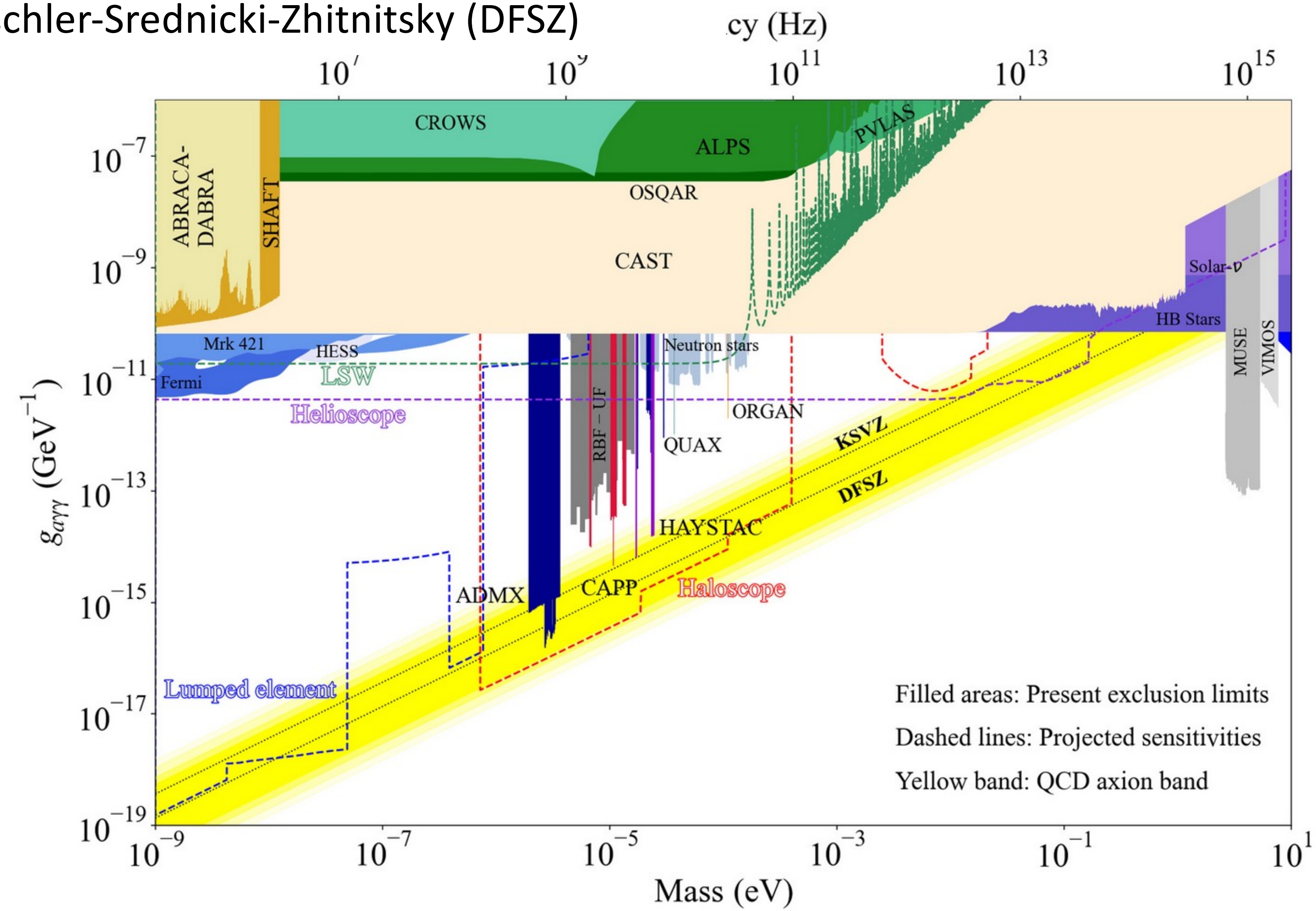


Fig. 3. Up-to-date experimental exclusion limits on the axion-photon coupling versus axion mass.

The projected sensitivities are represented by dashed lines. Two theoretical models are represented by the diagonal dashed lines with the uncertainty band in yellow. Major features of the individual experiments are described in the text. The acronyms of the experiments which are not discussed in the review include CROWS (CERN Resonant Weakly interacting sub-electron volt particle Search), PVLAS (Polarization of the Vacuum with Laser), HESS (High Energy Stereoscopic System), HB (horizontal branch) stars, MUSE (Multi Unit Spectroscopic Explorer) and VIMOS (Visible Multi-Object Spectrograph).

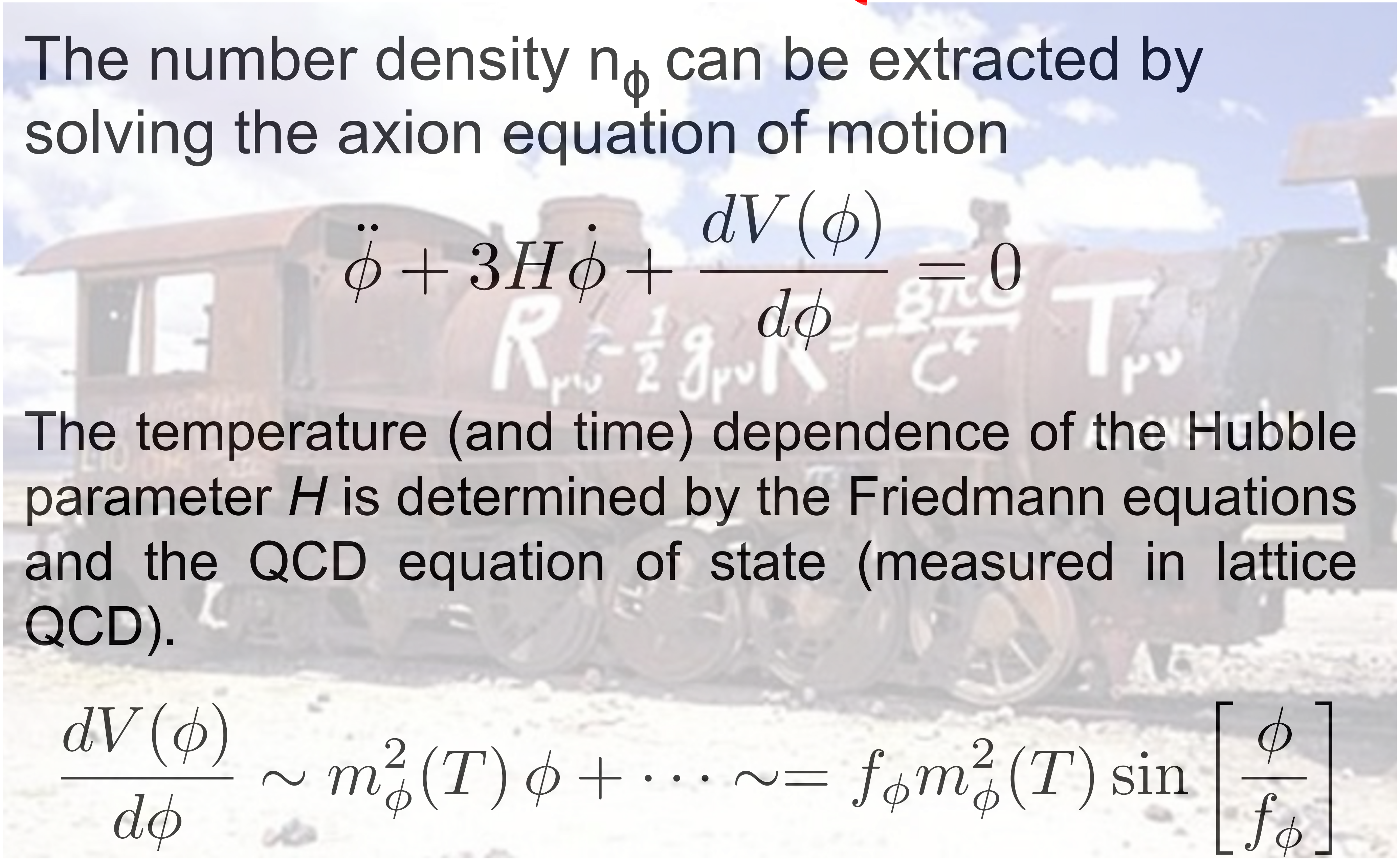
THE AXION PHENOMENOLOGY

Basic Formula:

$$\Omega_\phi = \frac{86}{33} \frac{\Omega_\gamma}{T_\gamma} \frac{n_\phi^\star}{s^\star} m_\phi \, ,$$

where Ω_γ and T_γ are the present abundance and temperature of photons while n_ϕ*/s* is the ratio between the comoving axion number density $n_\phi = m_\phi \, \phi$^2 and the entropy density computed at a late time t* such that the ratio n_ϕ/s became constant

THE AXION EVOLUTION EQUATION



The number density n_ϕ can be extracted by solving the axion equation of motion

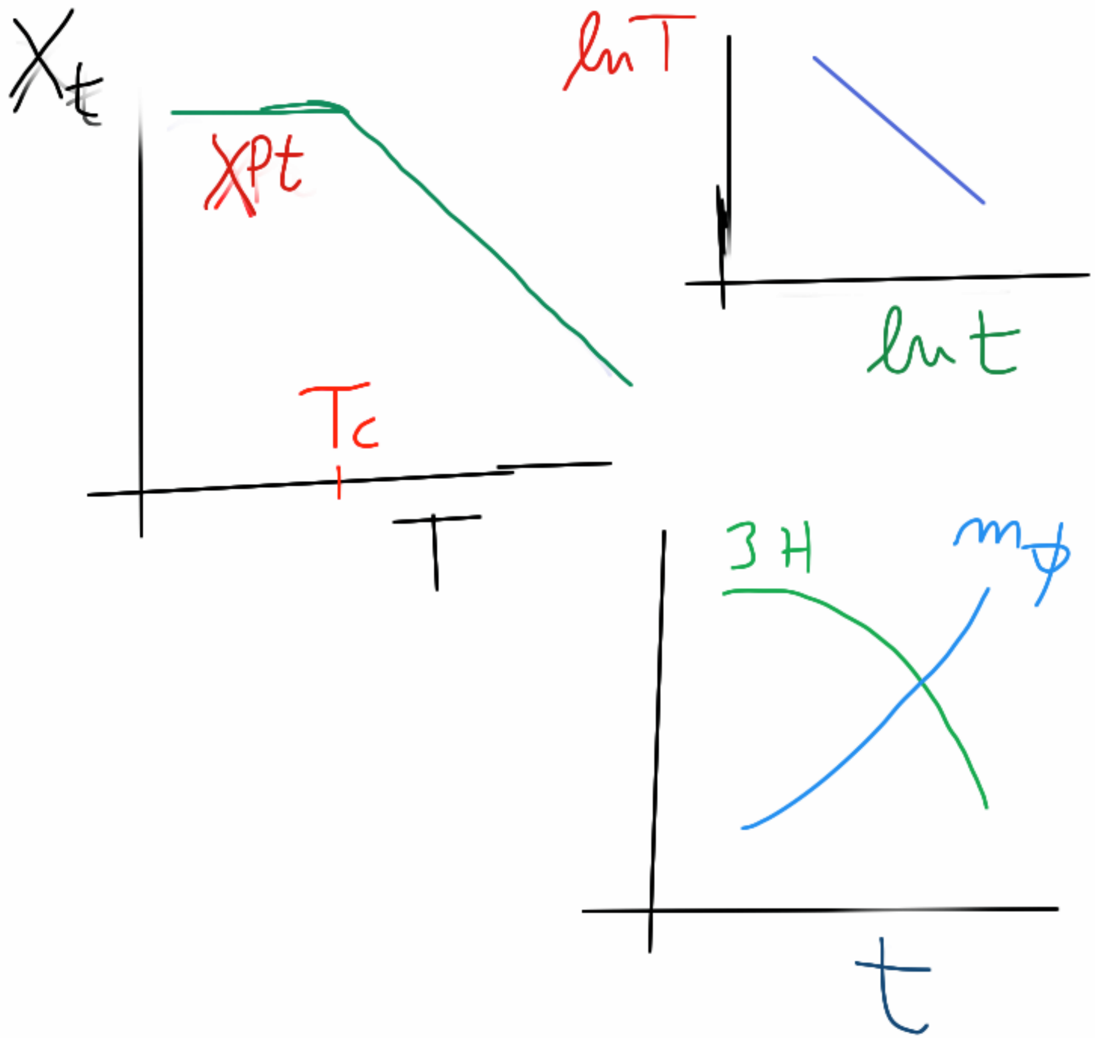
$$\ddot{\phi} + 3H\dot{\phi} + \frac{dV(\phi)}{d\phi} = 0$$

