Topological properties of strong interactions: from vacuum structure to axion phenomenology

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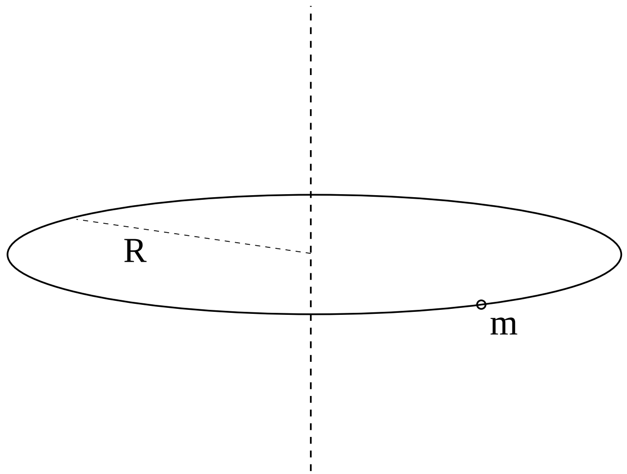
SUMMARY

- Strong interactions are described by QCD, a theory blessed by asymptotic freedom at high energies, which however becomes non-perturbative at low energies
- The existence of configurations with non-trivial topology, and the possible association with a CP-violating θ parameter, are among the most interesting non-perturbative features
- They also open a possible new window towards new physics beyond the standard model. Why is $\theta = 0$ in nature? $\Longrightarrow$ Peccei-Quinn mechanism and axions
- I will review issues related to topology and θ-dependence in QCD, focussing on numerical results from lattice QCD simulations
- I will first describe a simple QM model where most concepts about θ dependence are easily introduced

The free particle on a circle

alias: the simplest QM problem with non-trivial topological structure and numerical challenges



We will consider the path integral formulation for a free particle constrained on a circle of radius R

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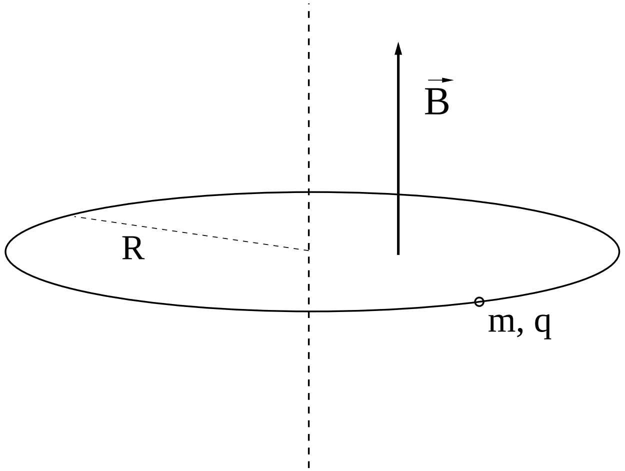

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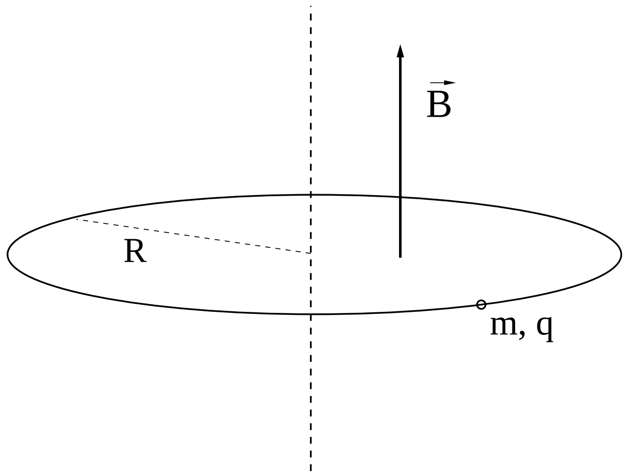

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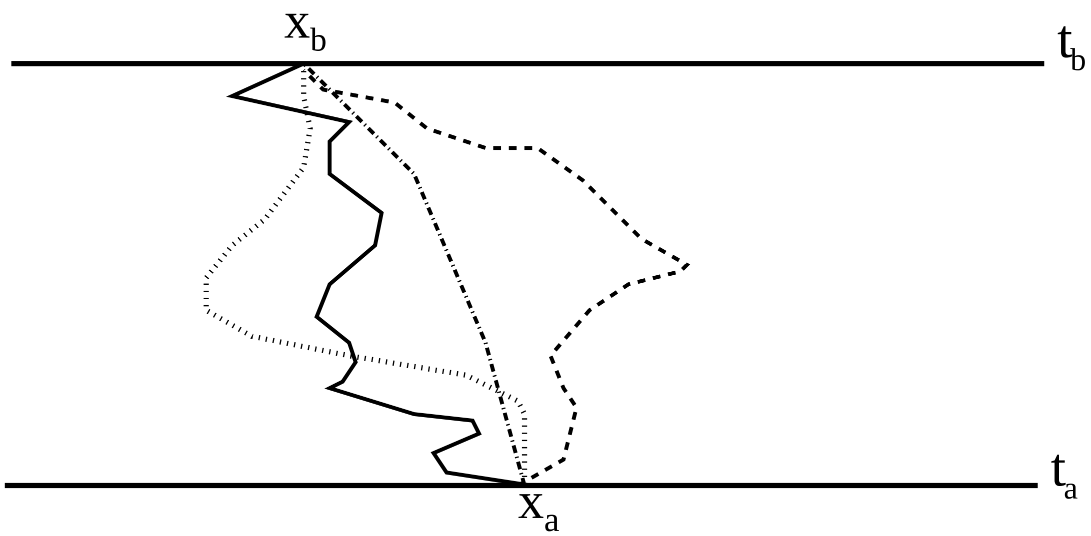
- This is a great example, where basic issues concerning topology and θ-dependence in gauge theories can be discussed in a simplified framework

- Even if everything is analitically computable here, as we try to study it by Monte-Carlo simulations, we face the same problems and failures as in QCD

Feynman path integral in a few words



The starting point is rewriting the probability amplitude for going from point x_a to point x_b in time $t_b - t_a$

$$\langle x_b | e^{-iH(t_b - t_a)/\hbar} | x_a \rangle = \mathcal{N} \int_{x(t_{a/b}) = x_{a/b}} \mathcal{D}x(t) \exp\left(\frac{iS[x(t)]}{\hbar}\right)$$

All possible paths contribute,"weighted" by an oscillating phase factor $\exp\left(\frac{iS[x(t)]}{\hbar}\right)$, where S is the classical action associated with each path.

$$S[x(t)] = \int_{t_a}^{t_b} dt' \mathcal{L}(x(t'), \dot{x}(t'))$$

The thermal partition function can be given a path integral formulation as well

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = \sum_n e^{-\beta E_n} = \int dx \langle x| e^{-\frac{H}{k_B T}} |x\rangle$$

the trace can be taken over energy eigenstates, but also over position eigenstates

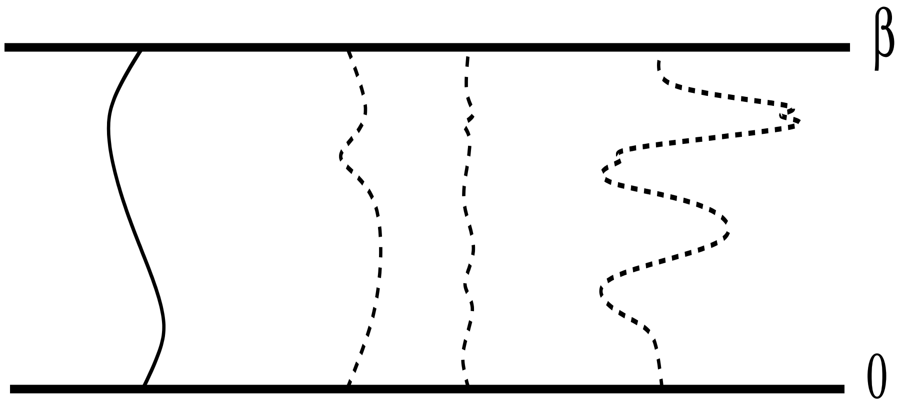
same amplitude as before if $|x_a\rangle = |x_b\rangle = |x\rangle$ **and** $\beta = \frac{1}{k_B T} = i(t_b - t_a)/\hbar$**.**

$$Z = \mathcal{N} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)$$

τ **is the Euclidean time,** $\tau \in [0, \hbar/(k_B T)]$**. Integration is over paths periodic in** τ**.**

S_E **is the Euclidean action, obtained from** S **after Wick rotation** $t \to -i\tau$

$F = -\frac{1}{\beta} \log Z$ **is the free energy of the system, which in the** $T \to 0$ **limit (**$\beta\hbar \to \infty$**) coincides with the ground state energy**



Z is a sum over periodic paths, weighted by factor $\exp(-\frac{S_E}{\hbar})$.

