

# Lattice QCD and its phenomenological applications

## Introduction to Lattice QCD - 2

2-8 July 2023, Aussois, France

Maria Paola Lombardo

INFN Firenze [lombardo@fi.infn.it](mailto:lombardo@fi.infn.it)



## Introduction to Lattice QCD – II

More on Euclidean formulation

Light quarks - chiral symmetry (and confinement)

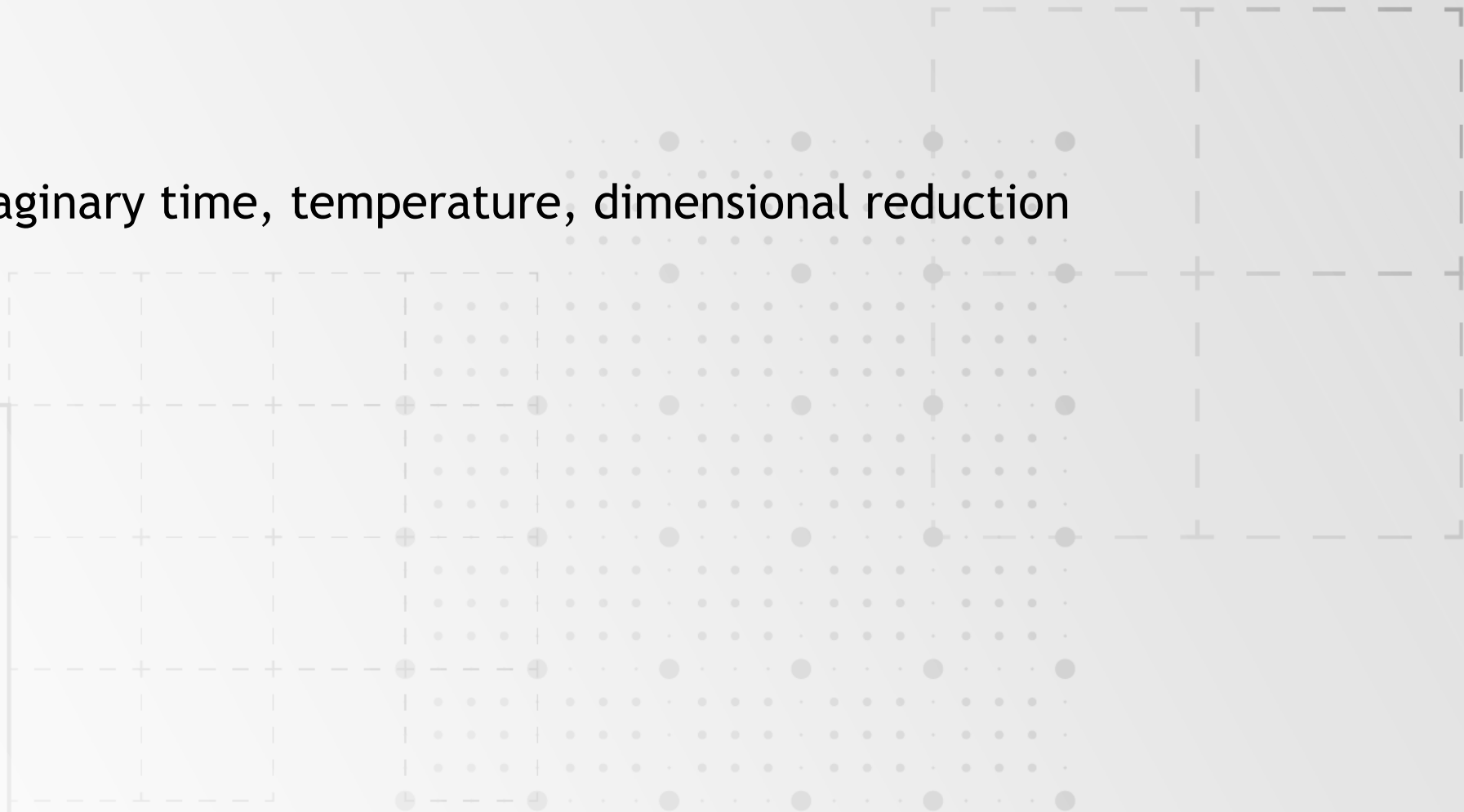
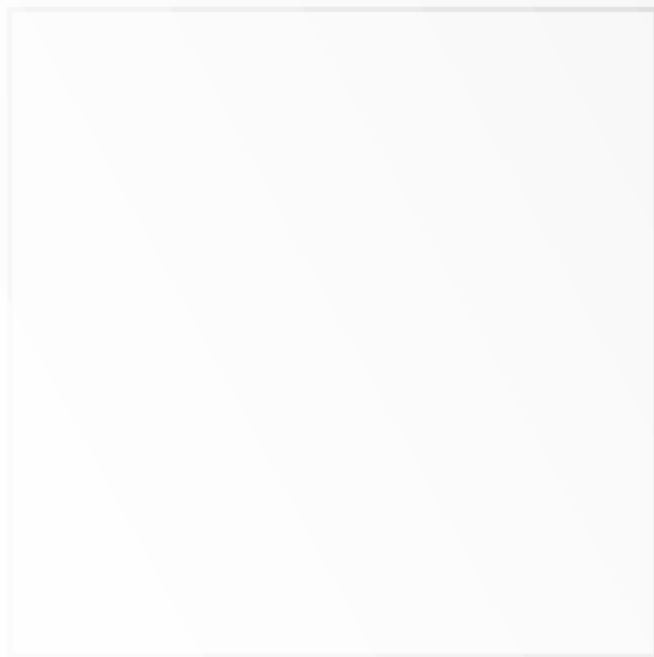
Theta term, strong CP problem, topology, axion (brief recap)

Topology

Heavy quarks

Lattice QCD and axion cosmology

Imaginary time, temperature, dimensional reduction



## Euclidean Field Theory $\rightarrow$ Classical Statistical System

$$\langle \phi_a | e^{-iHt} | \phi_a \rangle = \int d\pi \int_{\phi(x,0)=\phi_a(x)}^{\phi(x,t)=\phi_a(x)} d\phi e^{i \int_0^t dt \int d^3x (\pi(\vec{x},t) \frac{\partial \phi(\vec{x},t)}{\partial t} - H(\pi, \phi))}$$

$$\mathcal{Z} = \text{Tr} e^{-\beta(H - \mu \hat{N})} = \int d\phi_a \langle \phi_a | e^{-\beta(H - \mu N)} | \phi_a \rangle$$

$$\beta \equiv \frac{1}{T} \rightarrow it$$

Imaginary time

and

Inverse  
Temperature

d-dimensional space

Table 1

The equivalences between a Euclidean field theory and Classical Statistical Mechanics.

Euclidean Field Theory	Classical Statistical Mechanics
Action	Hamiltonian
unit of action $\hbar$	units of energy $\beta = 1/kT$
Feynman weight for amplitudes	Boltzmann factor $e^{-\beta H}$
$e^{-S/\hbar} = e^{-\int \mathcal{L} dt/\hbar}$	
Vacuum to vacuum amplitude	Partition function $\sum_{conf.} e^{-\beta H}$
$\int \mathcal{D}\phi e^{-S/\hbar}$	
Vacuum energy	Free Energy
Vacuum expectation value $\langle 0   \mathcal{O}   0 \rangle$	Canonical ensemble average $\langle \mathcal{O} \rangle$
Time ordered products	Ordinary products
Green's functions $\langle 0   T[\mathcal{O}_1 \dots \mathcal{O}_n]   0 \rangle$	Correlation functions $\langle \mathcal{O}_1 \dots \mathcal{O}_n \rangle$
Mass $M$	correlation length $\xi = 1/M$
Mass-gap	exponential decrease of correlation functions
Mass-less excitations	spin waves
Regularization: cutoff $\Lambda$	lattice spacing $a$
Renormalization: $\Lambda \rightarrow \infty$	continuum limit $a \rightarrow 0$
Changes in the vacuum	phase transitions

Table by Rajan Gupta

## Boundary conditions for the fields

$$\mathcal{Z} = \int d\phi d\psi e^{-S(\phi, \psi)}$$

$$S(\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$

### Bosons : periodic

$$G_B(\vec{x}, \vec{y}; \tau, 0) = Tr\{\hat{\rho} T_\tau[\hat{\phi}(\vec{x}, \tau)\hat{\phi}(\vec{y}, 0)]\} / \mathcal{Z}$$

where  $T_\tau$  is the imaginary time ordering operator:

$$T_\tau[\hat{\phi}(\tau_1)\hat{\phi}(\tau_2)] = \hat{\phi}(\tau_1)\hat{\phi}(\tau_2)\theta(\tau_1 - \tau_2) + \hat{\phi}(\tau_2)\hat{\phi}(\tau_1)\theta(\tau_2 - \tau_1)$$

Use now the commuting properties of the imaginary time ordering evolution and H:

$$[T_\tau, e^{-\beta H}] = 0$$

together with the Heisenberg time evolution

$$e^{\beta H} \phi(\vec{y}, 0) e^{-\beta H} = \phi(\vec{y}, \beta)$$

to get:

$$G_B(\vec{x}, \vec{y}; \tau, 0) = G_B(\vec{x}, \vec{y}; \tau, \beta)$$

## Fermions

$$T_\tau[\hat{\psi}(\tau_1)\hat{\psi}(\tau_2)] = \hat{\psi}(\tau_1)\hat{\psi}(\tau_2)\theta(\tau_1 - \tau_2) - \hat{\psi}(\tau_2)\hat{\psi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$\hat{\psi}(\vec{x}, 0) = -\hat{\psi}(\vec{x}, \beta) \quad \text{Antiperiodic}$$

## Fermions

$$T_\tau[\hat{\psi}(\tau_1)\hat{\psi}(\tau_2)] = \hat{\psi}(\tau_1)\hat{\psi}(\tau_2)\theta(\tau_1 - \tau_2) - \hat{\psi}(\tau_2)\hat{\psi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$\hat{\psi}(\vec{x}, 0) = -\hat{\psi}(\vec{x}, \beta) \quad \text{Antiperiodic}$$

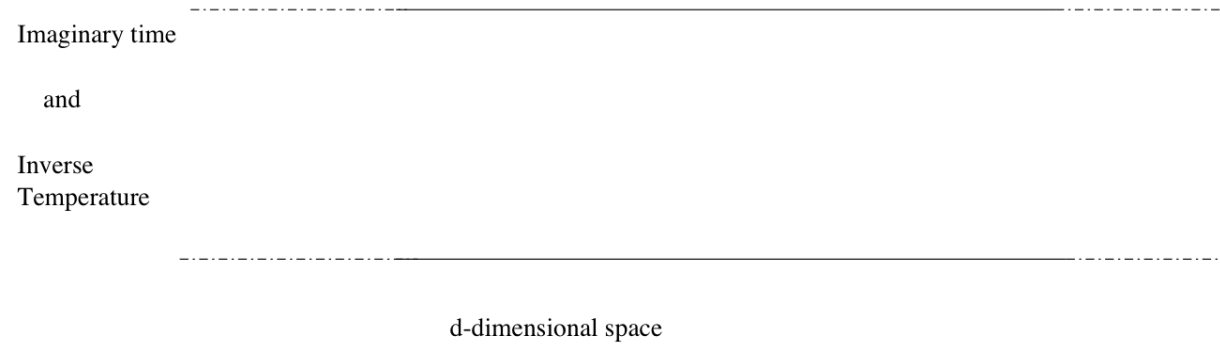
## Bosons

$$T_\tau[\hat{\phi}(\tau_1)\hat{\phi}(\tau_2)] = \hat{\phi}(\tau_1)\hat{\phi}(\tau_2)\theta(\tau_1 - \tau_2) + \hat{\phi}(\tau_2)\hat{\phi}(\tau_1)\theta(\tau_2 - \tau_1)$$

$$G_B(\vec{x}, \vec{y}; \tau, 0) = G_B(\vec{x}, \vec{y}; \tau, \beta) \quad \text{Periodic}$$



# Dimensional Reduction



+ coarse graining

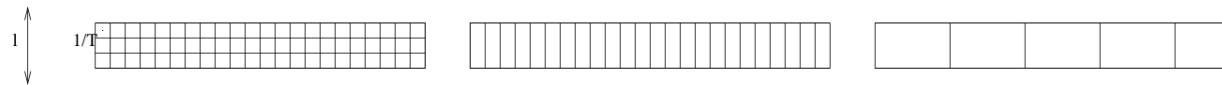


Figure 2: Sketchy view of the dimensional reduction from  $d+1$  to  $d$  dimensions (from the leftmost to the middle picture) and subsequent coarse graining (from middle to rightmost)

## Cases for Dimensional Reduction

- 1)  $T \gg \gg$  any mass  $\rightarrow$  High T Electroweak transition
- 2) Diverging correlation length  $\rightarrow$  second order transition, basis for universality  
High T QCD

## Mode expansion and Decoupling

$$\phi(x, t) = \sum_{\omega_n=2n\pi T} e^{i\omega_n t} \phi_n(x) \quad \text{Bosons}$$

$$\psi(x, t) = \sum_{\omega_n=(2n+1)\pi T} e^{i\omega_n t} \psi_n(x) \quad \text{Fermions}$$

In the expression for the Action

$$S(\phi, \psi) = \int_0^{1/T} dt \int d^d x \mathcal{L}(\phi, \psi)$$

the integral over time can then be traded with a sum over modes, and we reach the conclusion that a  $d+1$  statistical field theory at  $T > 0$  is equivalent to a  $d$ -dimensional theory with an infinite number of fields.

**When dimensional reduction is possible, only one boson field survives**

## Finite temperature at a glance

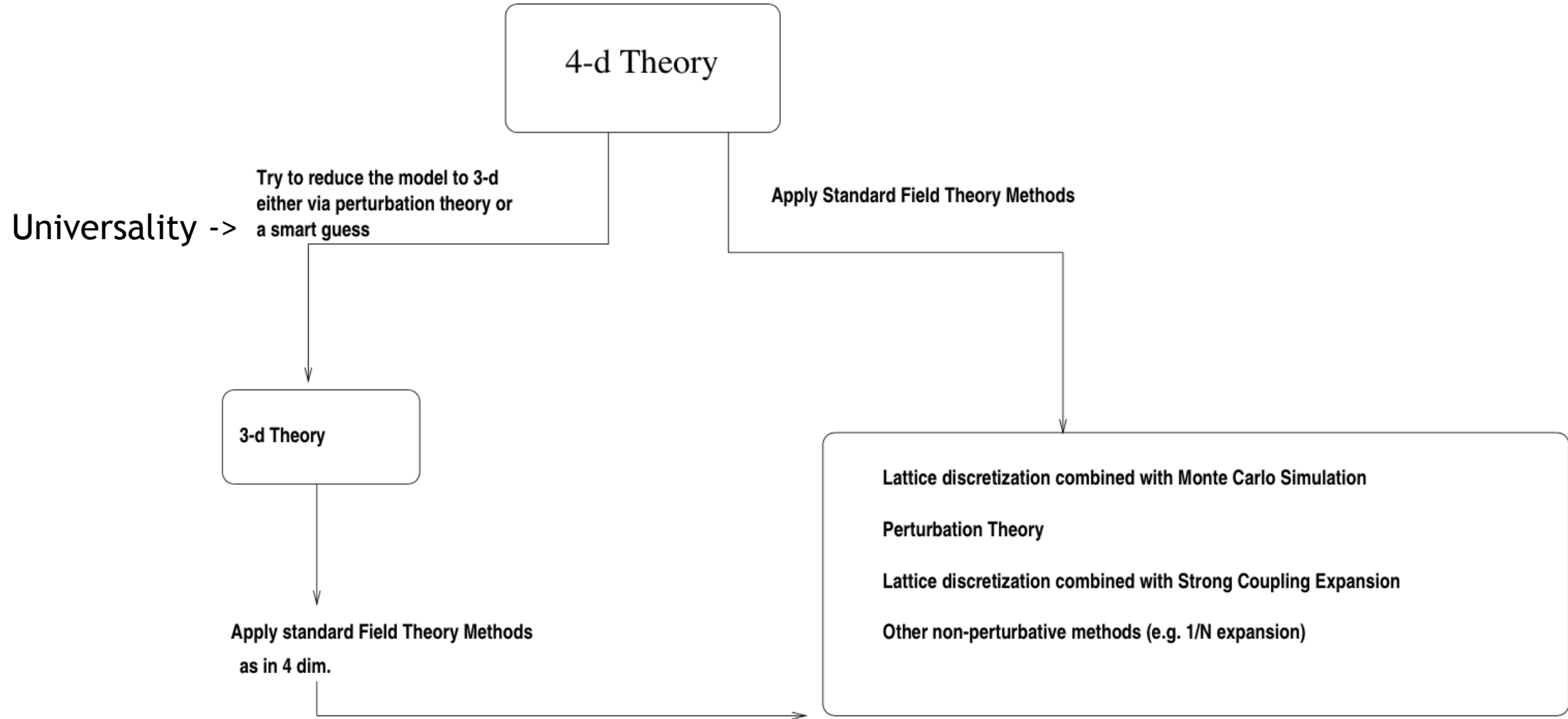
- The partition function  $\mathcal{Z}$  has the interpretation of the partition function of a statistical field theory in  $d+1$  dimension, where the temperature has to be identified with the reciprocal of the (imaginary) time.
- The fields' boundary conditions follows from the Bose and Fermi s

$$\begin{aligned}\phi(t = 0, \vec{x}) &= \phi(t = 1/T, \vec{x}) \\ \psi(t = 0, \vec{x}) &= -\psi(t = 1/T, \vec{x})\end{aligned}$$

i.e. fermionic and bosonic fields obey antiperiodic and periodic boundary conditions in time.

- “Dimensional reduction”, when ‘true’ means that the system become effectively 3-dimensional. In this case only the Fourier component of each Bose field with vanishing Matsubara frequency will contribute to the dynamics, while Fermions would decouple.
- The scenario above is very plausible and physically well founded, but it is by no means a theorem. Ab initio calculations can confirm or disprove it.

# Computational schemes at a glance





## Symmetry and pattern of breaking

Yang Mills

Massless QCD - light quarks

Interplay of chiral symmetry and confinement?

## symmetry of Yang-Mills

3-dimensional system of Polyakov loops

SU(3) : Z3 center symmetry breaking at  $T_c \rightarrow$  1st order 3 state Potts model

SU(2) : Z2 center symmetry breaking at  $T_c \rightarrow$  2nd order 2 state Potts model (Ising)

(a) Potts Model :



Q=2 (Ising model)



Q=3



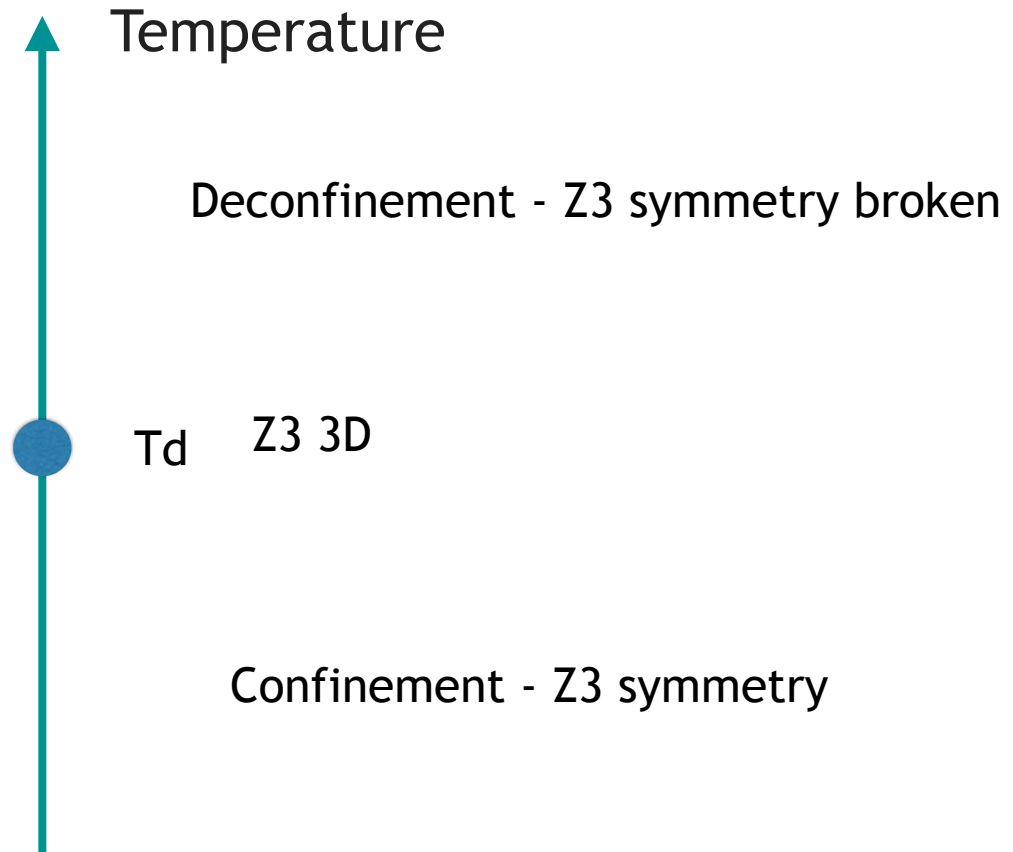
Q=4

Yang-Mills Theory       $N_c = 2$       – Ising 3D universality class

Source		$SU(2)$	Ising
$\langle  L  \rangle$	$\beta/\nu$	0.525(8)	0.518(7)
$D \langle  L  \rangle$	$(1 - \beta)/\nu$	1.085(14)	1.072(7)
	$1/\nu$	1.610(16)	1.590(2)
	$\nu$	0.621(6)	0.6289(8)
	$\beta$	0.326(8)	0.3258(44)
$\chi_\nu$	$\gamma/\nu$	1.944(13)	1.970(11)
$D\chi_\nu$	$(1 + \gamma)/\nu$	3.555(15)	3.560(11)
	$1/\nu$	1.611(20)	1.590(2)
	$\nu$	0.621(8)	0.6289(8)
	$\gamma$	1.207(24)	1.239(7)
	$\gamma/\nu + 2\beta/\nu$	2.994(21)	3.006(18)
$g_r$	$-g_r^\infty$	1.403(16)	1.41
$Dg_r$	$1/\nu$	1.587(27)	1.590(2)
$(\omega = 1)$	$\nu$	0.630(11)	0.6289(8)



# Phases of Yang-Mills



# Symmetries of QCD

$$\mathcal{L} = \sum_{a=1}^n \bar{q}_{La} \not{\partial} q_{La} + \bar{q}_{Ra} \not{\partial} q_{Ra} - m(\bar{q}_{La} q_{La} + \bar{q}_{Ra} q_{Ra}) + \theta \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu} + \mathcal{L}_{gauge}$$

With  $m = 0$ , invariant under  
 $q_L \rightarrow V_L q_L, q_R \rightarrow V_R q_R$ , with  $V \in U(n)$

Global symmetry:

$$U(n)_L \times U(n)_R \cong \underbrace{SU(n) \times SU(n)}_{\text{Spontaneously Broken}} \times U(1)_V \times U(1)_A$$

baryon  
number

Spontaneously Broken

Explicitly broken

Experimental evidence

$(n^2 - 1)$  pseudoGB

Heavy  $\eta'$

# Explicit breaking of axial symmetry: solution of the UA(1) puzzle

## Pseudoscalar spectrum

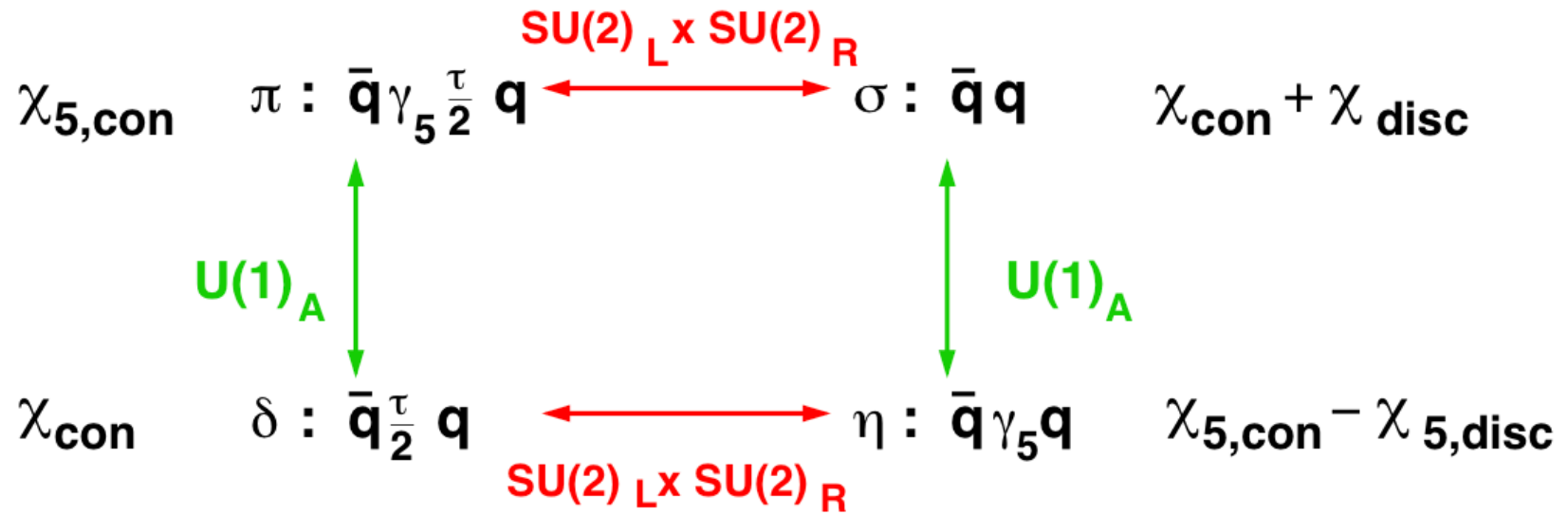
Particle name	Particle symbol $\blacklozenge$	Antiparticle symbol $\blacklozenge$	Quark content	Rest mass (MeV/c <sup>2</sup> ) $\blacklozenge$
Pion <sup>[6]</sup>	$\pi^+$	$\pi^-$	$u\bar{d}$	139.570 18 $\pm$ 0.000 35
Pion <sup>[7]</sup>	$\pi^0$	Self	$\frac{u\bar{u}-d\bar{d}}{\sqrt{2}}$ [a]	134.9766 $\pm$ 0.0006
Eta meson <sup>[8]</sup>	$\eta$	Self	$\frac{u\bar{u}+d\bar{d}-2s\bar{s}}{\sqrt{6}}$ [a]	547.862 $\pm$ 0.018
Eta prime meson <sup>[9]</sup>	$\eta'(958)$	Self	$\frac{u\bar{u}+d\bar{d}+s\bar{s}}{\sqrt{3}}$ [a]	957.78 $\pm$ 0.06
Kaon <sup>[12]</sup>	$K^+$	$K^-$	$u\bar{s}$	493.677 $\pm$ 0.016
Kaon <sup>[13]</sup>	$K^0$	$\bar{K}^0$	$d\bar{s}$	497.614 $\pm$ 0.024

