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Phys. Lett. B752 (2016) 175; quenched results Nature 539 (2016) 69; dynamical case



| Motivation | Wilson-flow & scale/topology | Quenched study | Dynamical case | Summary |
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| Outline | | | | |





Quenched study

4 Dynamical case



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Simple candidate for extension of SM:

- add a complex scalar field ϕ
- with symmetry breaking Mexican hat at high scale fa
- couple the Goldstone mode $arg(\phi)$ as dynamic θ angle to QCD
- (pseudo)Goldstone mode of the tilted potential is called axion

$$\mathcal{L}_{a} = \partial_{\mu}^{*} \phi \partial^{\mu} \phi - \frac{\lambda}{8} \left(\phi^{*} \phi - f_{a}^{2} \right)^{2} + \chi_{t} \frac{|\phi|}{f_{a}} \cos(\arg(\phi))$$

Full QCD can include an effective CP breaking θ term:

$$\mathcal{L}_{QCD} = \sum_{f} \bar{\psi}_{f} (D_{\mu} \gamma^{\mu} + m_{f}) \psi_{f} + \frac{1}{4} F^{a}_{\mu\nu} F^{a}_{\mu\nu} - i\theta \frac{g^{2}}{32\pi^{2}} \tilde{F}^{a}_{\mu\nu} F^{a}_{\mu\nu} \quad (1)$$

with $-\pi < \theta < \pi$, so naturally $\theta \sim \mathcal{O}(1)$

From experiments: $|\theta| < 10^{-10}$, unnatural \rightarrow fine-tuning?

Antrophic principle does not help: $|\theta| < 10^{-2}$ would be still fine

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interpret/introduce θ as a dynamical field with minimum at 0

- as phase of a global U(1) symmetric scalar field ϕ
- with spontaneous symmetry breaking potential

redefinition of the angular mode as $\arg(\phi) := \theta_{eff}$

$$\mathcal{Z} = \int \mathcal{D} A_{\mu} exp(-S_{QCD} - i heta_{eff} \cdot g^2/32\pi^2 \cdot ilde{F}^a_{\mu
u} F^a_{\mu
u})$$

Z reduced, F raised by phase cancellation unless $\theta_{eff}=0$ one can get the mass of the axion: $m_A^2 \propto \langle Q^2 \rangle \propto \chi_t$ effective potential for ϕ has a tilt & a minimum for $0 = \theta_{eff} = \arg(\phi) = 0$

$$\mathcal{L}_{a} = \partial_{\mu}\phi^{*}\partial^{\mu}\phi - \frac{\lambda}{8}\left(\phi^{*}\phi - f_{a}^{2}\right)^{2} + \chi_{t}\frac{|\phi|}{f_{a}}\cos(\theta_{eff})$$

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Two massive oscillations of ϕ

- heavy "string" mode in magnitude; with mass $m_s \approx \sqrt{\lambda} f_a$
- light "axion" mode in phase; with mass $m_a \approx \sqrt{\chi_t}/f_a$

Given χ_t , cosmology gives an abundance of axions

Axions can provide substantial/total amount of dark matter

Two axion production mechanisms:

- dynamics and decay of string/wall networks
- misalignment (sole ingredient in the pre-inflation case)

Topological Structures

Spontaneous symmetry breaking + causality:

different θ_{eff} in causally disconnected patches

 \Rightarrow Strings

with QCD potential $\theta_{eff} \rightarrow 0$ everywhere

 \Rightarrow Walls between Strings



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- string-like defects arise and form networks
 → axion radiation
- when χ_t becomes relevant, formation of walls between strings \rightarrow axion radiation
- walls accelerate annihilation of topological defects \rightarrow axion radiation

 χ_t influences string dynamics, needed as input for total axion production only in case of a post-inflationary Peccei-Quinn symmetry breaking

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| Misaligr | nment | | | |
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- alignment of misaligned neighbouring patches
 → axion radiation
- when χ_t becomes relevant, θ_{eff} "rolls" down to $\theta = 0$ \rightarrow axion radiation