For well behaved potentials that can be given a probabilistic interpretation

Thermal averages are then expectation values of path functionals over a thermal path probability distribution function $P[x(\tau)]$

$$\langle O\rangle_T = \frac{\mathrm{Tr}\left(e^{-\beta H}O\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)} = \frac{\int \mathcal{D}x(\tau)\exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)O[x(\tau)]}{\int \mathcal{D}x(\tau)\exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right)} \equiv \int \mathcal{D}x(\tau)P[x(\tau)]O[x(\tau)]$$

as $\beta \to \infty$, one recovers vacuum expectation values

Monte-Carlo computation of the path integral

- **After discretization (continuum $\rightarrow$ lattice), the number of integration variables is finite, the problem is numerically affordable.**

- **Huge number of variables $\Longrightarrow$ Optimal strategy: Monte-Carlo extraction of a sample of paths $x_1(\tau), x_2(\tau), \ldots, x_M(\tau)$ distributed according to $P[x(\tau)]$.**

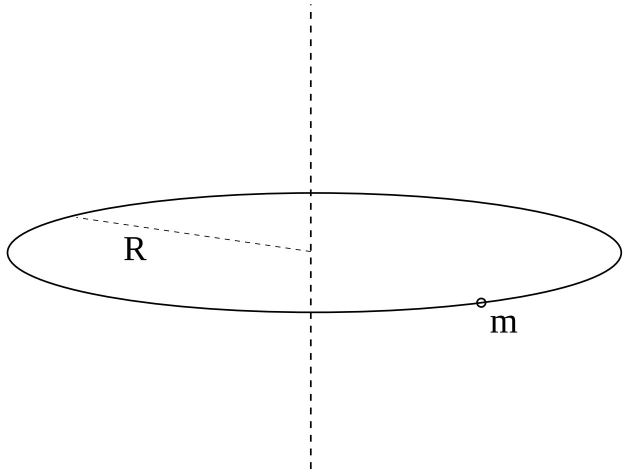
- **The sample average**

$$\bar{O} = \frac{1}{M} \sum_{i=1}^{M} O[x_i(\tau)]$$

is normally distributed around the true average $\langle O \rangle = \int \mathcal{D}x(\tau) P[x(\tau)] O[x(\tau)]$ with a statistical error of order $1/\sqrt{M}$ *(Central Limit Theorem)*

- **Of course, the discretization must be fine enough and one needs numerical results for several lattice spacings in order to extrapolate to the continuum limit**

Let us go back to the circle



In the standard approach Z is written a sum over energy/angular momentum eigenstates

$$Z = \sum_{n=-\infty}^{\infty} \exp\left(-\beta \frac{\hbar^2 n^2}{2mR^2}\right)$$

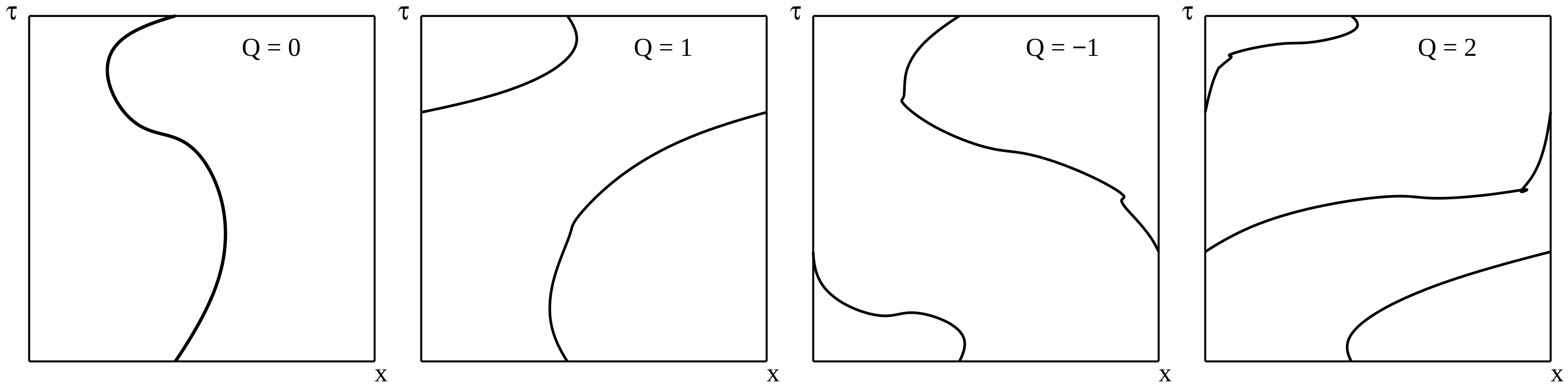
in the path integral approach

$$Z = \mathcal{N} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp\left(\frac{-S_E[x(\tau)]}{\hbar}\right) \quad ; \quad S_E[x(\tau)] = \int_0^{\beta\hbar} d\tau\, \frac{1}{2} m \left(\frac{dx}{d\tau}\right)^2$$

New feature: paths divide in topological classes

Boundary conditions in space $\Longrightarrow$ each path $x(\tau)$ contributing to Z is a continuous application from the temporal circle to the spatial circle.

how many times does the path wind around the circle before closing in eucl. time?



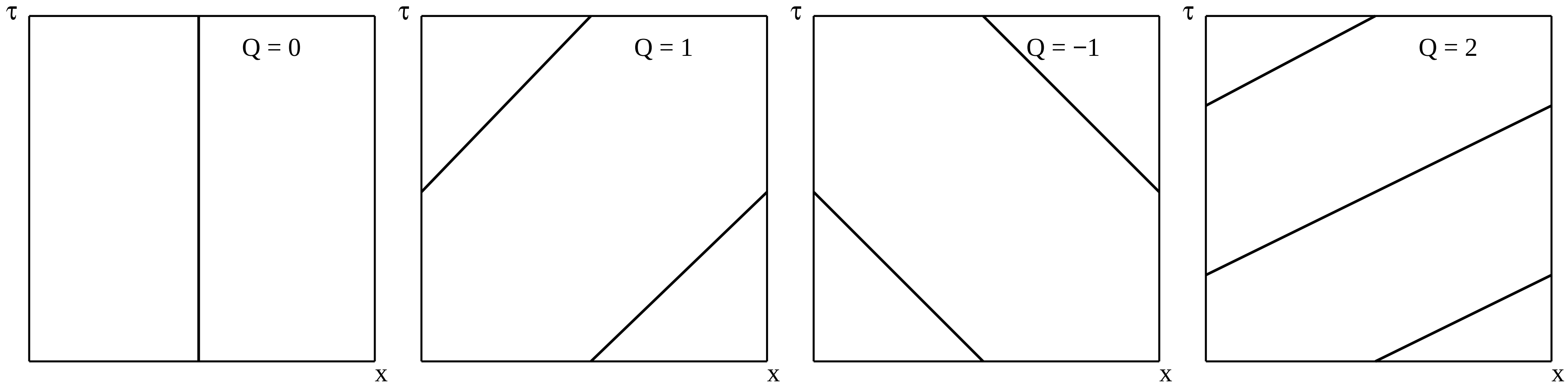
Paths are divided in homotopy classes according to their winding number Q which cannot be changed without cutting the path.

On the other hand, discontinuous paths have zero measure in the path integral

Wiener measure: first derivative divergent, but continuity is guaranteeed

The homotopy group is $\pi_1(S^1) = \mathbb{Z}$

Can we compute the contribution of each topological sector to the path integral? YES



- **The path integral over each sector can be done by integrating over classical solutions, which are minima of the Euclidean action**

- **In this simple case the integration can be done exactly, yielding a result proportional to $\exp(-S_Q/\hbar)$ where S_Q is the action of the classical path**

$$S_Q = \frac{1}{2} m \frac{(2\pi R Q)^2}{\beta\hbar}$$

- **We have therefore an expression for the weight of each sector, which is nothing but the probability distribution $P(Q)$ over the winding number Q**

$$P(Q) \propto \exp\left(-\frac{Q^2}{2\beta\hbar\chi}\right) \quad ; \quad \chi \equiv \frac{\hbar}{4\pi^2 m R^2}$$

Low and high T limits

$$Z = \sum_{n=-\infty}^{\infty} \exp\left(-\beta \frac{\hbar^2 n^2}{2mR^2}\right) \propto \sum_{Q=-\infty}^{\infty} \exp\left(-\frac{1}{\beta}\frac{Q^2}{2\hbar\chi}\right) = \sum_{Q=-\infty}^{\infty} \exp\left(-\frac{1}{\beta}\frac{2\pi^2 mR^2Q^2}{\hbar^2}\right)$$

the partition function can be written in terms of two different series, which are sort of dual to each other (β vs $1/\beta$ in the exponential)

- **low T (ground state physics)** ($\beta\hbar^2/(mR^2) \sim \hbar\beta\chi \gg 1$)