UA(1) puzzle



Pion, sigma => O(4) symmetry

Candidate universality class: O(4) in 3D



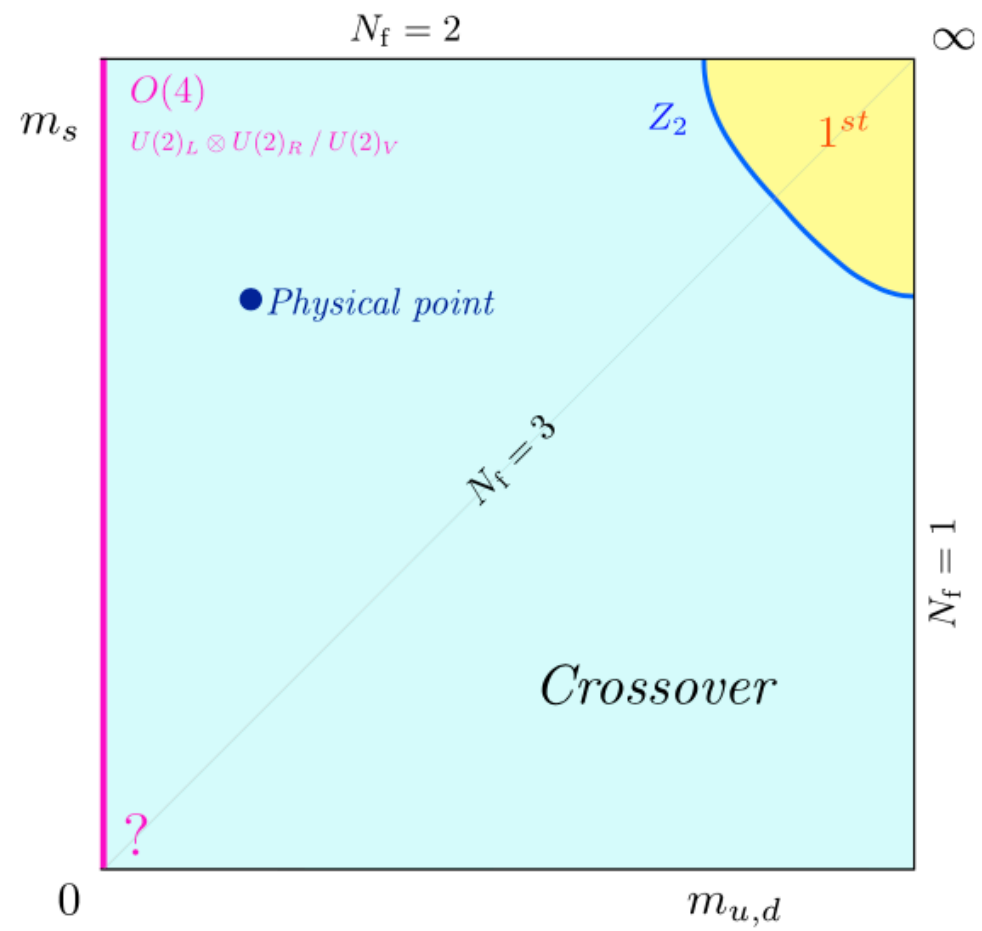
# Universality class of the high T transition:

theoretical (*lack of*) guidance

Parisen Toldin, Pelissetto, Vicari 2003

$N_f$	$U(1)_A$ broken	$U(1)_A$ restored
1	crossover or 1 <sup>st</sup> ord	$O(2) \rightarrow \mathbb{Z}_2$ or 1 <sup>st</sup> ord
2	$O(4) \rightarrow O(3)$ or 1 <sup>st</sup> ord Pisarski, Wilczek 1984	$U(2)_L \otimes U(2)_R \rightarrow U(2)_V$ or 1 <sup>st</sup> ord
$\geq 3$	1 <sup>st</sup> ord ?	1 <sup>st</sup> ord

Challenged by Cuteri, Philippsen, Sciarra 2020-2022



$$SU(n) \times SU(n)$$

$$M \quad \tilde{m}_\ell \rightarrow 0 \quad \begin{cases} A \left( \frac{T_c^0 - T}{T_c^0} \right)^\beta, & T < T_c^0 \\ 0, & T \geq T_c^0 \end{cases}$$

$$\chi_M \quad \tilde{m}_\ell \rightarrow 0 \quad \begin{cases} \infty, & T \leq T_c^0 \\ C \left( \frac{T - T_c^0}{T_c^0} \right)^{-\gamma}, & T > T_c^0 \end{cases}$$

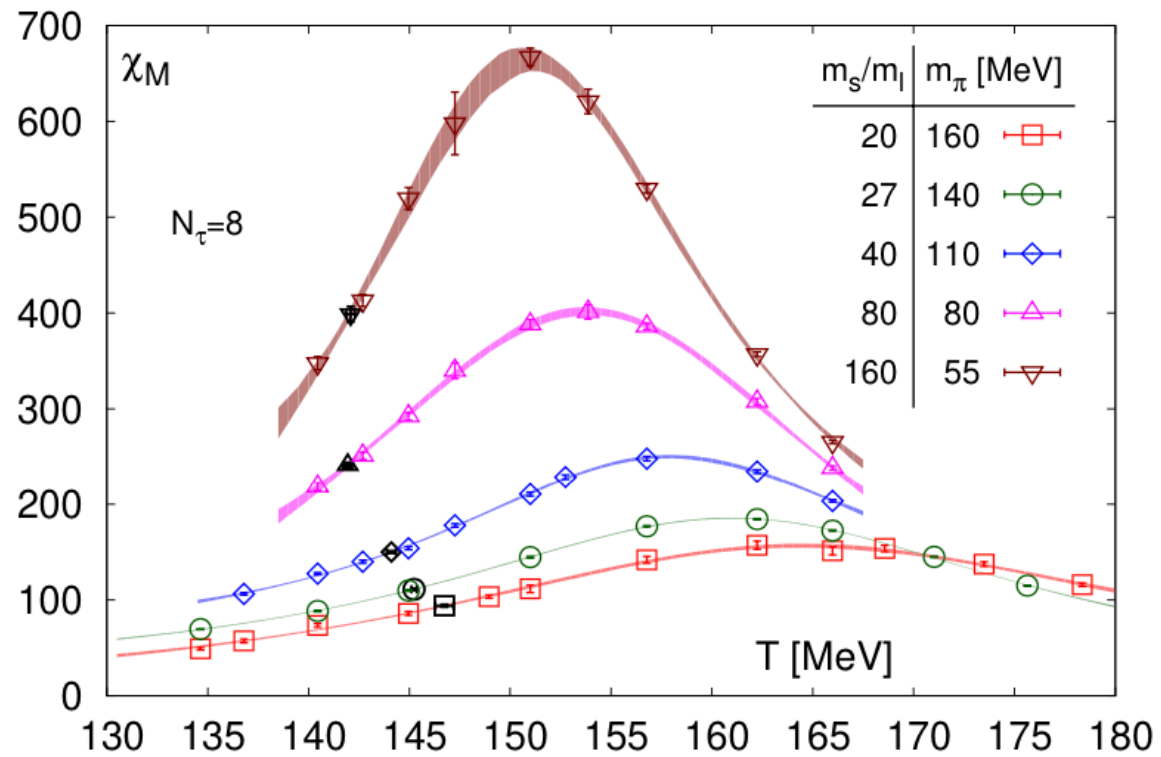
$$SU(n) \times SU(n)$$

$$T_c^0 = 132_{-6}^{+3} \text{ MeV}$$

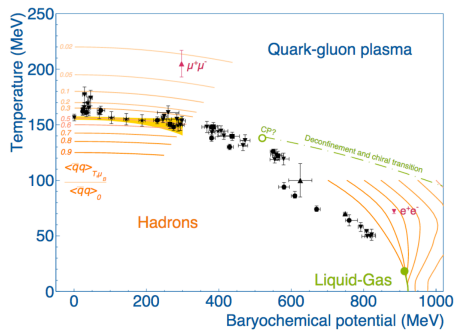
$$T_{pc} = 156.5(1.5) \text{ MeV}$$

O(4) universality

With physical quark masses







Physical trajectory

Goldstone singularity

$T$

$T_c$

Phases of massless QCD:  
imprinting  
on observations?



Universality class +  
scaling window

$m_s$

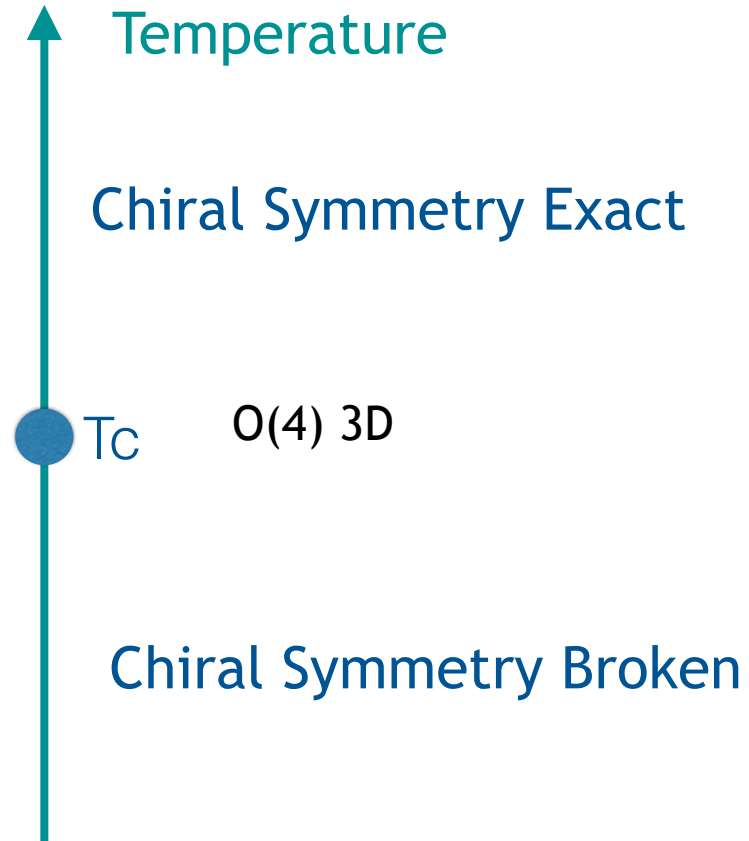
$m_{u,d}$

Fate of :  $U(1)_A$  ?

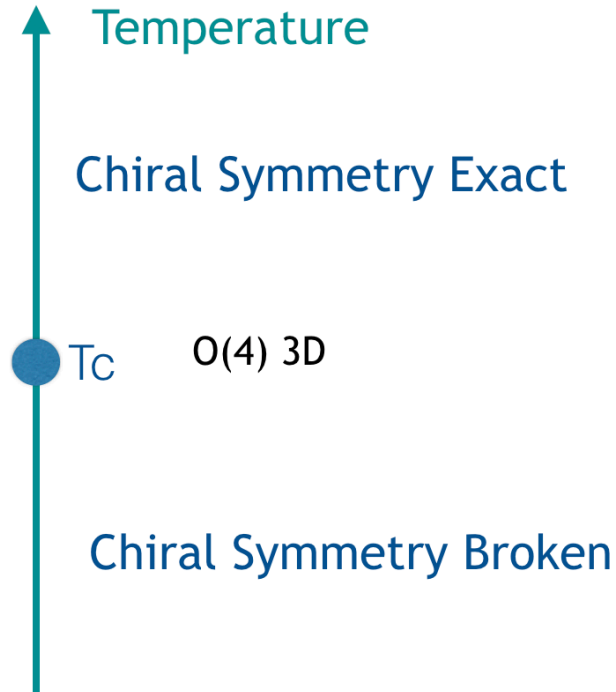
Probably still broken above  $T_c$

The fate of the anomaly and its impact on the transition remains an important open problem

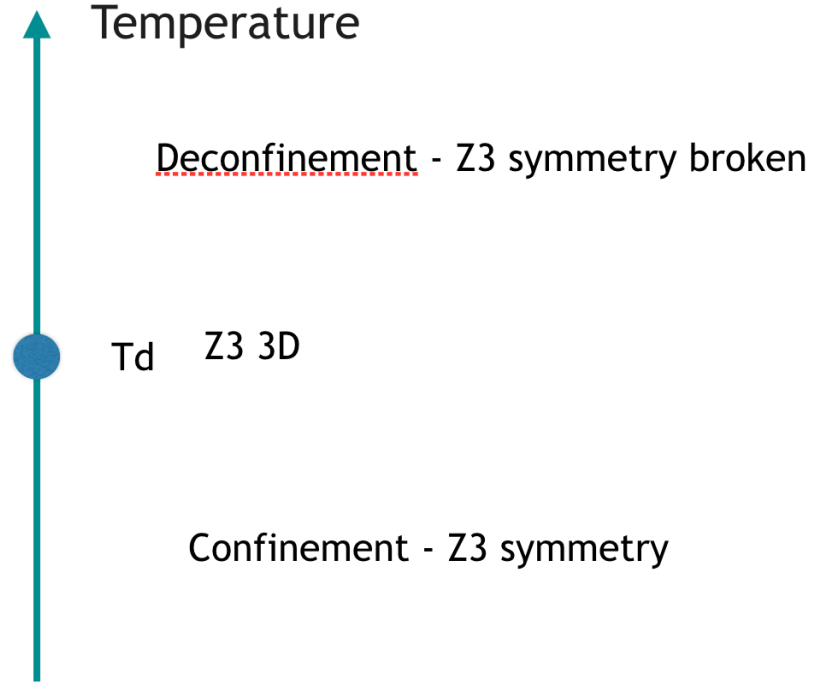
# Phases of massless QCD



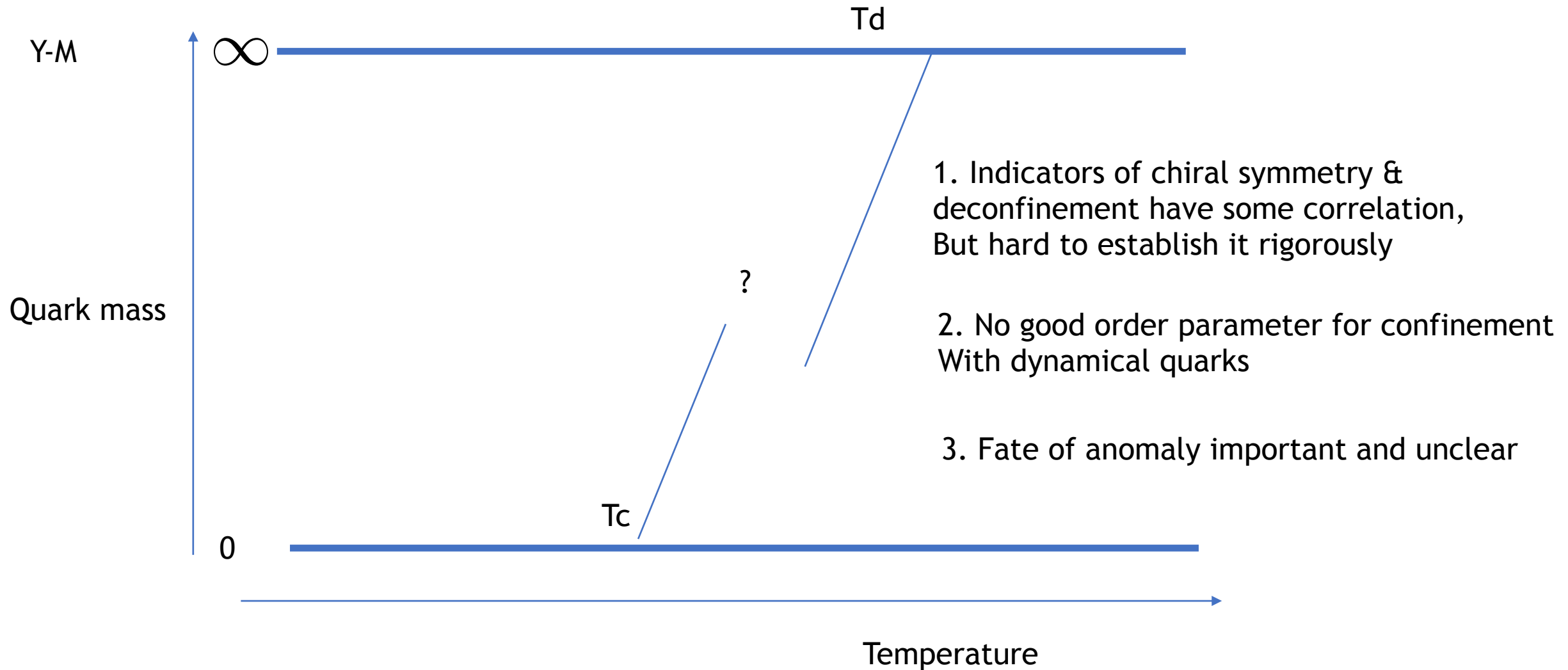
# Phases of massless QCD

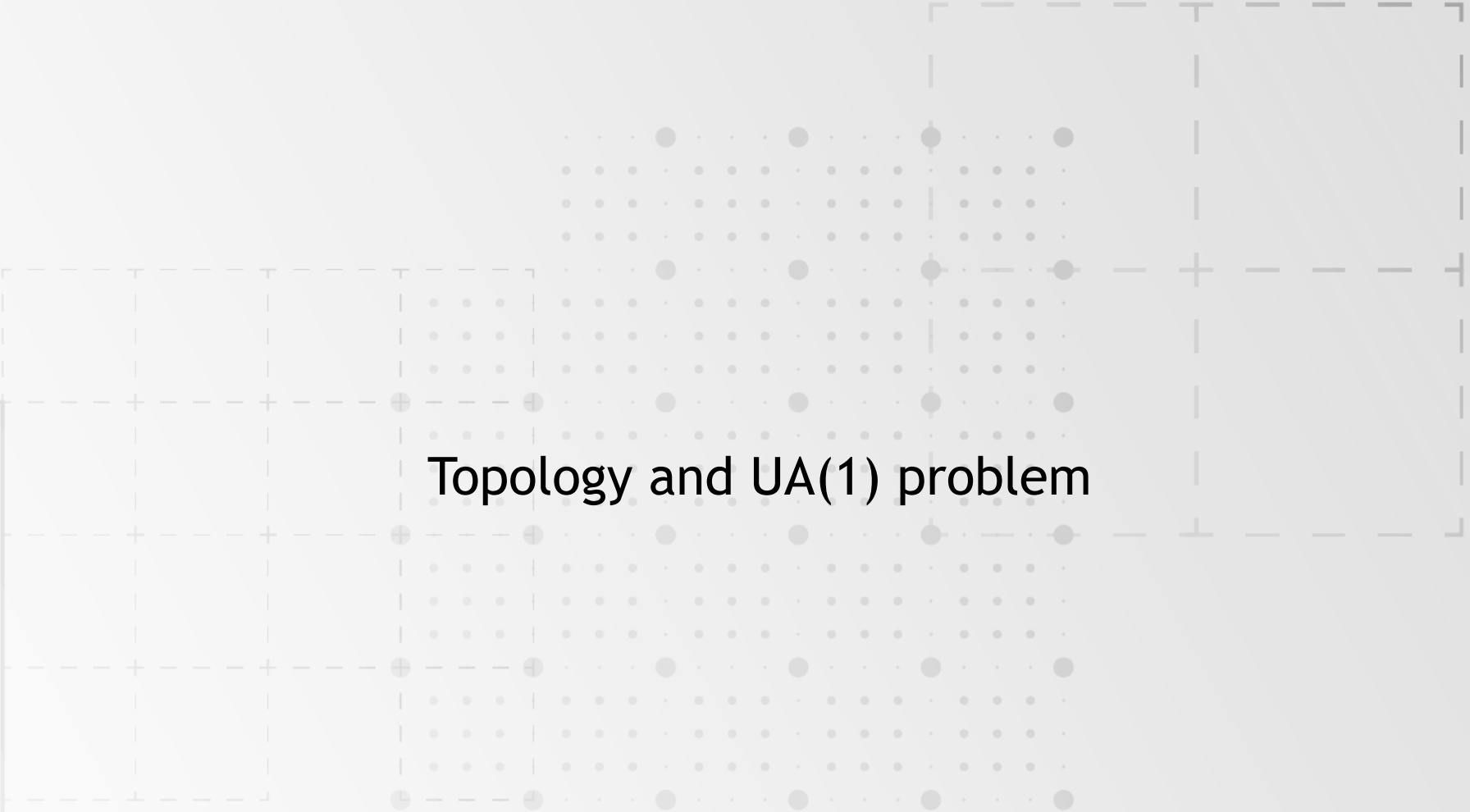
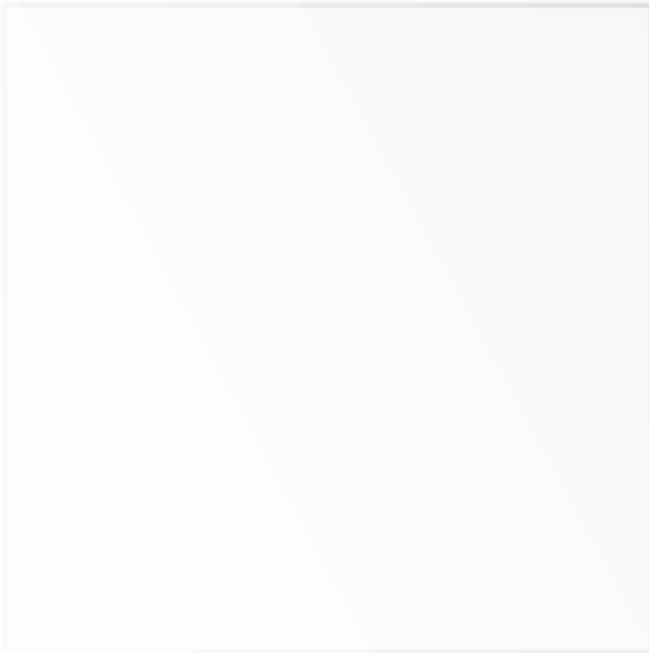


# Phases of Yang Mills



# Phases of QCD in the temperature, mass plane





Topology and UA(1) problem

Focus on the  $\theta$  term

$$\mathcal{L} = \mathcal{L}_{\text{QCD}} + \theta \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu}$$
$$\frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu} = q(x)$$

$$Q = \sum q(x)$$



Q — topological charge

**CP-violating term**

|

## GCPF and $\theta$

The GCPF of QCD is now a function of  $\theta$ :

$$\mathcal{Z}(\theta, T) = \int \mathcal{D}[\Phi] e^{-T \sum_t \int d^3x \mathcal{L}(\theta)} = e^{-VF(\theta, T)}.$$

The energy density  $F(\theta, T)$  is related with the probability of finding configurations with given topological charge  $Q = \int d^4x q(x)$ :

$$P_Q = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-i\theta Q} e^{-VF(\theta)},$$

so the coefficients  $C_n$  of the Taylor expansion

$$F(\theta, T) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{\theta^{2n}}{2n!} C_n$$

are given by the cumulants of the topological charge:

$$C_n = (-1)^{n+1} \frac{d^{2n}}{d\theta^{2n}} F(\theta, T) \Big|_{\theta=0} = \langle Q^{2n} \rangle_{conn}.$$



Topology,  $\eta'$  and solution of the  $U_A(1)$  problem

It can be proven that

$$\frac{1}{32\pi^2} \int d^4x F \tilde{F} = Q \quad \text{Gluonic definition}$$

and

$$Q = n_+ - n_- \quad \text{Fermionic definition}$$

The  $\eta'$  mass may now be computed from the decay of the correlation

$$\langle \partial_\mu j_5^\mu(x) \partial_\mu j_5^\mu(y) \rangle \propto \frac{1}{N^2} \langle F(x) \tilde{F}(x) F(y) \tilde{F}(y) \rangle$$

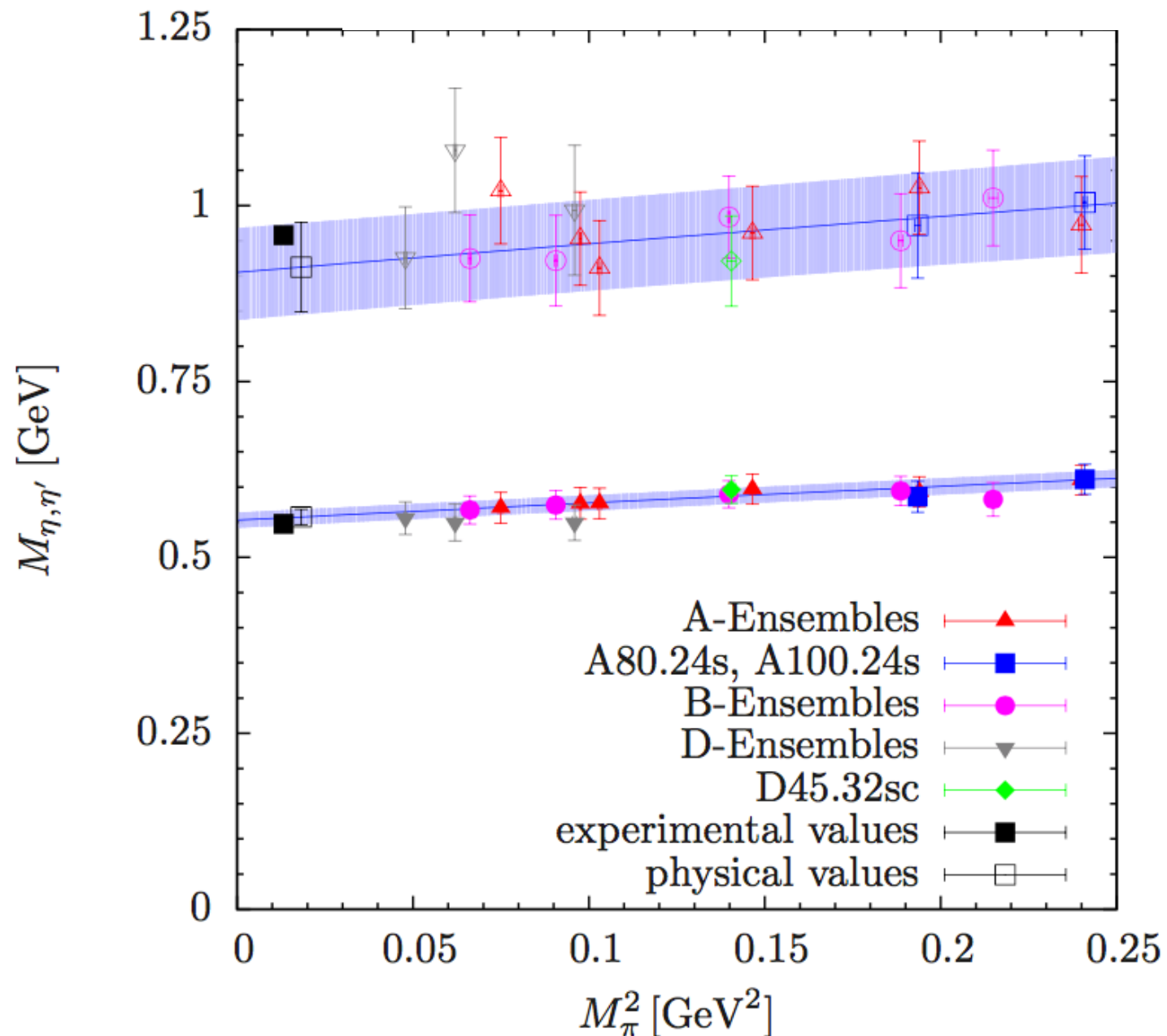
which at leading order gives the Witten-Veneziano formula

$$m_{\eta'}^2 = \frac{2N_f}{F_\pi^2} \chi_t^{\text{qu}}$$

Successful  
at T=0

Topology observable effects:

EVIDENCES OF THE EXPLICIT  $U(1)_A$  BREAKING.