 χ_t influences field dynamics, needed as input for total axion production



Evolution in the expanding universe



Integral

$$Q = \int_{\mathcal{M}} \mathrm{d}^4 x q(x)$$

over the topological charge density

$$q(x) = \frac{1}{4\pi^2} \epsilon_{\mu\nu\rho\sigma} \text{tr} \left(F_{\mu\nu}(x) F_{\rho\sigma}(x) \right)$$

- discretized in finite volume on $\mathcal{M} = \mathbb{T}^4$
- sectors with different Q separated by infinite action barrier in continuum
- problem for ergodicity of MC algorithms with small "step" size in field space ▲御▶ ▲ 国▶ ▲ 国▶ … 르

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Topological Susceptibility

Integral of qq correlator

$$\chi = \int_{\mathcal{M}} \mathsf{d}^4 x \langle q(0) q(x)
angle$$

With global translation symmetry on $\mathcal{M}=\mathbb{T}^4$

$$\chi = rac{1}{V_4} \langle Q^2
angle$$

- measurement must sample sectors with $Q \neq 0$
- difficult close to continuum
- difficult when $\chi V_4 = \langle Q^2 \rangle \ll 1$

Choice of the action: improvement

no consensus: which action offers the most cost effective approach our choice: tree-level $O(a^2)$ -improved Symanzik gauge action



2/4-level (stout) staggered or 2/3 (HEX) Wilson or overlap fermions



with tree-level O(a) clover improved fermions (Wilson):

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Scale settings and the static potential

- raw output of lattice QCD: physical quantities in lattice unit \Rightarrow measure a dimensionful quantity Q (M_{Ω} or f_{K}) the lattice spacing is given by $a=(aQ^{lat})/Q^{exp}$
- today erros below 2% for several lattice predictions it depends crucially on the error of the lattice spacing need for a controlled/small error lattice spacing determination
- not necessarily directly accesable for experiments e.g. potential popular choices are:
- string tension (strictly speaking doesn't exist: string breaking) the Sommer-scale $r_x^2 \cdot dV/dr = C_x$ originally re with $C_x = 1.65$ or MII C choice re with $C_x = 1$

String tension and Sommer scale from the potential

let us take $Q = \sigma$, the string tension

$$\sigma = \lim_{R \to \infty} \frac{\mathrm{d}V(R)}{\mathrm{d}R}$$

"Experimental value:" $\sqrt{\sigma} =$ 465 MeV

$$V(R) = -\lim_{T \to \infty} \frac{1}{T} \ln[W(R,T)], \qquad W(R,T) =$$



Static $q - \bar{q}$ potential V(r)

 $r_{\chi}^2 \cdot dV(r)/dr = C_{\chi}$ we need interpolation for the derivative

Sommer-scale, Omega mass, f_{π} and f_{K}

unfortunately, the calculations of $r_0 \& r_1$ are quite involved far more complicated than fitting the masses of particles

complications are reflected in the literature MILC: $r_1=0.3117(22)$ fm (better than 1% accuracy) RBC/UKQCD: $r_1=0.3333(93)(1)(2)$ fm 7% difference and 2.3 σ tension between them

another popular way is to use the Omega baryon mass the experimental value of M_{Ω} is well known more CPU demanding & sensititve to the strange quark mass mismatched strange quark mass leads to a mismatched scale

difficulties with f_{π} (chiral extrapolation) & f_{K} (mismatched m_{s})

suggestion of M. Luscher: use the Wilson flow to set the scale

Gauge field flow

flow equation: $\dot{V}_t = Z(V_t)V_t$, where Z is the staple equivalent to a series of infinitesimal stout smearing steps

M. Luscher, JHEP 1008 (2010) 071

as a representative example $E = G^a_{\mu\nu}G^a_{\mu\nu}/4$ is considered

above the cut-off (small t): lattice and continuum quite different



observed "linearity" for $t^2 \langle E \rangle$ one can extract it by $t \cdot dt^2 \langle E \rangle / dt$ instead $t^2 \langle E \rangle = 0.3$ (M. Luscher) $t \cdot dt^2 \langle E \rangle / dt = 0.3$ (w_0 scale) it should have less scaling violation the non-universal part (cut-off) shrinks

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How far can we go with conventional brute force?