  - only lowest energy levels (lowest $|n|$) contribute

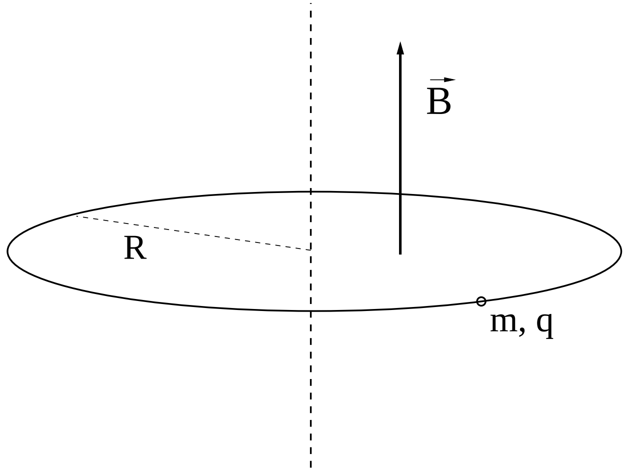
  - all Q values contribute and they are $\sim$ Gaussian distributed with variance $\sigma = \hbar\beta\chi$

- **high T:** ($\beta\hbar^2/(mR^2) \sim \hbar\beta\chi \ll 1$)

  - all energy levels n contribute, they are $\sim$ Gaussian distributed with variance $\sigma = 1/(4\pi^2\beta\hbar\chi)$

  - only lowest winding numbers contribute

And now the magnetic field, alias the θ-term



A uniform magnetic field across the circle implies a tangential gauge potential $A = BR/2$, hence

$$L = \frac{1}{2}mv^2 + qAv = \frac{1}{2}mv^2 + \frac{qBR}{2}v$$

while the energy levels change into

$$E_n = \frac{(\hbar^2 n^2 - qB^2R^4/2)^2}{(2mR^2}$$

In the Euclidean path integral formalism ($t \rightarrow -i\tau$) that amounts to adding the following term to the Euclidean action S_E:

$$i\frac{qBR}{2\hbar}\int_0^{\beta\hbar} d\tau \frac{dx}{d\tau} = i\frac{qBR}{2\hbar}\, 2\pi RQ = i\theta Q \quad ; \quad \theta \equiv \frac{\pi qBR^2}{\hbar}$$

Notice: a total derivative in the Lagrangian, does not change the classical equations, but leads to a global contribution which is constant in each topological sector

How the partition function changes

$$Z = \sum_{n=-\infty}^{\infty} e^{-\beta E_n} = \sum_{n=-\infty}^{\infty} e^{-\frac{\beta\hbar\chi}{2}(2\pi n-\theta)^2} = \mathcal{N} \int \mathcal{D}x(\tau) e^{-S_E[x(\tau)]/\hbar} e^{i\theta Q} \propto \sum_{Q=-\infty}^{\infty} e^{-\frac{1}{2\hbar\chi\beta}Q^2} e^{i\theta Q}$$

- **θ-dependence of the free energy $F(\theta) = -\log Z(\theta)/\beta$ here is related to the magnetic properties of the system. General features:**
  - $F(\theta + 2\pi) = F(\theta)$ (**θ is an angular variable**) ; $F(-\theta) = F(\theta)$
  - $Z(\theta) \leq Z(0) \implies F(\theta) \geq F(0)$ (**Vafa-Witten theorem**) $\implies$ **diamagnetism**

- **in the path integral formalism, a complex weight appears, which hinders the application of Monte-Carlo simulations. This is usually known as the sign problem.**

- **It afflicts other theories with a topological term. Here, it disappears when resumming Z in terms of other variables (n): such a rewriting is still a mirage in other cases**
  Then, how to investigate θ-dependence in the path-integral approach?

Taylor expansion approach

$$F(\theta) - F(0) = \frac{1}{2}F^{(2)}\theta^2 + \frac{1}{4!}F^{(4)}\theta^4 + \ldots \quad ; \qquad F^{(2n)} = \left.\frac{d^{2n}F}{d\theta^{2n}}\right|_{\theta=0}$$

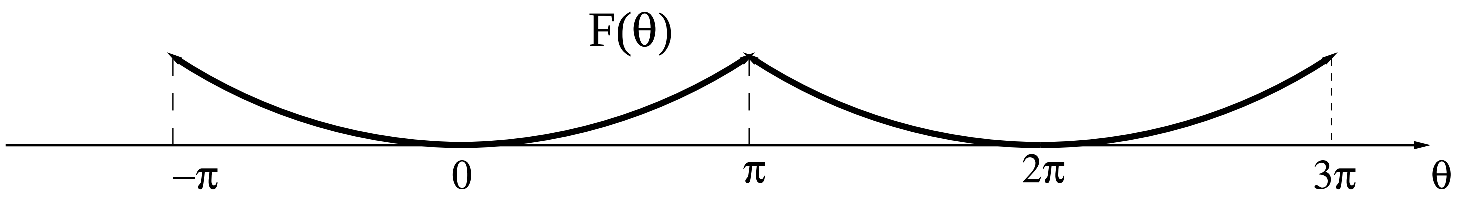
Taylor coefficients: cumulants of the Q distribution $P(Q) \propto e^{-Q^2/(2\hbar\beta\chi)}$ at $\theta = 0$

$$F^{(2)} = \frac{\langle Q^2\rangle_c}{\beta\hbar} = \frac{\langle Q^2\rangle - \langle Q\rangle^2}{\beta\hbar} \; ; \quad F^{(4)} = -\frac{\langle Q^4\rangle_c}{\beta\hbar} = -\frac{\langle Q^4\rangle - 3\langle Q^2\rangle^2}{\beta\hbar} \; ; \quad F^{(2n)} = -(-1)^n\frac{\langle Q^{2n}\rangle_c}{\beta\hbar}$$

as $\hbar\beta\chi \to \infty$ (vacuum), Q is purely Gaussian, only $F^{(2)} \neq 0$ (topological susceptibility)

$$F(\theta) - F(0) = \frac{\chi}{2}\theta^2$$

that, when combined with the expected periodicity and symmetries, gives rise to a multibranched function with quantum phase transitions at $\theta = \pi$ or odd multiples of it



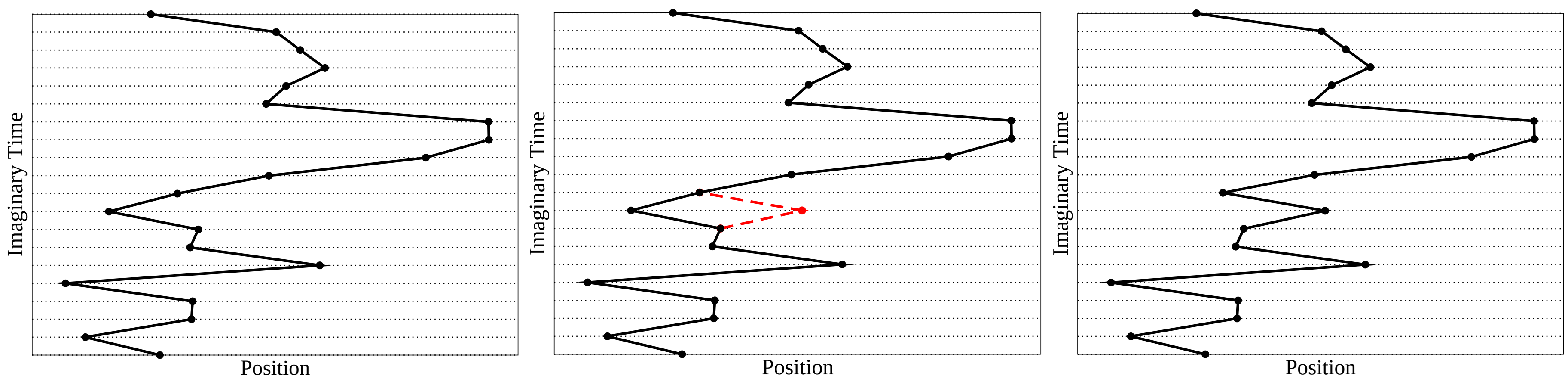
In terms of energy levels, at π we have a level crossing associated with the quantum phase transition, which disappears as soon as $T \neq 0$

In the opposite, hight T limit, $\hbar\beta\chi \ll 1$, only the lowest topological sectors contribute, taking just $Q = 0, 1, -1$:

$$Z(\theta) \propto 1 + 2e^{-1/(2\hbar\beta\chi)} \cos\theta \implies F(\theta) - F(0) \simeq -\frac{2}{\beta} e^{-1/(2\hbar\beta\chi)} \cos\theta$$