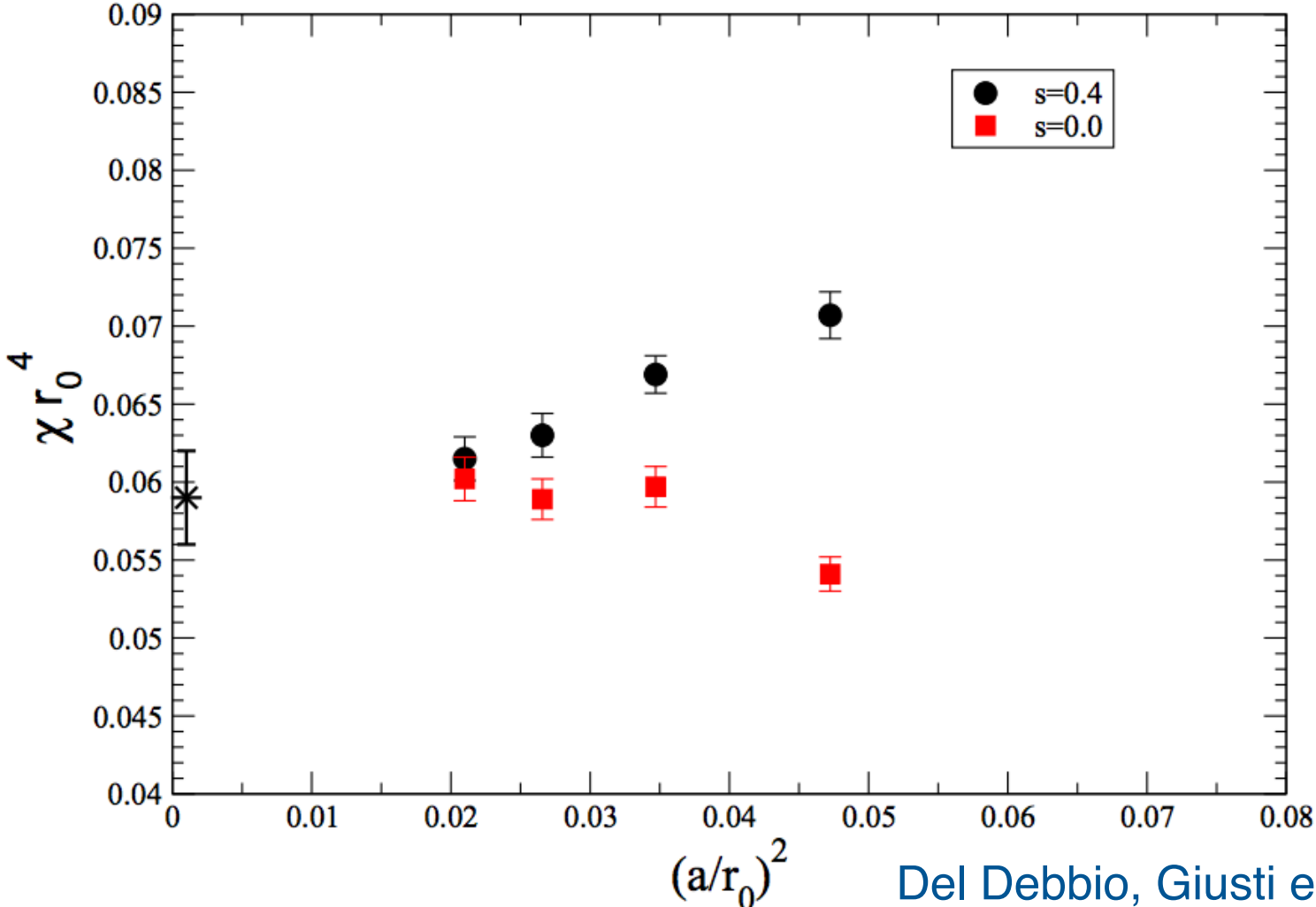


ETMC 2017

Topology observable effects:

EVIDENCES OF THE EXPLICIT  $U(1)_A$  BREAKING.

$\chi = (191 \pm 5 \text{ MeV})^4$ , Yang-Mills Topological Susceptibility



Del Debbio, Giusti et al. (2015)



Strong CP problem and the QCD axion

## LATTICE QCD AND $\theta$ TERM

Lattice simulations rely on a sampling of the phase space weighted with the  $e^{-S}$ , where  $S$  the Euclidean action.

$$Z = \int \mathcal{D}[U] e^{-S_{lat}[U]}$$

- ▶ Sign problem: In Euclidean space-time the Minkowskian Lagrangian becomes *complex* for real values of  $\theta$ .
- ▶ Way out: Taylor expansion around  $\theta = 0$  or an analytic continuation from imaginary values of  $\theta$  Bonati, D'Elia et al. 2019.

In the following, topological susceptibility and cumulants will be measured at  $\theta = 0$ :

$$\chi_{top}(T) \equiv \left. \frac{\partial^2 F(\theta, T)}{\partial \theta^2} \right|_{\theta=0}$$

# Topology and the Strong CP problem

How 'large' is  $\theta$  ?

The QCD Lagrangian admits a CP violating term

$$\mathcal{L} = \mathcal{L}_{QCD} + \theta \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu},$$

$\frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu}$  is the topological charge density  $q(x)$ ,

$\tilde{F}^{\mu\nu} = \frac{1}{2} \varepsilon^{\mu\nu\rho\sigma} F_{\rho\sigma}$ , and  $\theta q(x)$  is known as the  $\theta$ -term.

Without the  $\theta$ -term strong interactions conserve CP. With the  $\theta$ -term the neutron acquires an electric dipole moment  $d_n$ :

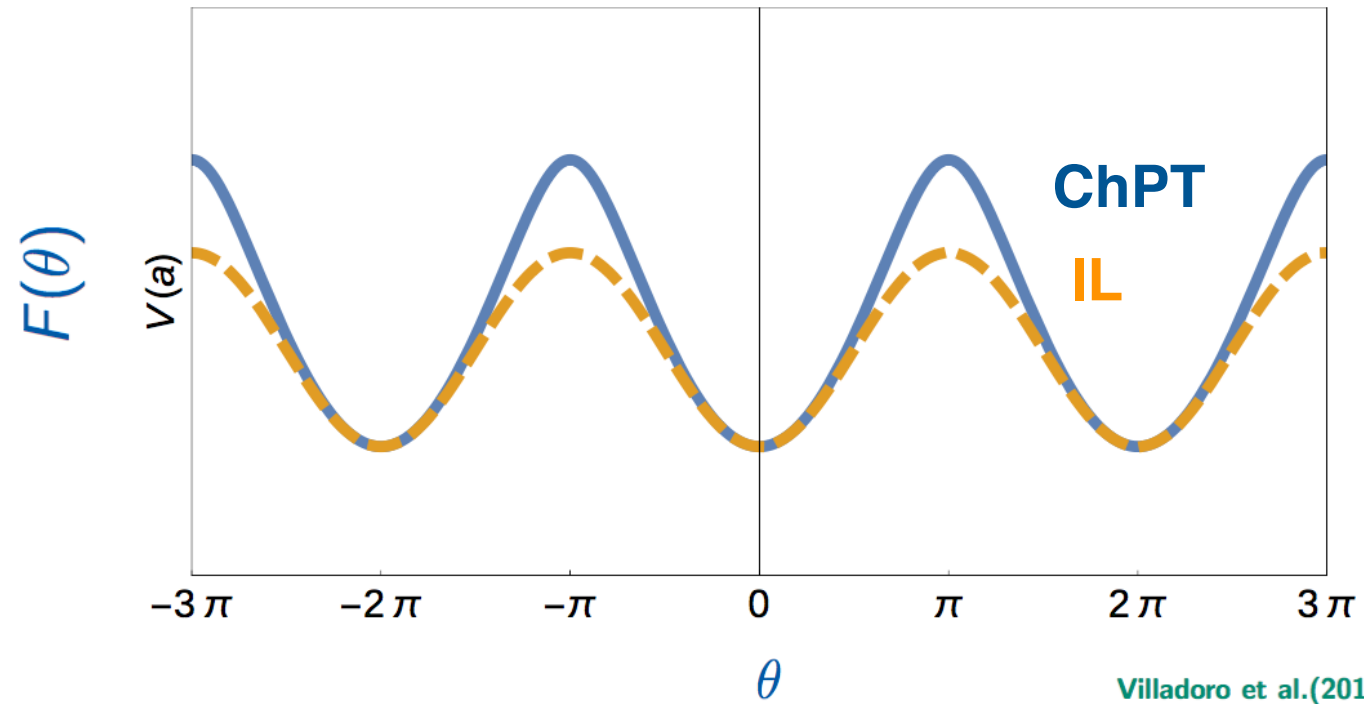
with QCD sum rules:  $d_n = 2.4 \times 10^{-16} \theta$  e cm

chiral perturbation theory:  $d_n = 3.3 \times 10^{-16} \theta$  e cm

Experiments:  $|d_n| < 1.8 \times 10^{-26}$  e cm at a 90% C.L.,

$$\theta < 0.5 \times 10^{-10}.$$

The free energy  $F(\theta, T)$  has a minimum at  $\theta = 0$   
BUT this does not solve the strong CP problem



Villadoro et al.(2015) (adapted)

## Solution of the strong CP problem: the axion

Suppose  $\theta$  were a dynamical parameter: in such a case, dynamics would force its value to zero, thus solving the strong CP problem. Postulate Axion! a pseudo-Goldstone boson of a spontaneously broken symmetry known as the Peccei-Quinn (PQ) symmetry, which couples to the QCD topological charge, with a coupling suppressed by a scale  $f_A$ .

Axion field  $a(x) = f_A\theta(x)$  is now a space-time dependent  $\theta$  parameter.

The axion–QCD Lagrangian:

$$\mathcal{L} = \mathcal{L}_{QCD} + \theta \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu} + \partial_\mu^2 a^2 + \frac{a}{f_A} \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu}.$$

Assume a shift symmetry:  $a \rightarrow a + \alpha$ . The  $\theta$  dependence has been traded with a dependence on the axion field, whose minimum is at zero:

**This solves the strong CP problem. !**

---



## The axion mass

At leading order in  $1/f_A$  – well justified as  $f_A \gtrsim 4 \times 10^8$  GeV – the axion can be treated as an external source, and its mass is given by

$$m_A^2(T) f_A^2 = \left. \frac{\partial^2 F(\theta, T)}{\partial \theta^2} \right|_{\theta=0} \equiv \chi_{top}(T) .$$

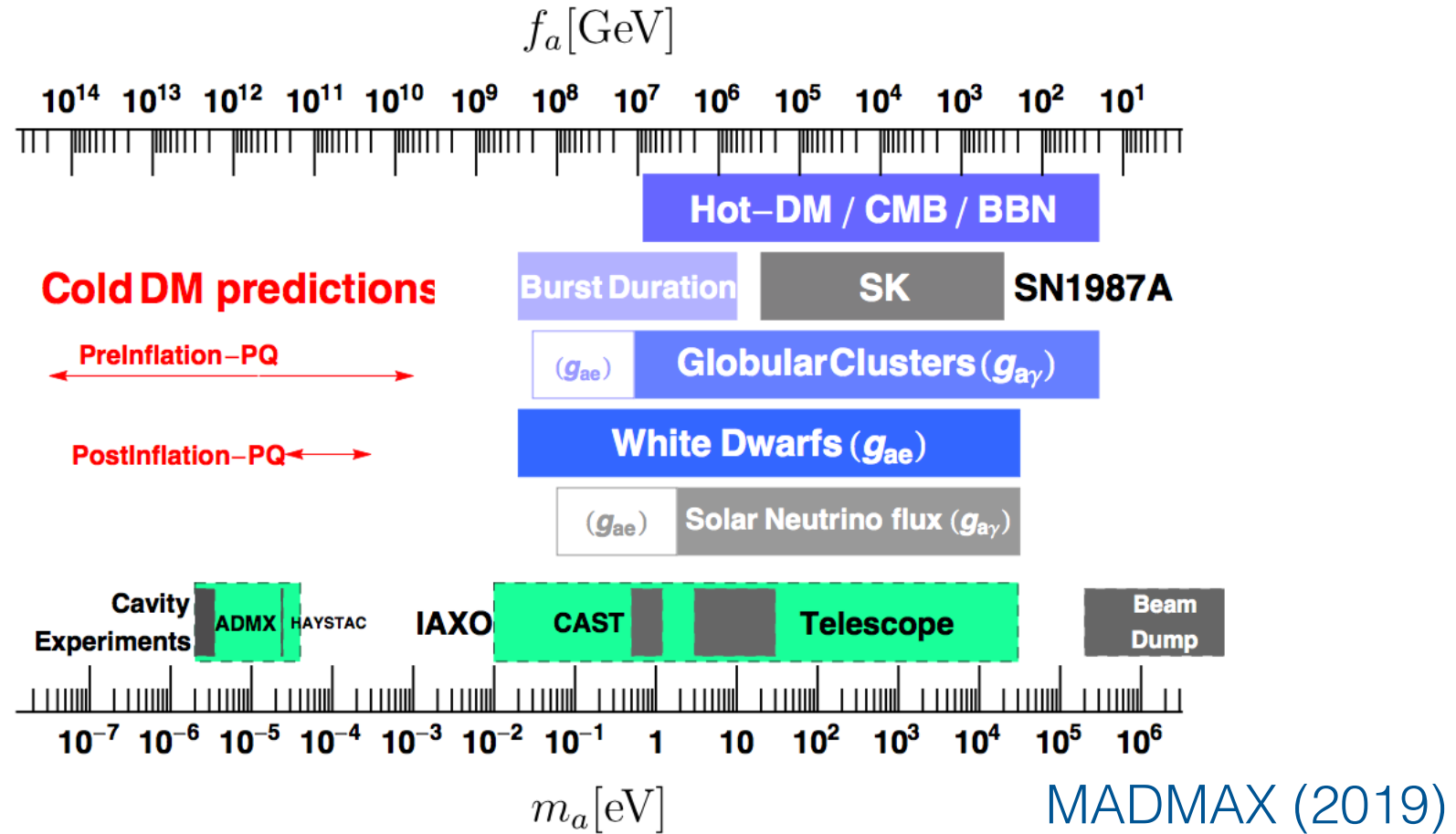
At zero and low temperature, chiral perturbation theory gives:

$$m_A^2 = \frac{m_u m_d}{(m_u + m_d)^2} \frac{m_\pi^2 f_\pi^2}{f_A^2} ,$$

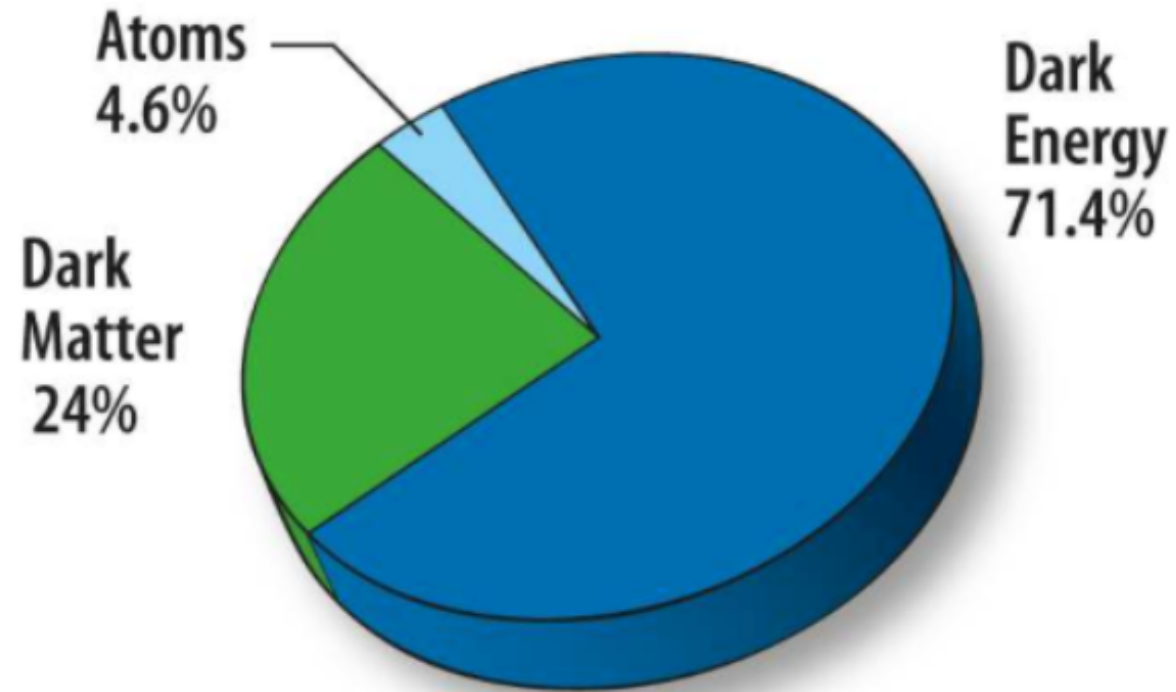
In very brief summary, the essence of this discussion is the close relation between axion mass and topological susceptibility:

$$m_A^2 f_A^2 = \chi_{top} ,$$

# QCD axion mass landscape



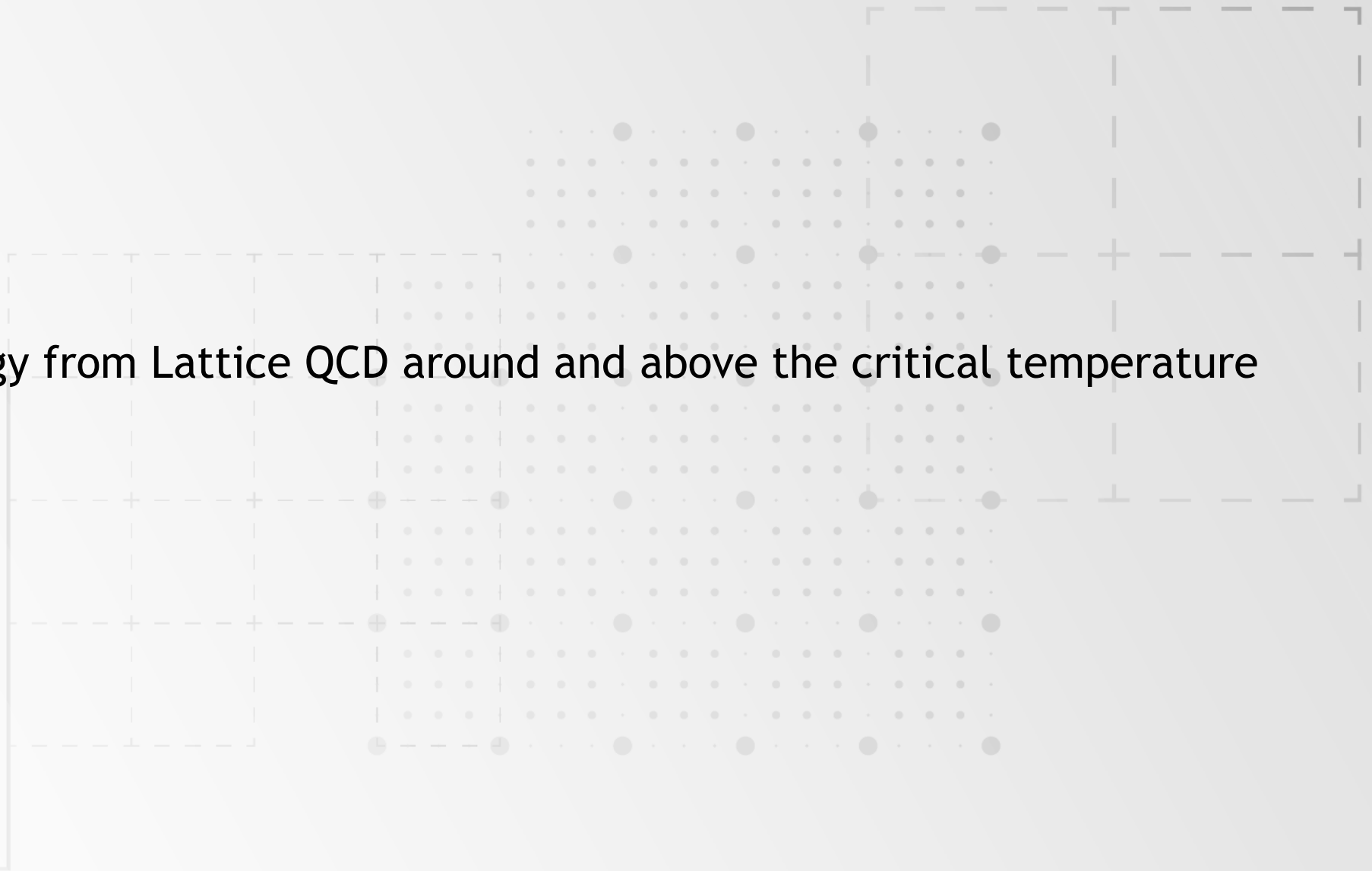
## Candidate to Dark Matter: QCD axion



TODAY

To constrain the axion mass values,  
It is necessary to know the  
Topological susceptibility at high temperatures

Topology from Lattice QCD around and above the critical temperature



## Analytic knowledge

At zero and low (below or around  $T_c$ ) temperatures  $F(\theta, T)$  can be computed by considering low energy effective Lagrangians  
Finite temperature corrections have been computed, and their validity stretches till  $T \simeq T_c$ .

In the Quark Gluon Plasma phase the basic expression for  $F(\theta, T)$  comes from dilute gas approximation (DIGA) and high temperature perturbation theory at leading order:

$$F(\theta, T) - F(0, T) \simeq T^{4-\beta_0} \left( \frac{m_l}{T} \right)^{N_{f,l}} (1 - \cos \theta),$$

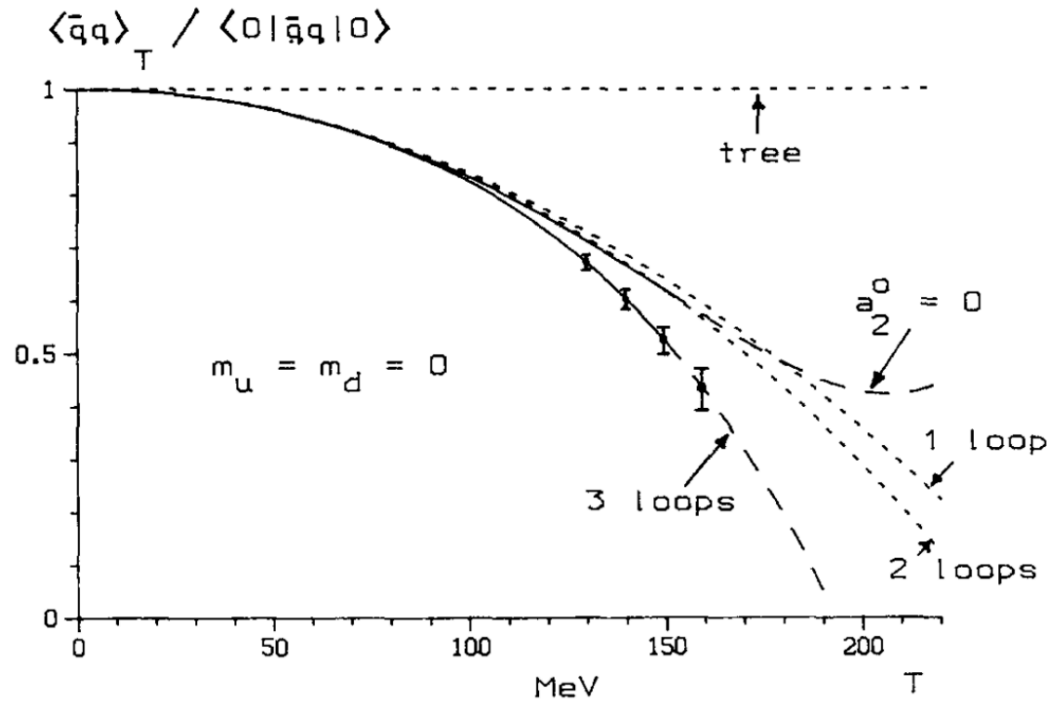
where  $\beta_0 = 11N_c/3 - 2N_f/3$  and  $N_{f,l}$  is the number of light flavors.

Intermediate temperatures, around  $T_c$ :  
Lattice simulations

# From chiral perturbation theory

$$\frac{\chi_{top}(T)}{\chi_{top}} \stackrel{\text{NLO}}{=} \frac{m_\pi^2(T) f_\pi^2(T)}{m_\pi^2 f_\pi^2} = \frac{\langle \bar{q}q \rangle_T}{\langle \bar{q}q \rangle}$$

$$\langle \bar{q}q \rangle \stackrel{m \rightarrow 0}{=} \langle 0 | \bar{q}q | 0 \rangle \left( 1 - \frac{T^2}{8F^2} - \frac{T^4}{384F^4} - \frac{T^6}{288F^6} \ln \frac{\Lambda_q}{T} + O(T^8) \right)$$



For axion applications we need  $T$  approx. 500-600 MeV

1) Comparison with DIGA: Only instanton-anti-instanton pair contribute

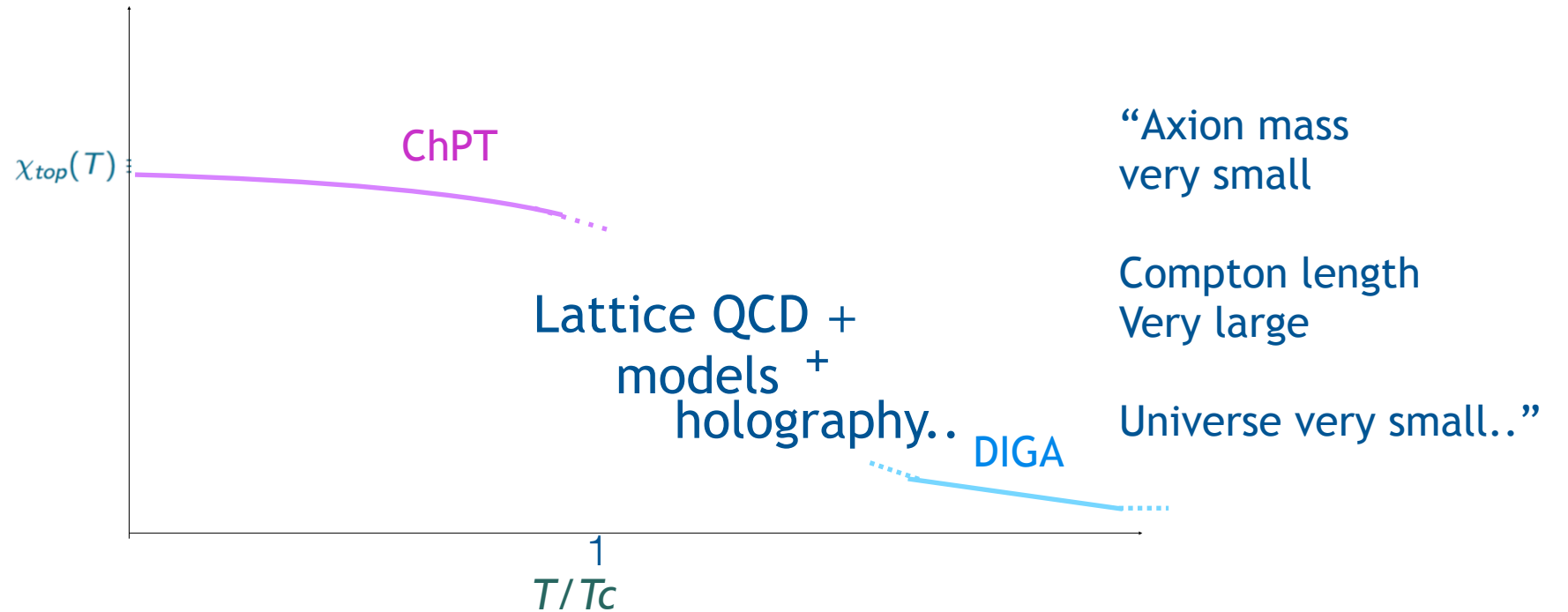
$$F(\theta, T) - F(0, T) \simeq T^{4-\beta_0} \left(\frac{m_l}{T}\right)^{N_{f,l}} (1 - \cos \theta),$$

where  $\beta_0 = 11N_c/3 - 2N_f/3$  and  $N_{f,l}$  is the number of light flavors.