 \rightarrow test it in the "cheap" quenched case

- learn how to control all errors and apply it for full QCD
- test bed to improve on the brute force strategy
- roughly the same temperature scaling as for full QCD
- estimate the costs for the full result

Alles:1996nm,Gattringer:2002mr etc. 1st gen results Berkowitz:2015aua large volume/statistics up to $2.5T_c$ Kitano:2015fla HMC up to $2T_c$



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| Lattice | Setup | | | |

Pure SU(3)

- Symanzik improved gauge action
- gluonic q(x) from clover field strength tensor $F_{\mu\nu}$
- update sweep: 1 heatbath + 4 overrelaxation

Parameters

- 0.1 $T_c \le T \le 4.0 T_c$
- $n_t = 5, 6, 8$
- spatial volume fixed in physical units $L_{x,y} = 2/T_c$
- $L_z = 2L_{x,y}$ to enable subvolume analysis

Simulations on the Wuppertal-QPACE machine

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| Renormalization of χ | | | | |

 $\chi(t)$ at finite Wilson-flow t is already renormalized [Luscher:2010iy]

- sufficient to perform a continuum limit at flow time fixed in physical units, e.g. t = w₀² (w₀²: flow time at which td/dt · [t²E(t)] = 0.3 [Borsanyi:2012zs])
- the choice of t influences the size of the lattice artefacts

• $\chi(t)$ has weak dependence on the choice of t

• we choose
$$t = w_0^2 \approx (0.176 \text{ fm})^2$$

• the finer the lattice the weaker the t-dependence



Continuum result: b=7.1(4)(2) & $\chi(4T_c)^{1/4}=17$ MeV



Quenched Lattice \leftrightarrow DIGA

correct *T* dependence normalization off by $\mathcal{O}(10)$ fixed by comparison to lattice

how $\chi_t(T)$ determines m_A ? start with an m_A e.g. 30μ eV m_A (T=0) gives the value of f_A

known: Hubble constant H(T) fix T_{osc} by $3H(T_{osc}) = m_A(T_{osc})$

using T_{osc} calculate the amount of dark matter

if it is too much/little iterate



Calibrated guess for dynamical with DIGA

- dynamic case with DIGA
- quenched calibrated K-factor is $\mathcal{O}(10)$
- cosmology can be used axionic dark matter & m_A can be determined
- K-factor uncertainty means a factor two in m_A
- dream: predict m_A ADMX experiment: tune it (eventually even find it)

Unquenched QCD 2-loop RGI DIGA K = 1 (blue), $K = 9.22\pm0.6$ (gray) ($\kappa = 0.6-2$) IILM from Ref. [10] (dashed red)



Cost of the conventional algorithm at relative error $\delta \chi_t$

$$costs \propto rac{1}{(\delta\chi_t)^2\chi_t(T)}$$

relative cost $(4T_c)/(1T_c)$ (our highest T was $4T_c$: not enough)

from measured
$$\chi_t(T)$$
 $4^{7.1} \approx 2 \times 10^4$ from measured $\delta\chi_t$ $10^5 - 10^6$

- quenched $\chi_t(T = 0)$ calculated \sim 20 years ago
- Moores law leads to a factor of $\sim 10^5$ in 24 years

 \Rightarrow Just possible to do (dynamical case is probably hard)

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About costs: dynamical QCD

Dynamic relative cost $(7T_c)/(1T_c)$ $(7T_c \sim 1200 MeV)$

from estimated
$$\chi_t(T)$$
 $7^{7-8} \approx 10^6 - 10^7$ increasing τ_{int} with T $10^7 - 10^9$