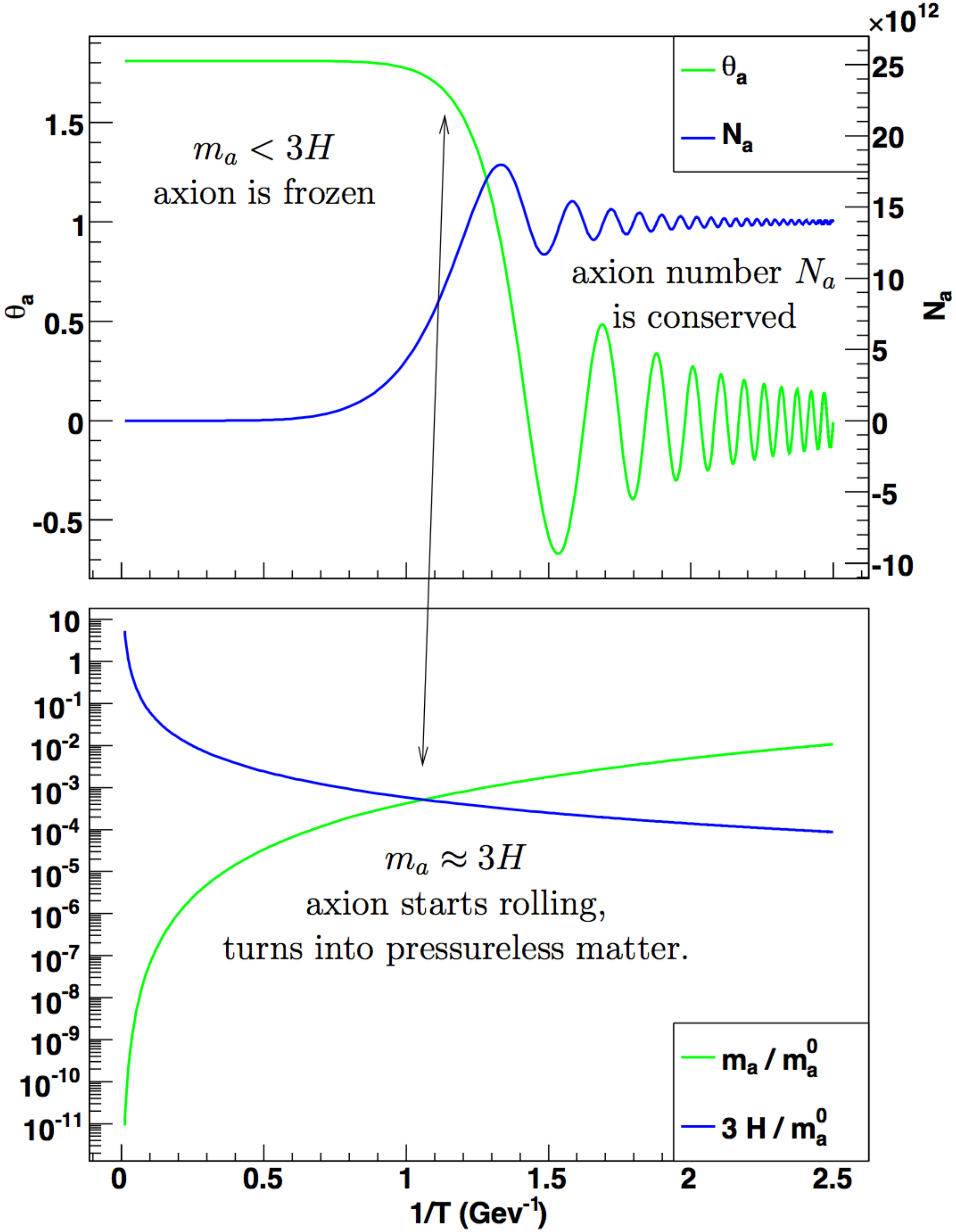
The temperature (and time) dependence of the Hubble parameter *H* is determined by the Friedmann equations and the QCD equation of state (measured in lattice QCD).

$$\frac{dV(\phi)}{d\phi} \sim m_\phi^2(T)\,\phi + \cdots \sim= f_\phi m_\phi^2(T) \sin\left[\frac{\phi}{f_\phi}\right]$$

At high temperatures the Hubble friction wins and the field is frozen to its initial value φ_0. As the Universe cools the pull from the potential wins over the friction (this happens when T ≈ Tosc m_φ (Tosc) ≈ 3 H(Tosc)) and the axion starts oscillating around the minimum.

Shortly after H becomes negligible and the mass term is the leading scale in the evolution equation





Wantz and Shellard

when H becomes negligible and the mass term is the leading scale the approximate WKB solution has the form

$$\phi(t) \sim A(t)\cos\left(\int_{t_0}^{t} dt' m_\phi(t')\right) =$$

$$\phi_0 \left(\frac{(m_\phi)_0 R_0^3}{m_\phi(t) R^3(t)}\right)^{1/2} \cos\left(\int_{t_0}^{t} dt' m_\phi(t')\right)$$

where R(t) is the cosmic scale factor. Since the energy density is given by $\rho_\phi = m^2_\phi A^2/2$, the solution implies that what is conserved in the comoving volume is not the energy density but $N_\phi = \rho_\phi R^3/m_\phi$, which can be interpreted as the number of axions.

Through the conservation of the comoving entropy S, it follows that n^*_ϕ / s^* *becomes adiabatic invariant.*

The biggest uncertainty comes therefore from the temperature dependence of the axion potential $V(\phi)$

THE AXION AT NON ZERO TEMPERATURE

That is WHEN LQCD ENTERS THE GAME

Chiral Lagrangians allow to study the temperature dependence of the axion potential and its mass to finite temperatures below the crossover region $T_c \sim 150$ MeV.

Around T_c there is no known reliable perturbative expansion under control and non-perturbative methods, such as lattice QCD are required.

S. Borsanyi et al., Phys. Lett. B 752, 175 (2016) [arXiv:1508.06917 [hep-lat]]
C. Bonati, M. D'Elia, H. Panagopoulos and E. Vicari, Phys. Rev. Lett. 110, 252003 (2013) [arXiv:1301.7640 [hep-lat]].
C. Bonati, JHEP 1503, 006 (2015) [arXiv:1501.01172 [hep-lat]]
G. Y. Xiong, J. B. Zhang, Y. Chen, C. Liu, Y. B. Liu and J. P. Ma, Phys. Lett. B 752, 34 (2016) [arXiv:1508.07704
A. Trunin, F. Burger, E.-M. Ilgenfritz, M. P. Lombardo and M. Muller-Preussker, arXiv:1510.02265 [hep-lat].
M. I. Buchoff et al., Phys. Rev. D 89, 054514 (2014) [arXiv:1309.4149 [hep-lat]].

Axion properties at zero and finite T from Lattice QCD

$SU(3)$ 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].

C. Bonati, M. D'Elia, G. Martinelli, F. Negro, F. Sanfilippo, A. Todaro
arXiv:1807.07954 [hep-lat]

\+ ......

At zero and non zero temperature T the Axion Potential can be derived from the dependence of the vacuum free energy F[θ,T] on θ

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

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

mass term

Quartic coupling

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

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

Thus for example the axion mass is related to the topological susceptibility

$$m_\phi^2 = \frac{1}{f_\phi^2}\,\chi_t = \frac{1}{f_\phi^2}\int d^4x\,\langle Q(x)Q(0)\rangle$$

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.

Analytical expectations

For $T \ll \Lambda_{QCD}$ we can trade θ-dependence for m-dependence by using a $U(1)_A$ transformation, and perform computations with ChPT (see e.g. Grilli di Cortona, Hardy, Pardo Vega, Villadoro 1511.02867 for NLO).

For $T \gg \Lambda_{QCD}$ semiclassical (DIGA) *and* perturbative computations become reliable and (Gross, Pisarski, Yaffe 1981)

$$\begin{aligned} \mathrm{DIGA}: &\quad F(\theta, T) - F(0, T) \simeq \chi(T)(1 - \cos\theta) \\ \mathrm{PT}: &\quad \chi(T) \propto m^{N_f} T^{4 - \frac{11}{3}N - \frac{1}{3}N_f} \end{aligned}$$

(see also Boccaletti, Nogradi 2001.03383).

The value of $\chi(T)$ for T of the order of GeVs is relevant for axion phenomenology, and Lattice QCD appears to be the only first principle method available to reliably investigate this range of temperatures (Berkowitz et al. 1505.07455).

Numerical problems

Lattice QCD simulations with physical light quarks are notoriously complicated from the computational point of view.

1) Huge lattice artifacts problem: The study of $\chi(T)$ in the high temperature phase is much worst, since topological observables are extremely sensitive to the explicit chiral symmetry breaking of the lattice fermion discretization;

2) Small box problem: At high T we have $\chi(T) \to 0$ the probability P(Q) of observing a configuration with charge Q gets strongly peaked at Q = 0

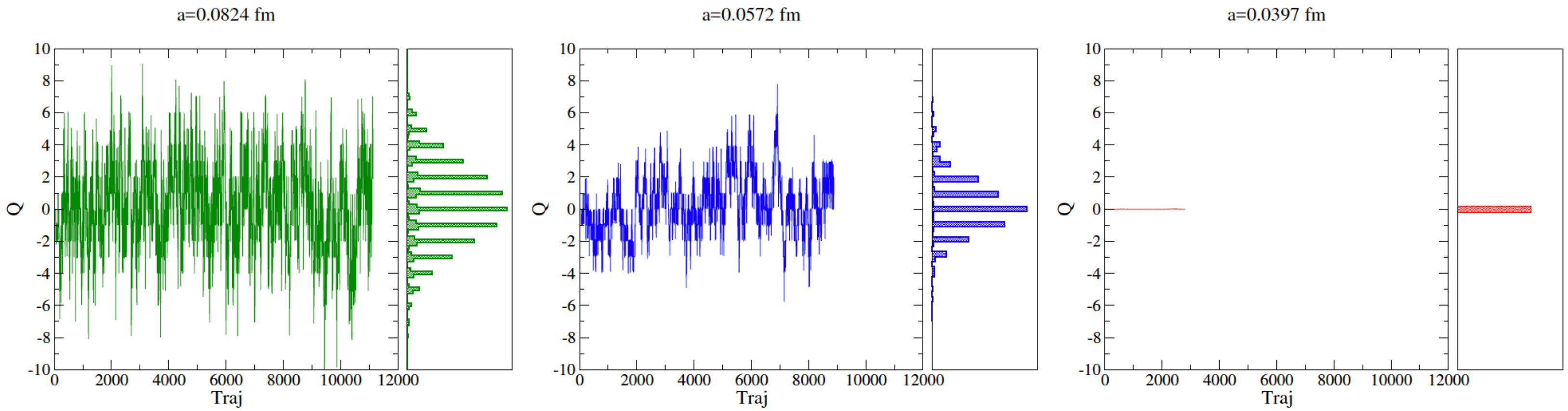
3) Freezing problem: As the continuum limit is approached autocorrelation times grows exponentially fast with the inverse lattice spacing, and simulations get stuck in a fixed topological sector

2) And 3)

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

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

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

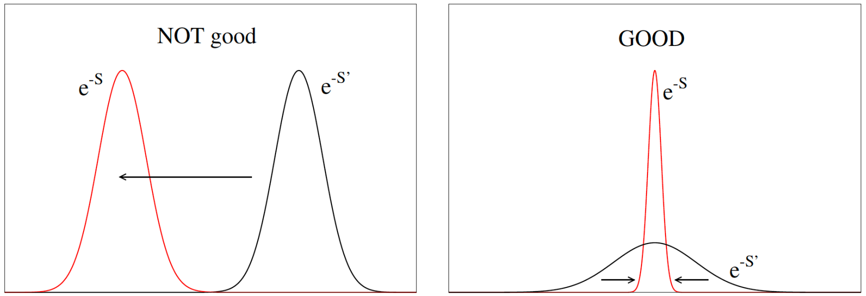
If the sampling of e^{-S} is "difficult" and the sampling of $e^{-S'}$ is "easy", it is more efficient to use the r.h.s. than the l.h.s.

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

To solve the small box problem we use the multicanonical approach - Bonati et al. 1807.07954: a modified distribution is sampled and the results are a posteriori re-weighted (in a stochastically exact way) to extract expectation values for the original distribution.

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.

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.

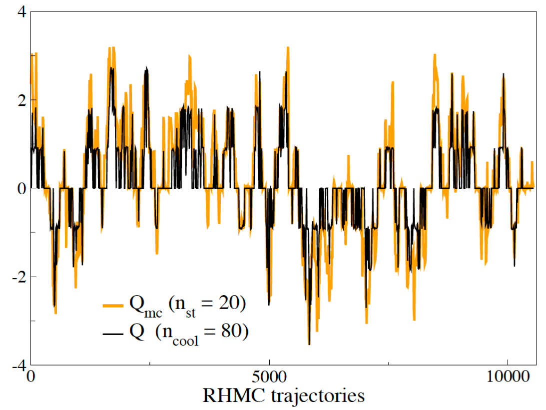


Figure 5. Monte-Carlo history of the topological charges obtained after 80 cooling steps and after 20 stout-smearing steps (with $\rho_{st} = 0.1$), for the run on the $32^3 \times 8$ lattice at $\beta = 4.14$, adopting a bias potential as in Eq.(2.12), with $B = 6$ and $C = 2$, and illustrated in Fig. 3.

Correlation 0.86

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):

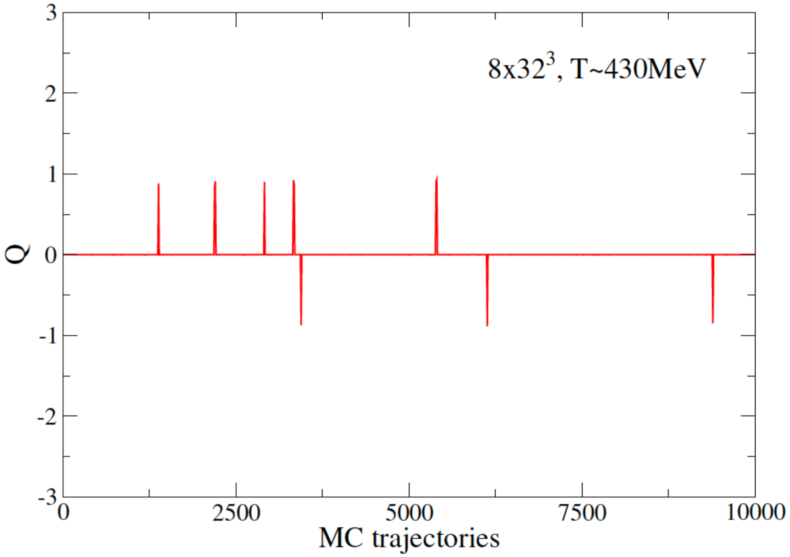
$V(Q) = bQ^2$: most natural choice at $T = 0$ but at high T it tends to oversample the large $|Q|$ region (pitfall danger)

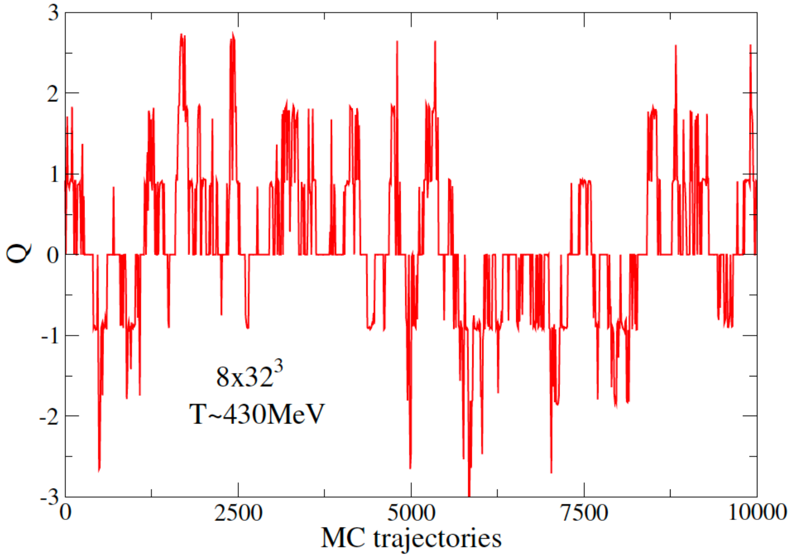
$V(Q) = b|Q|$: DIGA inspired choice, problems at $Q = 0$ likely due to the non-differentiability

$V(Q) = \sqrt{b^2 Q^2 + \epsilon}$: 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.