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

2) Fate of the eta'

What do we know about  $\chi_{top}(T) \equiv \left. \frac{\partial^2 F(\theta, T)}{\partial \theta^2} \right|_{\theta=0}$



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



# Lattice topology Michael Mueller-Preussker(2015)

- ▶ Gluonic: Luscher(2010), Bonati, d'Elia et al (2014), Alexandrou et al . (2015)

$$Q = \frac{a^4}{32\pi^2} \varepsilon_{\mu\nu\rho\sigma} \sum_n \text{Tr}[F_{lat}^{\mu\nu}(n) F_{lat}^{\rho\sigma}(n)],$$

Need smooth configurations, using smearing, cooling, gradient flow..

$$\dot{V}_\mu(n, \tau) = -g^2 [\partial_{n,\mu} S_G(V(\tau))] V_\mu(n, \tau), \quad V_\mu(n, 0) = U_\mu(n),$$

Pros: Easy

Cons: suffers very much from lattice artifacts

- ▶ Fermionic: Atiyah Singer(1971,1984)

$$Q = \frac{1}{32\pi^2} \varepsilon_{\mu\nu\rho\sigma} \int \text{Tr}[F^{\mu\nu}(x) F^{\rho\sigma}(x)] d^4x = n_+ - n_-$$

Pros: not affected but UV fluctuations

Cons: very high computational cost

- ▶ Fermionic - simple but approximate: Kogut et al.(1996), Petreczky, Sharma(2016)

$$\chi_{top} = \frac{\langle Q^2 \rangle}{V} = m_l^2 \chi_{5, disc}$$

$$\chi_{top}(T \gtrsim T_c) = m_l^2 \chi_{disc} = m_l^2 \frac{V}{T} (\langle (\bar{\psi}\psi)^2 \rangle_l - \langle \bar{\psi}\psi \rangle_l^2).$$

- ▶ Fermionic - simple but approximate: Kogut et al.(1996),Petreczky, Sharma(2016)

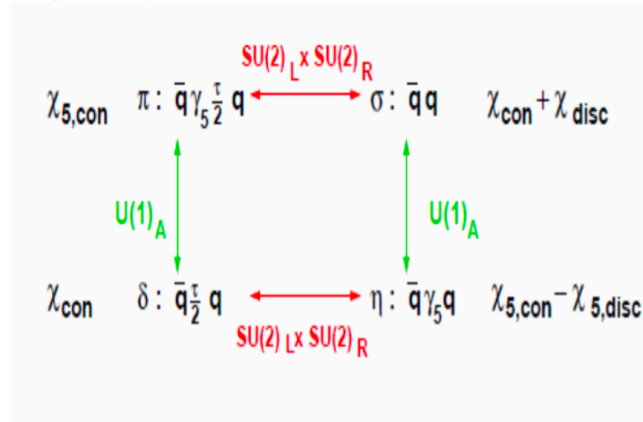
$$\chi_{top} = \frac{\langle Q^2 \rangle}{V} = m_l^2 \chi_{5,disc}$$

$$\chi_{top}(T \gtrsim T_c) = m_l^2 \chi_{disc} = m_l^2 \frac{V}{T} (\langle (\bar{\psi}\psi)^2 \rangle_l - \langle \bar{\psi}\psi \rangle_l^2). \text{ Above } T_c$$

□

Recall:

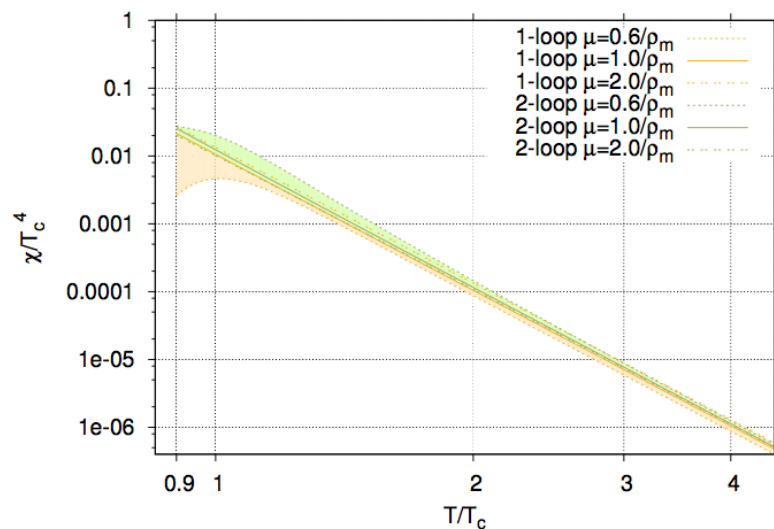
- ▶ Degeneracy pattern for two flavors: MILC plot



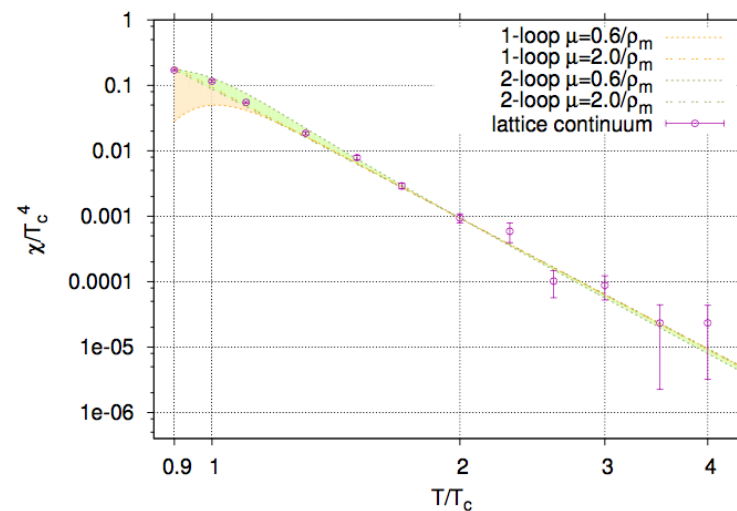
# Yang-Mills

Borsanyi et al. 2015

## Two loop RG DIGA



## Lattice results



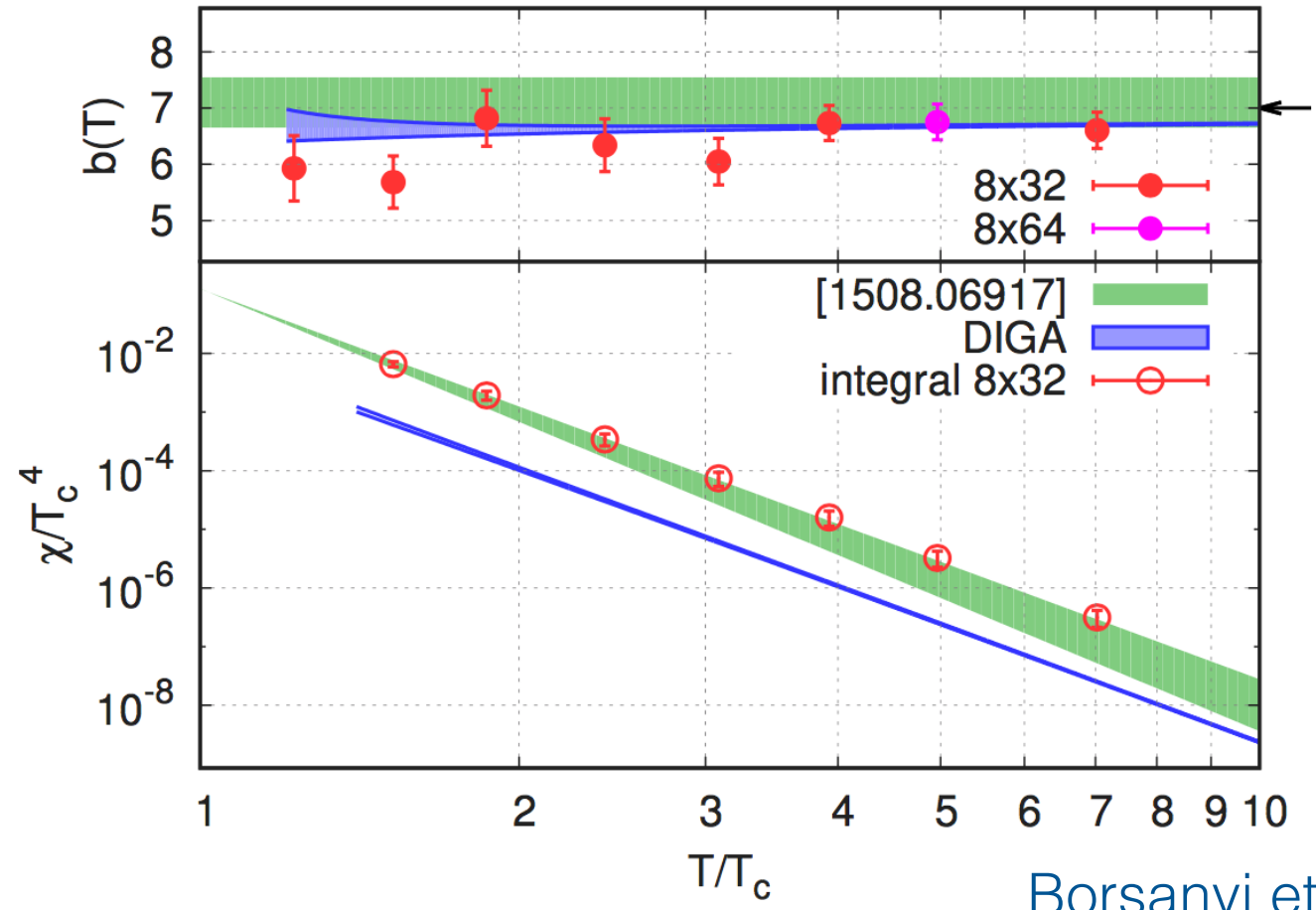
Exponent OK

One order of magnitude discrepancy  
in the absolute value

$T/T_c$	1.5	2	3	4	5
$b(\kappa = 0.6)$	-6.04	-6.26	-6.43	-6.50	-6.55
$b(\kappa = 1)$	-6.37	-6.46	-6.55	-6.59	-6.62
$b(\kappa = 2)$	-6.55	-6.59	-6.64	-6.67	-6.69

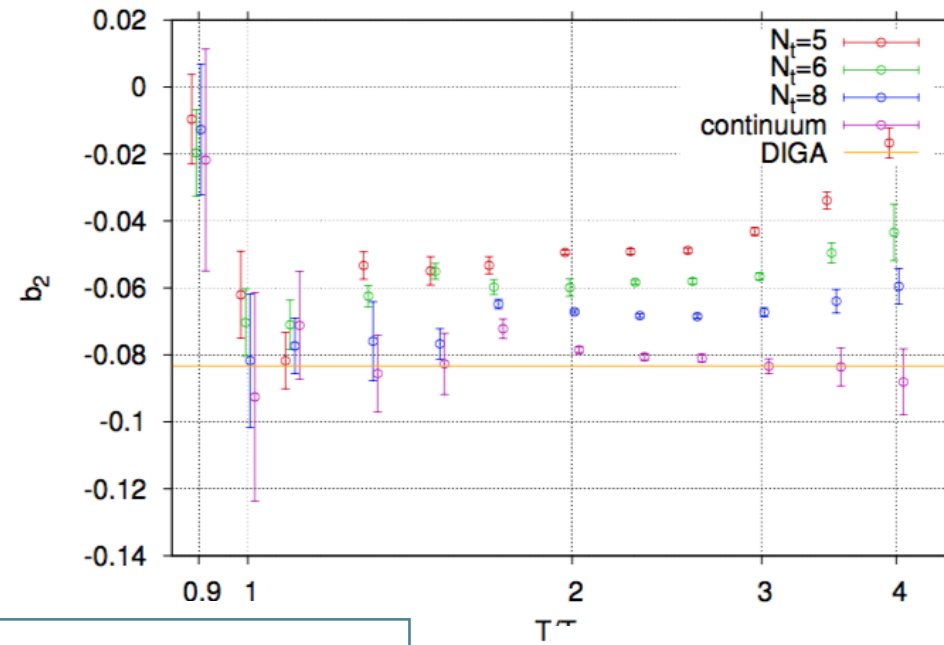
Table 2: Temperature slopes of the topological susceptibility predicted in the two-loop RGI DIGA, for a range of renormalization scales  $\mu$ .

$T/T_c$	1	2	3	4	5
$\alpha_{\overline{\text{MS}}}(1/\rho_m)$	0.36	0.23	0.19	0.17	0.16



Borsanyi et al. 2016

# Beyond topological susceptibility



$$V(A, T) = \frac{1}{2} \chi(T) \theta^2 \left[ 1 + b_2(T) \theta^2 + \dots \right] \Big|_{\theta=A/f_A},$$

$$b_2(T) = - \frac{\langle Q^4 \rangle_T - 3 \langle Q^2 \rangle_T^2}{12 \langle Q^2 \rangle_T} \Big|_{\theta=0}.$$

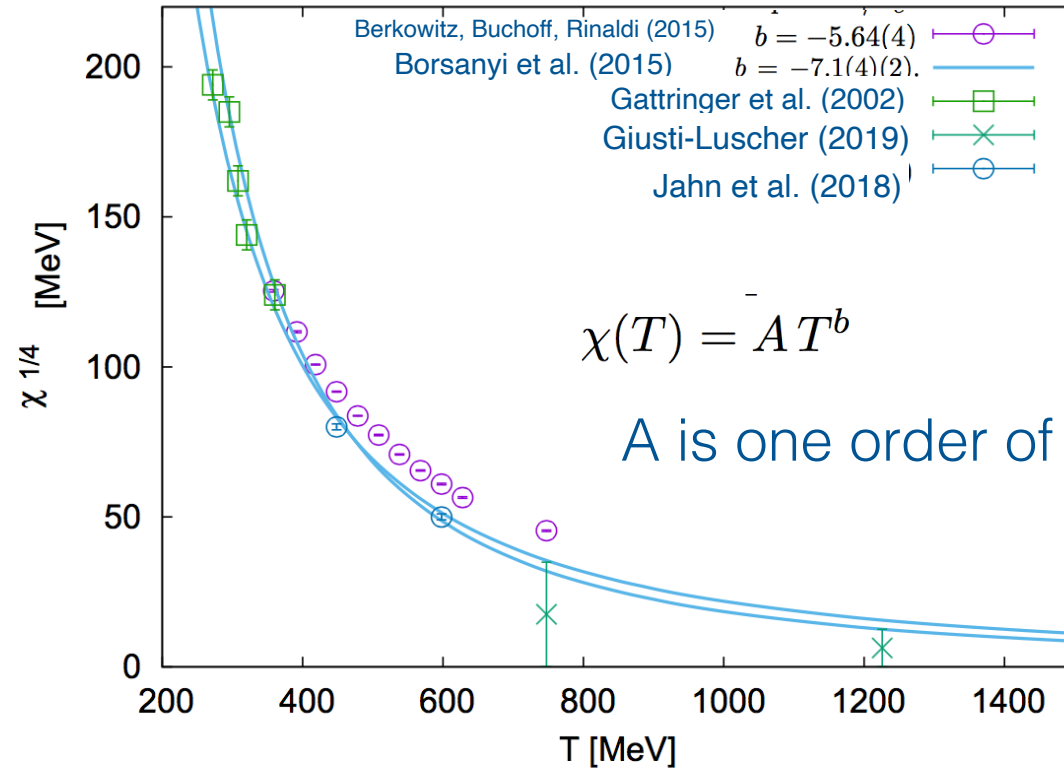
Bonati, D'Elia, Panagopoulos, Vicari 2013

$$C_n = (-1)^{n+1} \frac{d^{2n}}{d\theta^{2n}} F(\theta, T) \Big|_{\theta=0} = \langle Q^{2n} \rangle_{conn}.$$

Borsanyi et al. 2016

# Yang-Mills - summary

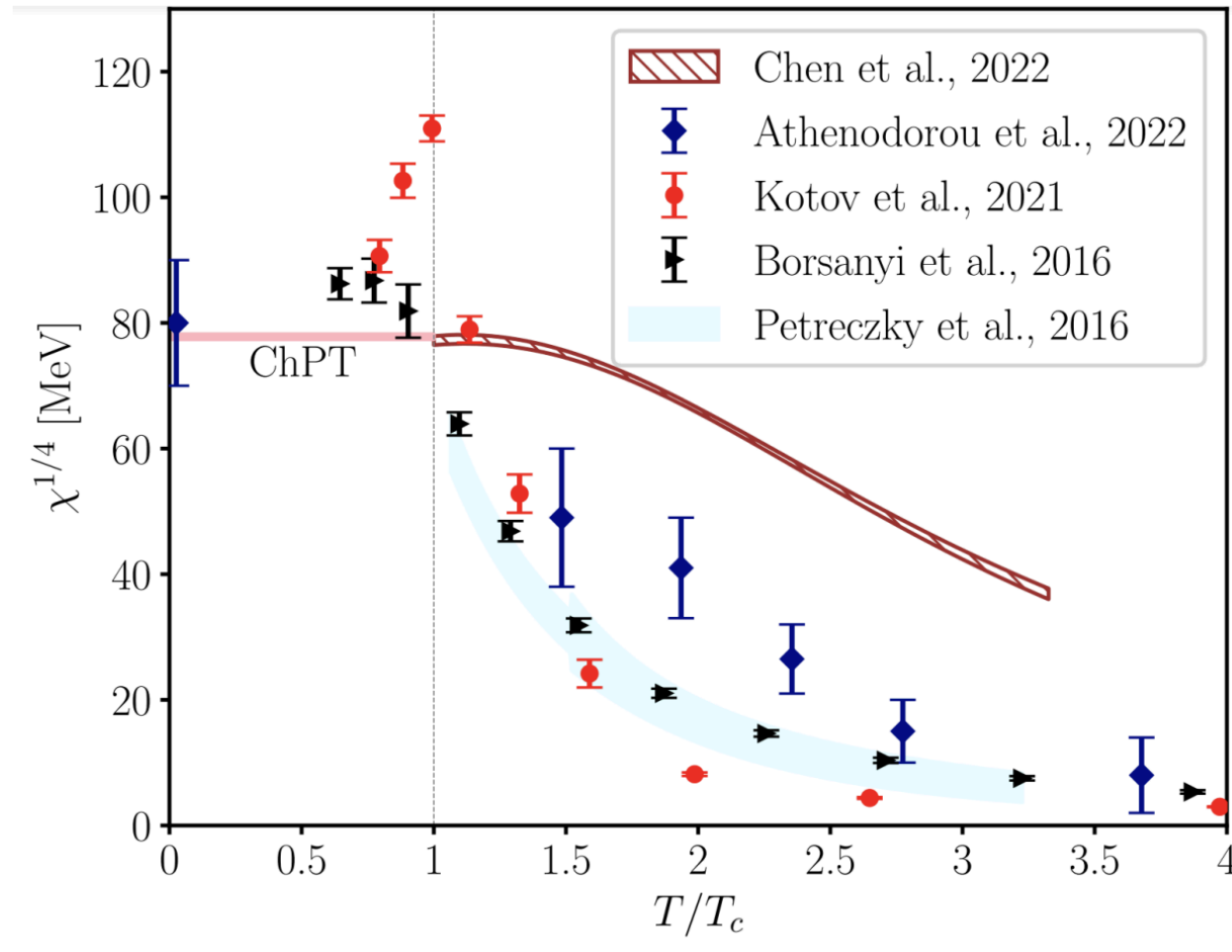
1



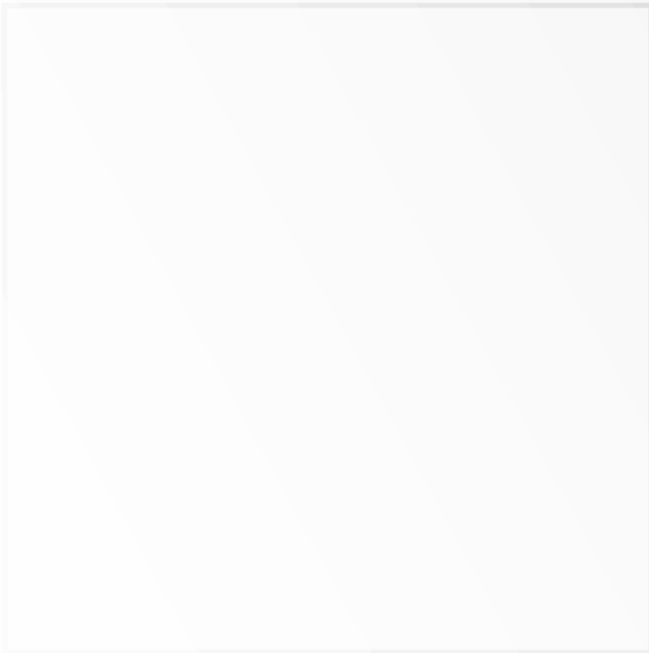
$$\chi(T) = AT^b$$

A is one order of magnitude off!

# QCD - summary

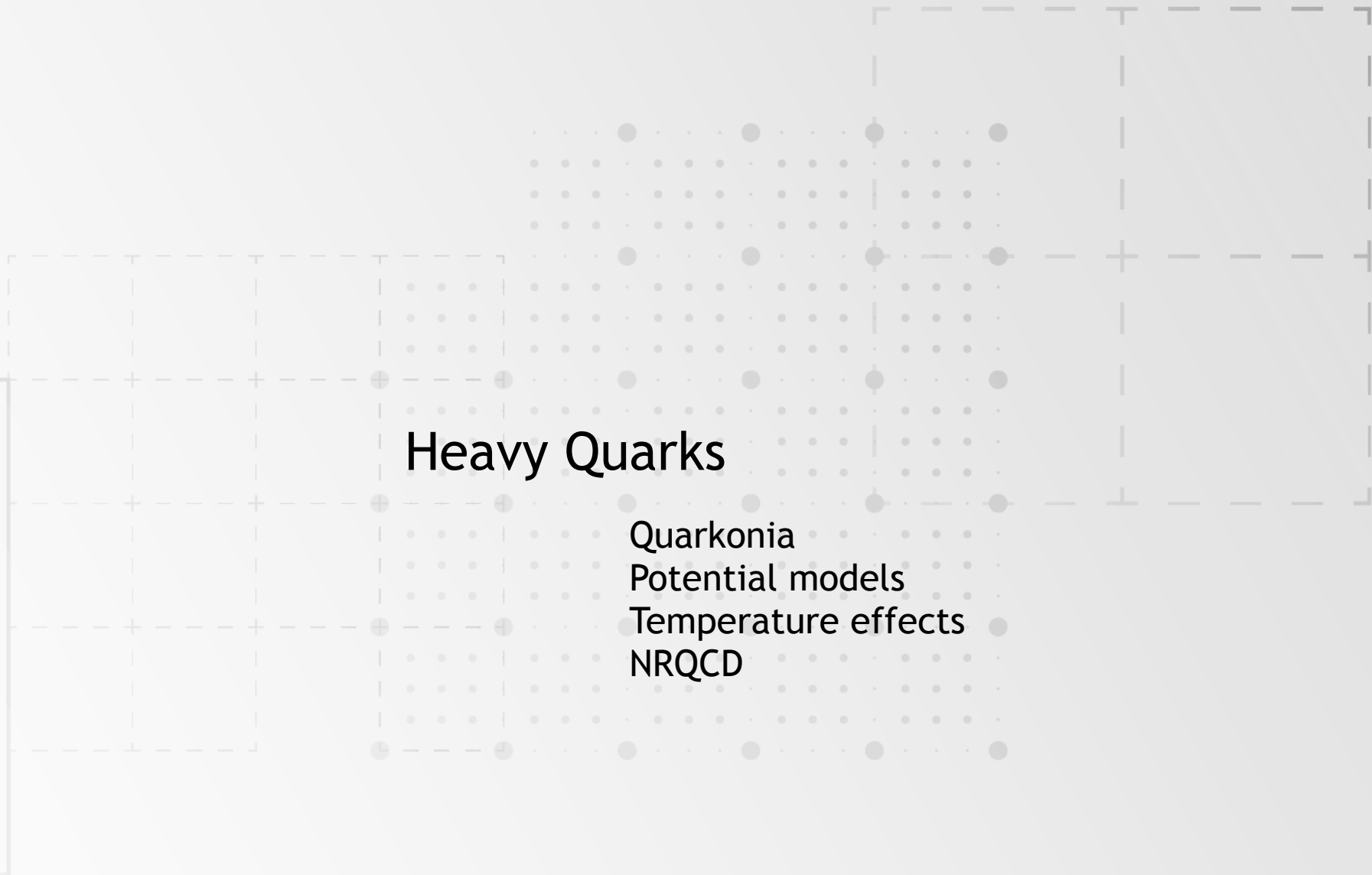


Plot by  
Claudio Bonanno



# Heavy Quarks

- Quarkonia
- Potential models
- Temperature effects
- NRQCD





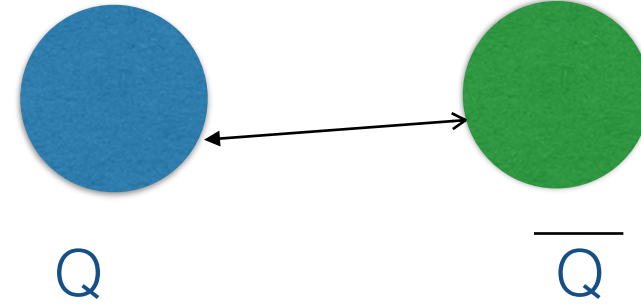
Quarkonia: heavy quarks  $\Rightarrow$  non-relativistic potential theory

Jacobs et al. 1986

Schrödinger equation  $\left\{ 2m_c - \frac{1}{m_c} \nabla^2 + V(r) \right\} \Phi_i(r) = M_i \Phi_i(r)$

with confining (“Cornell”) potential  $V(r) = \sigma r - \frac{\alpha}{r}$

$$E(r) = 2m + \frac{1}{2mr^2} + V(r),$$



Minimizing the energy:

$$\frac{1}{mr_{J/\psi}^3} - \frac{\alpha_{\text{eff}}}{r_{J/\psi}^2} - \sigma = 0$$