• dynamic $\chi_t(T = 0)$ in 2010, Moore factor of ~ 10

 \Rightarrow conventional dynamical study not possible (needs 35 years)



C.Bonati, M.d'Elia, G.Martinelli et al. JHEP 229 03, 155 (2016)

• brute force fully dynamic in the continuum up to $\approx 4 T_c$



Result: $b \sim 3$ unexpected (DIGA etc. $b \sim 8$) for T>2 GeV is larger than DIGA by 7-8 orders of magnitude one order of magnitude shift for the axion dark matter window crosses quenched result at $4T_c$ (for quenched $\chi_t^{1/4}(4T_c)=17$ MeV) \Rightarrow further study is obviously necessary

Consequences of the non-scaling behaviour

for large '*a*' no proper a^2 scaling (e.g. due to large m_{π} splitting) how do we monitor it, how to be sure being in the scaling regime? dimensionless combinations in the $a \rightarrow 0$ limit:

 $T_c r_0$ or T_c / f_K for the remnant of the chiral transition



 N_t =4,6: inconsistent continuum limit

*N*_t=6,8,10: consistent continuum limit (stout-link improvement)

independently which quantity is taken one obtains the same T_c signal: extrapolation is safe, we are in the a^2 scaling regime

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Introduction to the dynamical case

- $\bullet~$ Strong CP problem $\rightarrow~$ axion $\rightarrow~$ dark matter candidate
- Two important inputs for axion production: equation of state & topological susceptibility at high T
- Determine topological susceptibility at high temperatures at the physical point using fixed *Q* integral
- Exact zero modes of the Dirac operator for Q ≠ 0 are crucial
 → large discretization effects with staggered fermions
- Possible solutions
 - 1) eigenvalue reweighting
 - 2) using chiral fermions
- In the following we use
 - 1) for the 3 flavor theory and
 - 2) for going down to the physical point

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Effective number of degrees of freedom including all SM particles

$$ho = rac{\pi^2}{30} g_
ho T^4 \qquad s = rac{2\pi^2}{45} g_s T^3 \qquad c = rac{2\pi^2}{15} g_c T^3$$



The challenge of computing the susceptibility

- large autocorrelation of *Q* on fine lattices (algorithmic problem)
- $\chi(T)$ decreases strongly with temperature
 - \rightarrow very few $Q \neq 0$ configurations (physical problem)
 - E.g. $\langle Q^2 \rangle = 10^{-6}$ means one $Q = \pm 1$ configuration per million.
 - Even $\mathcal{O}(\text{million})$ configurations can lead to large statistical errors
- $\chi(T)$ has large lattice artefacts



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T=0 instanton on the lattice: physical units



T=0 instanton on the lattice: lattice units



Goal: compute QCD topological susceptibility $\chi(T)$

- Temperature range: 0 < T < 2GeV
- Physical quark masses (m_u, m_d, m_s, m_c)
- Continuum limit
- Using
 - $N_f = 2 + 1 + 1$, with isospin splitting correction
 - staggered and overlap quarks
 - Lattices with *N*_t = 8, 10, 12, 16, 20



- Dilute gas of small ($r \approx 1/T$) instantons remain
- Zero modes in the light quark det suppress topology
- $\Rightarrow \chi(T)$ falls sharply above T_c

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T>0 instanton in the continuum



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Challenge #1: large cut-off effects

- Small-instanton zero modes badly captured by lattice Dirac operator
- Higher Q sectors not properly suppressed
- Cut-off effects much larger at higher T
- Solution: identify would-be zero eigenvalues and shift them to zero → reweighting

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T>0 instanton on the lattice: lattice units



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T>0 instanton on the lattice: physical units



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Challenge #1: large cut-off effects

- Small-instanton zero modes badly captured by lattice Dirac operator
- Higher Q sectors not properly suppressed
- Cut-off effects much larger at higher T
- Solution: identify would-be zero eigenvalues and shift them to zero → reweighting