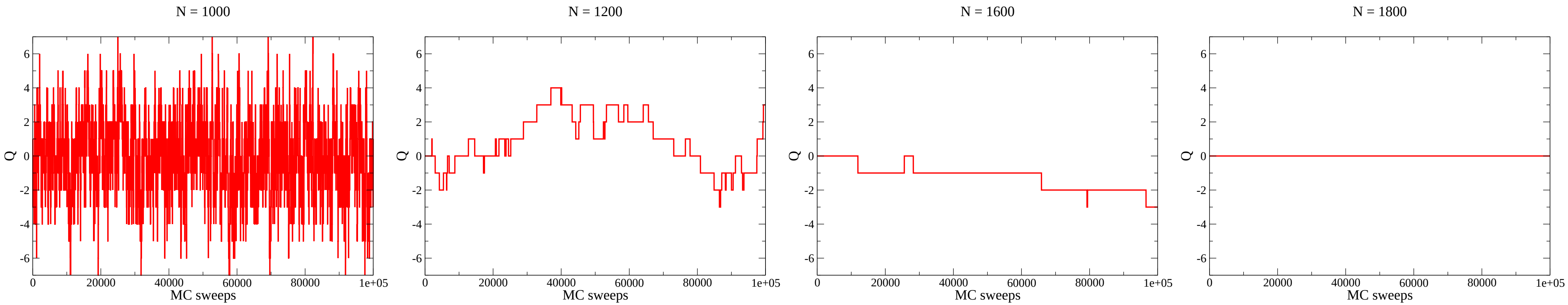
i.e. a smooth, periodic behavior in θ

Problems in numerical sampling of topological modes



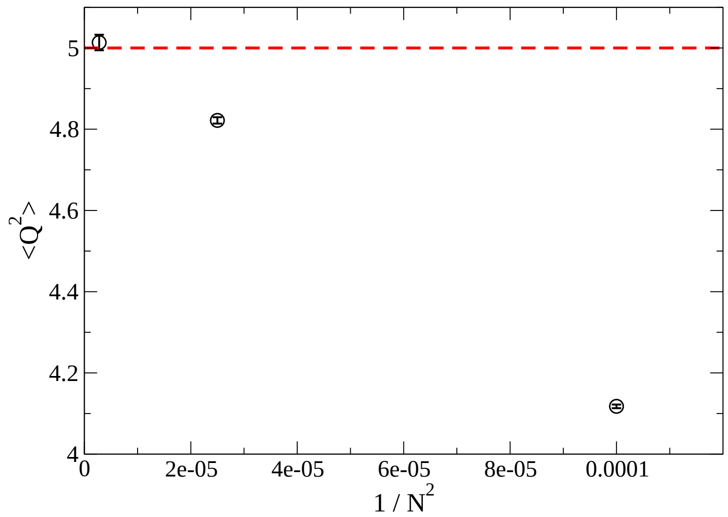
Apart from the sign problem, the study of θ-dependence faces other numerical challenges:

- **standard algorithms update the path configuration by small local steps**
- **in the continuum limit, paths evolve *almost continuously* in configuration space**
- **how is it possible, in this limit, to change topological sector? One should move across unlikely "discontinuous paths", which in the continuum limit have zero measure.**
- **standard algorithms become slower and slower in moving from one topological sector to the other, until they become completely non-ergodic.**



Set of MC histories (100K sweeps, Metropolis algorithm), obtained at fixed $\hbar\beta\chi = 5$ varying the number of temporal slices N

Critical slowing down proceeds fast towards complete freezing of topological modes



Luckily enough, in this case numerical results approach the continuum limit quite earlier (finest point $N = 600$)

Back to QCD

QCD is a bit less trivial than a particle on a circle, its Euclidean action reads:

$$S_{QCD} = \int d^4x \, \mathcal{L}_{QCD} = \int d^4x \left(\sum_f \bar{\psi}_f \left(D_\mu \gamma_\mu + m_f \right) \psi_f + \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} \right)$$

ψ_f **are quark fields (six flavors of spin 1/2, in the fundamental repres. of the** $SU(3)$ **gauge group)**

A^a_μ **are gluonic gauge fields (8 spin 1, color charged bosonic particles)**

$G^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu - g f^{abc} A^b_\mu A^c_\nu$ **is the field strength tensor**

$D_{\mu\, ij} = \partial_\mu \delta_{ij} + i g T^a_{ij} A^a_\mu$ **is the covariant derivative** g **is the color gauge coupling**

Also in this case relevant gauge field configurations divide in homotopy classes, characterized by an integer winding number $Q = \int d^4x \; q(x)$

$$q(x) = \frac{g^2}{64\pi^2} G^a_{\mu\nu}(x) \tilde{G}^a_{\mu\nu}(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu}(x) G^a_{\rho\sigma}(x)$$

$$GG \propto \vec{E}^a \cdot \vec{E}^a + \vec{B}^a \cdot \vec{B}^a \;\; ; \quad G\tilde{G} \propto \vec{E}^a \cdot \vec{B}^a$$

Homotopy group: $\pi_3(SU(3)) = \mathbb{Z}$ **(actually,** $\pi_3(SU(N_c)) = \pi_3(SU(2)) \; \forall \; N_c$**)**

Classical solutions with non-trivial winding around the gauge group: instantons

characterized by various parameters: position, radiud ρ, . . .

Effective action known only perturbatively. The 1-loop one-instanton contribution is

$$\exp\left(-\frac{8\pi^2}{g^2(\rho)}\right)$$

where $g(\rho)$ is the running coupling at the instanton scale ρ.

- **by asymptotic freedom, works well for small instantons, which are then exponentially suppressed, implying the validity of a dilute instanton gas approximation (DIGA)**

- **however, perturbation theory breaks down for large instantons ($1/\rho \lesssim \Lambda_{QCD}$), which become dominant, overlap with each other, and break DIGA**

QCD at non-zero θ

Also in this case, we can modify the theory introducing a θ-parameter coupled to Q:

$$Z(\theta) = \int [\mathcal{D}A][\mathcal{D}\bar{\psi}][\mathcal{D}\psi]\, e^{-S_{QCD}}\, e^{i\theta Q}$$

θ is a super-selection parameter: different θ, different Hilbert space

$G\tilde{G}$ is renormalizable, the theory at $\theta \neq 0$ is well defined, but presents explicit breaking of CP symmetry ($\tilde{G} \propto \vec{E} \cdot \vec{B}$)

As for the 1D-model, the free energy density $F(\theta) = -T \log Z/V$ is a periodic even function of θ, $F(\theta) \geq F(0)$, which can be expanded around $\theta = 0$ (assuming analyticity)

$$F(\theta) - F(0) = \frac{1}{2} F^{(2)} \theta^2 + \frac{1}{4!} F^{(4)} \theta^4 + \ldots \quad ; \qquad F^{(2n)} = \left. \frac{d^{2n} F}{d\theta^{2n}} \right|_{\theta=0} = -(-1)^n \frac{\langle Q^{2n} \rangle_c}{V_4}$$

$V_4 = V/T$ **is the 4D volume**

A common parametrization

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

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

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

The probability distribution $P(Q)$ of the different topological sectors now is not known: it is a non-perturbative property of QCD

Coefficients b_{2n} parametrize deviations of the distribution of topological charge from a Gaussian in the theory at $\theta=0$.

A substantial difference with respect to the toy-model: we have fermions around

An axial $U(1)_A$ rotation of the fermion fields move θ from the gluon to the quark sector (same concept as for the axial anomaly). For any flavor:

$$\psi_f \to e^{i\alpha\gamma_5}\psi_f \qquad \text{and} \qquad \bar{\psi}_f \to \bar{\psi}_f e^{i\alpha\gamma_5}$$

$$\Longrightarrow \quad \theta \to \theta - 2\alpha \qquad \text{and} \qquad m_f \to m_f e^{2i\alpha}$$

- **should any quark be massless (this is not the case), θ could be rotated away and θ-dependence would be trivial**

- **in the presence of light quarks (this is the case), θ-dependence can be reliably studied within the framework of chiral perturbation theory (χPT)**

Experimental bounds on the electric dipole of the moment set stringent limits to the amount of CP-violation in strong interactions.

$$|\theta| \lesssim 10^{-10}$$

So: why do we bother with θ-dependence at all?