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

1) Lattice artefacts

To reduce lattice artefacts we use the spectral projectors definition of the topological charge.

This definition was introduced in Giusti & Luscher 0812.3638 for Wilson-type fermion discretizations and was extended to the staggered case in Bonanno, Clemente, D'Elia, Sanfilippo 1908.11832.

At $T = 0$ the spectral projector definition was shown in Alexandrou et al. 1709.06596 to have much smaller discretization errors than the other commonly adopted discretizations. Possible explanation (still to be really understood): since the same Dirac operator is used in the weight of the configuration and in the measure, some discretization effects get cancelled.

Non-chiral fermions and would-be-zero modes

In the QCD path-integral, field configurations are weighted with the determinant of the Dirac operator:

$$\det\{\not{D} + m_q\} = \prod_{\lambda \in \mathbb{R}} (i\lambda + m_q)\,.$$

The Index Theorem relates the presence of zero-modes in the spectrum of $\not{D}$ to the topological charge of the gluon field:

$$Q = \mathrm{Index}\{\not{D}\} = \mathrm{Tr}\{\gamma_5\} = n_+ - n_-.$$

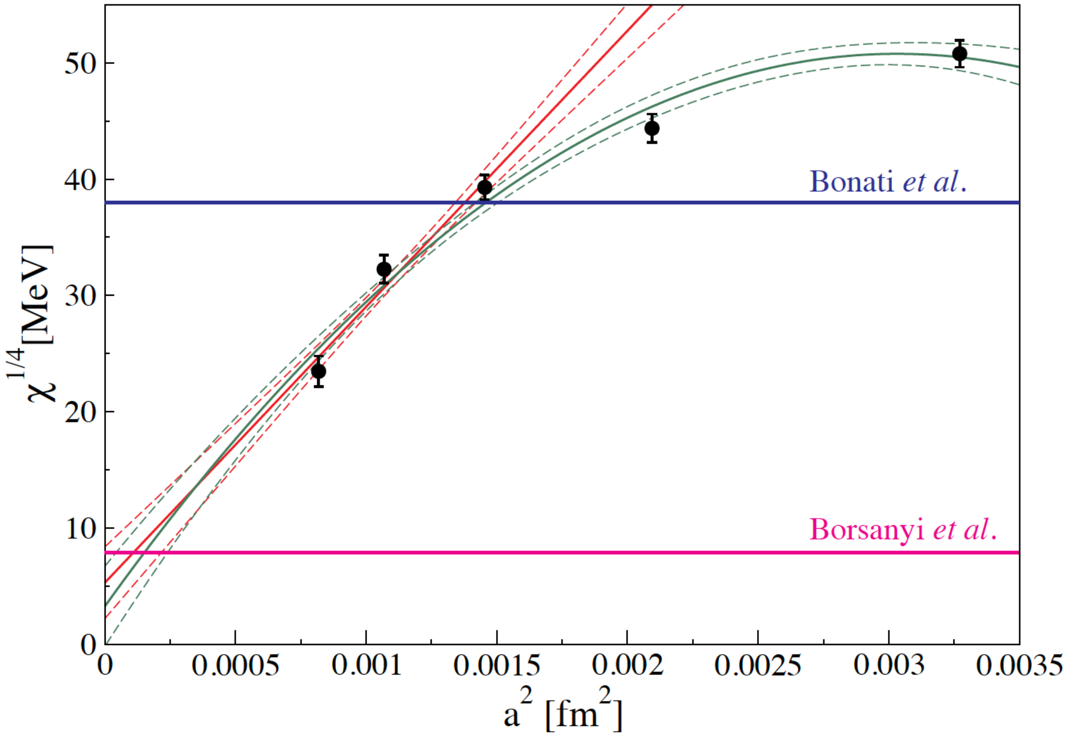
If a configuration has $Q \neq 0$, lowest eigenvalues are $\lambda_{min} = m_q$.

On the lattice, however, some fermionic discretizations (e.g., staggered) do not have exact zero-modes. $\Longrightarrow$ The determinant fails to efficiently suppress non-zero charge configurations.

$$\lambda_{min} = m_q \longrightarrow m_q + i\lambda_0, \qquad \lambda_0 \underset{a\to 0}{\to} 0.$$

Non-chiral fermions and large lattice artifacts

Bad suppression of non-zero charge configurations $\Longrightarrow$ large discretization corrections $\Longrightarrow$ continuum extrapolation not under control (Bonati et al., 2018):



In (Borsanyi et al., 2016) lattice artifacts affecting χ at high-T have been suppressed a posteriori by reweighting configurations with the corresponding continuum lowest eigenvalues of $\not{D}$.

Spectral projectors with staggered fermions

In the continuum, only zero-modes contribute to Q. This is not true on the lattice for staggered fermions, due to the absence of exact zero-modes:

$$Q = \mathrm{Tr}\{\gamma_5\} \longrightarrow \mathrm{Tr}\{\Gamma_5 \mathbb{P}_M\},$$

$$\mathbb{P}_M = \sum_{|\lambda_k| \leq M} u_k u_k^\dagger, \qquad i\not{D}_{stag} u_k = \lambda_k u_k.$$

To avoid a mode over-counting, taste degeneration has to be considered ($n_t = 2^{d/2}$):

$$Q_{0,stag} = \frac{1}{n_t} \mathrm{Tr}\{\Gamma_5 \mathbb{P}_M\}.$$

Lattice charge gets a renormalization $Z_Q^{stag} = \frac{Z_P}{Z_S}$, which can be derived from Ward identities for the flavor-singlet axial current:

$$Q_{stag} = \frac{Z_P}{Z_S} Q_{0,stag}, \qquad \left(\frac{Z_P}{Z_S}\right)^2 = \frac{\langle \mathrm{Tr}\{\mathbb{P}_M\}\rangle}{\langle \mathrm{Tr}\{\Gamma_5 \mathbb{P}_M \Gamma_5 \mathbb{P}_M\}\rangle}.$$

Choice of the cut-off mass M

The choice of the cut-off mass M is irrelevant in the continuum limit. Its renormalized value $M_R = M/Z_S$ must be kept constant as $a \to 0$ to guarantee $O(a^2)$ corrections:

$$\chi_{\mathrm{SP}}(a, M_R) = \chi + c_{\mathrm{SP}}(M_R)a^2 + o(a^2).$$

To avoid the direct computation of Z_S for each lattice spacing, one can observe that, for staggered fermions:

$$m_{q,R} = m_q/Z_S.$$

If a Line of Constant Physics is known, it is sufficient to keep

$$M/m_q = M_R/m_{q,R}$$

constant as $a \to 0$ to have M_R constant too.
Is there an optimal choice for M_R? One would like to have small corrections, i.e., $c_{\mathrm{SP}}(M_R) \ll c_{\mathrm{gluo}}$.

Optimal choice for the cut-off mass M/m_q

Guiding principle: choose M/m_q to include all relevant Would-Be Zero-Modes (WBZMs) in spectral sums. E.g., look at chirality: $r_\lambda = |u_\lambda^\dagger \Gamma_5 u_\lambda|$ vs λ/m_q.

However, distinguishing between WBZMs and non-chiral modes is ambiguous → choose cut-off to include "chiral enough" modes.

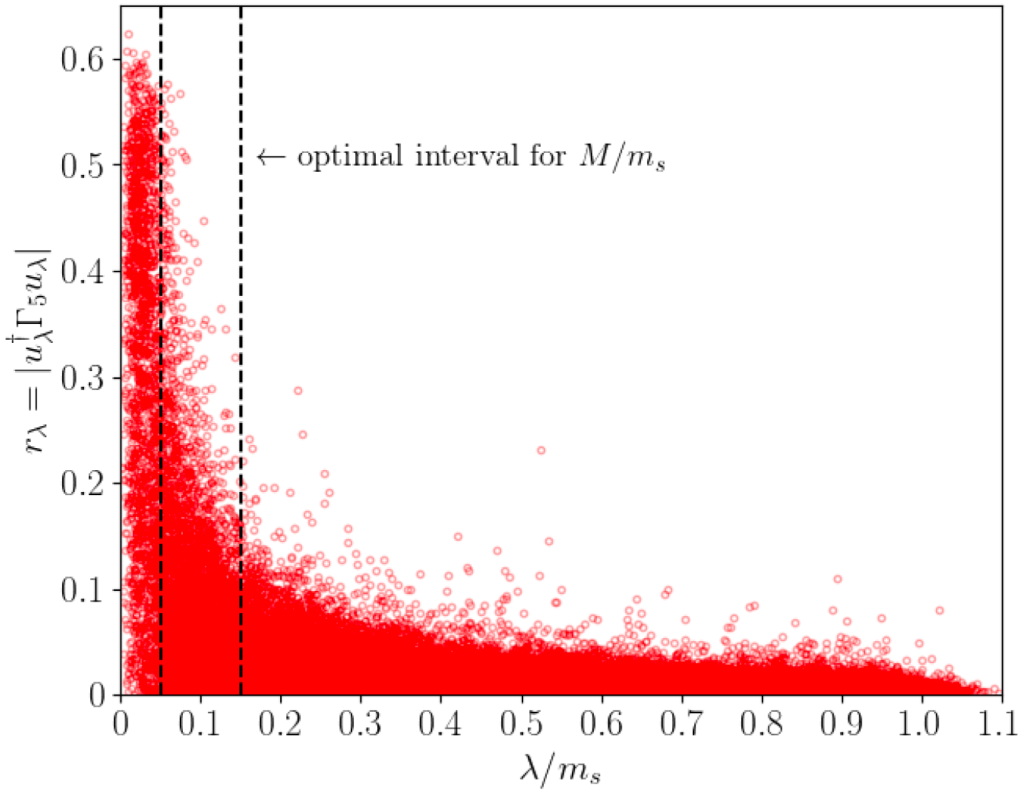


Figure refers to: $N_f = 2{+}1$ QCD, $T \simeq 0$, $V = 48^4$, $a \simeq 0.057$ fm, $m_q = m_s$.

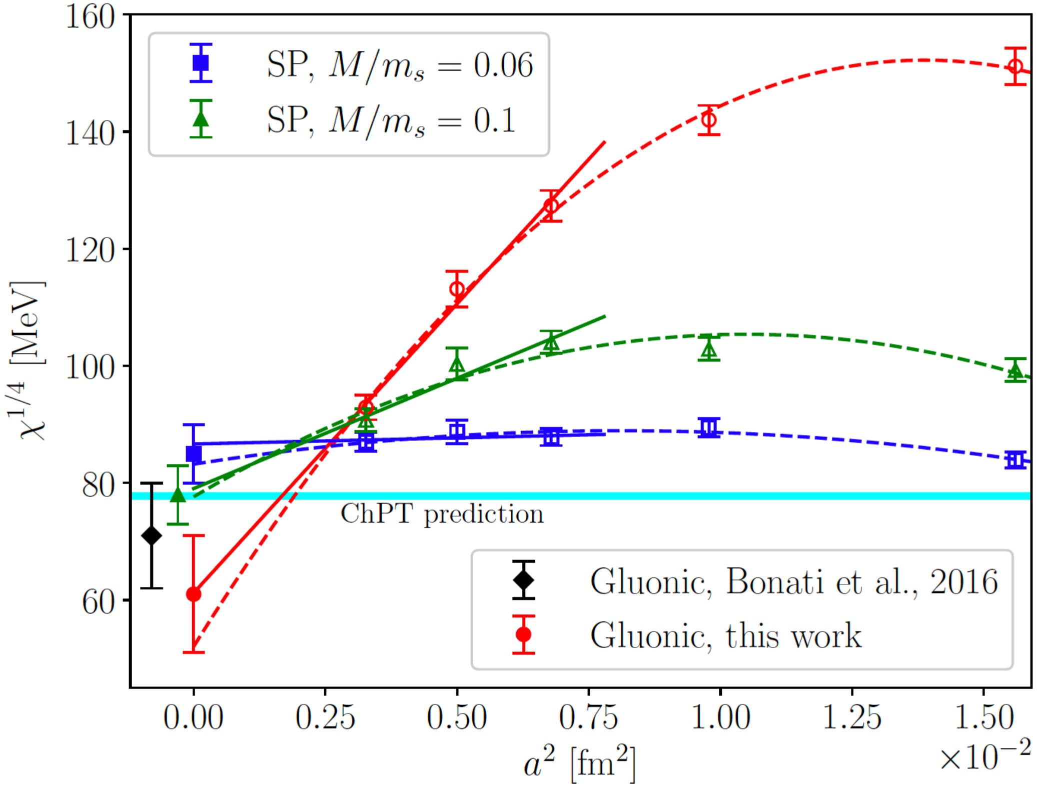
Vertical lines: optimal choices for $M/m_s \in [0.05, 0.15]$.

Continuum limit of $\chi^{1/4}$ at $T = 0$

Lattice Setup: $N_f = 2+1$ rooted stout staggered fermions at physical point.