Relation between the parameters of the potential, the mass and the radius

Quarkonia: heavy quarks  $\Rightarrow$  non-relativistic potential theory

Jacobs et al. 1986

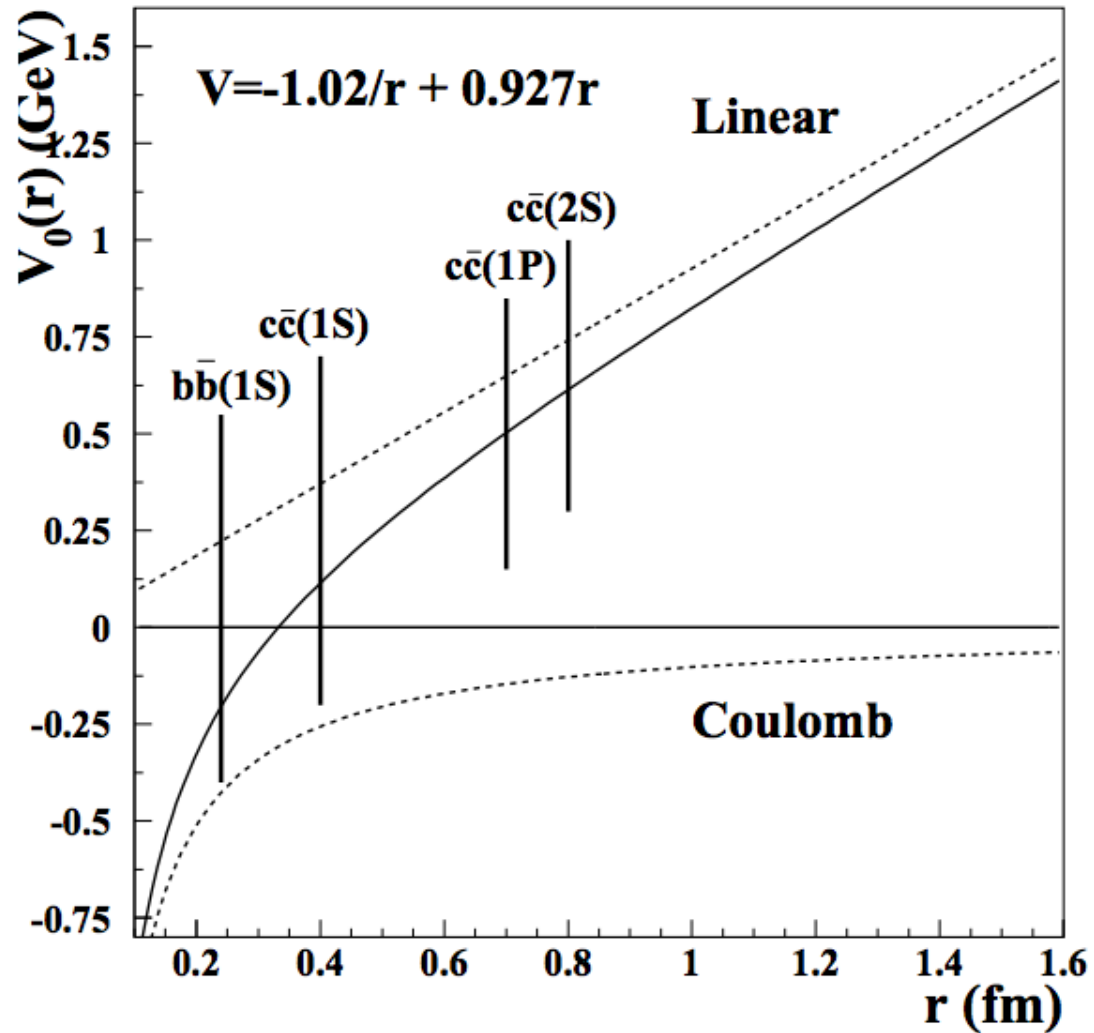
Schrödinger equation  $\left\{ 2m_c - \frac{1}{m_c} \nabla^2 + V(r) \right\} \Phi_i(r) = M_i \Phi_i(r)$

with confining (“Cornell”) potential  $V(r) = \sigma r - \frac{\alpha}{r}$

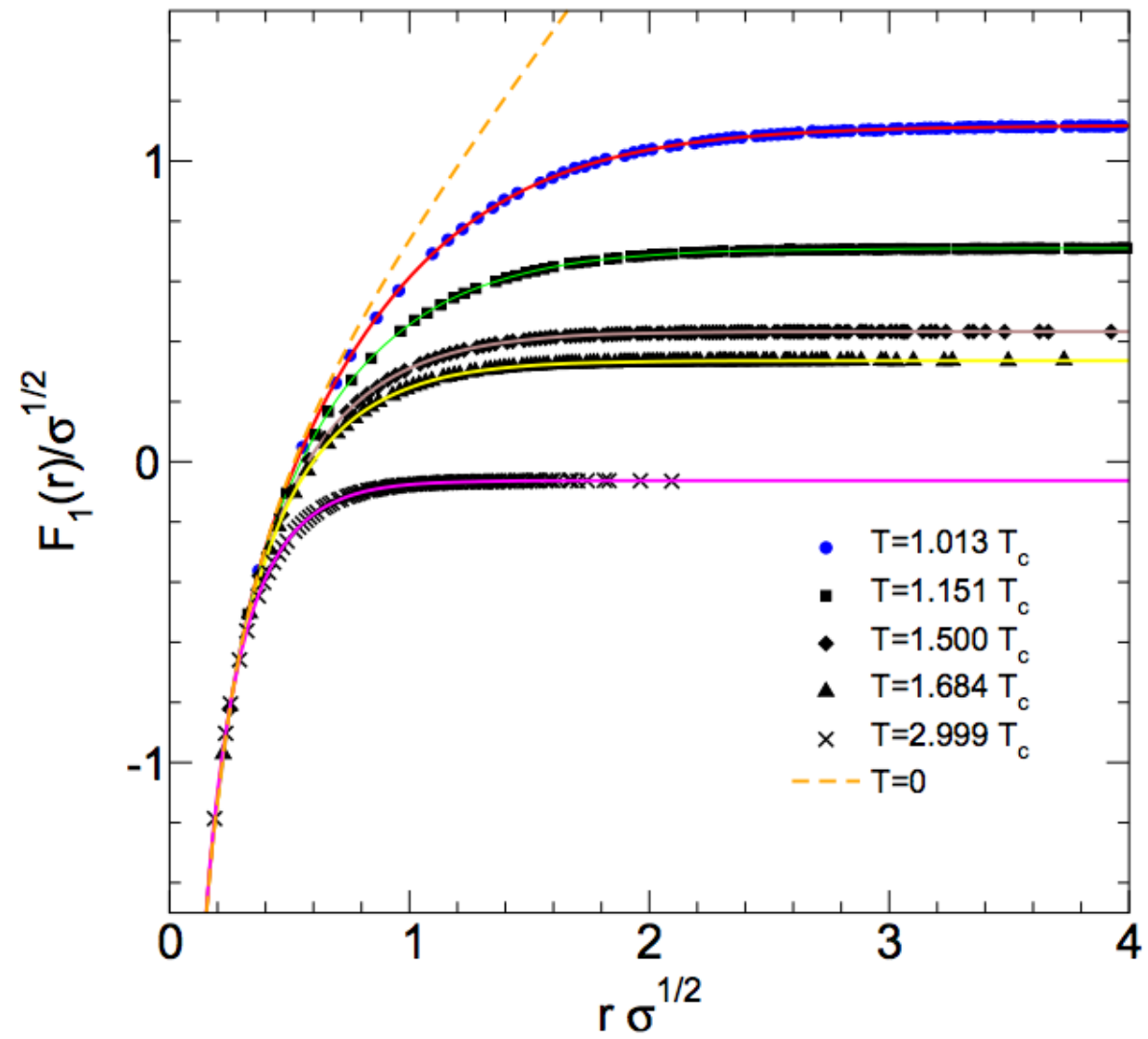
state	$J/\psi$	$\chi_c$	$\psi'$	$\Upsilon$	$\chi_b$	$\Upsilon'$	$\chi'_b$	$\Upsilon''$
mass [GeV]	3.10	3.53	3.68	9.46	9.99	10.02	10.26	10.36
radius [fm]	0.25	0.36	0.45	0.14	0.22	0.28	0.34	0.39

# Bound by Coulombic part vs confining binding

Potential probes gauge dynamics



# Temperature effects

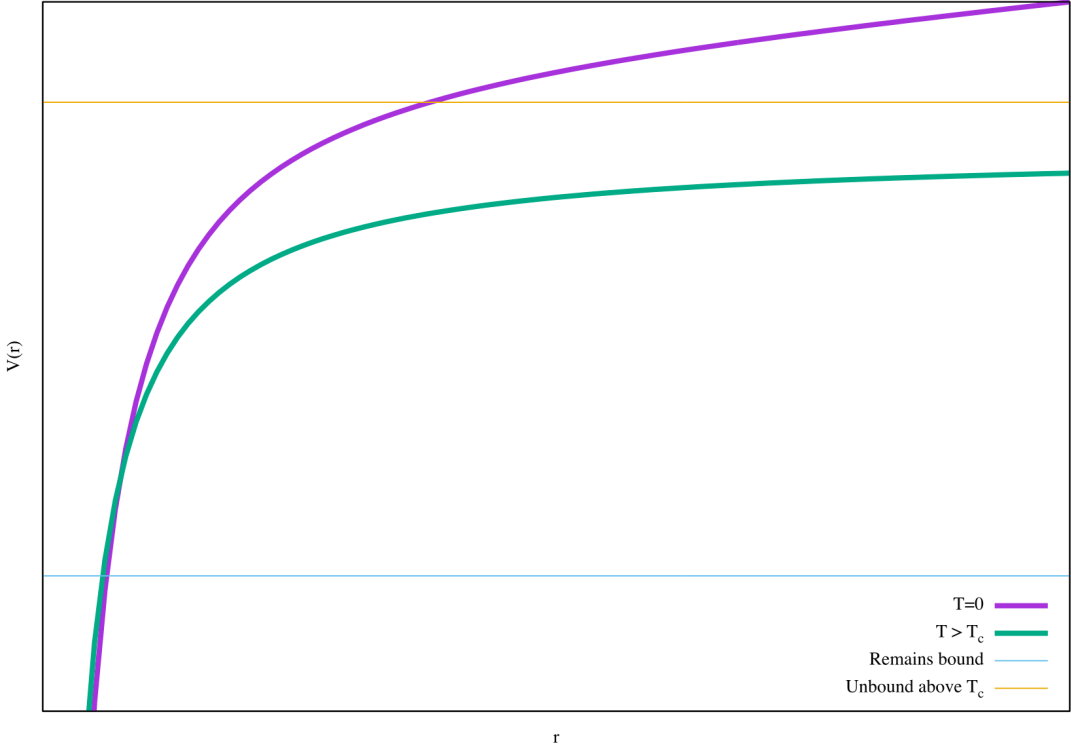


# Heavy quark potential from: models + high T p.t.

## High temperature Debye Screening

$$V(r) = \sigma r - \frac{\alpha}{r} \xrightarrow{T} V(r) \sim \frac{e^{-m_D^0 r}}{4\pi r},$$

$$m_D^0 = \left( \frac{N}{3} + \frac{N_f}{6} \right)^{1/2} gT$$



Caveat: recent works challenge this picture

Potential model recipe:

- 1) Find Potential as a function of temperature
- 2) Solve Schroedinger eq. as a function of T
- 3) Check who remains bound (binding energy)

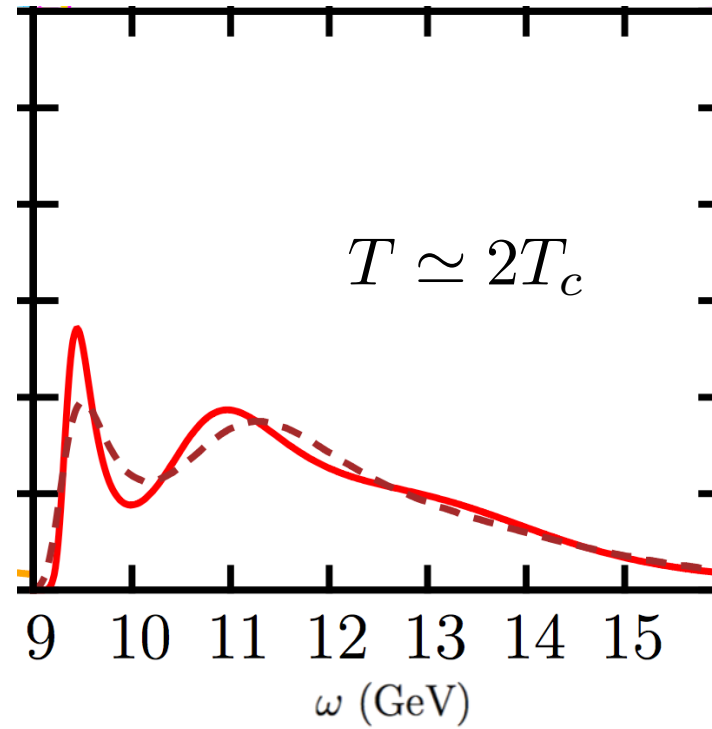
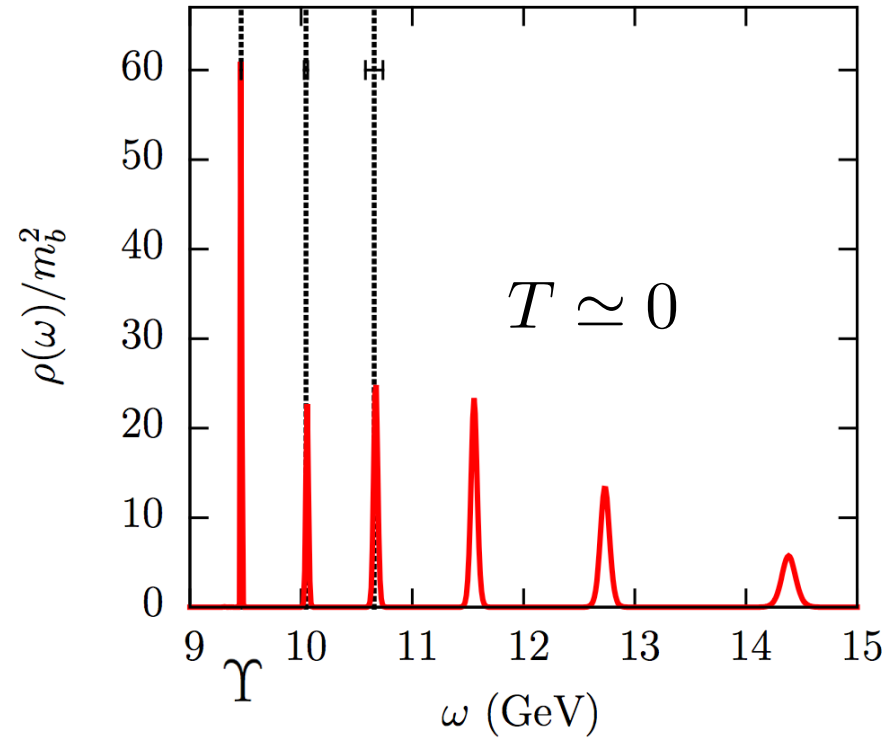
Various uncertainties ..

# Compromise: Bottomonium via NRQCD

Zero temperature NRQCD works beautifully for the spectrum

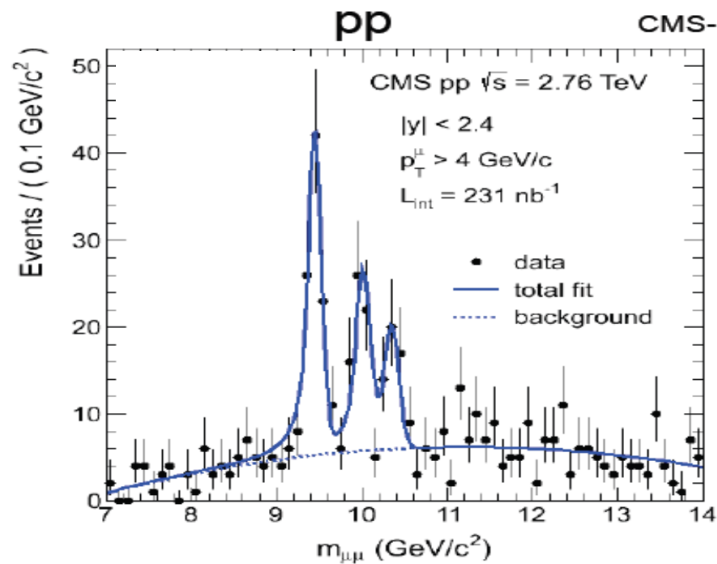
$n^{S+1}L_J$	State	$a_\tau M$	$E_0 + M$ (MeV)	$M_{\text{expt}}$ (MeV)
$1^1S_0$	$\eta_b$	0.20549(4)	9409(12)	9398.0(3.2)
$2^1S_0$	$\eta'_b$	0.311(3)	10004(21)	9999(4)
$1^3S_1$	$\Upsilon$	0.21460(5)	9460*	9460.30(26)
$2^3S_1$	$\Upsilon'$	0.318(3)	10043(22)	10023.26(31)
$1^1P_1$	$h_b$	0.2963(4)	9920(15)	9899.3(1.0)
$1^3P_0$	$\chi_{b0}$	0.2921(4)	9896(15)	9859.44(52)
$1^3P_1$	$\chi_{b1}$	0.2964(4)	9921(15)	9892.78(40)
$1^3P_2$	$\chi_{b2}$	0.2978(4)	9928(15)	9912.21(40)

# Bottomonium spectral functions from the lattice



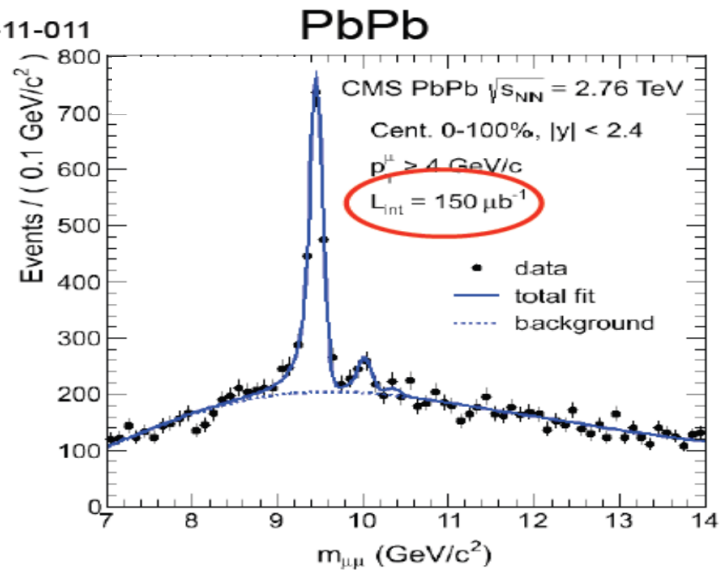


# Bottomonium as a probe of QGP



$$N_{R(2S)}/N_{R(1S)}|_{\text{pp}} = 0.56 \pm 0.13 \pm 0.01$$

$$N_{R(3S)}/N_{R(1S)}|_{\text{pp}} = 0.21 \pm 0.11 \pm 0.02$$



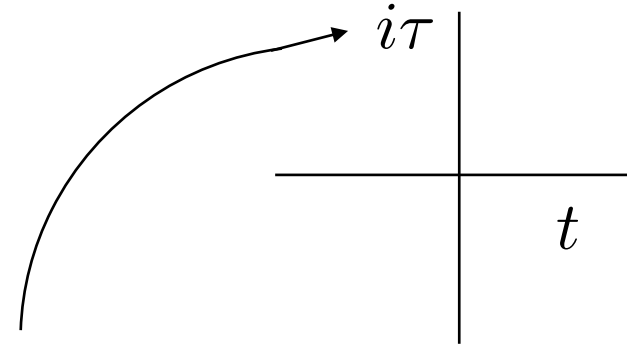
$$N_{R(2S)}/N_{R(1S)}|_{\text{PbPb}} = 0.12 \pm 0.03 \pm 0.01$$

$$N_{R(3S)}/N_{R(1S)}|_{\text{PbPb}} < 0.07$$

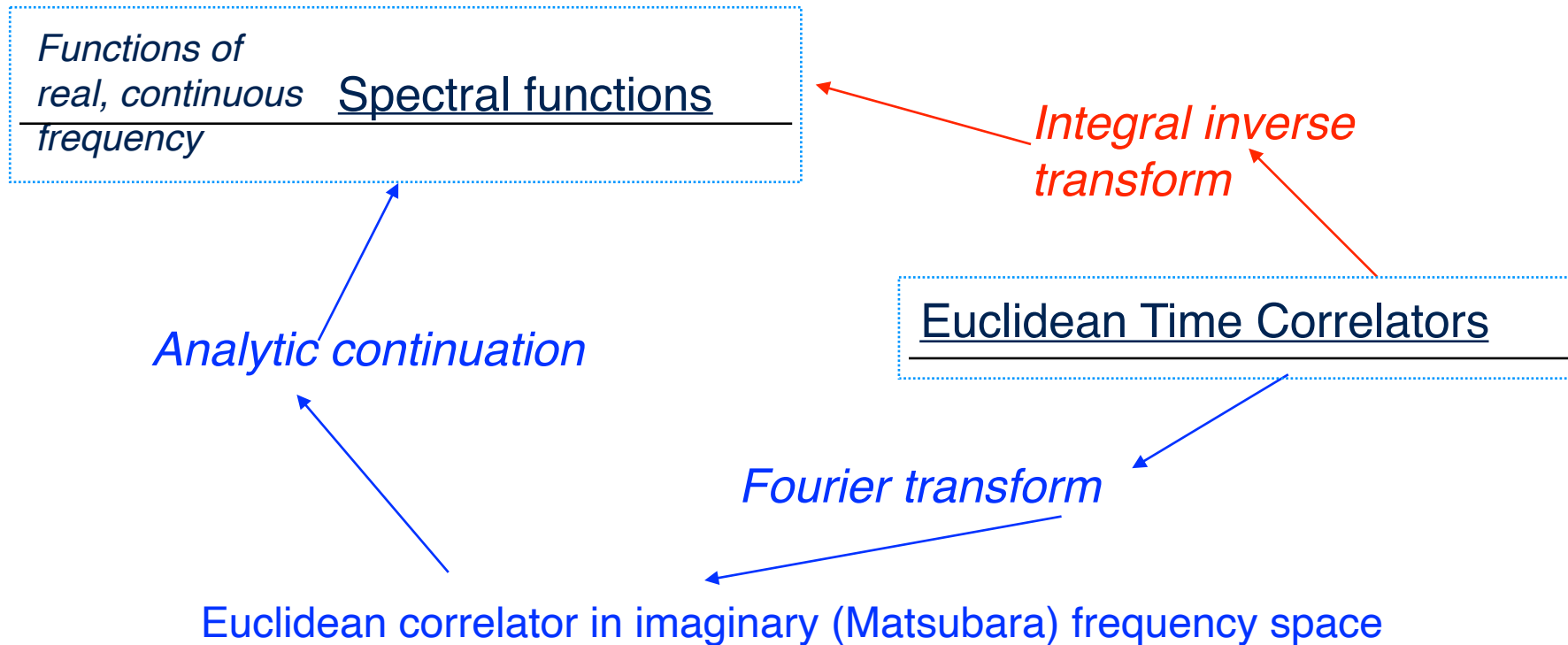
CMS

Eur.Phys.J. C76 (2016) no.3, 107

Objects of interest: Spectral functions



Computed on the lattice: Euclidean (imaginary) Time Correlators



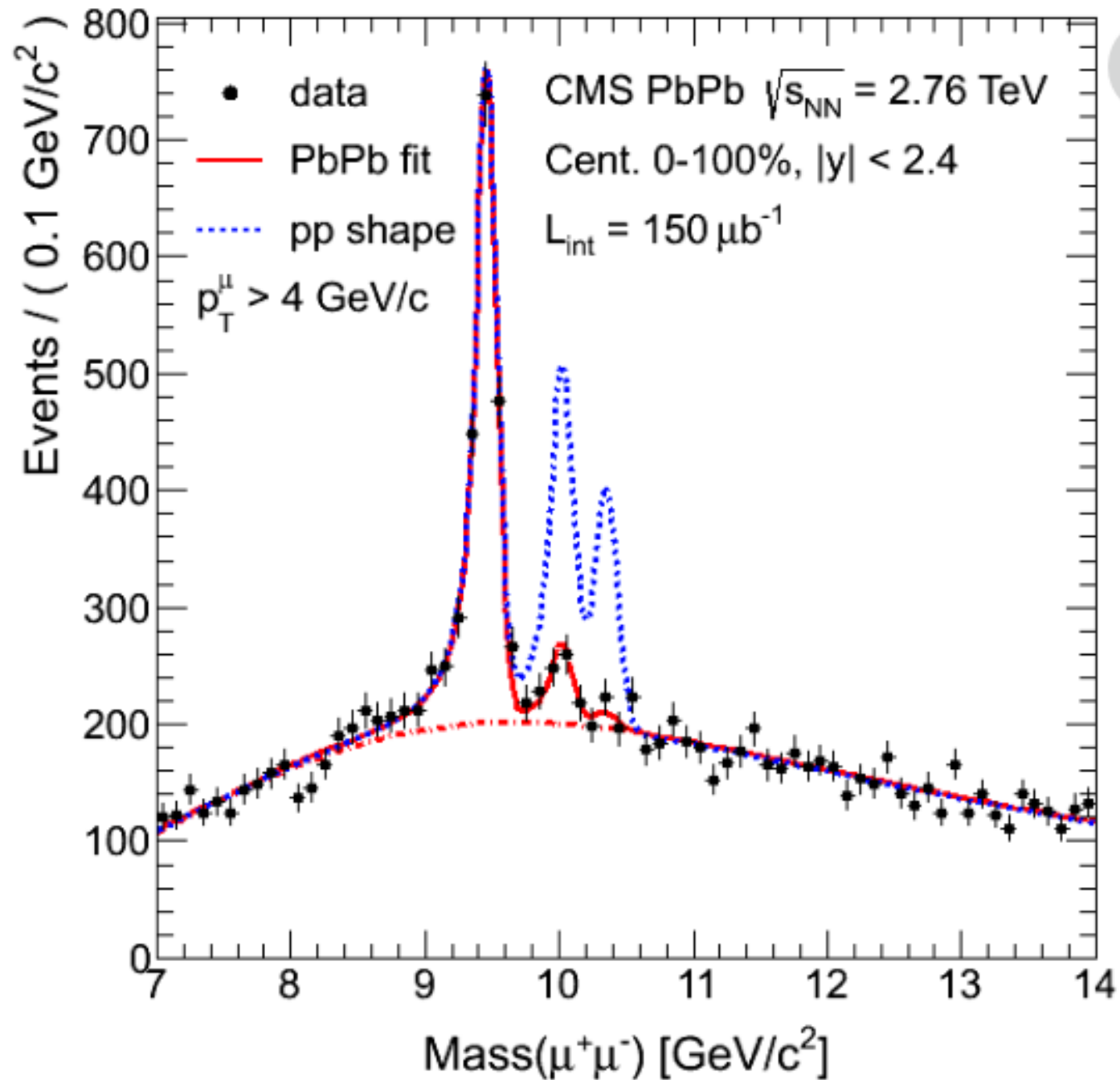
Relativistic

$$D(\tau) = \int_0^{\infty} \frac{e^{-\tau\omega} + e^{-(\beta-\tau)\omega}}{1 - e^{-\beta\omega}} S(\omega) d\omega$$

Non-relativistic

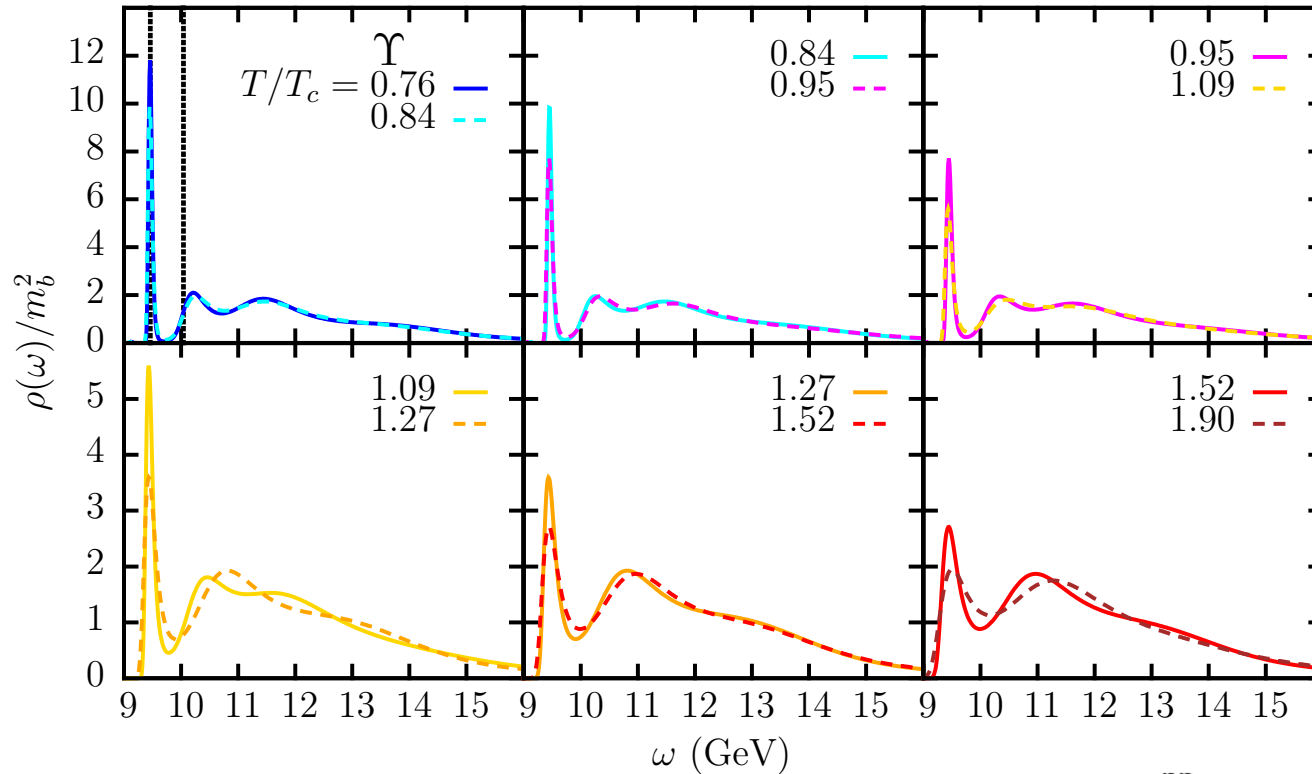
$$D(\tau) = \int_{-M_0}^{\infty} e^{-\tau\omega} S(\omega) d\omega$$

Inverse Laplace:  
makes life easier..