Challenge #2: tiny χ hard to measure

- No statistics for $Q \neq 0$ sectors (dictated by physics)
- Topology change slow on fine lattices (algorithmic)

• Solution:

Derivative of $\chi(T)$ much easier to measure than χ

- Measure $\chi(T_0)$ at low enough T_0
- Using $d\chi/dT$ integrate up to $T \rightarrow$ integral method Also suggested for the quenched case by [Frison et al '16]

Topological susceptibility at T=300 MeV



Topological susceptibility at T=300 MeV



Topological susceptibility at T=300 MeV



Topological susceptibility at T=300 MeV



- Would-be zero eigenvalues too big
- Weight in det is

Lattice: $\lambda_0 + m_f$ Instead of continuum: m_f

• Even if $a \propto 1/T$ (fix N_t , increase β)

 λ_0/m increases with T

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Strong cut-off effects are related to the lack of exact zero-modes.

- In the continuum non-trivial sectors are suppressed by the contribution of zero-modes to the fermion determinant, ie. by the quark mass.
- On the lattice the suppression is altered: $m \rightarrow m + \lambda_0$, where λ_0 is a would be zero-mode. Weaker suppression $\rightarrow \chi(T)$ overestimated.
- To improve 1. identify would be zero-modes
 - 2. restore the continuum weight \rightarrow reweight

$$w[U] \sim \frac{m}{m+\lambda_0}$$

T=300 MeV: susceptibility after reweighting

Topological susceptibility at T=300 MeV



Topology changing streams

simulation time history of the topological charge 3+1 flavor staggered simulation at T=400 MeV

cutoff effects: N_t =6 fluctuates more than N_t =12 for N_t =6 the rewighting factor is more substantial



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• Weight in det is $\lambda_0 + m_f$ instead of m_f

Solution: identify would-be zero modes and shift them to 0

- Compute topological charge Q with Wilson flow [Lüscher '10]
- Identify 4|Q| would-be zero eigenvalues λ₁, λ₂...λ_{4|Q|}
- Modify quark determinant by reweighting with factor

$$w[U] = \prod_{f} \prod_{n=1}^{4|Q|} \left(\frac{m_f}{\lambda_n[U] + m_f}\right)^{1/4}$$

• Approaching the continuum it is getting better $w[U] \rightarrow 1$

Quenched study

Distribution of the would-be zero modes

 $N_f = 2 + 1 + 1$ staggered quarks, T = 240 MeV



Average reweighting factors

 $N_f = 3 + 1$ staggered quarks, T = 300 MeV



Challenge #2: tiny χ hard to measure

- No statistics for $Q \neq 0$ sectors (dictated by physics)
- Topology change slow on fine lattices (algorithmic)

• Solution:

Derivative of $\chi(T)$ much easier to measure than χ

- Measure $\chi(T_0)$ at low enough T_0
- Using $d\chi/dT$ integrate up to $T \rightarrow$ integral method Also suggested for the quenched case by [Frison et al '16]

Instead of waiting for tunneling events, we make simulations in fixed *Q* sectors. How to get

$$Z_1/Z_0 = ?$$

First calculate derivative of $\log Z_1/Z_0$:

$$b_1(T) \equiv \frac{d\log Z_1/Z_0}{d\log T}$$

Use fixed N_t -approach, ie. $T = (aN_t)^{-1}$ is changed by β :

$$b_1(T) = \frac{d\beta}{d\log a} \left(\langle S_g \rangle_1 - \langle S_g \rangle_0 \right)$$

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Fixed *Q* simulation: extra acc/rej step at the end of each update, as lattice spacing decreased the acceptance gets better.

Test in quenched case: pure Wilson action upto $7 \cdot T_c$ and 8×64^3



standard method: extrapolation using a fit; integral method; Dilute Instanton Gas Approximation: exponent agrees nicely, but order of magnitude difference in χ .