Expected continuum scaling for Spectral Projectors (SP):

$$\chi_{\rm SP}^{1/4}(a, M/m_s) = \chi^{1/4} + c_{\rm SP}(M/m_s)a^2 + o(a^2).$$



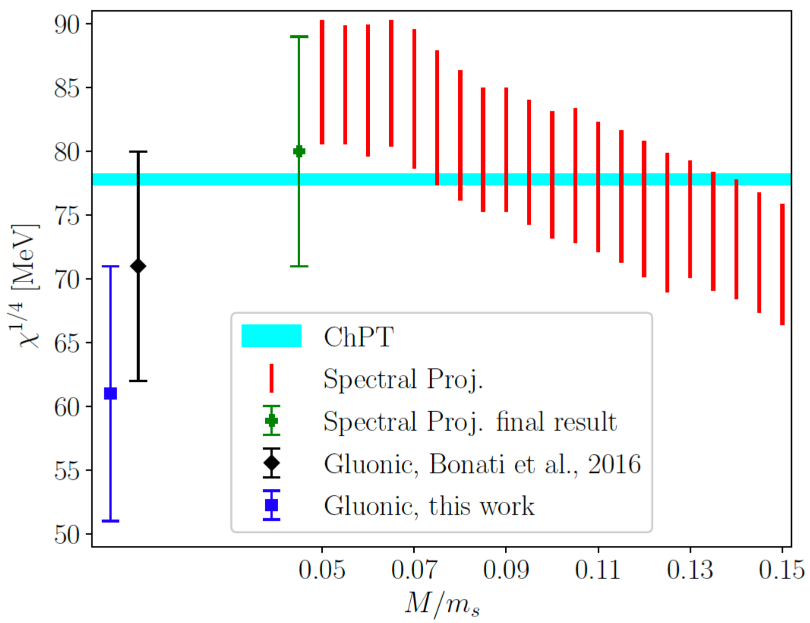
M/m_s inside optimal interval $\rightarrow$ reduction of lattice artifacts: $c_{\rm SP}(0.06)/c_{\rm gluo} \sim 1 \cdot 10^{-2}$, $c_{\rm SP}(0.1)/c_{\rm gluo} \sim 3 \cdot 10^{-1}$.

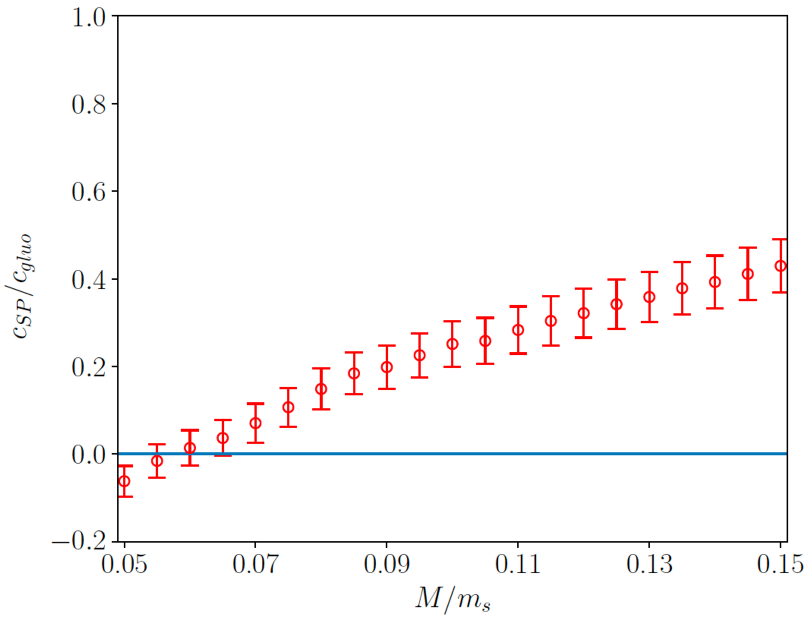
Spectral determination: very good agreement with gluonic and leading order Chiral Perturbation Theory (ChPT) determinations.

Continuum extrapolation $T = 0$ vs M/m_s

Choosing M/m_s inside the optimal range we observe:

- good agreement within the errors for determinations obtained for different values of M/m_s (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation (Fig. on the right)

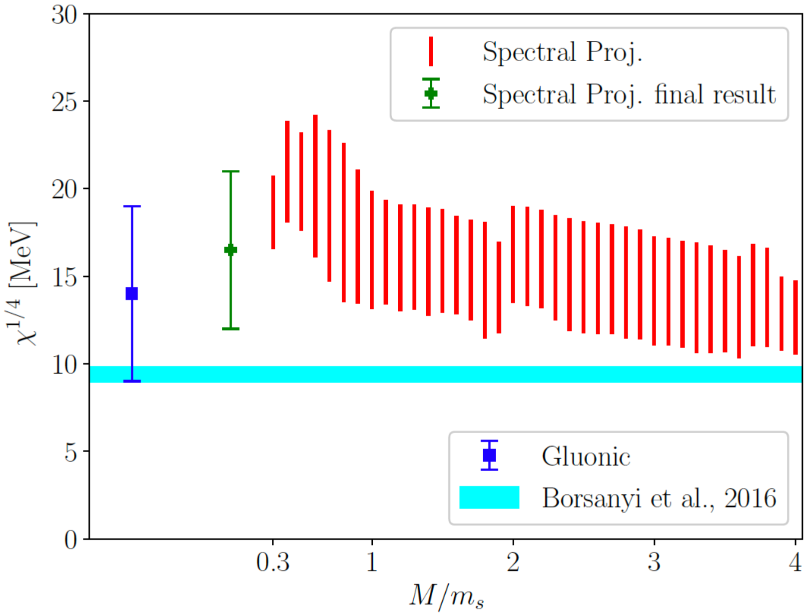


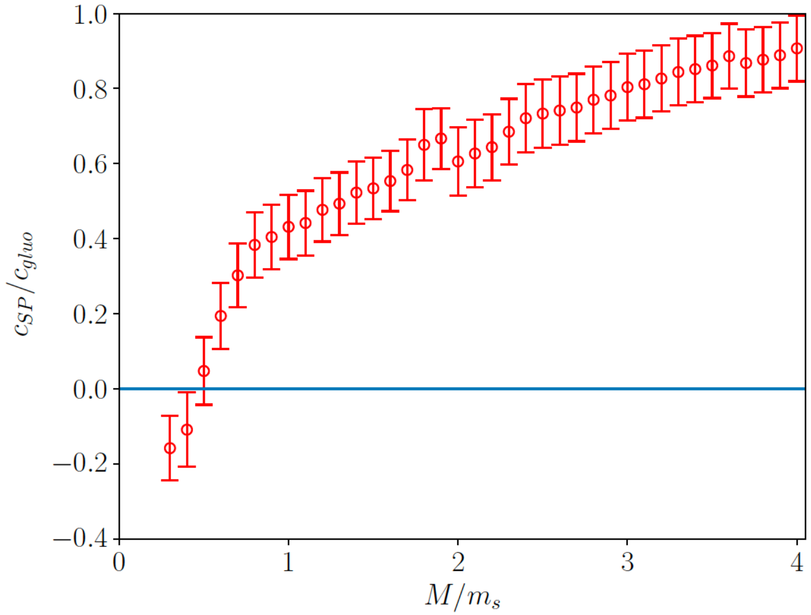


Continuum extrapolation $T = 430$ vs M/m_s

Choosing M/m_s inside the optimal range we observe:

- good agreement within the errors for determinations obtained for different values of M/m_s (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation can be achieved with suitable choice of M/m_s (Fig. on the right)





Chirality vs M/m_s at finite T

Same strategy as $T = 0$: consider $r_\lambda = |u_\lambda^\dagger \Gamma_5 u_\lambda|$ vs λ/m_s to estimate optimal range for M/m_s.

At finite T more clear separation of WBZMs compared to $T = 0$ case, although some ambiguity is still present.

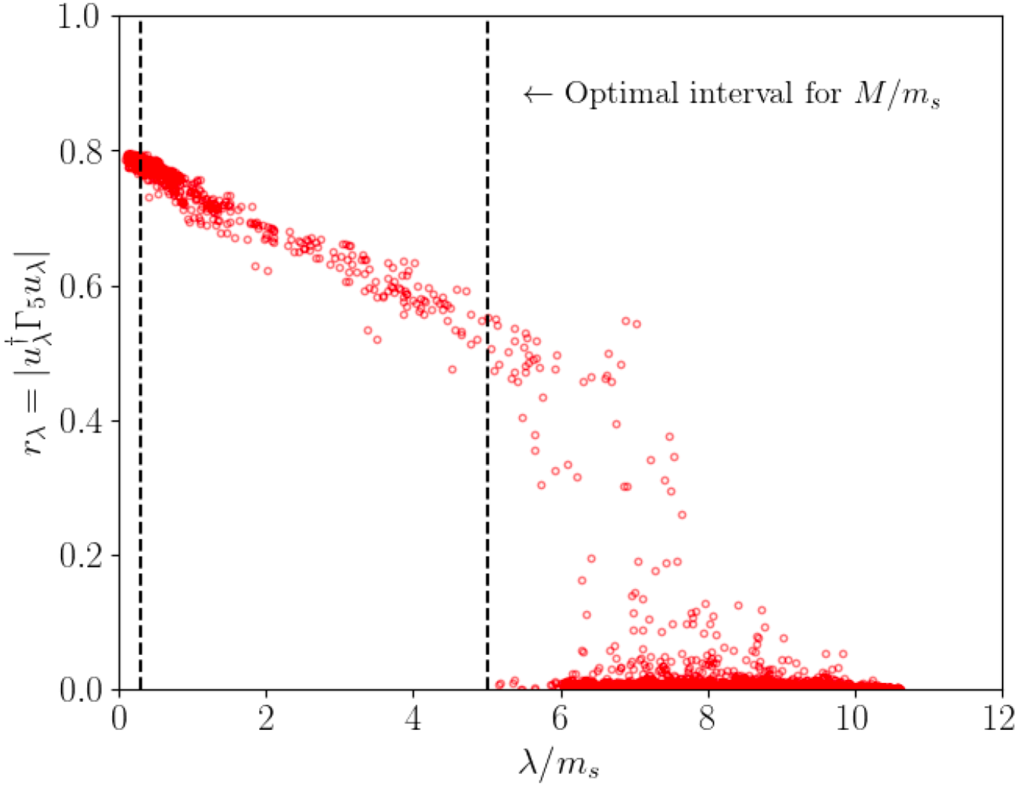


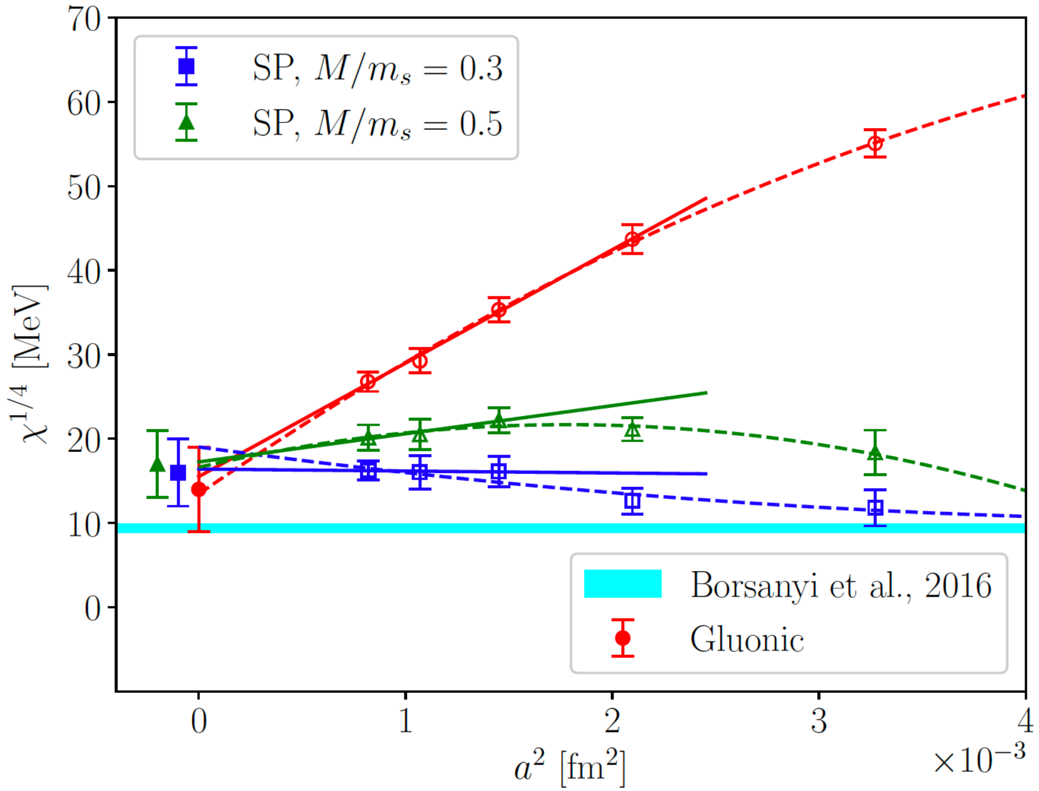
Figure refers to: $N_f = 2{+}1$ QCD, $T \simeq 430$ MeV, $V = 48^3 \times 16$, $a \simeq 0.0286$ fm, $m_q = m_s$.

Vertical lines: optimal choices for $M/m_s \in [0.3, 5]$.