# Upsilon's spectral functions from MEM (NRQCD)

FASTSUM

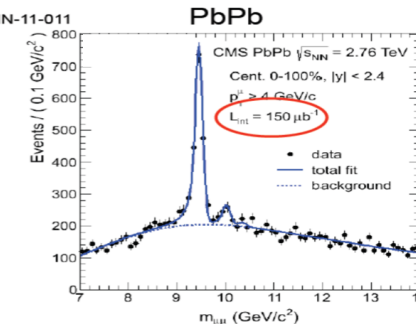
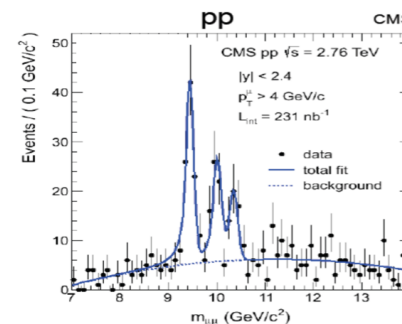


Persistence of  
the ground state  
at all temperatures

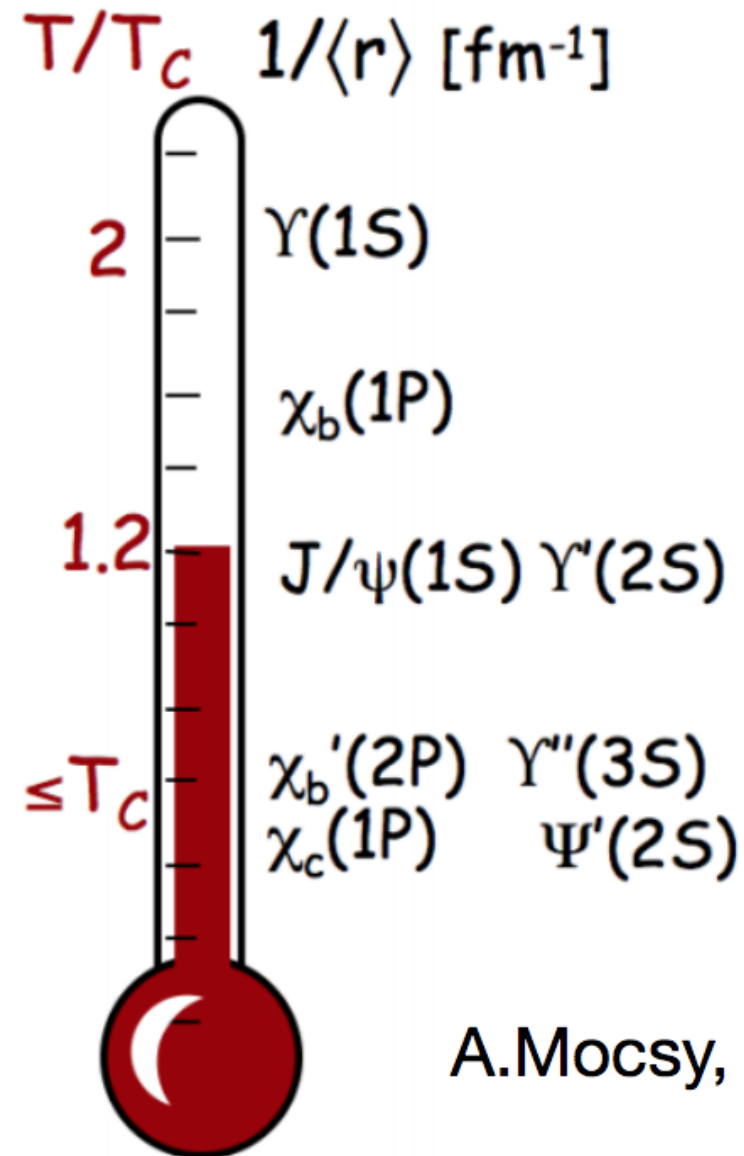
Melting of  
excited states

Modifications of  
the ground state

Pattern reminiscent of experimental observations



The picture of sequential melting is qualitatively correct, but quantitative uncertainties remain – cross checks from different methods important



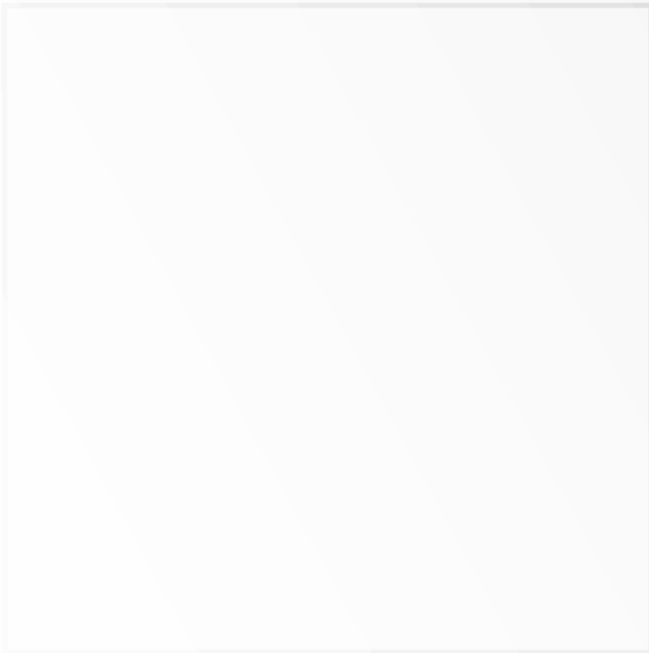
A.Mocsy, arXiv:0811.0337

Review by C.Allton:

<https://www.ggi.infn.it/talkfiles/slides/slides5843.pdf>

# Study of Numerical Methods

- |   |   |  |
|---|---|--|
| 1. Exponential (Conventional $\delta$ f'ns)       | } | Maximum Likelihood<br>(Minimise $\chi^2$ ) |
| 2. Gaussian Ground State (+ $\delta$ f'n excited) |   |  |
| 3. Moments of Correlation F'ns                    |   | Direct Method - "no" fit                   |
| 4. BR Method                                      | } | Bayesian Approaches                        |
| 5. Maximum Entropy Method                         |   |  |
| 6. Kernel Ridge Regression                        |   | Machine Learning                           |
| 7. Backus Gilbert                                 |   | from Geophysics                            |

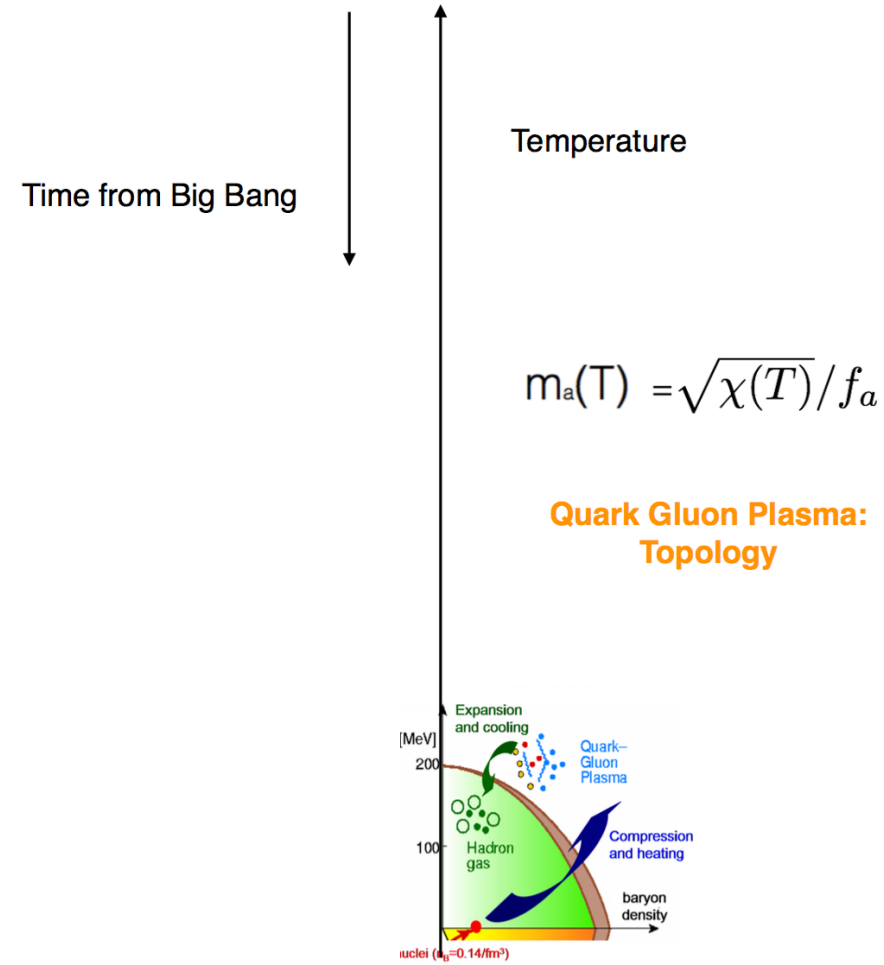


Axion cosmology and lattice



$$T_c \text{ Peccei Quinn} \simeq 10^7 - 10^8 \text{ GeV}$$

$$T_c \text{ Electroweak} \simeq 160 \text{ GeV (SM)}$$



Peccei-Quinn transition: spontaneous breaking of a U(1) symmetry

[aside: possible gravitational waves..]

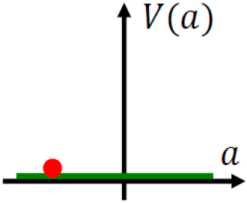
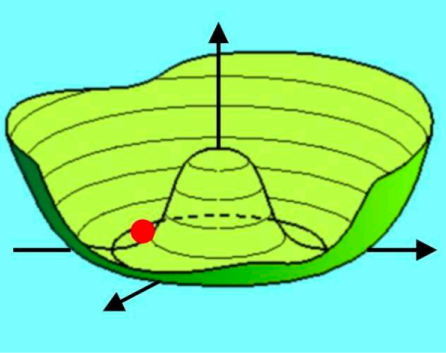
Low energy effective Lagrangian for the axion:

$$\mathcal{L} = \mathcal{L}_{QCD} + \theta \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu} + \partial_\mu^2 a^2 + \frac{a}{f_A} \frac{g^2}{32\pi^2} F_{\mu\nu}^a \tilde{F}_a^{\mu\nu}.$$

Axion: Goldston boson of U(1) broken symmetry

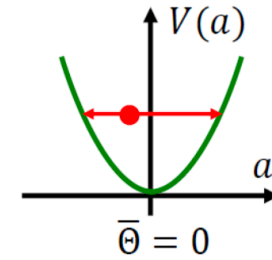
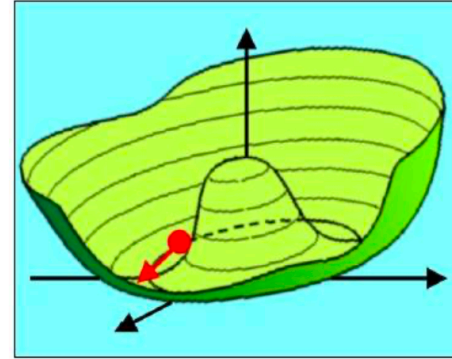
$T \sim f_a$  (very early universe)

- $U_{PQ}(1)$  spontaneously broken
- Axion fields settles in the "Mexican hat"
- Axion field frozen at initial value  $a(t_i) = \theta_i f_a$



Graphic by A.Mirizzi

Axion mass: U(1) symmetry explicitly broken by topological fluctuations



$$m_A^2(T) f_A^2 = \left. \frac{\partial^2 F(\theta, T)}{\partial \theta^2} \right|_{\theta=0} \equiv \chi_{top}(T) .$$

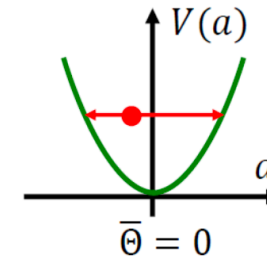
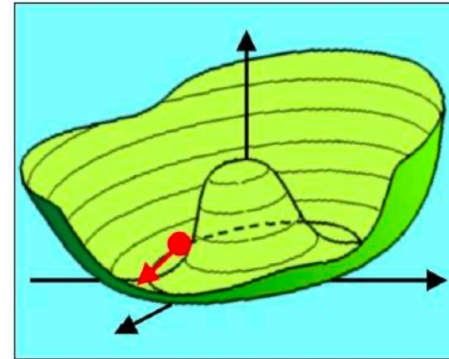
Axion mass: U(1) symmetry explicitly broken by topological fluctuations

When does the explicit breaking become effective?

$T \sim 1 \text{ GeV}$  ( $H \sim 10^{-9} \text{ eV}$ )

- Axion mass turns on quickly
- Field start oscillating when  $m_a \geq 3H$
- Classical field oscillations (axion at rest)

Vacuum realignment



$$m_A^2(T) f_A^2 = \left. \frac{\partial^2 F(\theta, T)}{\partial \theta^2} \right|_{\theta=0} \equiv \chi_{top}(T) .$$

## Axion cosmology (...just a glimpse..)

$$1) \quad H^2 = \frac{1}{3M_p^2} \left( \frac{\pi^2}{30} g_{*,R} T^4 + f_a^2 \left( \frac{1}{2} \dot{\theta}_a^2 + m_a^2(T) (1 - \cos \theta_a) \right) \right)$$

$$\ddot{\theta} + 3H\dot{\theta}_a + m_a^2(T) \sin \theta_a = 0$$

$$2) \quad \frac{\dot{\rho}_a}{f_a^2} = 2m_a \dot{m}_a (1 - \cos \theta_a) - 3H\dot{\theta}_a^2,$$

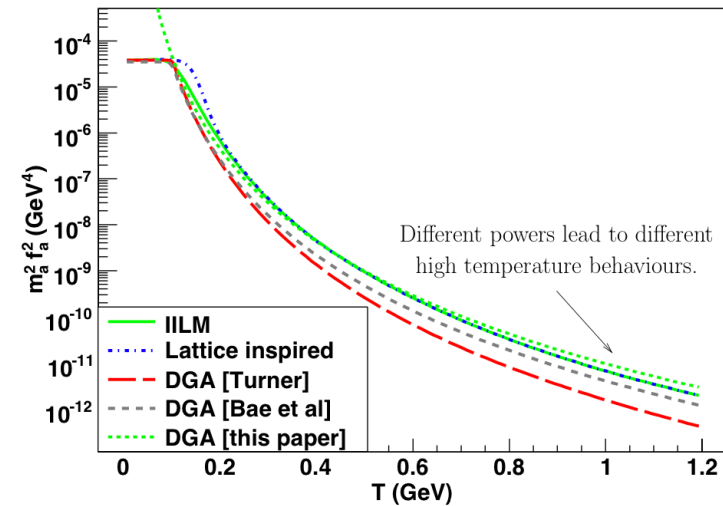
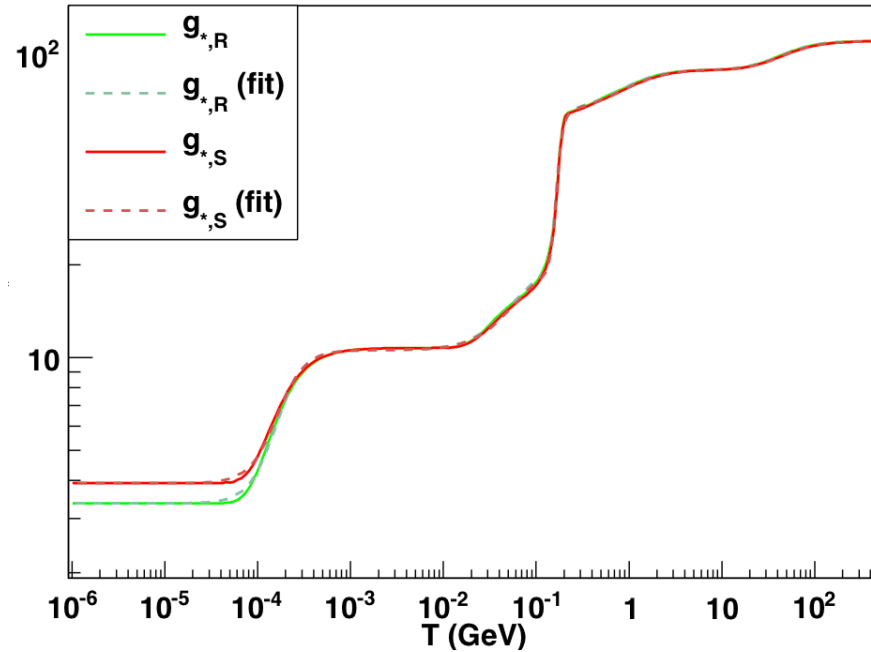
Freezout at:  $3H(T) = m_a(T)$

3) After freezout:

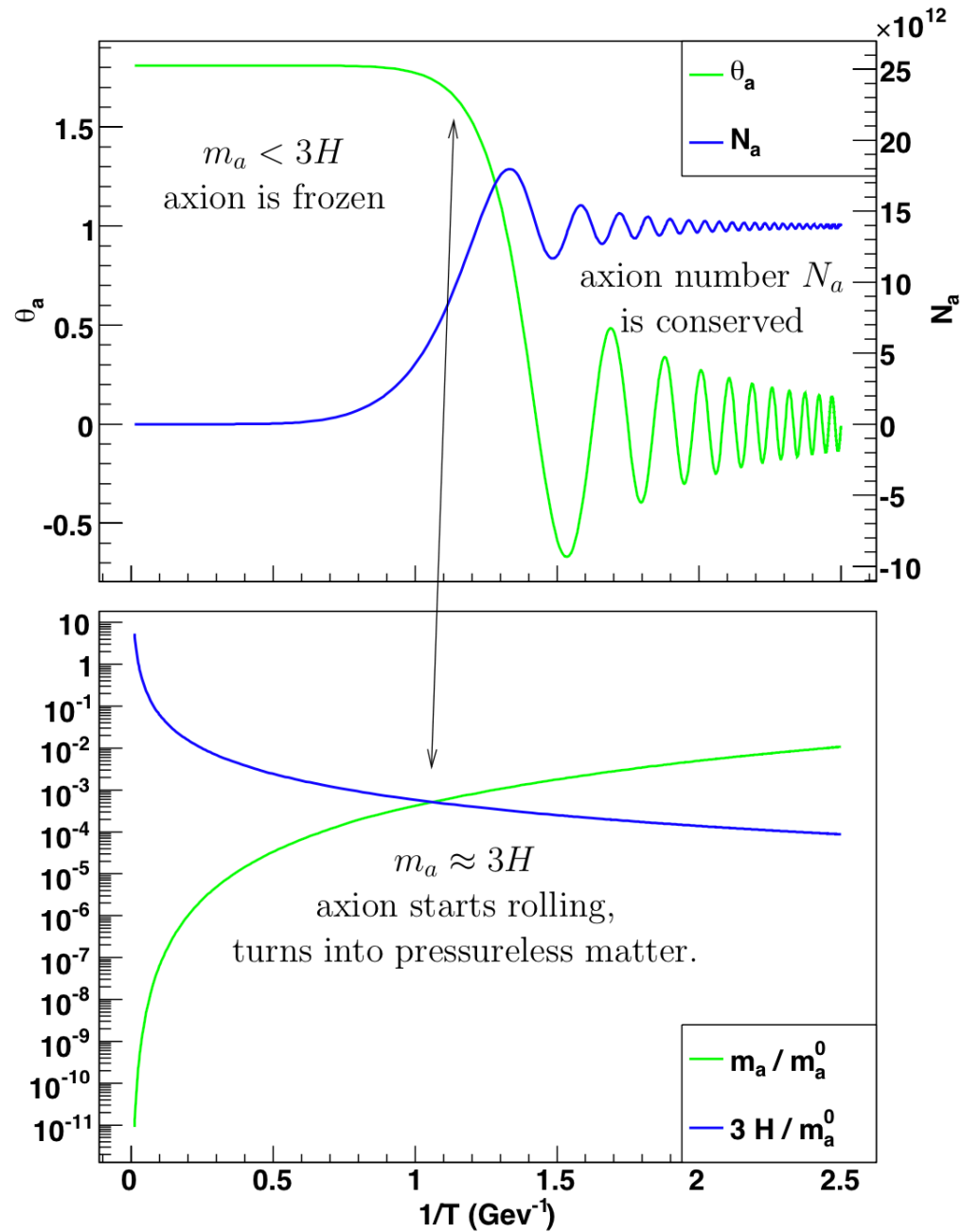
Axions oscillate in their potential  
Bose condensed gas with

$s$  ( $s = \text{entropy}$ ) - - -

$$\rho_a(\text{today}) = \rho_a(T) \frac{m_a(\text{today})}{m_a(T)} \frac{s(\text{today})}{s(T)}$$



Basic work: [Wantz-Shellard 2009](#)



Missing ingredient:  
Exact knowledge of  
 $\chi(T)$

Needed to find freezout  
Conditions

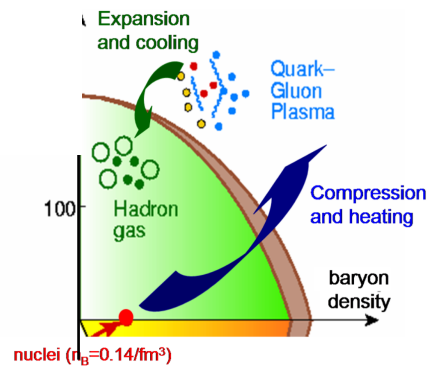
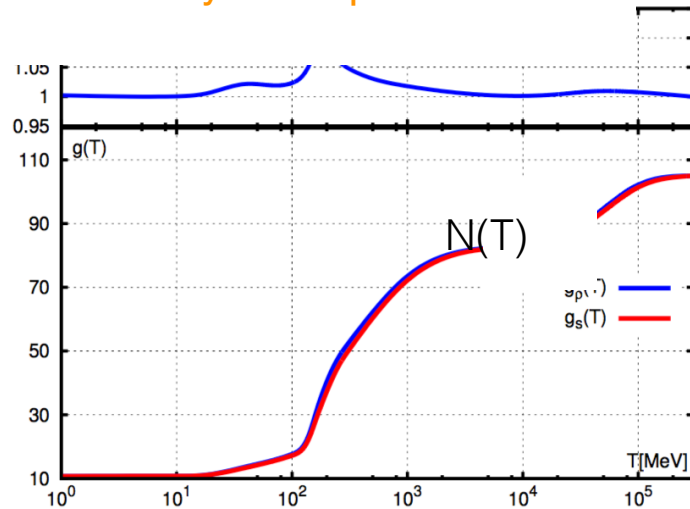
Time from Big Bang

Temperatures

$150 \text{ MeV} < T < 500 \text{ MeV}$

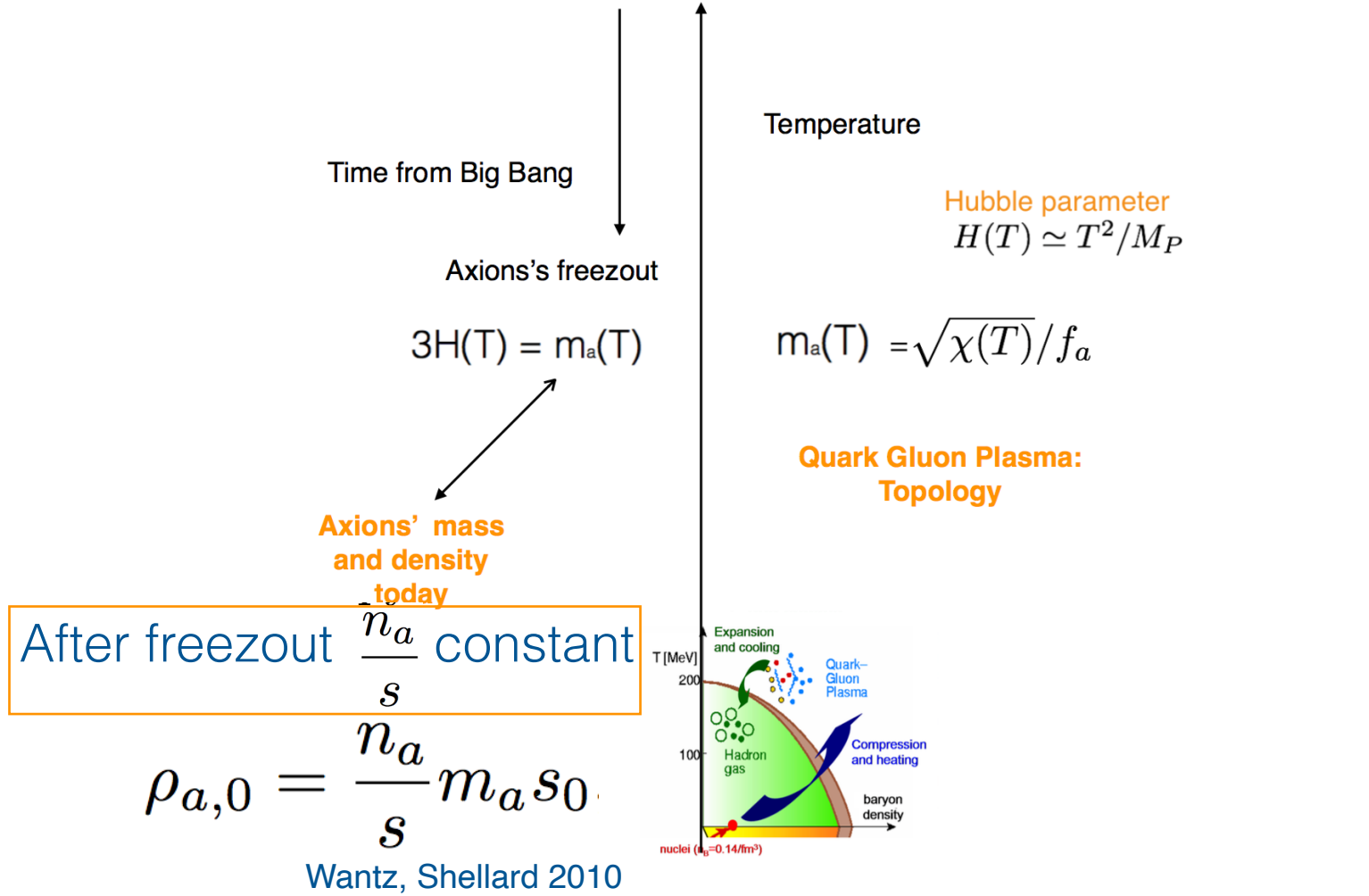
..and beyond

Temperature and Time from BigBang are linked by the Equation of State



$$T_c \text{ Peccei Quinn} \simeq 10^7 - 10^8 \text{ GeV}$$

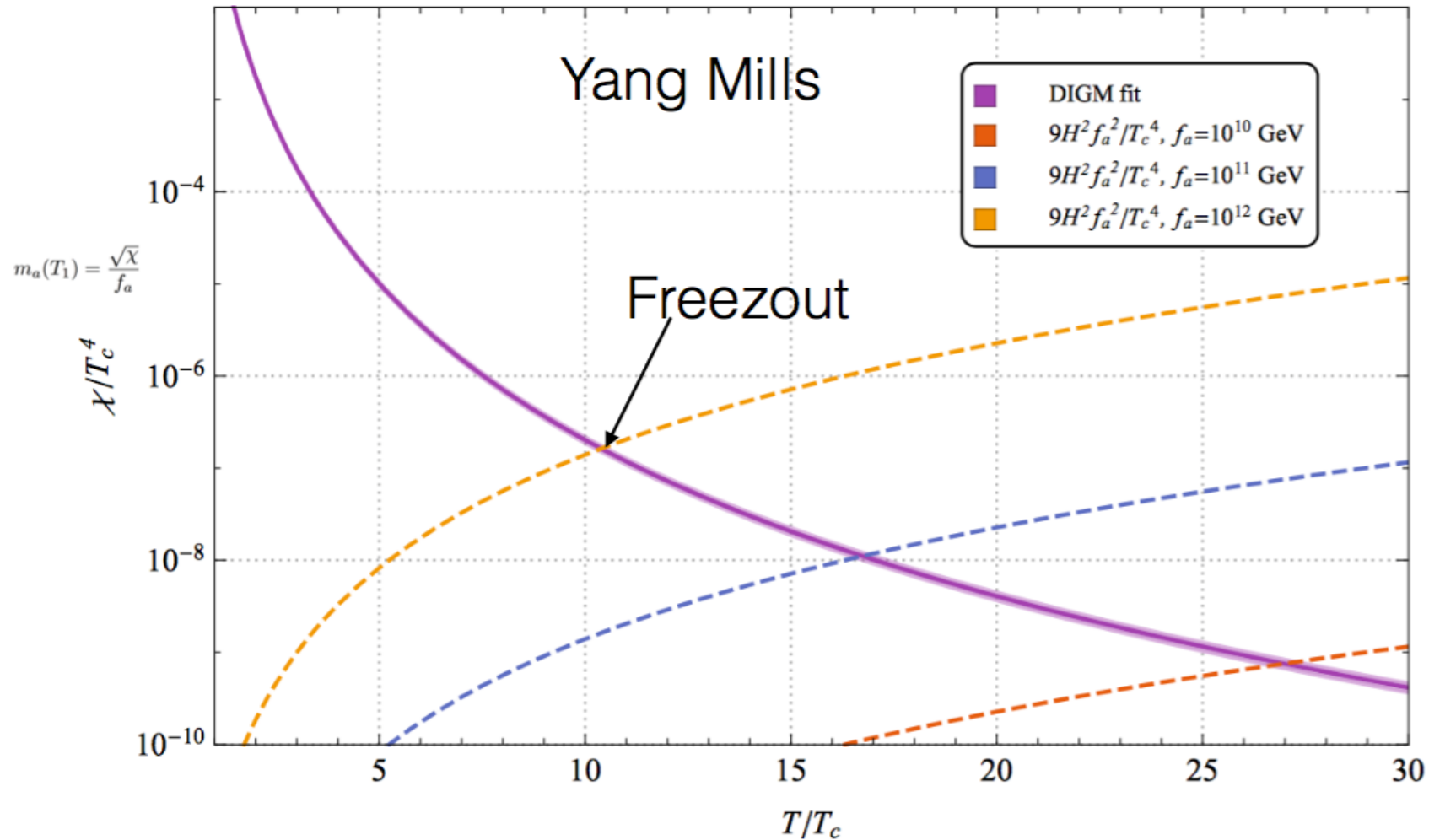
$$T_c \text{ Electroweak} \simeq 160 \text{ GeV (SM)}$$





Axion freezout :  $3H(T) = m_a(T) = \sqrt{\chi(T)}/f_a$

Berkowitz Buchoff Rinaldi 2015



Axion density at freezout controls axion density today

# From exponent $d$ to axion mass in three steps

1.