Fixed Q integral with fermions

At high temperatures $\chi(T) \sim T^{-b}$ only Q = 0, 1 contribute

$$b_{1} = -\frac{d\beta}{d\log a} \langle S_{g} \rangle_{1-0} - \sum_{f} \frac{d\log m_{f}}{d\log a} m_{f} \langle \overline{\psi}\psi_{f} \rangle_{1-0}$$

• S_g : small cutoff effects, huge statistics \rightarrow staggered $N_f = 3$ • $m_f \langle \overline{\psi} \psi_f \rangle_{1-0}$: large cutoff effects \rightarrow

staggered reweighting for $N_f = 3$, overlap for $N_f = 2 + 1$



Mass integration with chiral fermions

 There is an exact index theorem on the lattice for fermions which satisfy the Ginsparg-Wilson relation

 $\{D, \gamma_5\} = aD\gamma_5D$

- lattice artifacts can be largely reduced
- overlap construction with $H_W = \gamma_5(1 D_W)$: $D = (m_0 - m/2)(1 + \gamma_5 \text{sgn}(H_W)) + m$,
- much more expensive than staggered fermions, but condensate difference can be computed
- we find that $m_f \langle \overline{\psi} \psi_f \rangle_{1-0} = N_f$ for $T \ge 300$ MeV within errors
- this gives the mass exponent required to integrate down to the physical point





Z. Fodor Lattice QCD for axion cosmology

How many sectors are needed?

for large temperatures (above 300 MeV & N_f =3) χ_t is small for not too large volumes only q=0,1 and 2 (for N_f =2+1 even less)



reach saturation ($LT_c \gtrsim 2$) \Rightarrow it is V independent

for small T one needs more sectors χ_t is not that small one should control the contribution of the various sectors.

Volume dependence of χ at T=180 MeV for a \rightarrow 0







Distribution determined by one parameter: $V\chi$

Measure Z_1/Z_0 for any volume $V \rightarrow$ full distribution $\rightarrow \chi$

Topological susceptibility at the physical point

very few topology changes (hard): S. Borsanyi et al. Nature 539 (2016) 69



absolute lower limit (all DM from misalignment): $m_A \gtrsim 28(2) \ \mu eV$ assuming 50-99% other (e.g. strings): $m_A = 50 - 1500 \ \mu eV$

Comparison with other work



- Bonati et.al (1512.06746): smaller exponent
- Petreczky, Schadler, Sharma (1606.03145): bosonic and fermionic definitions, consistent results with large errors
- Y. Taniguchi et al., (1611.02411) gives 7.2(0.9) and 7.3(1.7)

Constraints on the axion mass



- Pre-inflation scenario: *m_A* unambiguously determines the Θ₀ initial condition of our Universe
- Post-inflation: Θ_0 average equivalent to $\Theta \approx 2.15$ absolute lower limit (all DM from misalignment): $m_A \ge 28(2) \ \mu eV$ assuming 50-99% other (e.g. strings): $m_A = 50 - 1500 \ \mu eV$

Motivation

Wilson-flow & scale/topology

Quenched study

Hox gene regulation is central to the evolution of five-digit tetrapods from polydaetyl ancestors PAGE 89

AFRICA'S POWER

STRUGGLE

Can a continent bypass fossil

fuels and adout renewables

Dynamical case

nature

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Summary





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MELZO Lattice QCD for axion cosmology

There may be another

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- Axion: a solution to a) strong CP b) dark matter problems
- Calculating axion production in the early universe requires the EoS and $\chi({\rm T})$
- Brute force approach expensive: estimates using pure SU(3)
- Both were determined using lattice calculations up to high T
- Axion mass in the post-inflation scenario: lower bound: 28(2) μeV estimated mass range: m_A = 50 - 1500 μeV

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Calculated *T*-dependence of the QCD topological susceptibility

- Temperature range: 0 ≤ T ≤ 2 GeV (follow change of χ over 10 orders of magnitude)
- Physical quark masses
- Continuum limit

Main lesson: keep in mind the physics of the problem

- Large cut-off effects due to instanton zero-modes
- At high T: tiny $\chi \rightarrow$ ideal instanton gas