Continuum limit of $\chi^{1/4}$ at finite T ($T = 430$ MeV)

Same lattice setup of the $T = 0$ case. Also in this case, we consider the following continuum-scaling function for Spectral Projectors (SP):

$$\chi_{\mathrm{SP}}^{1/4}(a, M/m_s) = \chi^{1/4} + c_{\mathrm{SP}}(M/m_s)a^2 + o(a^2).$$



Spectral lattice artifacts are suppressed compared to the gluonic case when M/m_s is chosen in the previously determined optimal interval:

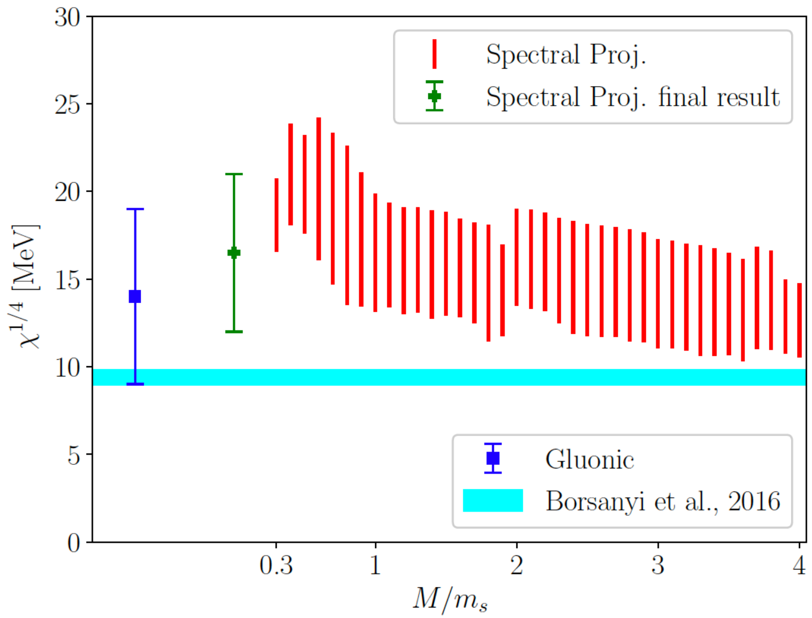
$c_{\mathrm{SP}}(0.3)/c_{\mathrm{gluo}} \sim 5 \cdot 10^{-2}$,

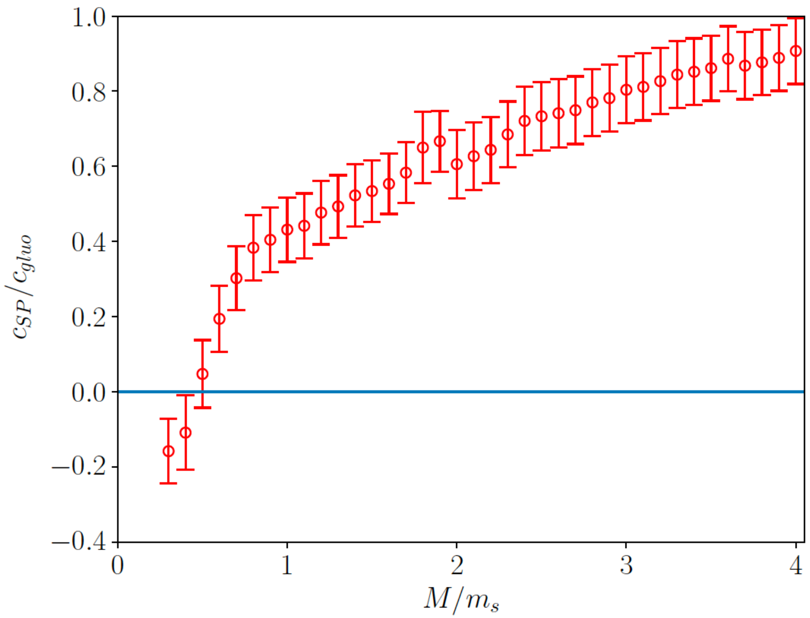
$c_{\mathrm{SP}}(0.5)/c_{\mathrm{gluo}} \sim 10^{-1}$.

Continuum extrapolation $T = 430$ vs M/m_s

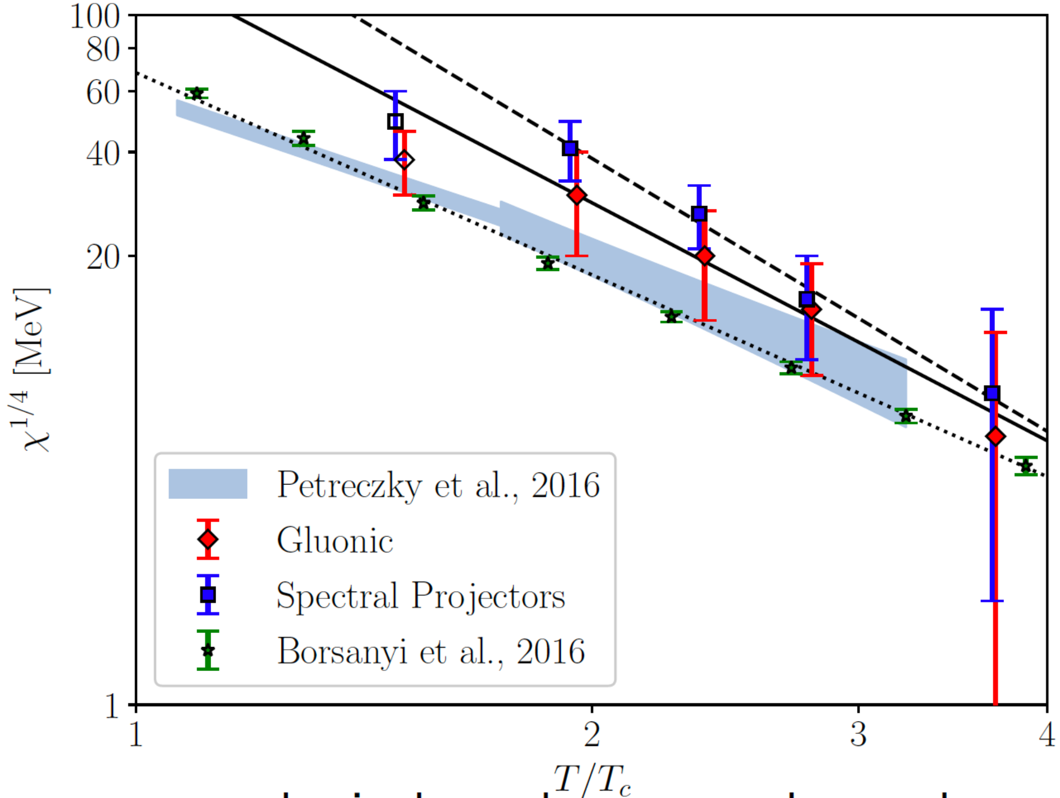
Choosing M/m_s inside the optimal range we observe:

- good agreement within the errors for determinations obtained for different values of M/m_s (Fig. on the left)
- significant reduction of lattice artifacts compared to the standard gluonic computation can be achieved with suitable choice of M/m_s (Fig. on the right)





All results and comparison with others groups



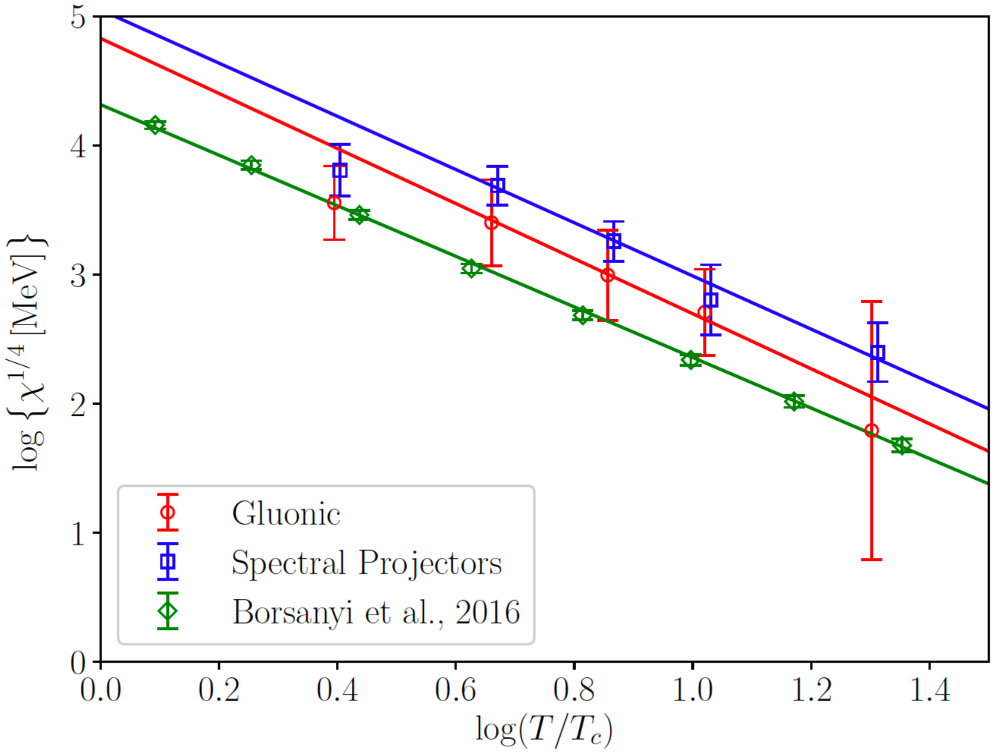
Borsanyi et al. 1606.07494: physical quark masses, thermodynamical integration at fixed Q and a posteriori near zero mode reweighting (note: no isospin symmetry breaking for all the data above).

Petreczky et al. 1606.03145: $m_\pi \simeq 160$ MeV, χ rescaled using DIGA expectations $\chi \propto m_\ell^2 \propto m_\pi^4$.

$\chi(T)$ for $T > T_c$ from Spectral Projectors

The Dilute Instanton Gas Approximation (DIGA) predicts:

$$\chi^{1/4}(T) \sim T^{-b}, \quad T \gg T_c, \qquad b_{\mathrm{DIGA}} \simeq 2.$$



Our data for $T \gtrsim 300$ MeV are in very good agreement with a decaying power-law, with exponents:

$$b_{\mathrm{SP}} = 2.06(41)$$
$$b_{\mathrm{gluo}} = 2.1(1.1)$$

Compare also with result from Borsanyi at al., 2016:

$$b = 1.96(2).$$

Best fit lines are $\sim$ parallel, SP prefactor of $\chi^{1/4}$ is $\sim$ a factor of 2 larger compared to previous results, i.e., an order of magnitude for χ.

see also Vicente Azcoiti 2101.06439 [hep-lat] and *Phys.Rev.D* 100 (2019) 7, 074511

- e-Print: 1907.01872 and refs. therein

Are we satisfied ? No,
too many systematic uncertainties and limitations remain

Conclusions and perspectives

We presented results for $\chi(T)$ in the high temperature regime of QCD, obtained by using the spectral projector discretization and the multicanonical algorithm.

pro: much better control on the systematics of the continuum extrapolation due to smaller lattice artifacts and to the presence of a new parameter.

con: errors still bigger than we hoped for...

A precise unbiased first-principle calculation of $\chi(T)$ is still an extremely challenging task. Larger statistics and smaller lattice spacings are required to settle this problem.

New algorithms to cope with the exponential critical slowing down of topological modes are being developed/tested.

Lattice QCD for Cosmology

Sz. Borsanyi, Z. Fodor, K.-H. Kampert, S. D. Katz, T. Kawanai, T. G. Kovacs, S. W. Mages, A. Pasztor, F. Pittler, J. Redondo, A. Ringwald, K. K. Szabo

Talks by Kalman SZABO and Dr. Szabolcs BORSANYI @ LATTICE 2016

1) Upgraded and extended analysis of the equation of state (energy and entropy density) as a function of T with nf=2+1+1 staggered fermions + bottom using perturbation theory

1) Study of the topological susceptibility up to quite large values of T

1) Detailed study of discretization errors

EFFECTIVE DEGREES OF FREEDOM AS A FUNCTION OF THE TEMPERATURE

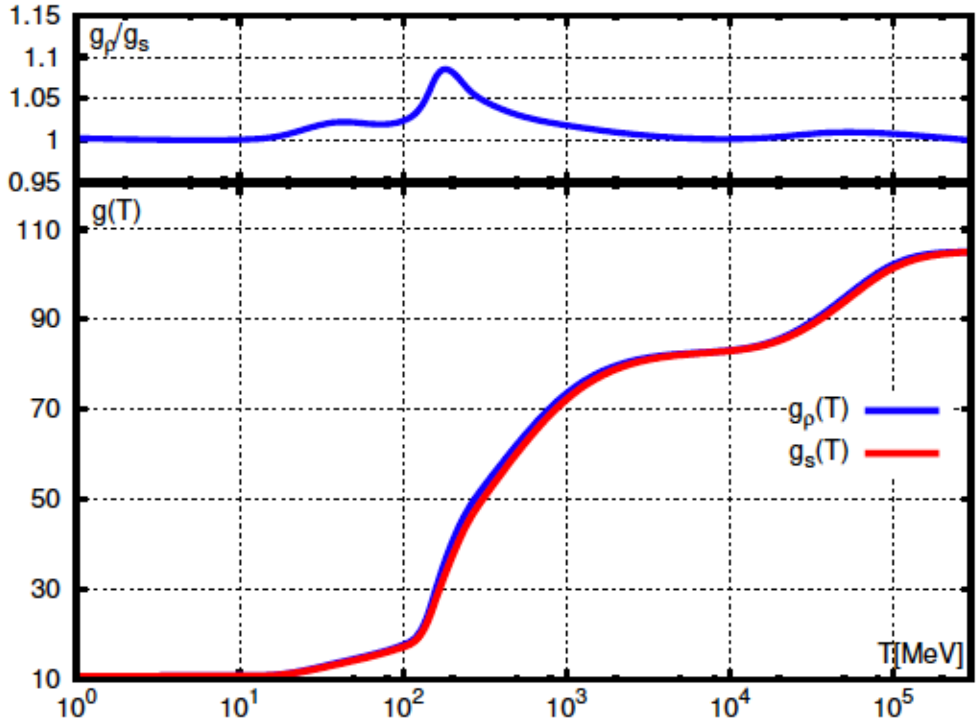


Figure 1: The effective degrees of freedom for the energy density (g_ρ) and for the entropy density (g_s). The line width is chosen to be the same as our error bars at the vicinity of the QCD transition where we have the largest uncertainties. At temperatures $T < 1$ MeV the equilibrium equation of state becomes irrelevant for cosmology, because of neutrino decoupling. The EoS comes from our calculation up to $T = 100$ GeV. At higher temperatures the electroweak transition becomes relevant and we use the results of Ref. [13]. Note that for temperatures around the QCD scale non-perturbative QCD effects reduce g_ρ and g_s by 10-15% compared to the ideal gas limit, an approximation which is often used in cosmology. For useful parametrizations for the QCD regime or for the whole temperature range see [17].