- **θ-dependence $\longleftrightarrow P(Q)$ at $\theta = 0$ $\Longrightarrow$ it enters phenomenology anyway.**
  e.g., Witten-Veneziano mechanism: $\chi^{YM} = f_\pi^2 m_{\eta'}^2/(2N_f)$

- **Strong CP-problem: why is $\theta = 0$?** $m_f = 0$ **is ruled out.**
  A possible mechanism (Peccei-Quinn) invokes the existence of a new scalar field (axion) whose properties are largely fixed by θ-dependence

- **Axions are popular dark matter candidates, so the issue is particularly important**

The QCD axion

Main idea: add a new scalar field a, with only derivative terms acquiring a VEV $\langle a \rangle$ and coupling to the topological charge density. Low energy effective lagrangian:

$$\mathcal{L}_{eff} = \mathcal{L}_{QCD} + \frac{1}{2}\partial_\mu a \partial^\mu a + \left(\theta + \frac{a(x)}{f_a}\right) \frac{g^2}{32\pi^2} G\tilde{G} + \dots$$

- a is the Goldstone boson of a spontaneously broken (Peccei-Quinn) $U(1)$ axial symmetry (various high energy models exist)
- coupling to $G\tilde{G}$ involves the decay constant f_a, supposed to be very large
- shifting $\langle a \rangle$ shifts θ by $\langle a \rangle / f_a$. However θ-dependence of QCD breaks global shift symmetry on $\theta_{eff} = \theta + \langle a \rangle / f_a$, and the system selects $\langle a \rangle$ so that $\theta_{eff} = 0$.
- Assuming f_a very large, a is quasi-static and its effective couplings (mass, interaction terms) are fixed by QCD θ-dependence. For instance

$$m_a^2(T) = \frac{\chi(T)}{f_a^2} = \frac{\langle Q^2 \rangle_{T,\theta=0}}{V_4 f_a^2}$$

knowing $F(\theta, T)$ fixes axion parameters during the Universe evolution

Predictions about θ-dependence - I

Dilute Instanton Gas Approximation (DIGA) for high T (Gross, Pisarski, Yaffe 1981)

- **instantons - antiinstantons treated as uncorrelated (non-interacting) objects**

  Poisson distribution with an average probability density p per unit volume

$$Z_\theta \simeq \sum \frac{1}{n_+! n_-!} (V_4 p)^{n_+ + n_-} e^{i\theta(n_+ - n_-)} = \exp\left[2 V_4 p \cos\theta\right]$$

$$F(\theta,T) - F(0,T) \simeq \chi(T)(1 - \cos\theta) \implies \quad b_2 = -1/12\,; \quad b_4 = 1/360\,; \ldots$$

- **Instantons of size $\rho \gg 1/T$ suppressed by thermal fluctuations, for high T instantons of effective perturbative action $8\pi/g^2(T)$ dominate. Including also leading order suppression due to light fermions and zero modes:**

$$\chi(T) \sim T^4 \left(\frac{m}{T}\right)^{N_f} e^{-8\pi^2/g^2(T)} \sim m^{N_f} T^{4 - \frac{11}{3} N_c - \frac{1}{3} N_f} \propto T^{-7.66} \quad (\text{for } N_f = 2)$$

Notice: perturbative limit implies diluteness, hence DIGA, however DIGA might be good before reaching the asymptotic perturbative behavior

Predictions about θ-dependence - II

Chiral Perturbation Theory (χPT) for low T

At low T, perturbation theory breaks down, however, by $U(1)$ axial rotations, θ can be moved to the light quark masses. Then, χPT can be applied as usual.

Result for the ground state energy **(Di Vecchia, Veneziano 1980)**

$$E_0(\theta) = -m_\pi^2 f_\pi^2 \sqrt{1 - \frac{4 m_u m_d}{(m_u + m_d)^2} \sin^2 \frac{\theta}{2}}$$

$$\chi = \frac{z}{(1+z)^2} m_\pi^2 f_\pi^2, \quad b_2 = -\frac{1}{12} \frac{1+z^3}{(1+z)^3}, \quad z = \frac{m_u}{m_d}$$

Explicitly

$$z = 0.48(3) \qquad \chi^{1/4} = 75.5(5)\,\mathrm{MeV} \qquad b_2 = -0.029(2)$$

$$z = 1 \qquad \chi^{1/4} = 77.8(4)\,\mathrm{MeV} \qquad b_2 = -0.022(1)$$

$$\Longrightarrow \qquad m_a \sim 10^{-5} \left(\frac{10^{12}\mathrm{GeV}}{f_a} \right)$$

Predictions about θ-dependence - III

Large-N_c for low T $SU(N_c)$ gauge theories (Witten, 1980)

$$L_{QCD}(\theta) = \frac{1}{4} G^a_{\mu\nu} G^a_{\mu\nu} + \theta \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} G^a_{\mu\nu} G^a_{\rho\sigma}$$

$g^2 N_c = \lambda$ **is kept fixed as** $N_c \to \infty \implies$ **if any non-trivial dependence on** θ **exist in the large-**N_c **limit, the dependence must be on** $\bar{\theta} = \theta/N_c$**.**

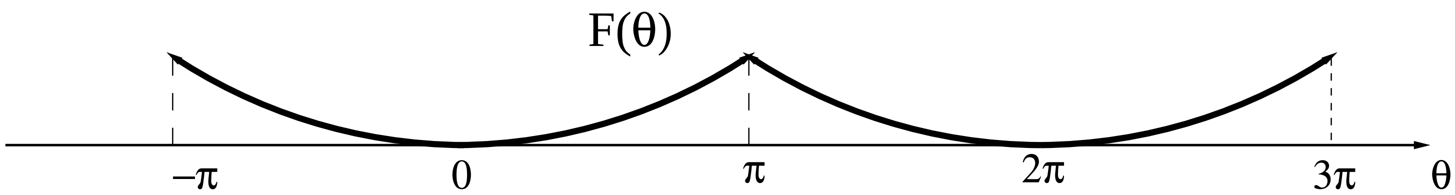
$$F(\theta, T) - F(0, T) = N_c^2 \bar{F}(\bar{\theta}, T)$$

$$\bar{F}(\bar{\theta}, T) = \frac{1}{2} \bar{\chi} \bar{\theta}^2 \left[1 + \bar{b}_2 \bar{\theta}^2 + \bar{b}_4 \bar{\theta}^4 + \cdots \right]$$

Matching powers of $\bar{\theta}$ **and** θ **we obtain**

$$\chi \sim N_c^0 \;\; ; \quad b_2 \sim N_c^{-2} \;\; ; \quad b_{2n} \sim N_c^{-2n}$$

$P(Q)$ **is Gaussian in the large** N_c**, as the toy model. Periodicity in** θ **enforces a multibranched structure with phase transitions at** $\theta = (2k+1)\pi$**.**



Numerical Results from Lattice QCD

main technical and numerical issues

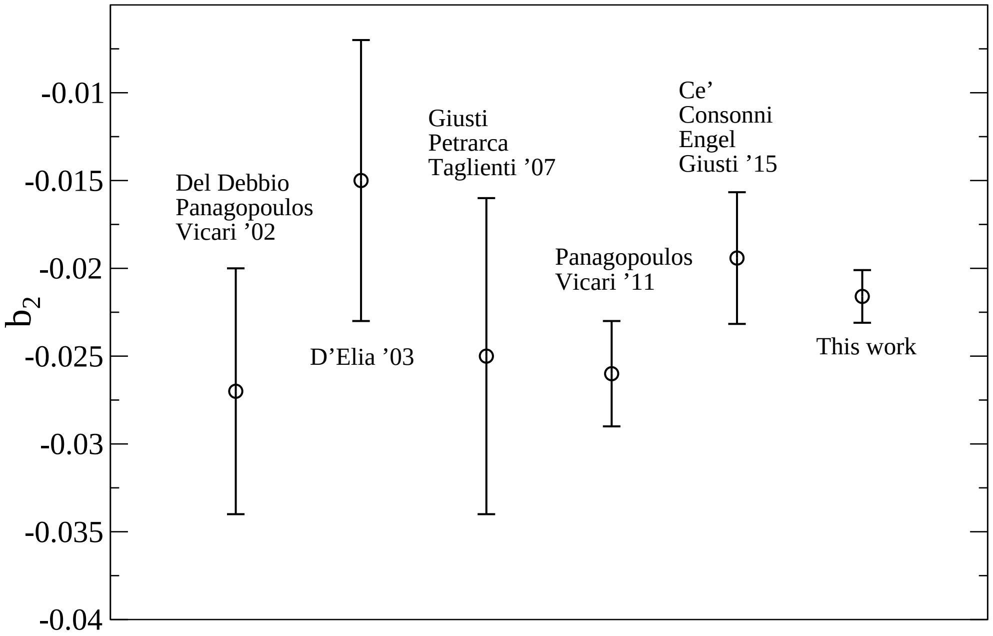
- **topological charge renormalizes, naive lattice discretizations are non-integer valued. Various methods devised leading to consistent results**
  - field theoretic compute renormalization constants and subtract
  - fermionic definitions use the index theorem to deduce Q from fermionic zero modes
  - smoothing methods use various techniques to smooth gauge fields and recover an integer valued Q (cooling, Wilson flow, smearing ...all substantially equivalent (see e.g. Panagopoulos, Vicari 0803.1593, Bonati, D'Elia 1401.2441)

- **Determination of higher cumulants is numerically challenging: need to detect deviations from a Gaussian, but as $V_4 \to \infty$ Gaussian modes dominate.**

- **Freezing of topological modes in the continuum**

Pure gauge results: $T = 0$

The value of the topological susceptibility is well know, with increasing refinement, since 20 years, and compatible with the Witten-Veneziano mechanism for $m_{\eta'}$, $\chi^{1/4} \sim 180$ MeV



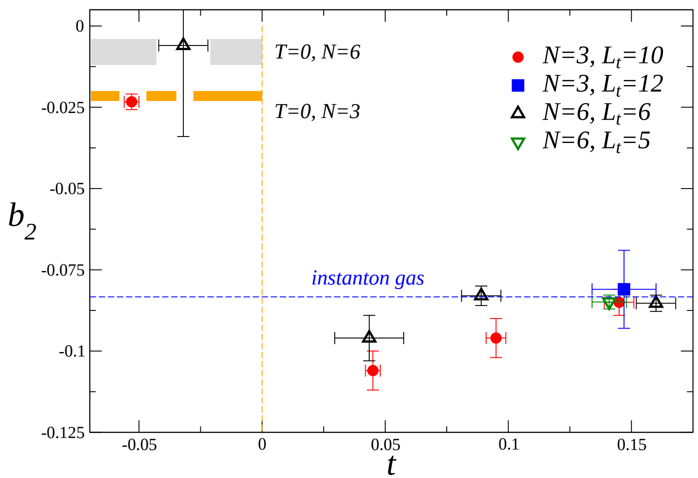
Determination of b_2 more difficult. Most recent determination for $SU(3)$ (Bonati, D'Elia, Scapellato, 1512.01544) obtained by introducing an external imaginary θ source to improve signal/noise.