TOPOLOGICAL SUSCEPTIBLITY
AS A FUNCTION OF THE TEMPERATURE

VERY GOOD AGREEMENT WITH DILUITE INSTANTON GAS APPROXIMATION

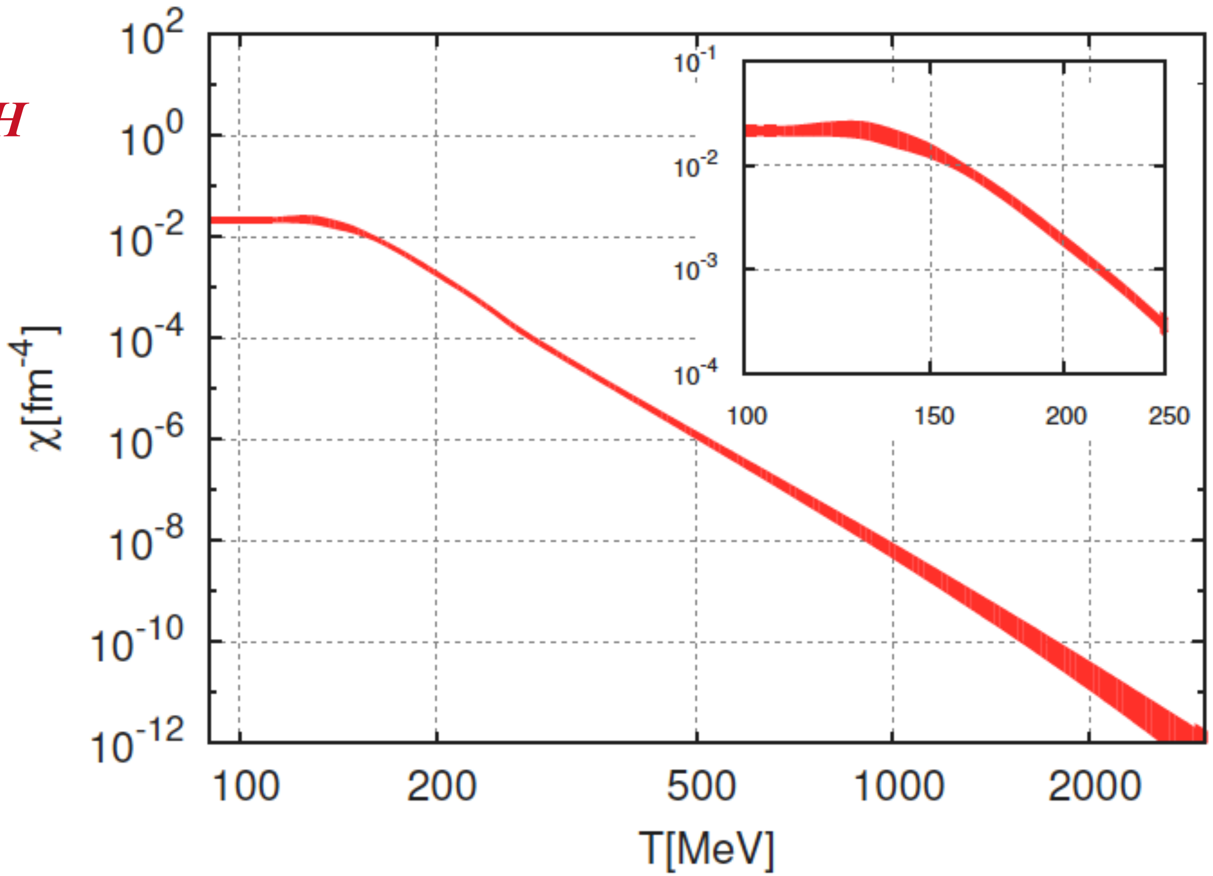
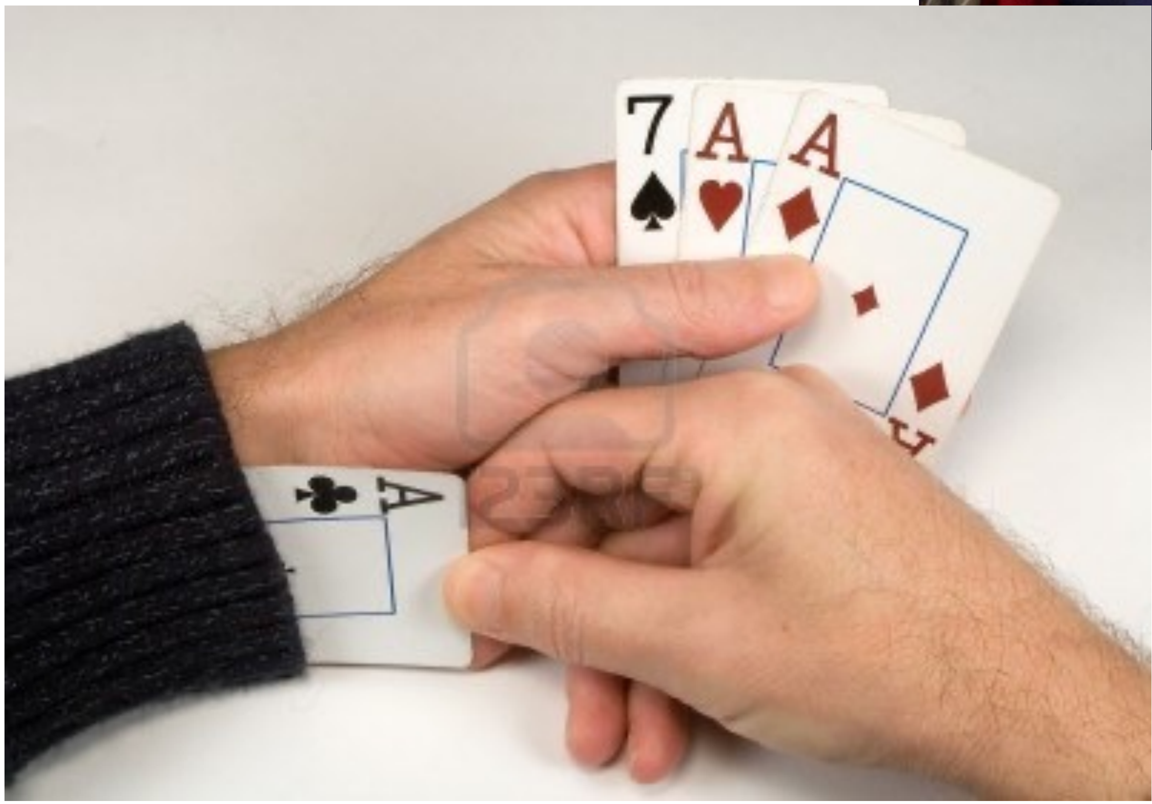


Figure 2: Continuum limit of $\chi(T)$. The insert shows the behaviour around the transition temperature. The width of the line represents the combined statistical and systematic errors. The dilute instanton gas approximation (DIGA) predicts a power behaviour of T^{-b} with b=8.16, which is confirmed by the lattice result for temperatures above ~ 1 GeV.

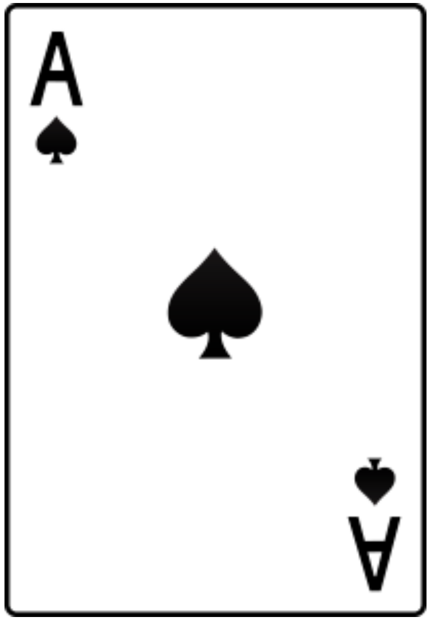
BUT …

THE FODOR TRUMP CARDS

or how these smart people obtained results as such large values of T



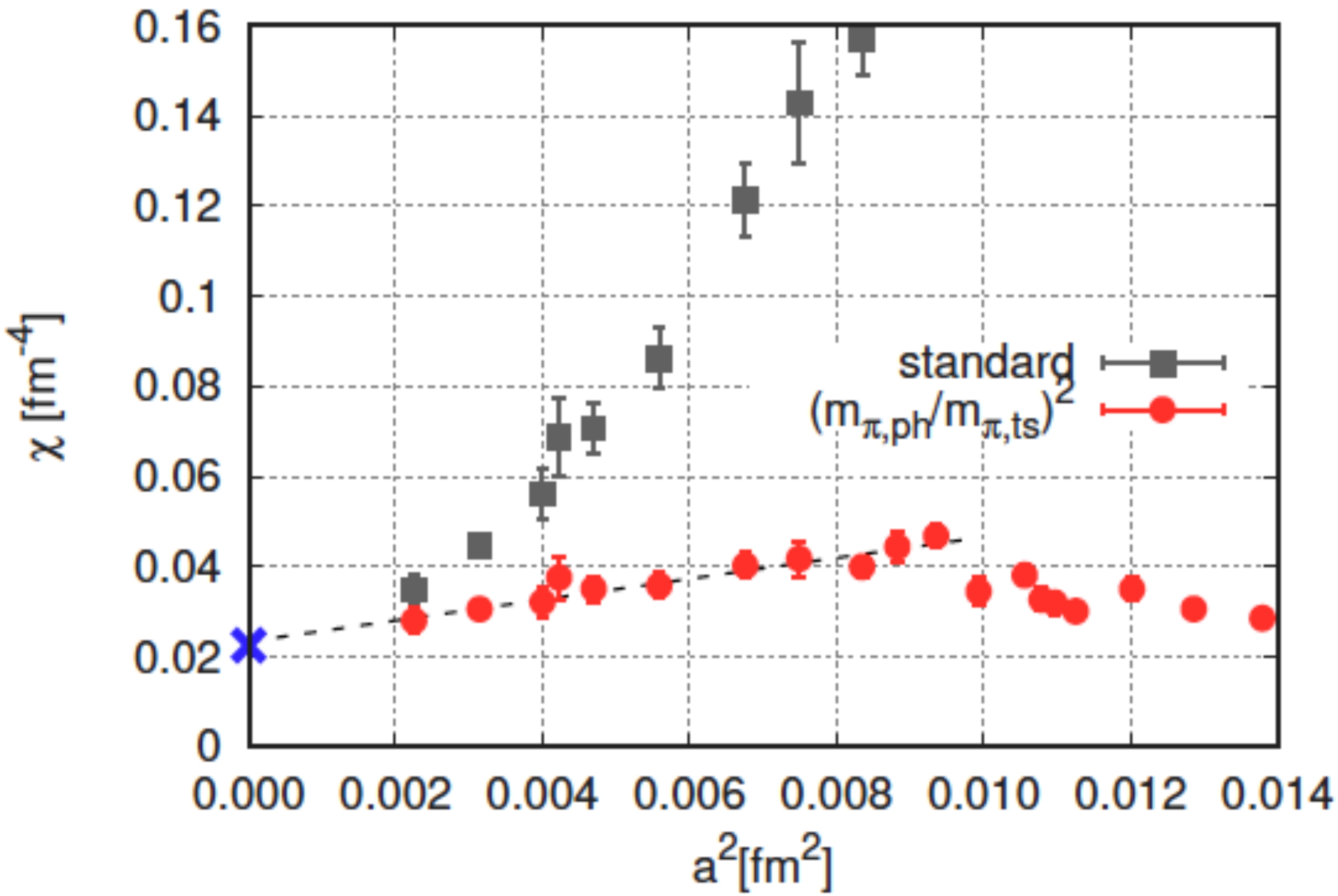
Some approximations have been used to compute the Equation of State (EOS)
But they will not be discussed here

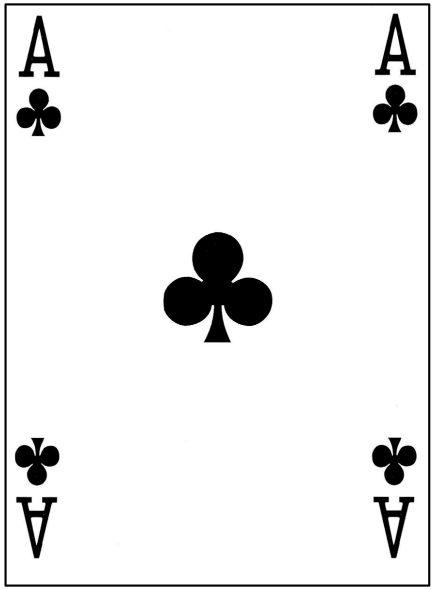


Trying to reduce discretization errors which for staggered fermions are rather large.
At zero temperature

$$\tilde{\chi} = \left(\frac{m_\pi}{m_{\pi I}} \right)^2 \chi$$

A serious study of the dependence on the quark masses is still missing however





Lines of Constants Physics (LCP) and $n_f = 3+1$ vs $n_f = 2+1+1$

$n_f = 2+1+1$

$$m_s = m_s^{\rm st}(\beta) \quad m_{ud} = R\, m_s^{\rm st}(\beta) \quad m_c = C\, m_s^{\rm st}(\beta)$$

$$a = a^{\rm st}(\beta) \quad 1/R = 27.63 \quad C = 11.85$$

then compute w_0

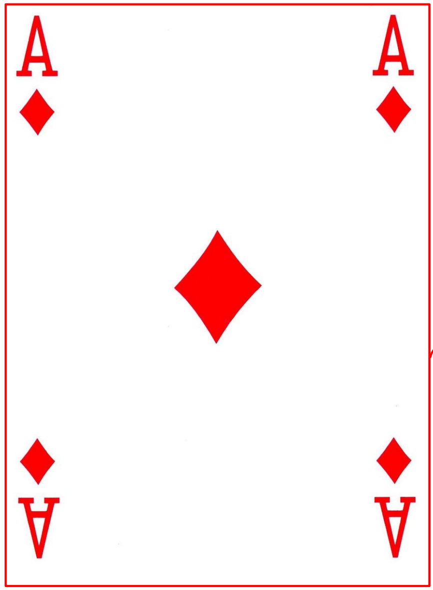
$n_f = 3+1$, with the same $m_s = m_s^{\rm st}(\beta)$

and obtain $m_\pi^{(3)}\, w_0^{(3)}$ and $w_0^{(3)}$

change lattice fermions, compute $m_s^{\rm fermions}(\beta)$

in such a way that $m_\pi^{(3)}\, w_0^{(3)}$ is the same

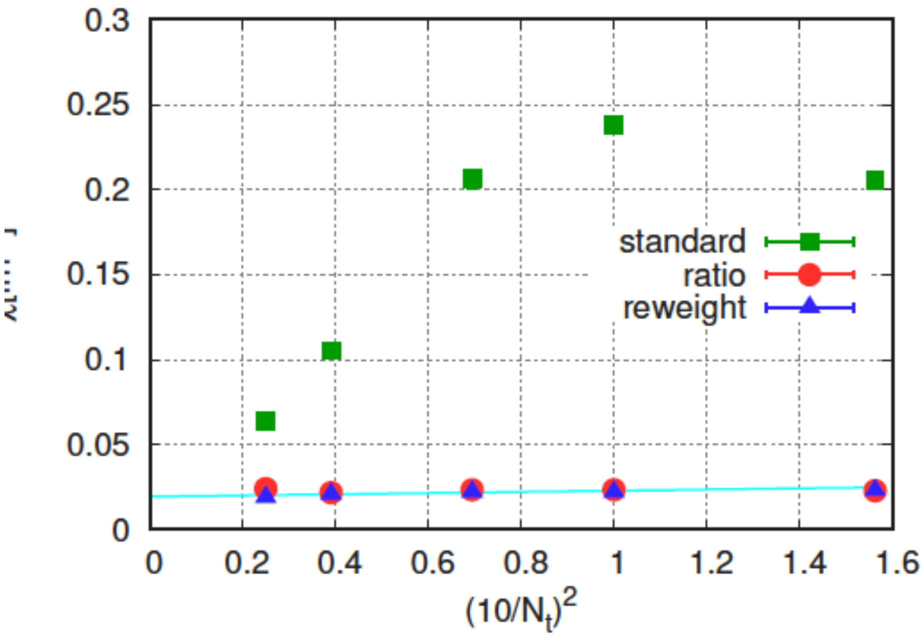
$$a^{\rm fermions} = \frac{w_0^{(3)}}{w_0^{\rm fermions}}\, a^{\rm st}(\beta)$$

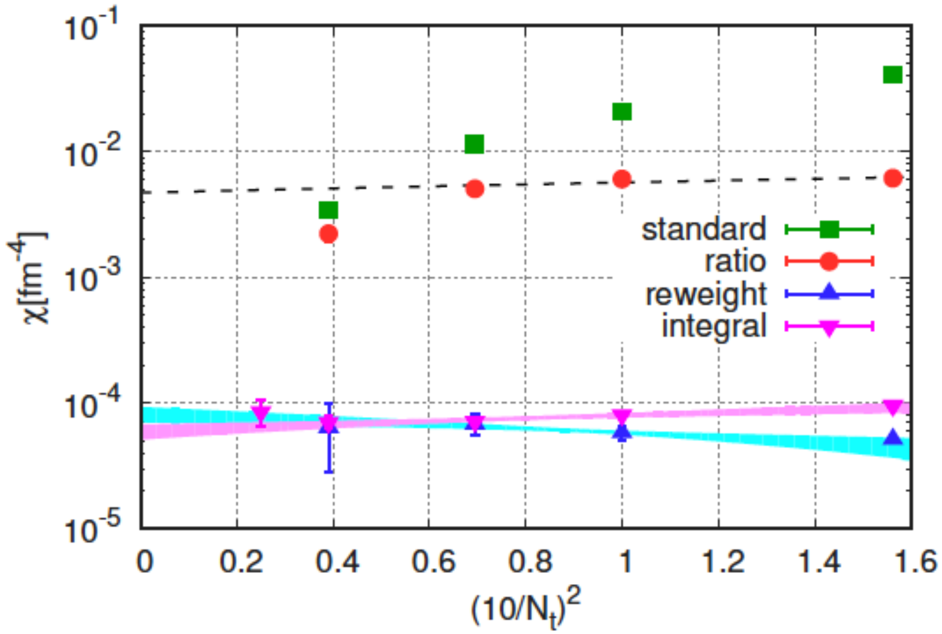


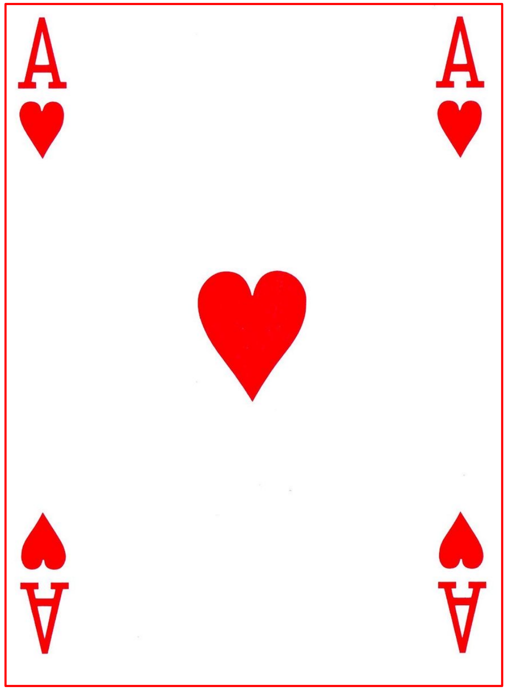
Reweighting of the chiral condensate to reduce discretization errors

$$w[U] = \prod_f \prod_{n=1}^{2Q[U]} \prod_{\sigma=\pm 1} \left(\frac{2\,m_f}{i\sigma\lambda_n[u] + 2\,m_f} \right)^{n_f/4}$$

The choice of Q[U] looks rather arbitrary and has a huge effect (1-2 order of magnitude)







BUT THE REAL TRUMP CARD IS:

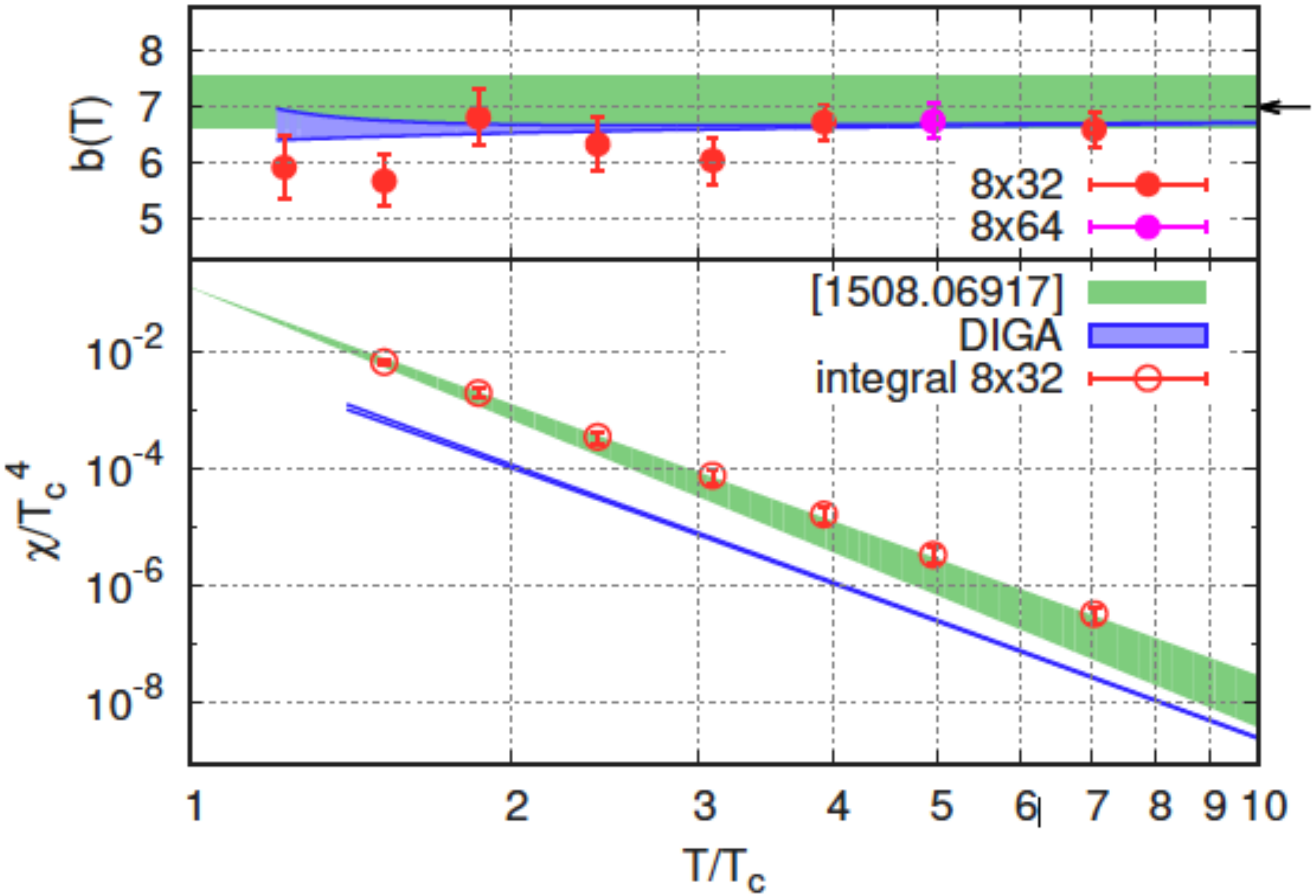
1) At high T calculation at fixed topological sector Q=0,1 only;
2) $Z_Q/Z_0(T)$ computed via average action and condensate

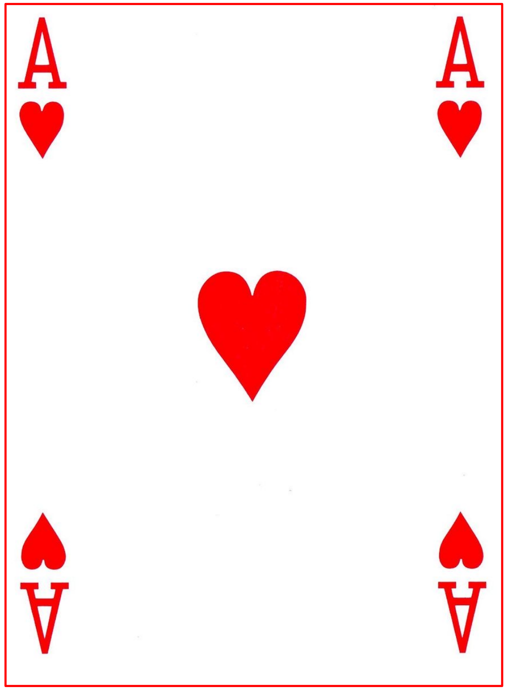
Compute $b_Q = \frac{d\log Z_Q/Z_0}{d\log T} =$

$$\frac{d\beta}{d\log a}\langle S_g\rangle_{Q-0} + \sum_f \frac{d\log\, m_f}{d\log a}\langle\bar{\psi}\psi_f\rangle_{Q-0}$$

$$\frac{Z_Q}{Z_0}(T) = e^{\int_{T_0}^{T} d\log T'\, b_Q(T')}\, \frac{Z_Q}{Z_0}(T_0)$$

QUENCHED CASE





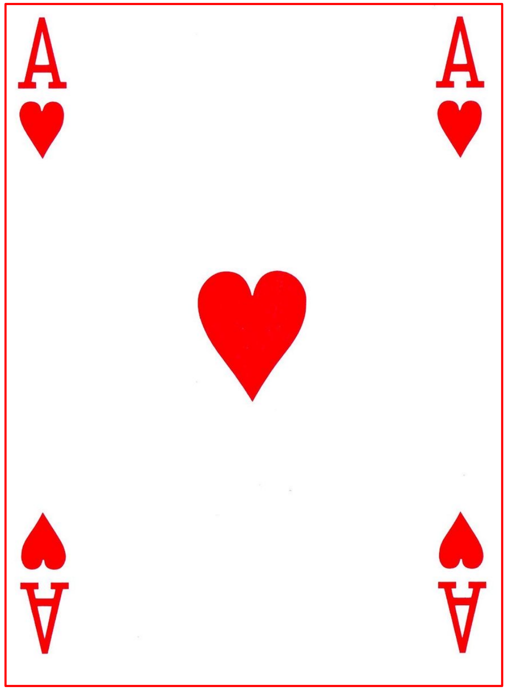
Somehow a circular argument: Freezing at high temperatures and small lattice spacing ➔ small Q ➔ only Q=0,1 -> diluite instanton gas

Freezing and or physical small volumes can mimic large discretization errors

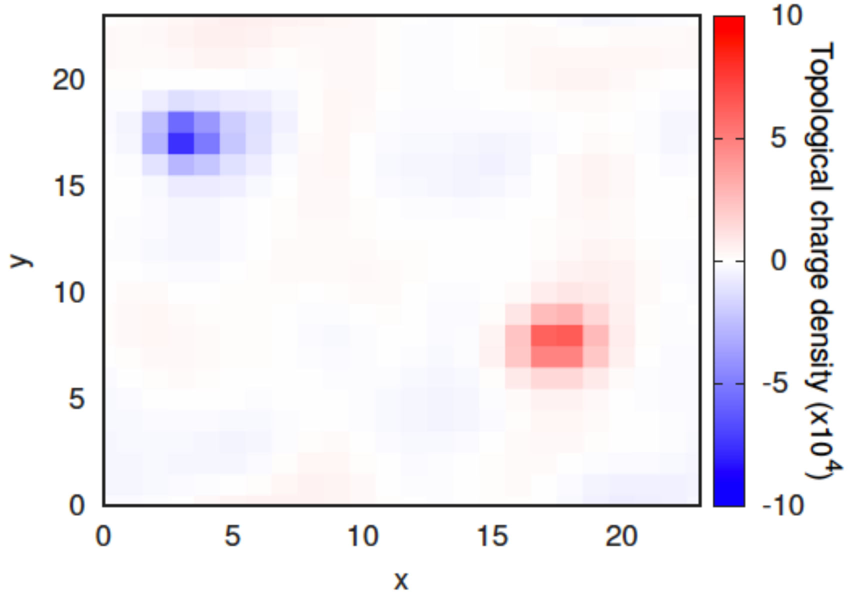
But it is not enough yet:

$$b_Q^{\mathrm{rw}} = \frac{d\log Z_Q^{\mathrm{rw}}/Z_0^{\mathrm{rw}}}{d\log T} = \frac{d\beta}{d\log a}\langle S_g\rangle_{Q-0}^{\mathrm{rw}} + \sum_f \frac{d\log m_f}{d\log a} m_f \langle\overline{\psi}\psi_f\rangle_{Q-0}^{\mathrm{rw+zm}},$$

$$\langle\overline{\psi}\psi_f\rangle_{Q-0}^{\mathrm{rw+zm}} = \langle\overline{\psi}\psi_f\rangle_{Q-0}^{\mathrm{rw}} + \frac{|Q|}{m_f} - \left\langle \frac{1}{2m_f}\sum_{n=1}^{2|Q|}\frac{4m_f^2}{\lambda_n^2[U]+4m_f^2}\right\rangle_Q^{\mathrm{rw}}.$$