Evidence for $1/N_c^2$ scaling still preliminary

Still upper bounds for b_4, for $SU(3)$ $|b_4| \lesssim 4 \times 10^{-4}$ (Bonati, D'Elia, Scapellato, 1512.01544)

Pure gauge results: Finite T, across and above T_c

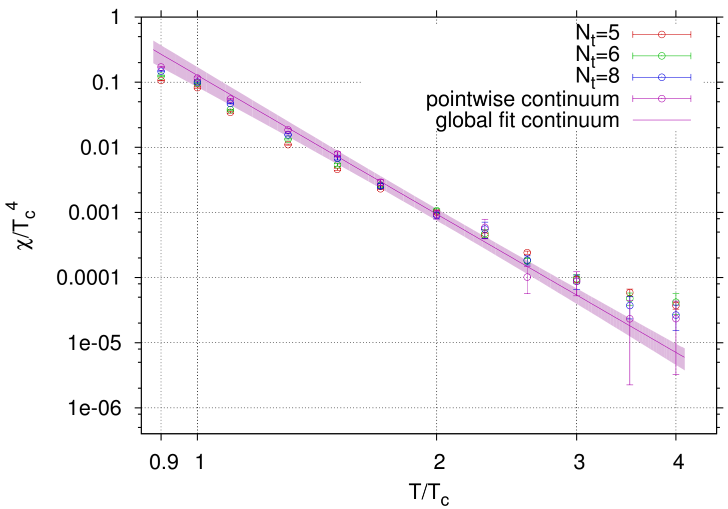
Topological activity stays almost unchanged till T_c and then χ drops suddenly: known since 20 years, but we had recent significant progress:



from Bonati, D'Elia, Panagopoulos, Vicari 1301.7640

DIGA values for higher cumulants reached quite soon, already for $T \gtrsim 1.1\,T_c$.

Small deviations compatible with repulsive instanton-instanton interactions



from S. Borsanyi et al. 1508.06917

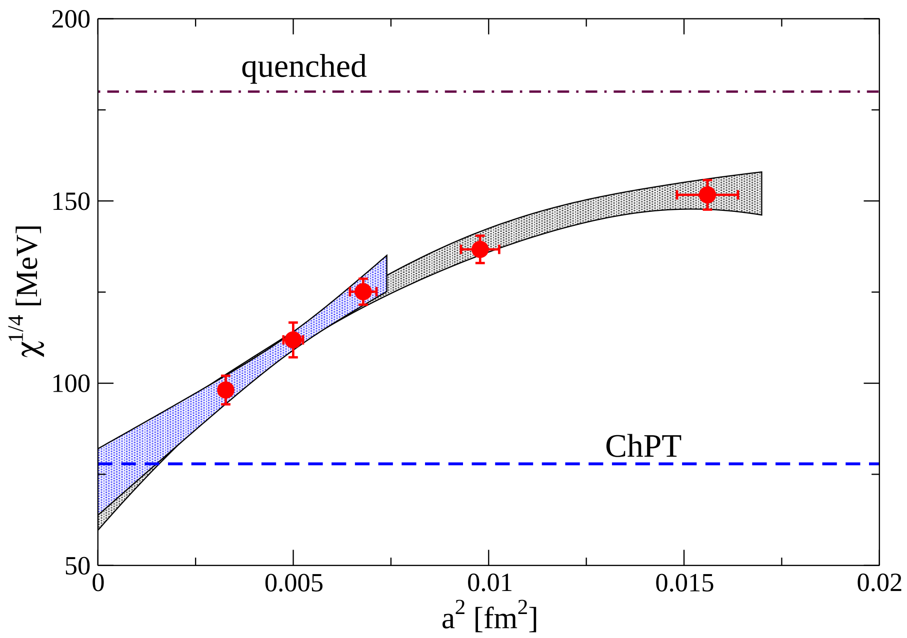
The perturbative power low behavior predicted for χ at high T has been verified

$\chi(T) \propto 1/T^b$, where $b = 7.1(4)(2)$ (perturbative prediction $b = 7$), but absolute value a factor 10 larger

Full QCD results

from C. Bonati et al., JHEP 1603 (2016) 155 [arXiv:1512.06746]

We have performed simulations of $N_f = 2 + 1$ QCD, with stout improved staggered fermions, a tree-level Symanzik gauge action, at the physical point (physical quark masses)

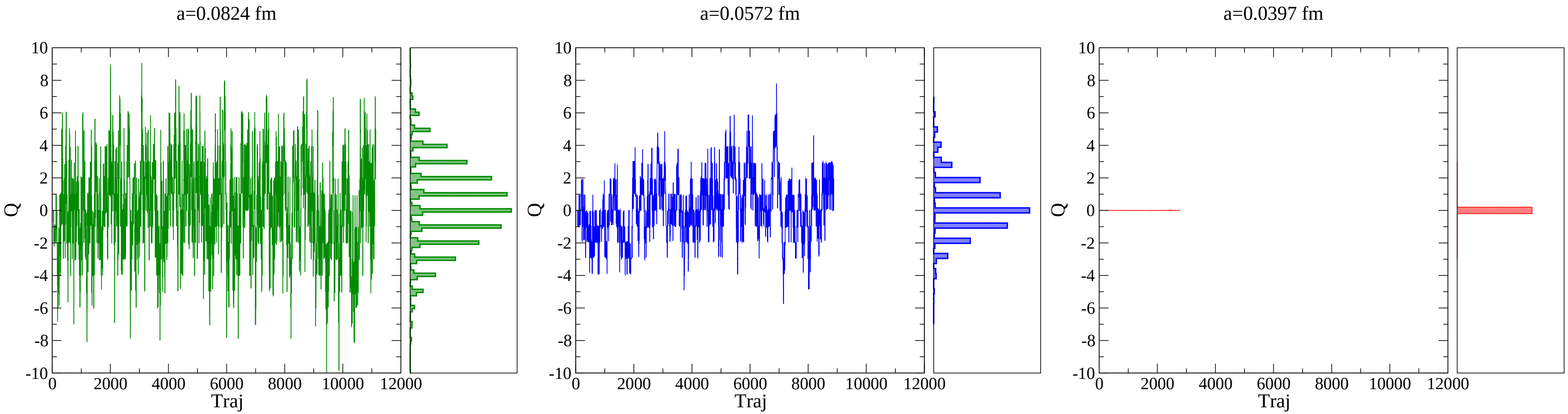


The approach to the continuum limit is quite slow and lattice spacing well below 0.1 fm are needed

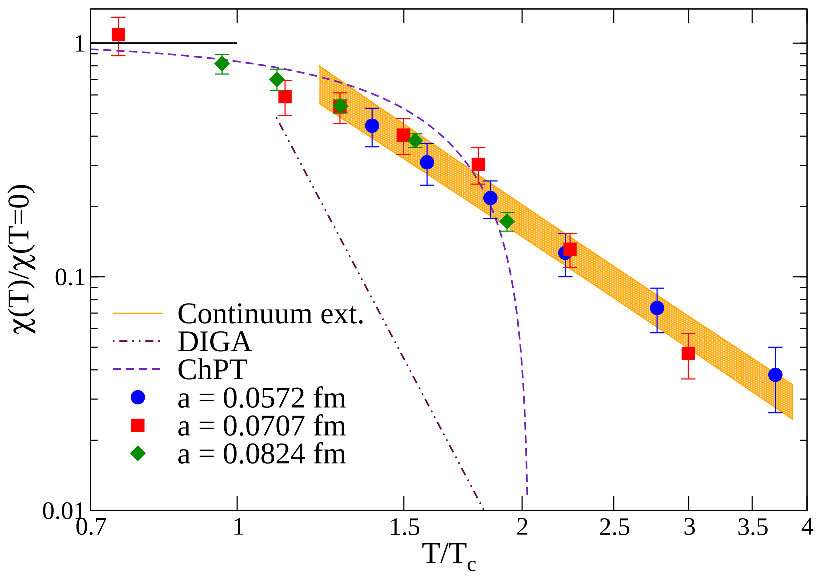
continuum limit compatible with ChPT ($73(9)\mathrm{MeV}$ against $77.8(4)\mathrm{MeV}$)

slow convergence to the continuum is strictly related to the slow approach to the correct chiral properties of fermion fields