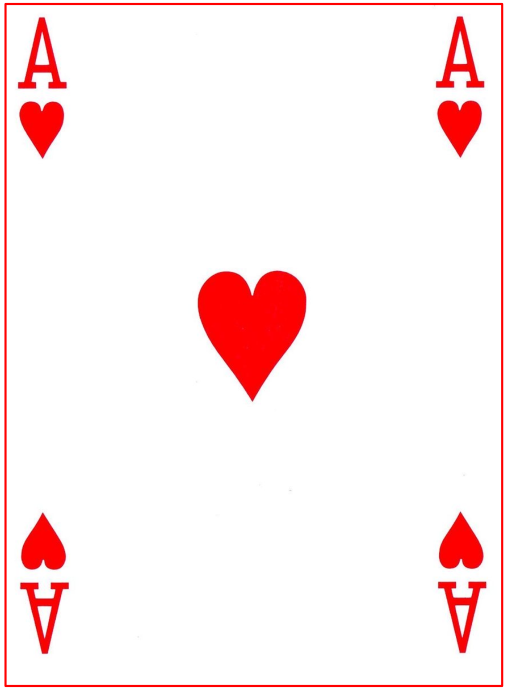


But it is not enough yet: by hand treatment of Instanton-Antistanton configurations



But it is not enough yet: 3+1 versus 2+1+1 T high temperatures (indeed they approximate with R^2)

$$\left.\frac{Z_1}{Z_0}\right|_{2+1+1} = \exp\left(\int_{m_{ud}^{phys}}^{m_s^{phys}} d\log m_{ud}\; m_{ud}\langle\overline{\psi}\psi_{ud}\rangle\right)\cdot \left.\frac{Z_1}{Z_0}\right|_{3+1}$$

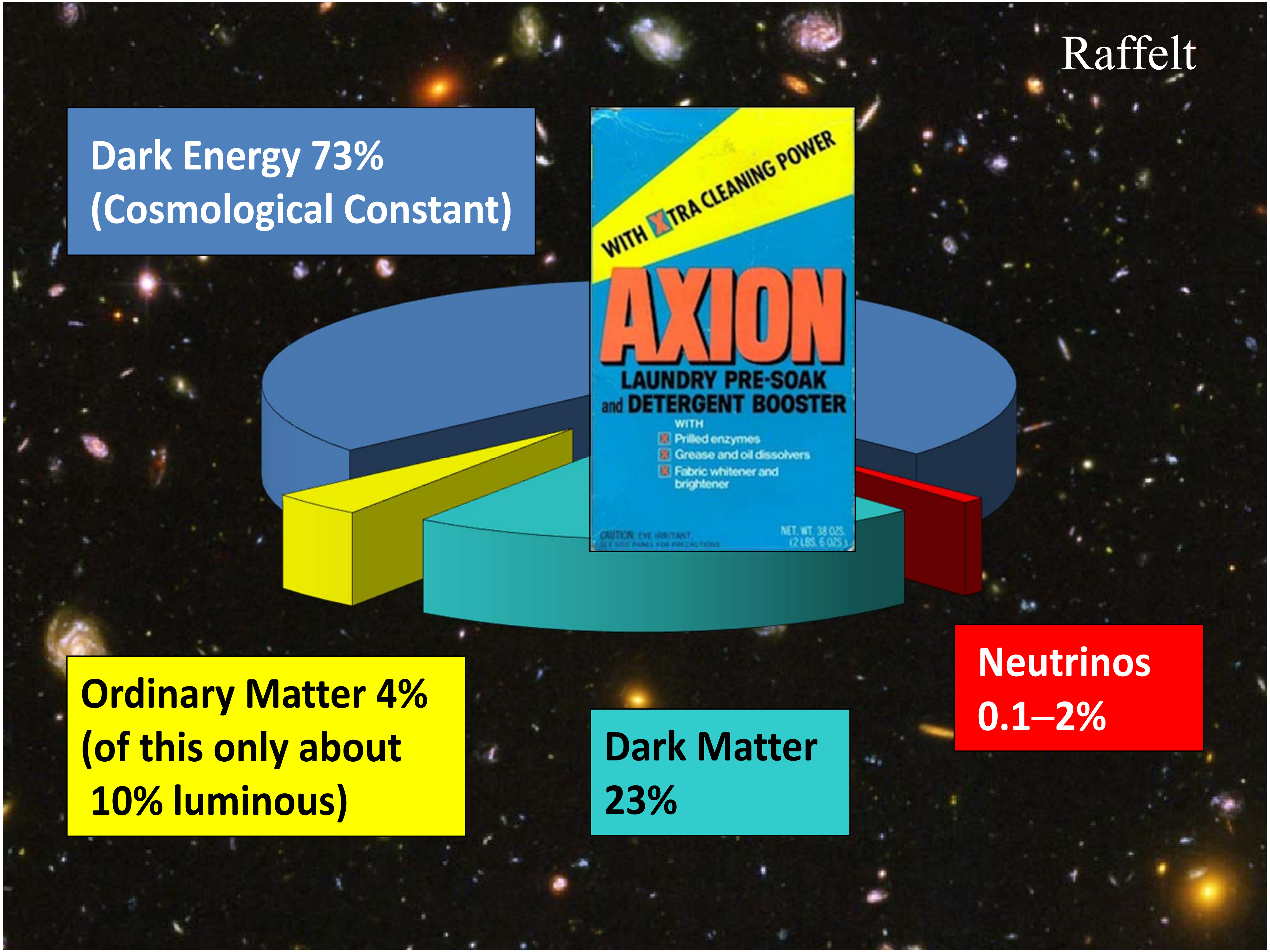


But it is not enough yet: since it is difficult to compute $\langle S_g \rangle_{1-0}$

they propose to compute $\langle S_g \rangle_{Q-0}$ with Q=2,3, etc

$$\langle S_g \rangle_{1-0} = \langle S_g \rangle_{Q-0} / |Q| \quad !!$$

Also a riscaling of the topological susceptibility of a factor
4 mu md /(mu+md)^2 = 0.88
by hand


Raffelt
Dark Energy 73%
(Cosmological Constant)
WITH XTRA CLEANING POWER
AXION
LAUNDRY PRE-SOAK
and DETERGENT BOOSTER
WITH
Prilled enzymes
Grease and oil dissolvers
Fabric whitener and brightener
NET. WT. 38 OZS.
(2 LBS. 6 OZS.)
Ordinary Matter 4%
(of this only about
10% luminous)
Dark Matter
23%
Neutrinos
0.1–2%

AXION RESULTS

Given that $b_2(T)$ converges relatively fast to the value predicted by a single cosine potential, we can assume $V(\phi)=-\chi_t(T)\cos(\phi/f_\phi)$ for $T \geq Tc$

Using the most conservative results for the fit

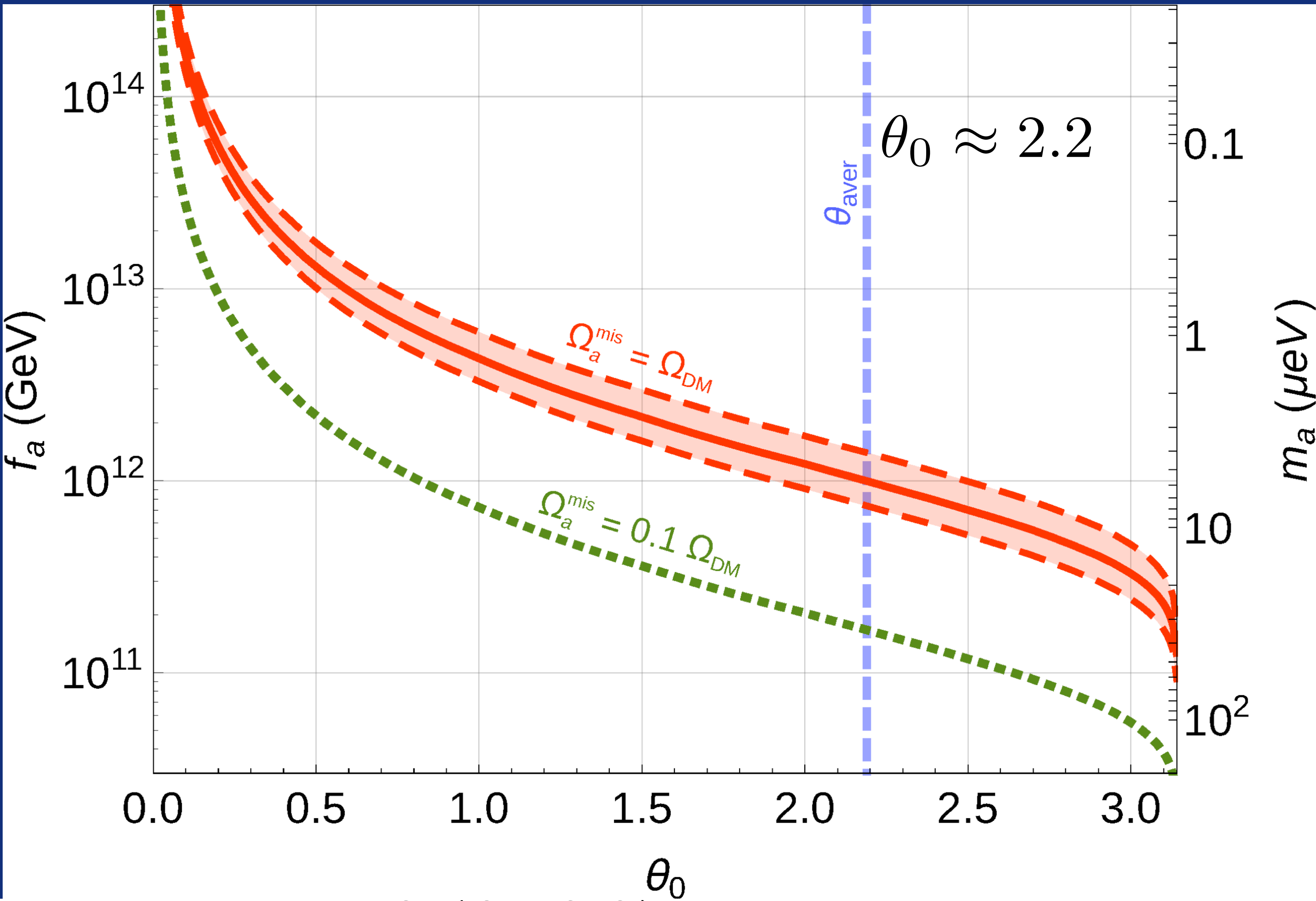
$$\chi(T)/\chi(0) = (1.8 \pm 1.5)(T_c/T)^{2.90\pm0.65}$$

we plot the prediction for the parameter f_ϕ as a function of the initial value of the axion field $\vartheta_0=\phi_0/f_\phi$ assuming that the axion contribution make up for the whole observed dark matter abundance

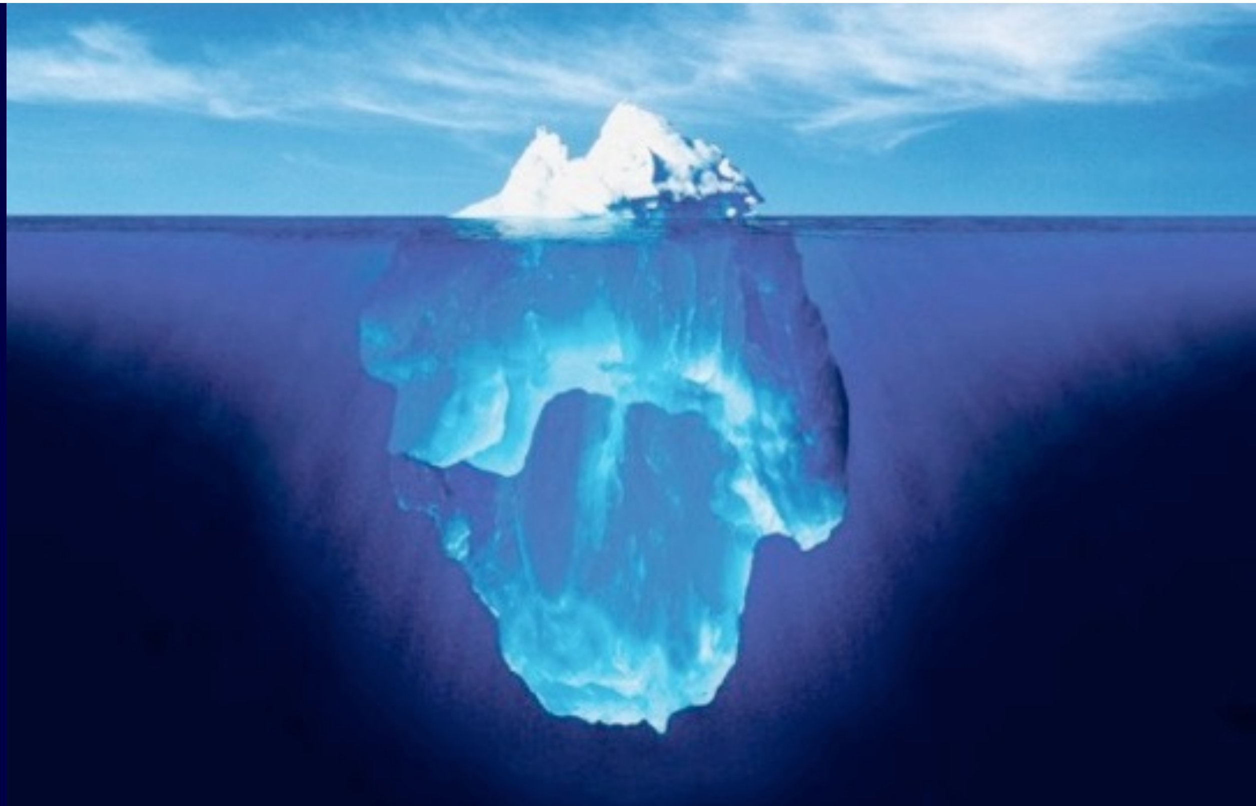
$$\Omega_{\rm DM} = 0.259(4)$$

Predictions for f_ϕ

(almost one order of magnitude larger than the instanton value)



$$f_\phi(\theta_0) = (1.00^{+0.40}_{-0.26}{}^{+0.07}_{-0.18} \pm 0.06) \cdot 10^{12}\ \text{GeV}$$



MAIN MESSAGE

In particular for the value of $f_\phi \approx 10^{12}$ GeV the axion field starts oscillating around Tosc=4.3 GeV. An even longer extrapolation is required for $f_\phi \approx 1.67\ 10^{11}$ GeV corresponding to Ω_ϕ=0.1 Ω_{DM}, where the axion starts oscillating around Tosc=7.2 GeV.

MAIN MESSAGE

The results however rely on the extrapolation of the axion mass fit formula up to few GeV

THE CONTROL OF THE LARGE T REGION IS VERY IMPORTANT