The need for quite small lattice spacings, in order to correctly extrapolate to the continuum limit, has brought us to the frontier of frozen topology



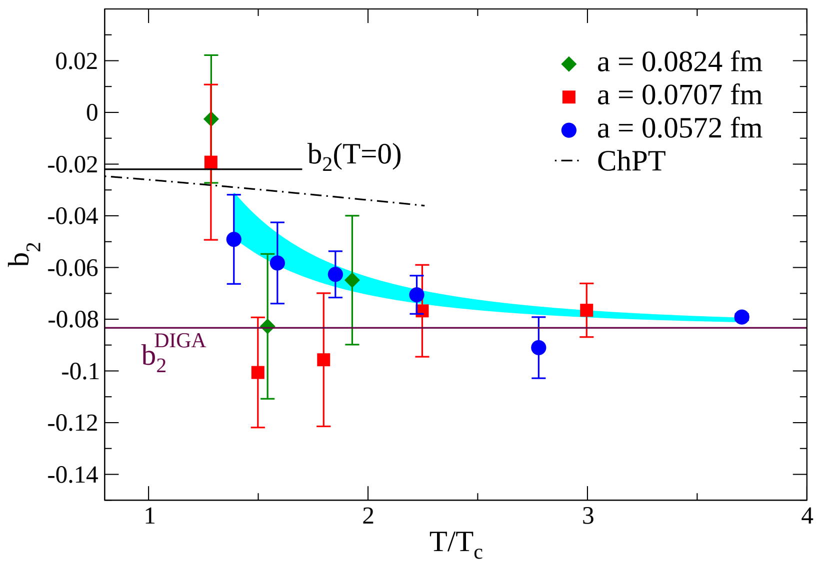
Finite T results provide some surprises



Cut-off effects strongly reduced in the ratio $\chi(T)/\chi(T=0)$

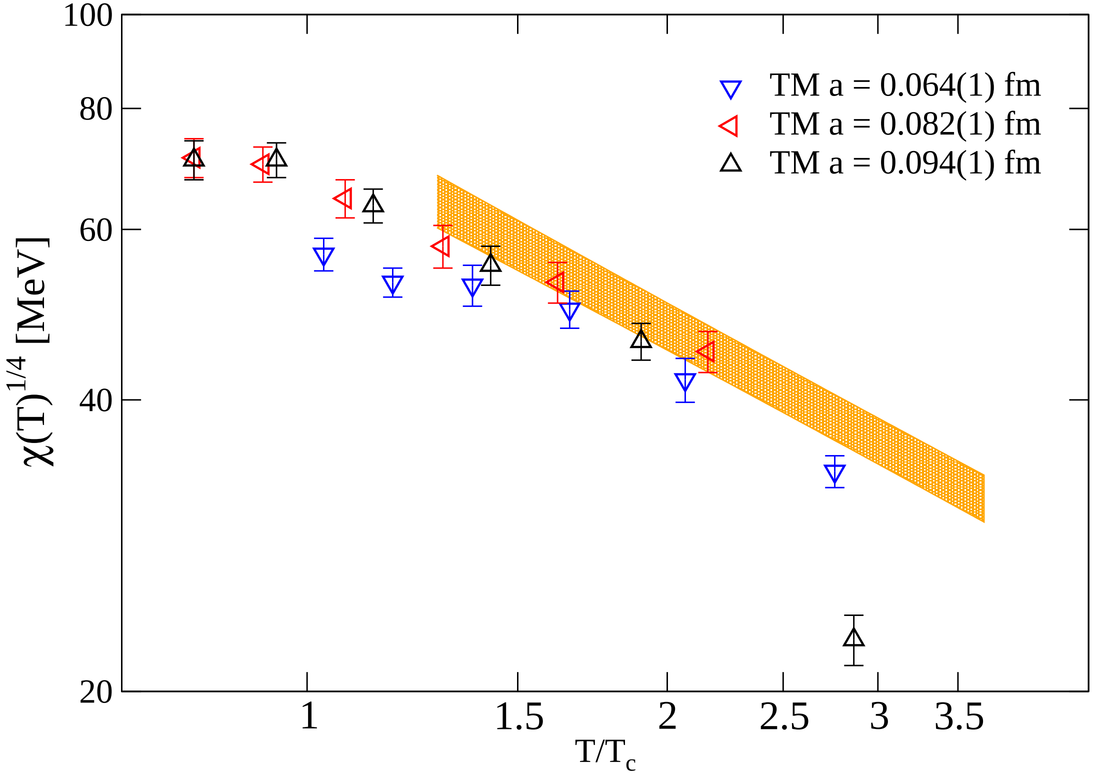
drop of the chiral susceptibility much smoother than perturbative estimate: $\chi(T) \propto 1/T^b$ with $b = 2.90(65)$ (DIGA prediction: $b = 7.66 \div 8$)

similar results in Trunin et al. 1510.02265



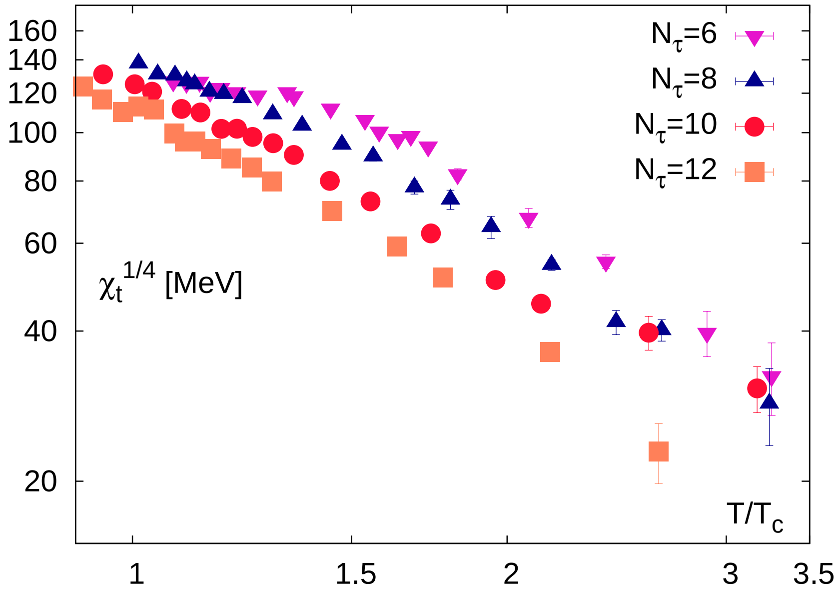
Values for b_2 converge faster to DIGA prediction, however deviations seem of opposite sign with respect to the quenched case:

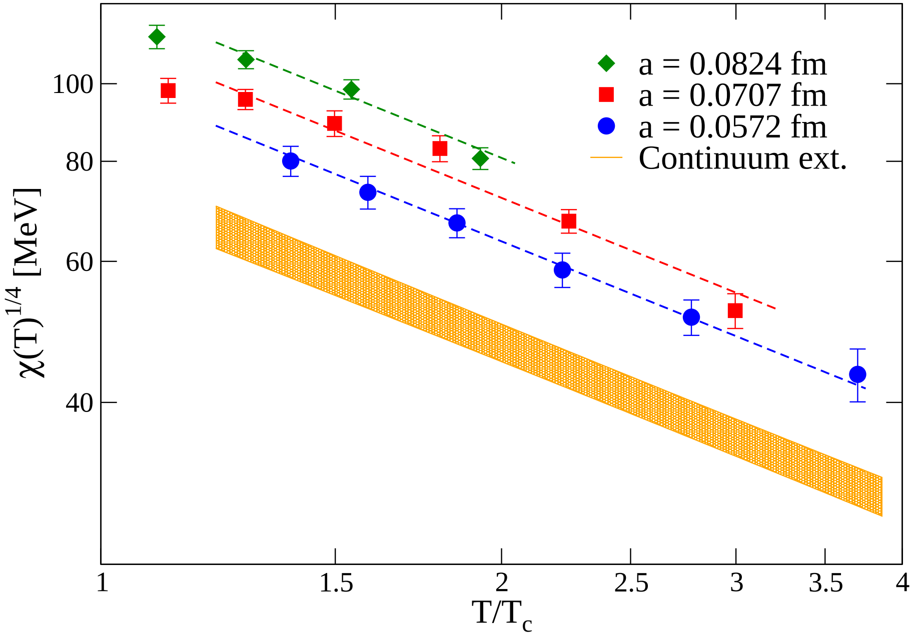
quark mediated attractive instanton-instanton interaction?



direct comparison with results from Trunin et al. 1510.02265 after rescaling according to the DIGA relation $\chi(T) \sim m_q^2 \sim m_\pi^4$

a recent update





arXiv:1606.0315 (Petreczky Schadler Sharma) **arXiv:1512.06746 (our work)**

Numerical simulations with HISQ staggered quarks report a slope more in line with perturbative DIGA expectations.

Main difference: finer lattice spacings at the higher temperature?

What are the consequences of our results for axion physics?

Main source of axion relics: misalignment. Field not at the minimum after PQ symmetry breaking. Further evolution (zero mode approximation, H = Hubble constant):

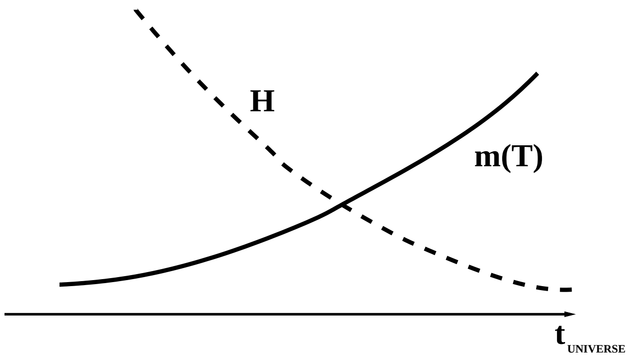
$$\ddot{a}(t) + 3H(t)\dot{a}(t) + m_a^2(T)a(t) = 0 \; ; \quad m_a^2 = \chi(T)/f_a^2$$

$T \gg \Lambda_{QCD}$ 2^{nd} term dominates $\Longrightarrow$ $a(t) \sim \mathrm{const}$

$m_a \gtrsim H$ oscillations start $\Longrightarrow$ adiabatic invariant

$N_a = m_a A^2 R^3 \sim$ number of axions ($\sim$ cold DM)

A = oscill. amplitude; R = Universe radius



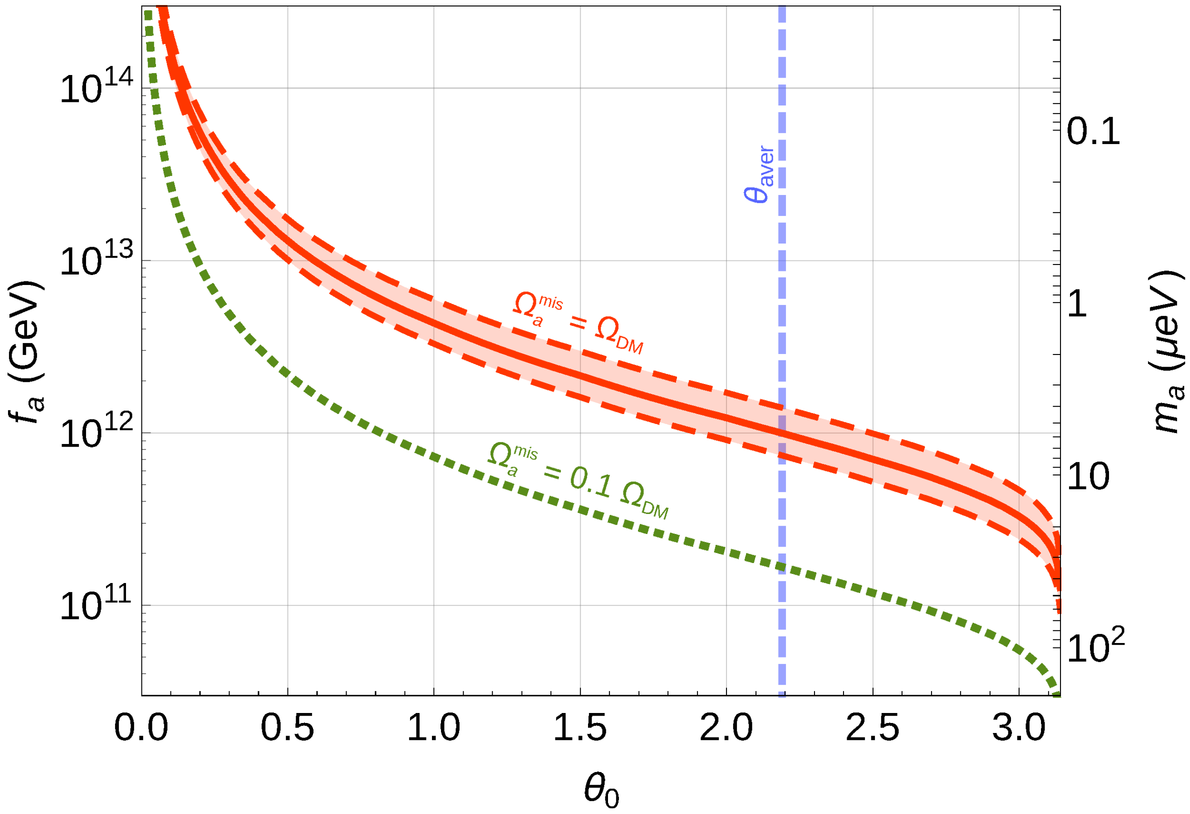
A larger $\chi(T)$ implies larger m_a and moves the oscillation time earlier (higher T, smaller Universe radius R)

Requiring a fixed N_a ($\Omega_{axion} \sim \Omega_{DM}$)

$\chi(T)$ grows $\Longrightarrow$ oscill. time anticipated $\Longrightarrow$ less axions $\Longrightarrow$ require larger f_a to maintain N_a

On the other hand, larger f_a means smaller m_a today

Our results translated in predictions for f_a, hence m_a at our times, depending on the required amount of axion dark matter. f_a factor 10 larger (m_a smaller) wrt perturbative DIGA predictions



An unknown variable is the initial misalignment θ_0. Moreover, if PQ symmetry breaks before inflation the initial value is constant, otherwise an average over the initial value has to be performed. **order of magnitude prediction for present $m_a \sim 10\ \mu\text{eV}$**

Conclusions and Discussion

- Our present results on θ dependence in the high T phase of $N_f = 2+1$ QCD with physical quark masses would shift the axion window by $\sim$ one order of magnitude.

- However, our results push the oscillation temperature to a few GeVs, while our results are limited to $T \sim 600$ MeV. We are relying on an extrapolation. Could perturbative DIGA sets in in the while?

- Need for lattice results at higher temperatures. But $T = 1/(N_t a)$, in order to reach $T \sim$ few GeVs with $N_t \sim 10$ we need $a \sim 10^{-2}$ fm.
  How to deal with topological charge freezing?
  How to correctly sample extremely rare events?

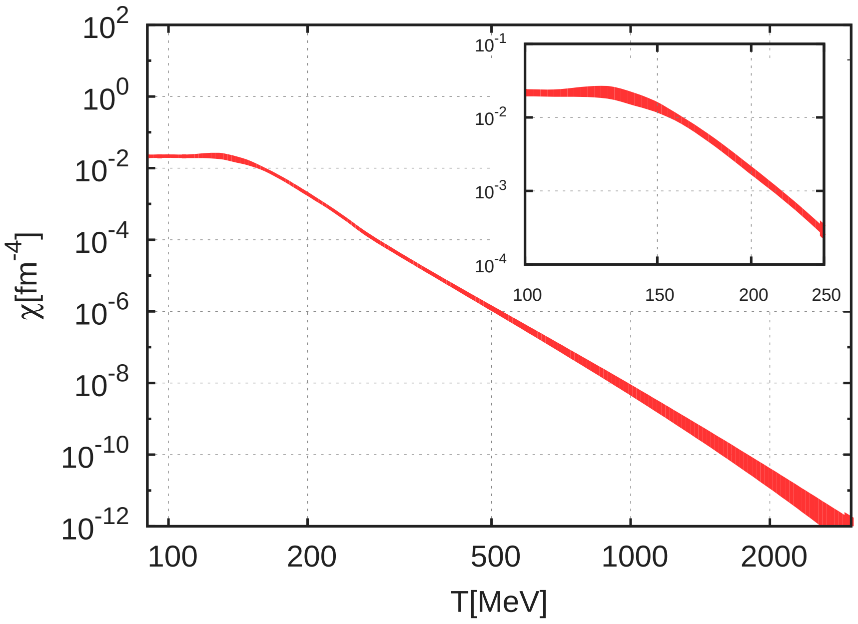
- We need new algorithms and strategies: open boundary conditions? (Luscher, Schaefer) Metadynamics?(Laio, Martinelli, Sanfilippo, arXiv:1508.07270) Non-orientable manifolds? (Mages et al., arXiv:1512.06804) ...

A recent new approach (arXiv:1606.07494):

in order to compute $F(\theta)$, we need to compute $P(Q,T) \propto Z_Q(T)$. Then one can compute $Z_Q(\bar{T})/Z_0(\bar{T})$ in an accessible temperature region and then integrate its derivative

$$\frac{d}{dT} \log \left(\frac{Z_Q(T)}{Z_0(T)} \right)$$

up to the desired T. In this case one needs simulations at fixed topology.



high T results in line with DIGA. In this case $m_a \sim 10^2 - 10^3\ \mu\text{eV}$

BACKUP SLIDES

comparison of cooling and the gradient flow on a couple of sample configurations and on the whole statistical ensemble