Time from Big Bang  
 ↓  
 Axions's freezeout  
 $3H(T) = m_a(T)$

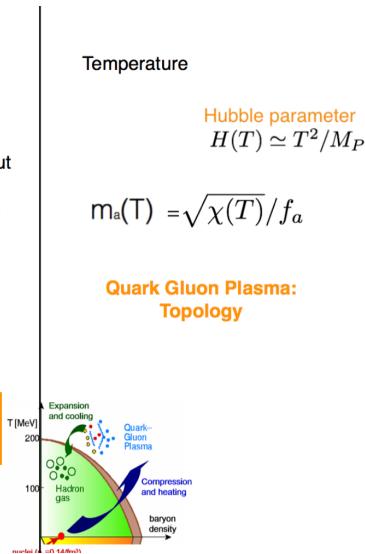
Axions' mass and density today

2.

After freezeout  $\frac{n_a}{s}$  constant

3.

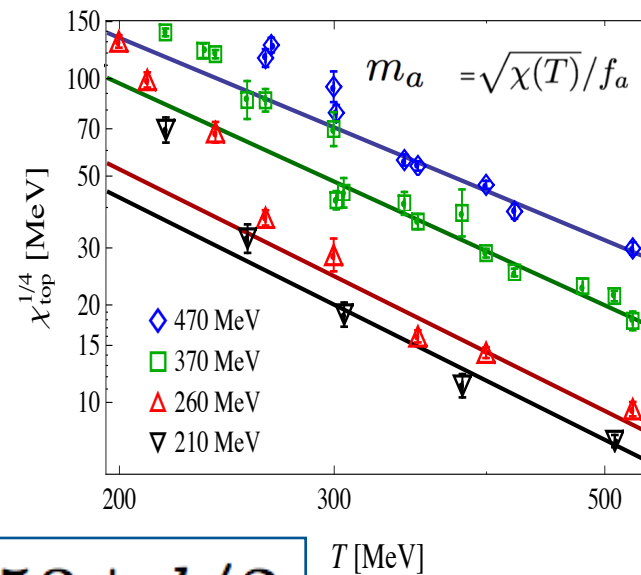
$$\rho_{a,0} = \frac{n_a}{s} m_a s_0$$



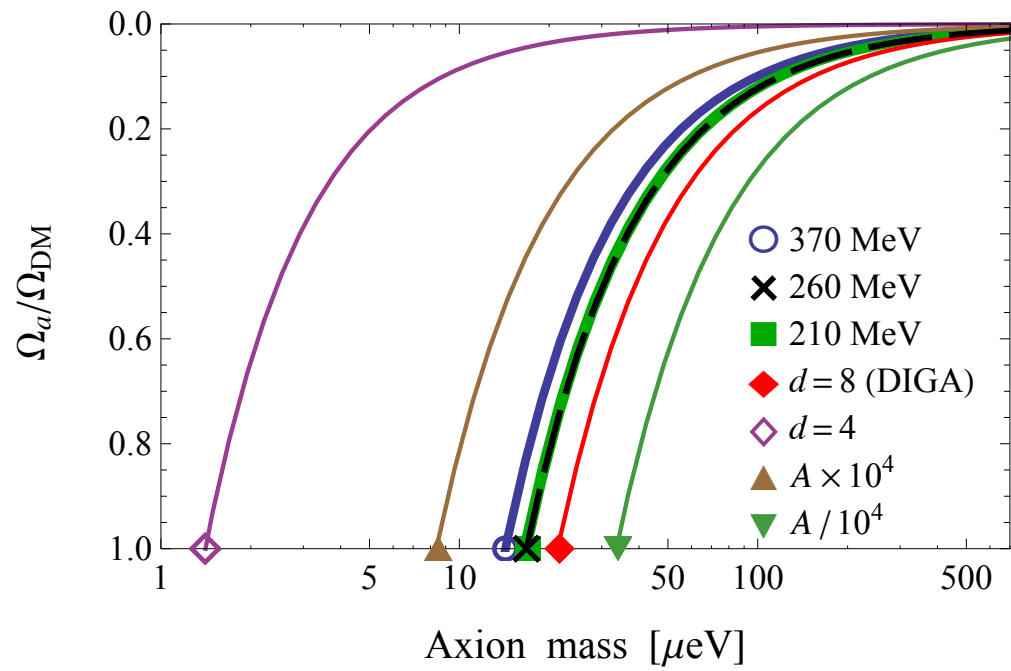
$$\chi_{\text{top}} \simeq A T^{-d}$$

$$d = (6.26, 6.88, 7.52, 7.48)$$

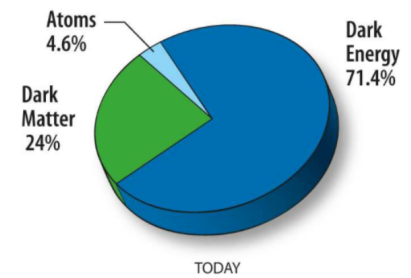
$$m_\pi = (470, 370, 260, 210) \text{ MeV}$$

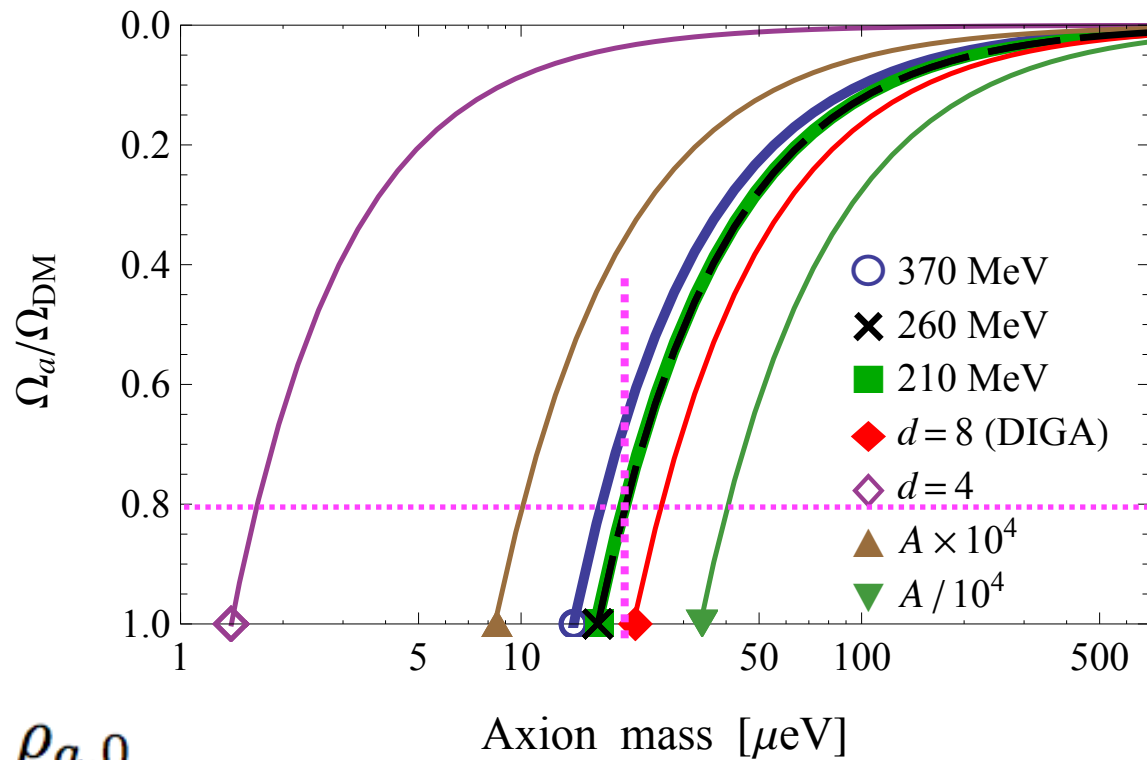


$$\rho_a(m_a) \propto m_a^{-\frac{3.053 + d/2}{2.027 + d/2}}$$



$$\Omega_a = \frac{\rho_{a,0}}{\rho_c};$$



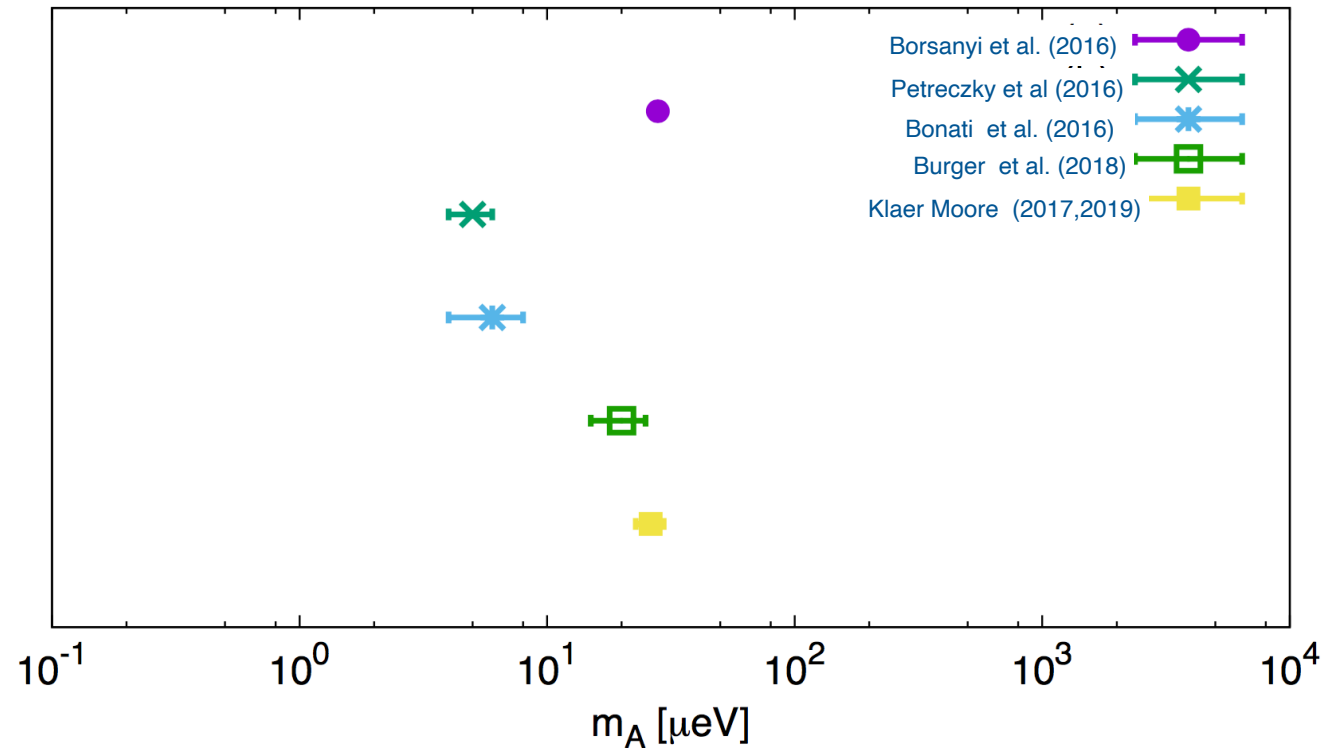


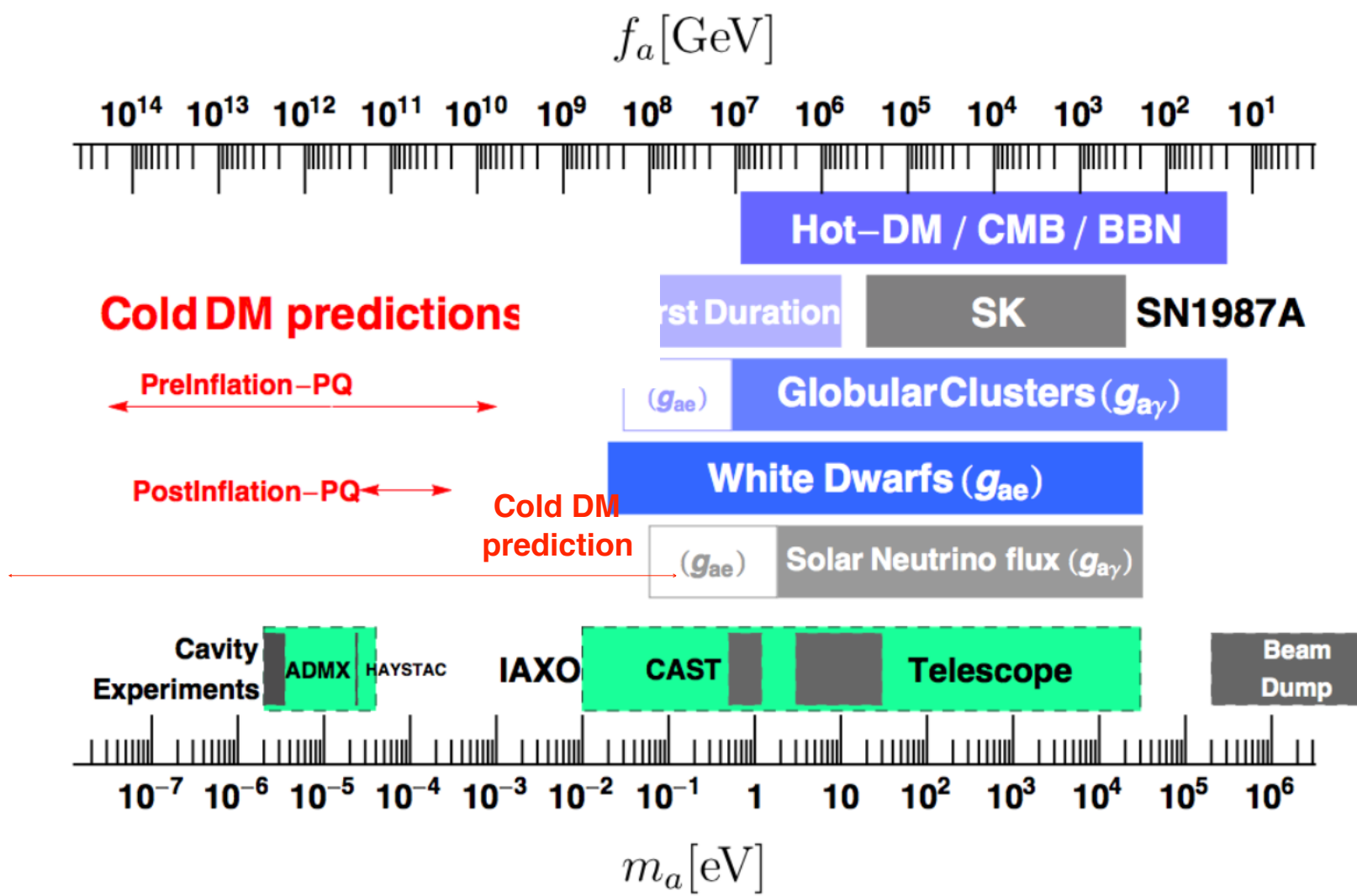
$$\Omega_a = \frac{\rho_{a,0}}{\rho_c};$$

Example: if axions constitute 80% DM,  
our results give a lower bound for the  
axion mass of

$$\simeq 30 \mu\text{eV}$$

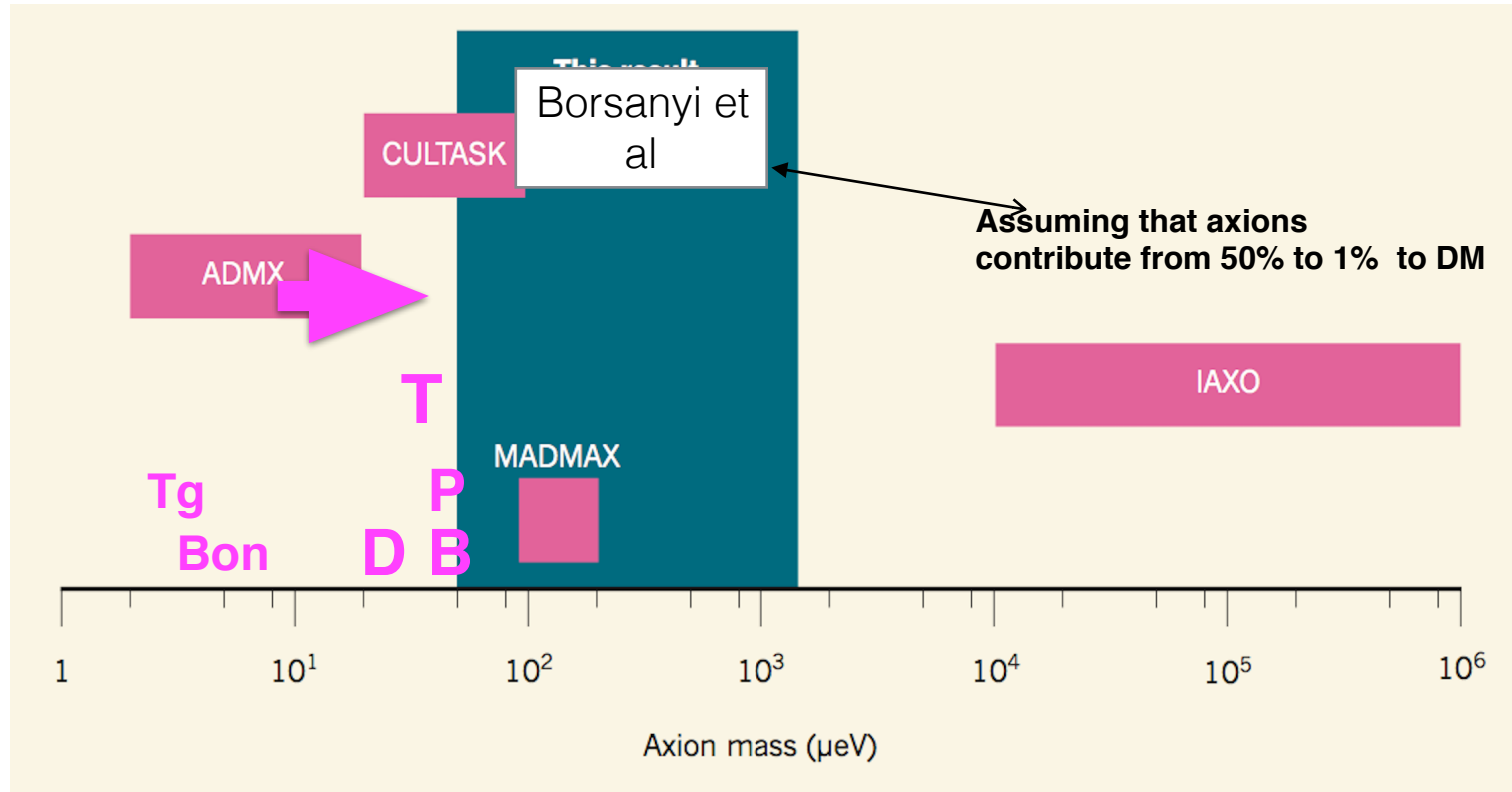
## Lower limits on post-infl. axion mass from lattice QCD





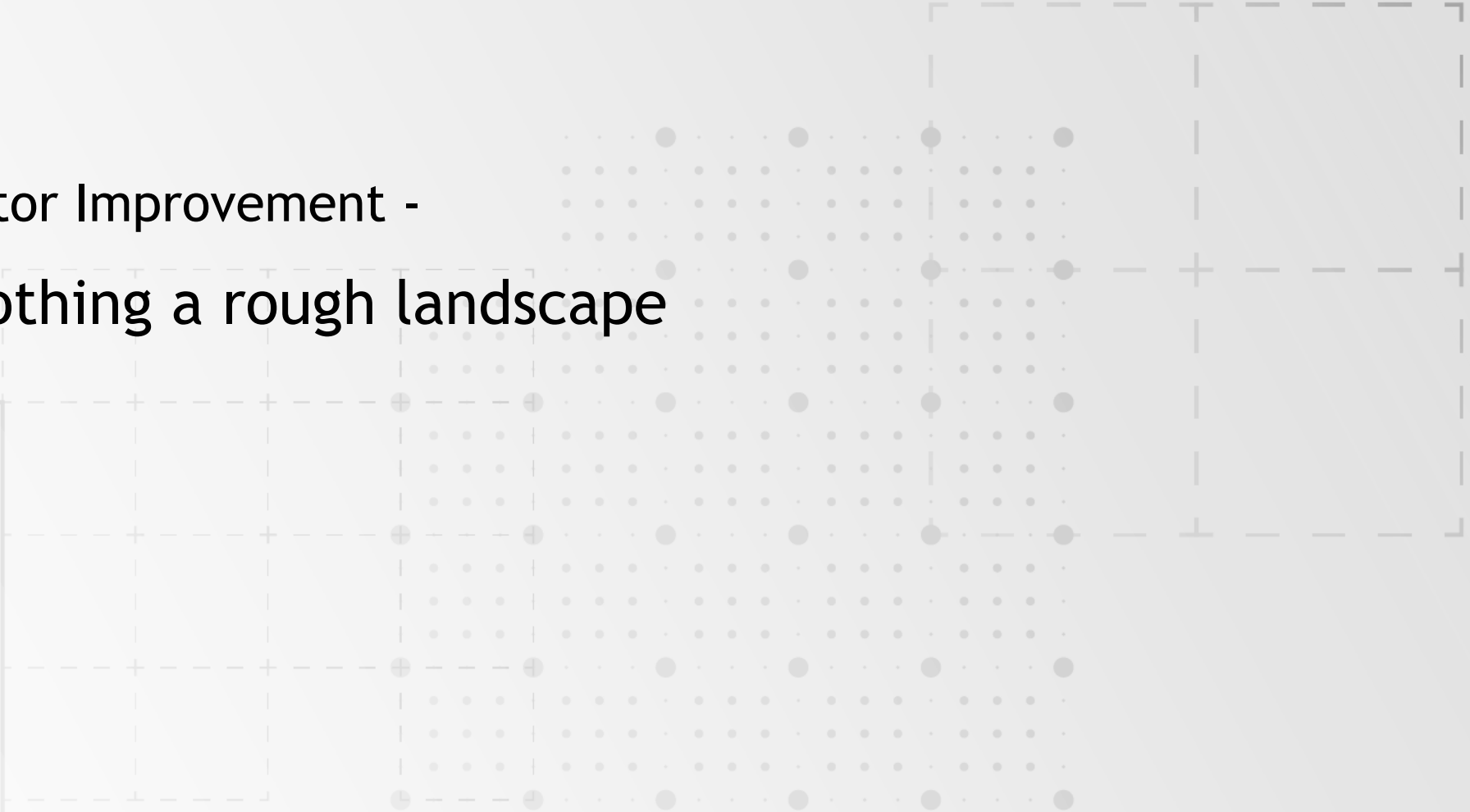
# Lower limits on the axion mass assuming that axions make 100% of DM:

Tg: TWEXT gluonic; Bon: Bonati et al.; D: DIGA, B: Borsanyi et al.,  
P: Petreczky et al., T: TWEXT, fermionic



Operator Improvement -

Smoothing a rough landscape





CERN-PH-TH/2010-143

# Properties and uses of the Wilson flow in lattice QCD

Martin Lüscher

*CERN, Physics Department, 1211 Geneva 23, Switzerland*

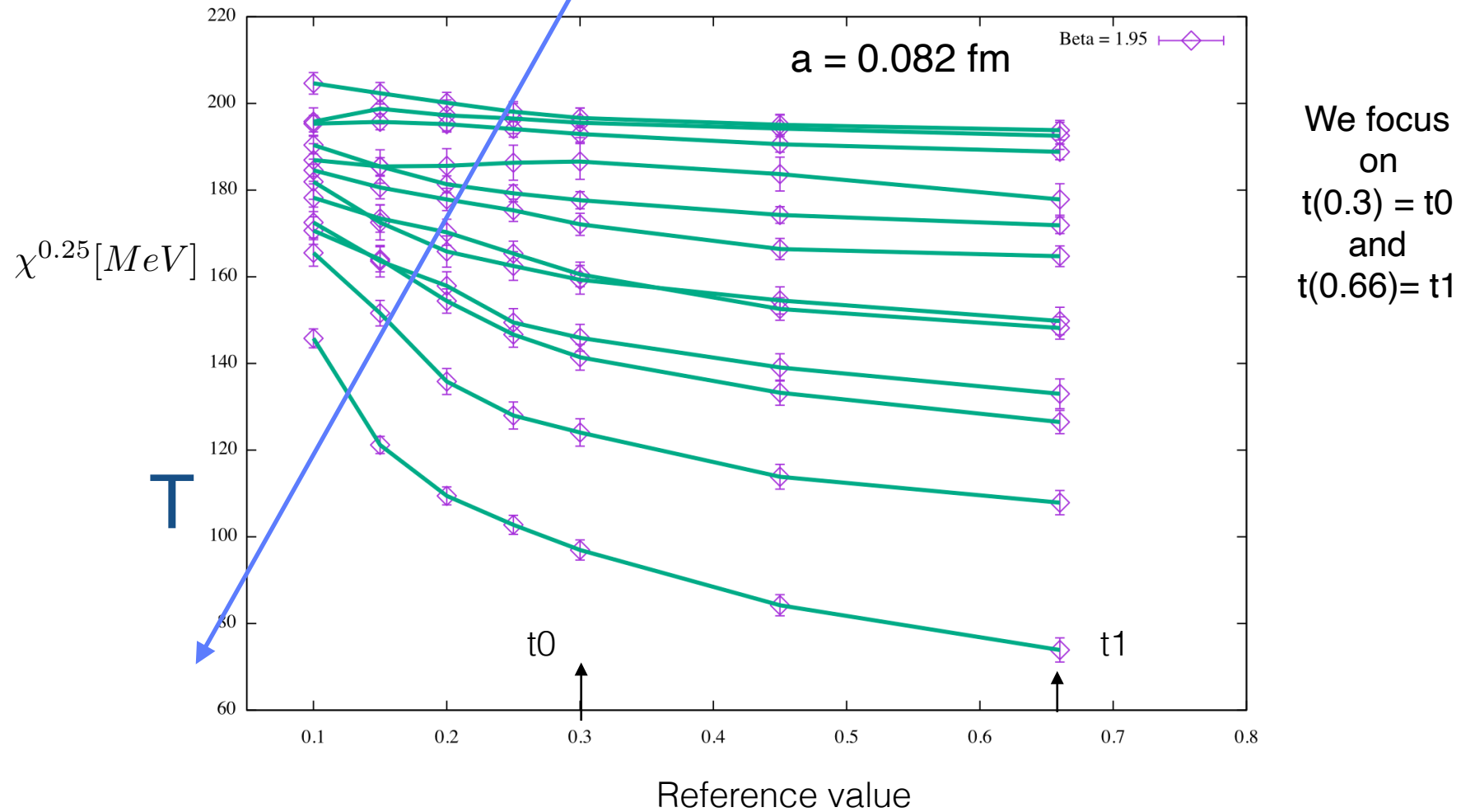
In a nutshell:

Evolves gauge fields towards minimum of the Action in fictitious time  $\tau_F$

Gaussian smearing over sphere with flow radius  $\sqrt{8\tau_F}$

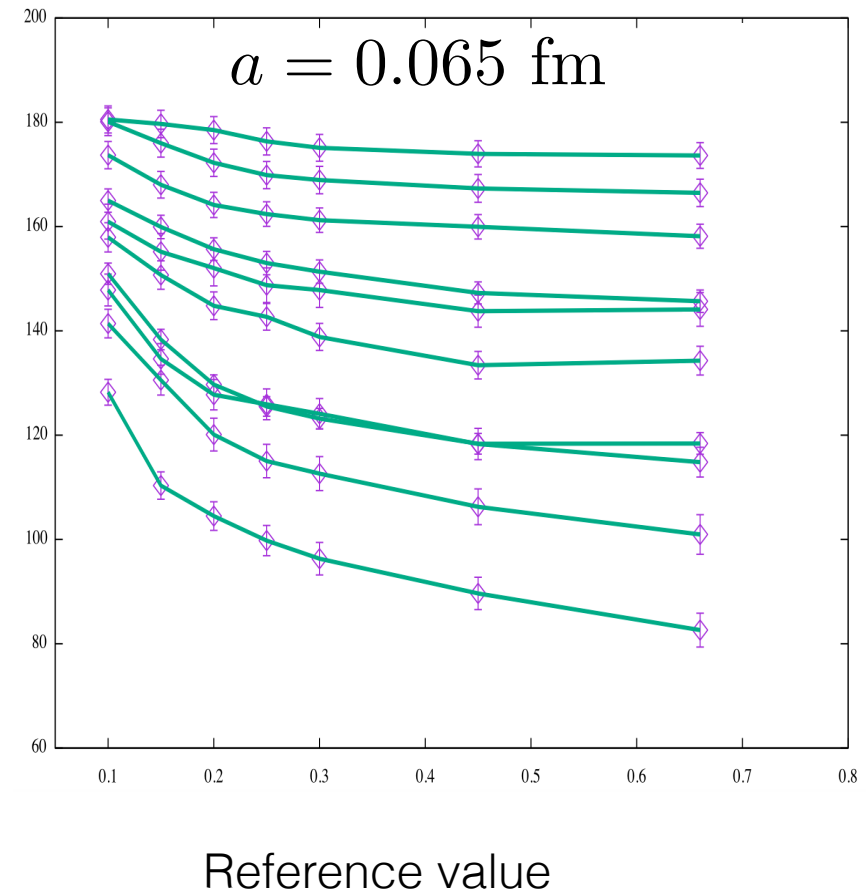
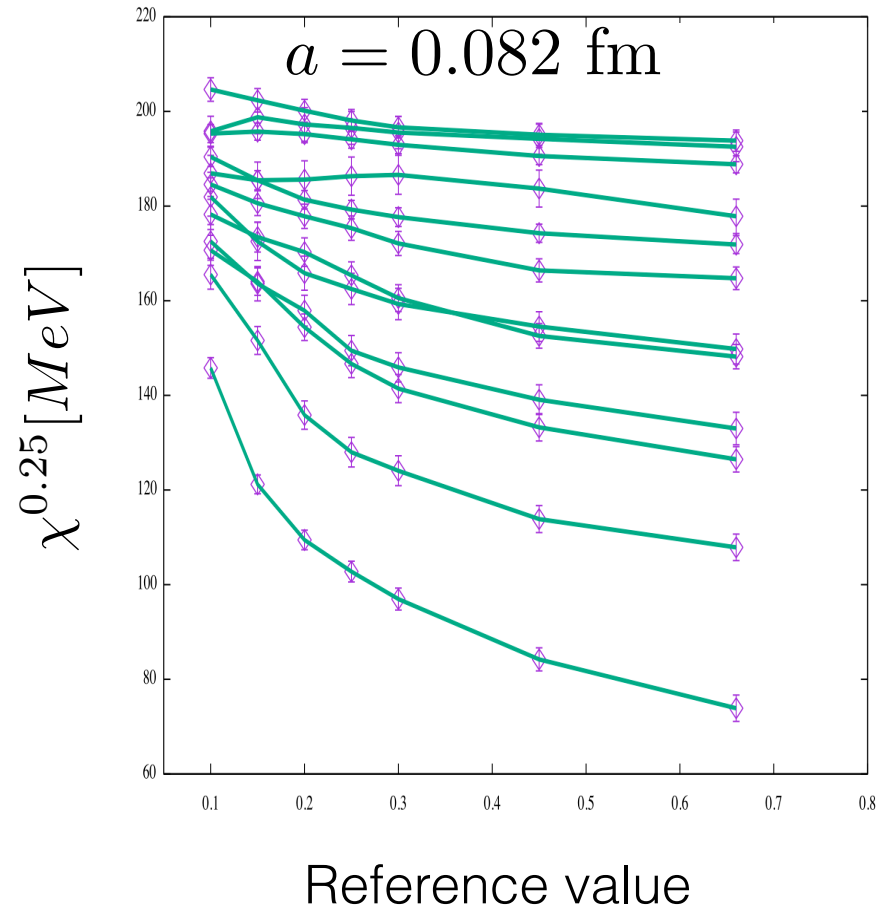
# Flowing towards the plateau

$$t^2 \langle E \rangle |_{t=t_x, x=0-6} = (0.3, 0.66, 0.1, 0.15, 0.2, 0.25, 0.45)$$



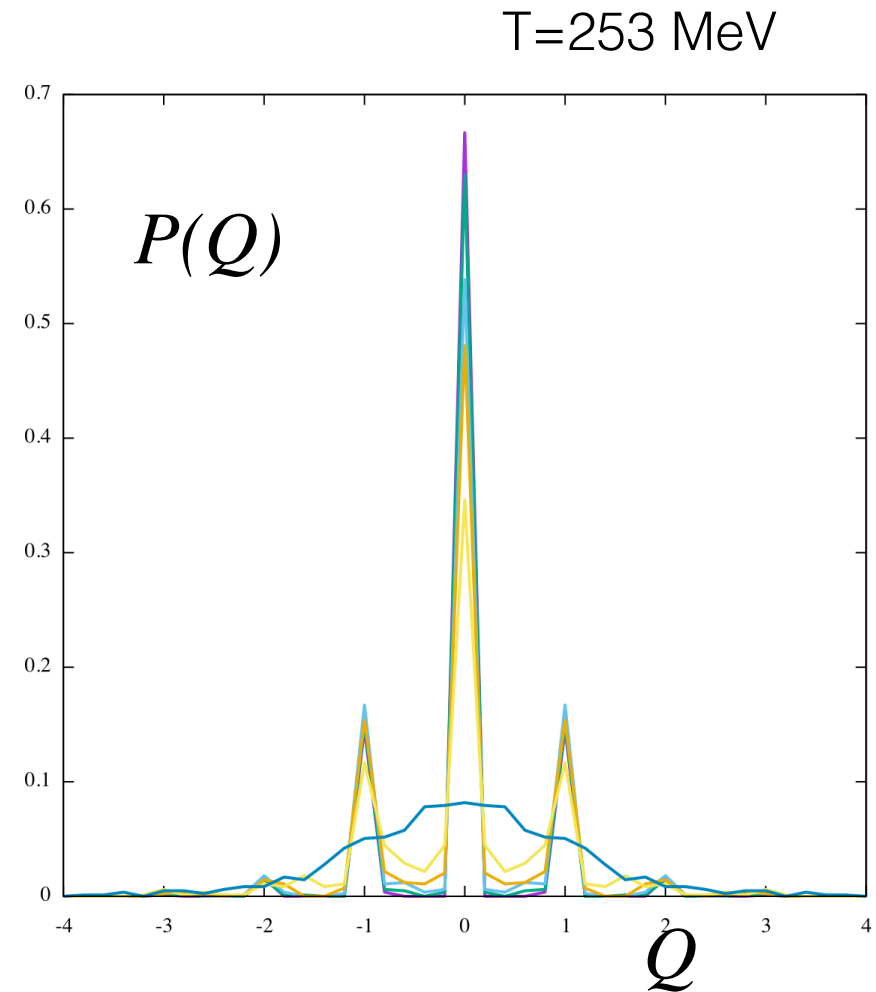
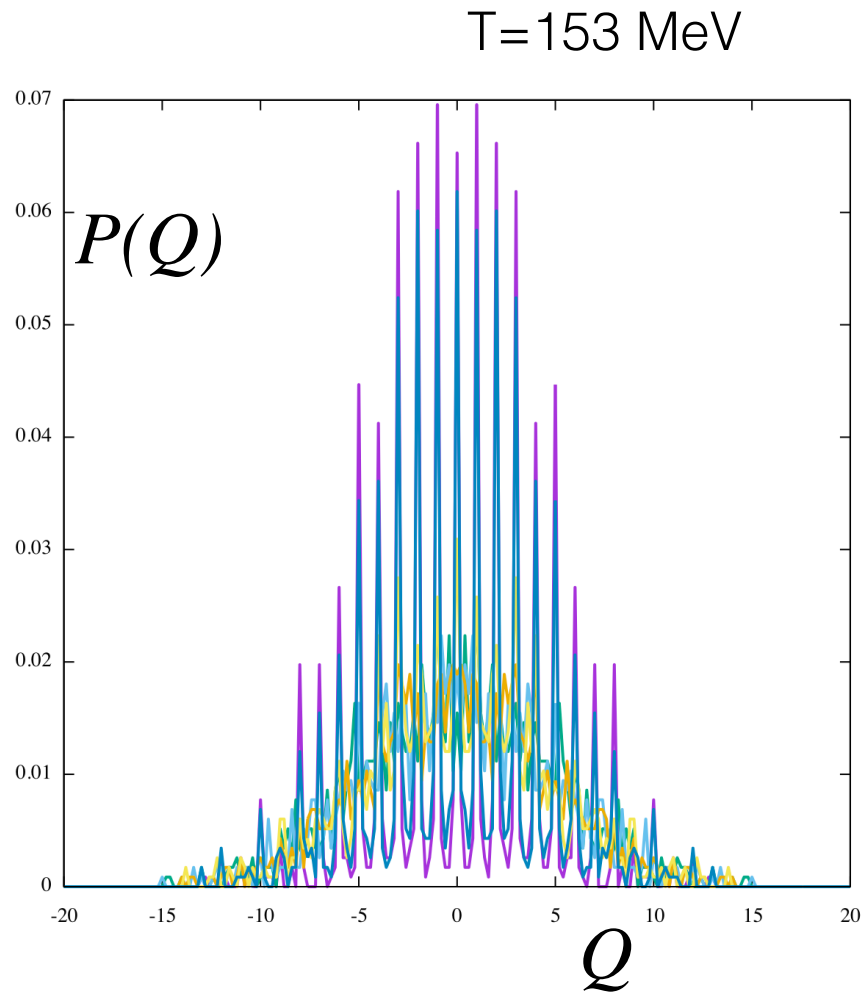
On finer lattices, plateau is almost reached:

Gradient method coincides with cooling



QCD: Distribution of the topological charge  $P(Q)$   
cluster around integers as cooling proceeds

(results for  $a = 0.06$  fm)



# Different smoothing methods

## Properties and uses of the Wilson flow in lattice QCD

PROCEEDINGS  
OF SCIENCE

Martin Lüscher

*CERN, Physics Department, 1211 Geneva 23, Switzerland*

### Comparison of the gradient flow with cooling in $SU(3)$ pure gauge theory

Claudio Bonati\* and Massimo D'Elia†

*Dipartimento di Fisica dell'Università di Pisa and INFN - Sezione di Pisa,  
Largo Pontecorvo 3, I-56127 Pisa, Italy*

The gradient (Wilson) flow has been introduced recently in order to provide a solid theoretical framework for the smoothing of ultraviolet noise in lattice gauge configurations. It is interesting to ask how it compares with other, more heuristic and numerically cheaper smoothing techniques, such as standard cooling. In this study we perform such a comparison, focusing on observables related to topology. We show that, already for moderately small lattice spacings, standard cooling and the gradient flow lead to equivalent results, both for average quantities and configuration by configuration.

### The topological susceptibility of the pure $SU(3)$ Yang–Mills vacuum on the lattice ☆

M. Campostrini, A. Di Giacomo, Y. Gündüç<sup>1,2</sup>, M.P. Lombardo,  
H. Panagopoulos and R. Tripiccion

*INFN, Sezione di Pisa and Dipartimento di Fisica dell'Università, I-56100 Pisa, Italy*

Received 2 August 1990

Using a “field theoretic” approach, we compute the topological susceptibility  $\chi$  of the pure gauge  $SU(3)$  theory on the lattice. We also apply an algorithm of gradual cooling, and use these two approaches as a cross-check on each other. The final value we find for  $\chi$  confirms results found earlier using an abrupt-cooling algorithm.

### String tension from smearing and Wilson flow methods

**Antonio González-Arroyo<sup>ab</sup>**

*<sup>a</sup>Instituto de Física Teórica UAM/CSIC, C/ Nicolás Cabrera 13-15  
Universidad Autónoma de Madrid, E-28048–Madrid, Spain*

*<sup>b</sup>Departamento de Física Teórica, C-15*

*Universidad Autónoma de Madrid, E-28049–Madrid, Spain*

*E-mail: antonio.gonzalez-arroyo@uam.es*

**Masanori Okawa<sup>\*c</sup>**

*<sup>c</sup>Graduate School of Science, Hiroshima University*

*Higashi-Hiroshima, Hiroshima 739-8526, Japan*

*E-mail: okawa@sci.hiroshima-u.ac.jp*

Recently, we proposed a new method to extract the string tension from 4-dimensionally smeared Wilson loops. In this talk, we first show that the results obtained using this smearing method are identical to those obtained by Wilson flow, once the time step is sufficiently small. We then demonstrate the practical advantage of our method by applying it to the calculation of string tension in  $SU(3)$  Yang-Mills theory.

## Smearing

Build a sequence of operators

$$\varphi^{(s)}(n) \rightarrow \varphi^{(s+1)}(n) = \varphi^{(s)}(n) + \epsilon \sum' \varphi^{(s)}(n')$$

Evolution in 'smearing time'  $\tau = s\epsilon$

$$\partial\varphi/\partial\tau = \nabla^2\varphi$$

In momentum space :

$$\exp(-Wk^2) \approx (W + \tau)^{-5/2}$$

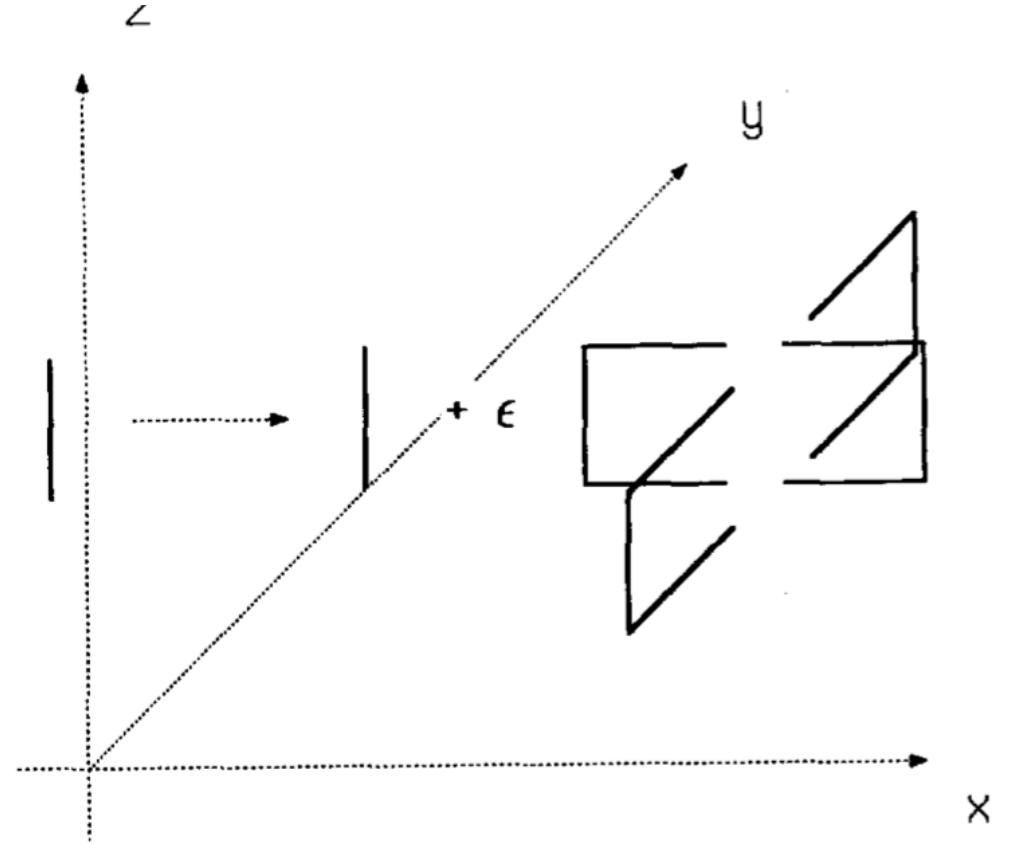


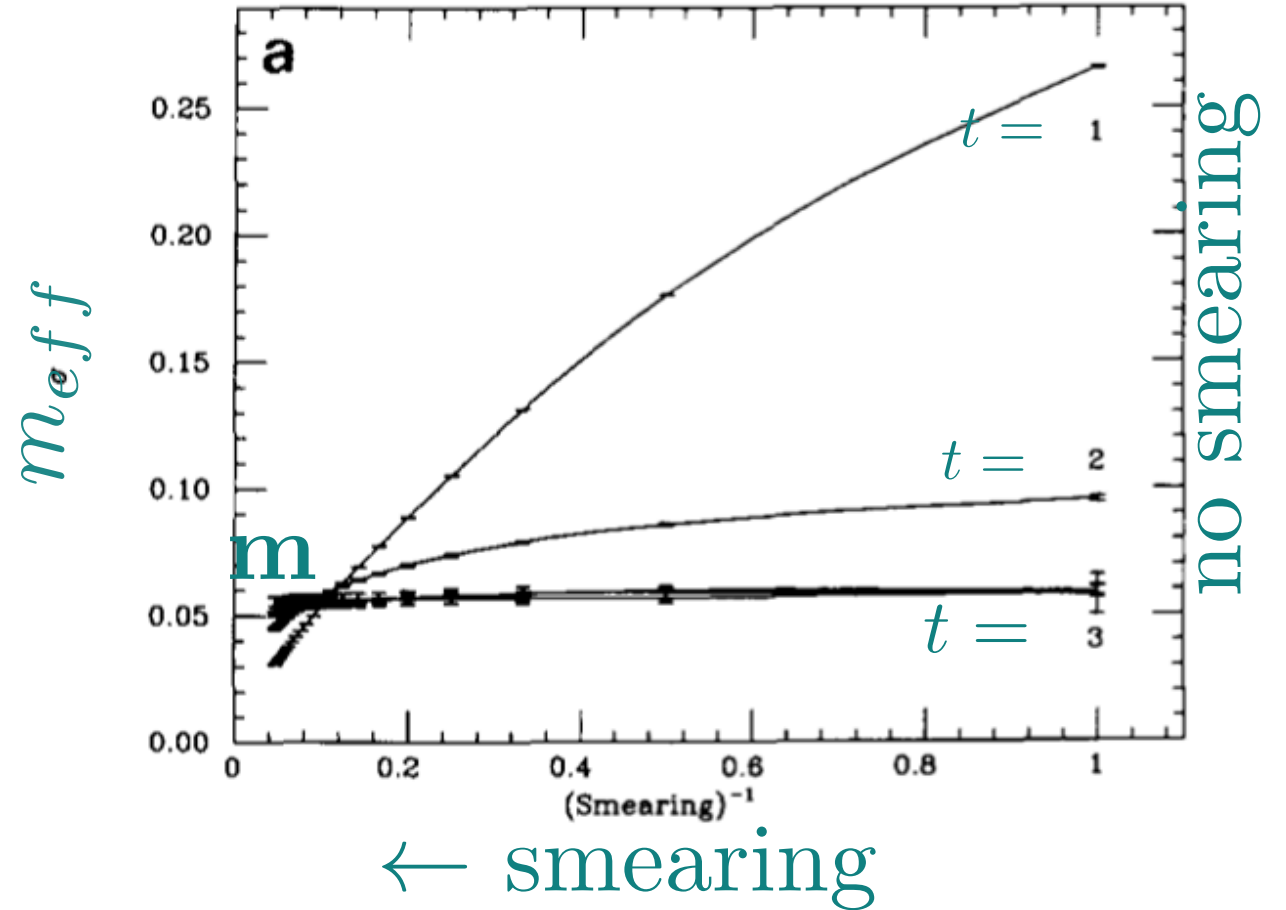
Fig. 1. The smearing procedure. We substitute a link with itself plus  $\epsilon$  times the sum of the incomplete neighboring space like

# Smearing at work

$$G(t)_{t \rightarrow \infty} \rightarrow e^{-\mathbf{m}t}$$

Define

$$m_{eff}(t) \equiv - \frac{d \ln G(t)}{dt}$$
$$m_{eff}(t)_{t \rightarrow \infty} \rightarrow \mathbf{m}$$



# Glueball masses

$$G(t) \equiv \langle O(t) \cdot O(0) \rangle - \langle O(t) \rangle \cdot \langle O(0) \rangle$$

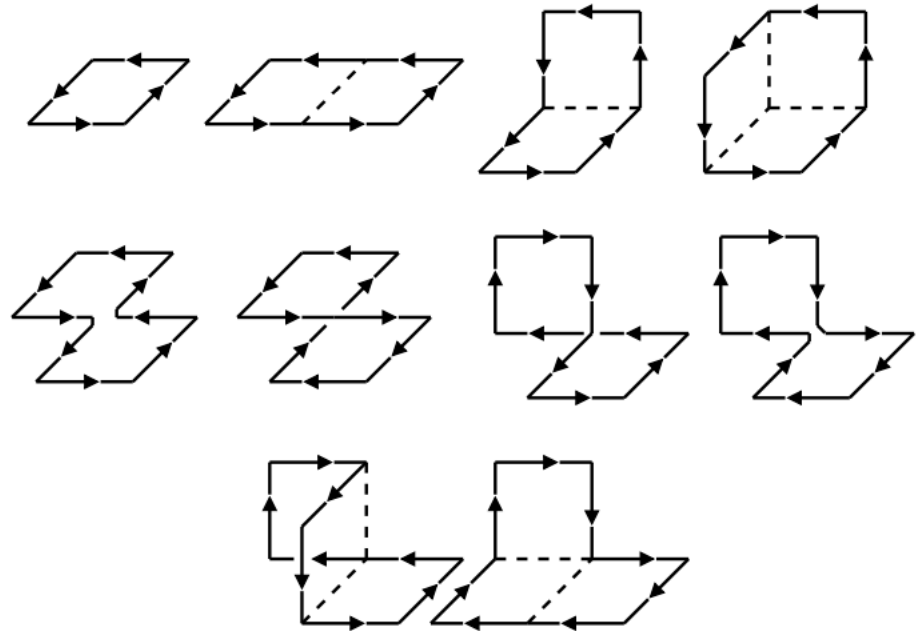
$\approx \exp(-mt)$  , Note:  $t$  Euclidean time!

$$G(t) = \int \delta(M - \omega) e^{-\omega t} \propto e^{-Mt}$$

Smearing

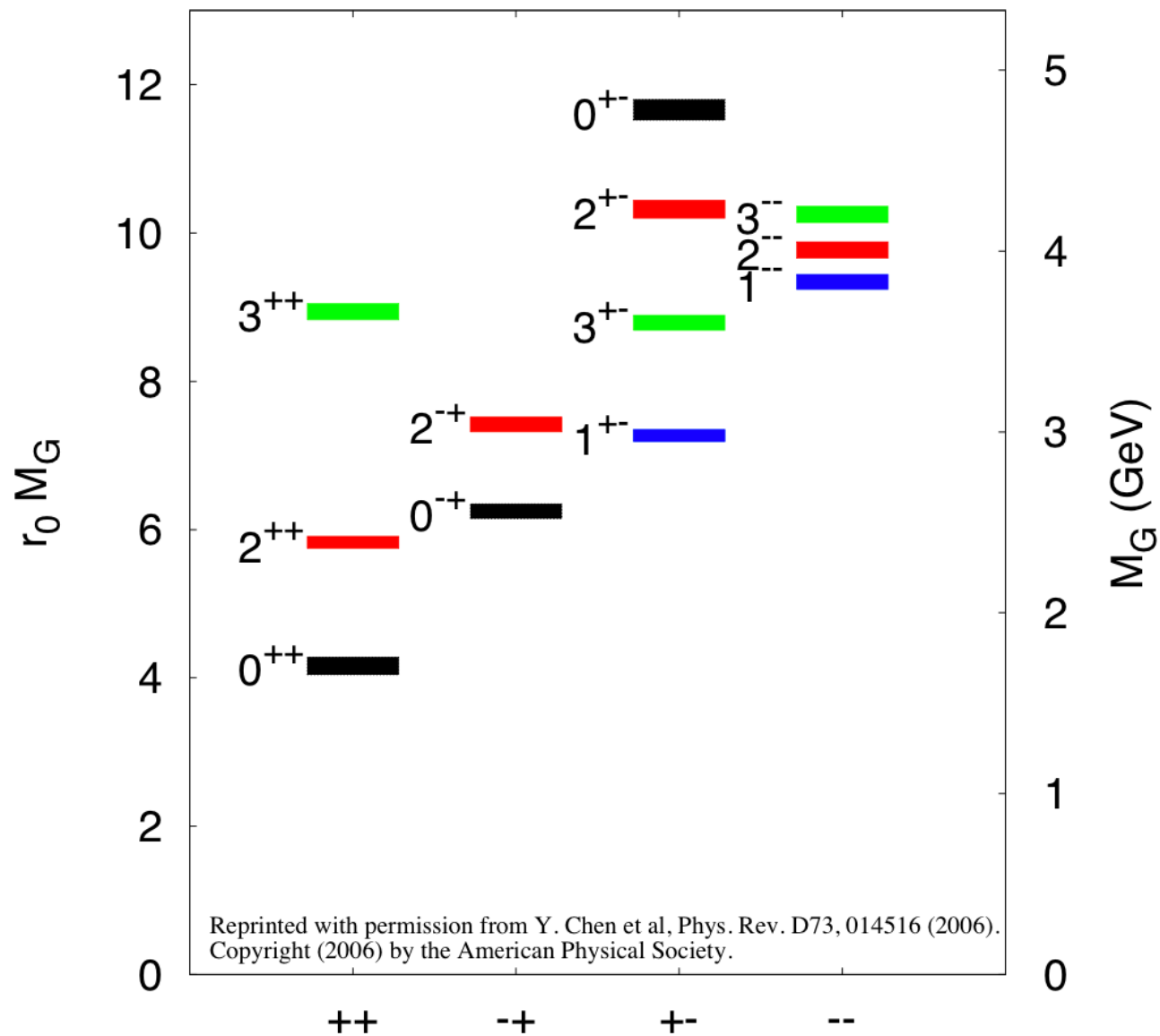
$$G_0^{(s)}(t) \equiv O^{(s)}(x,y) + O^{(s)}(y,z) + O^{(s)}(x,z) \quad 0^{++}$$

$$G_2^{(s)}(t) \equiv -2O^{(s)}(x,y) + O^{(s)}(y,z) + O^{(s)}(x,z) \quad 2^{++}$$

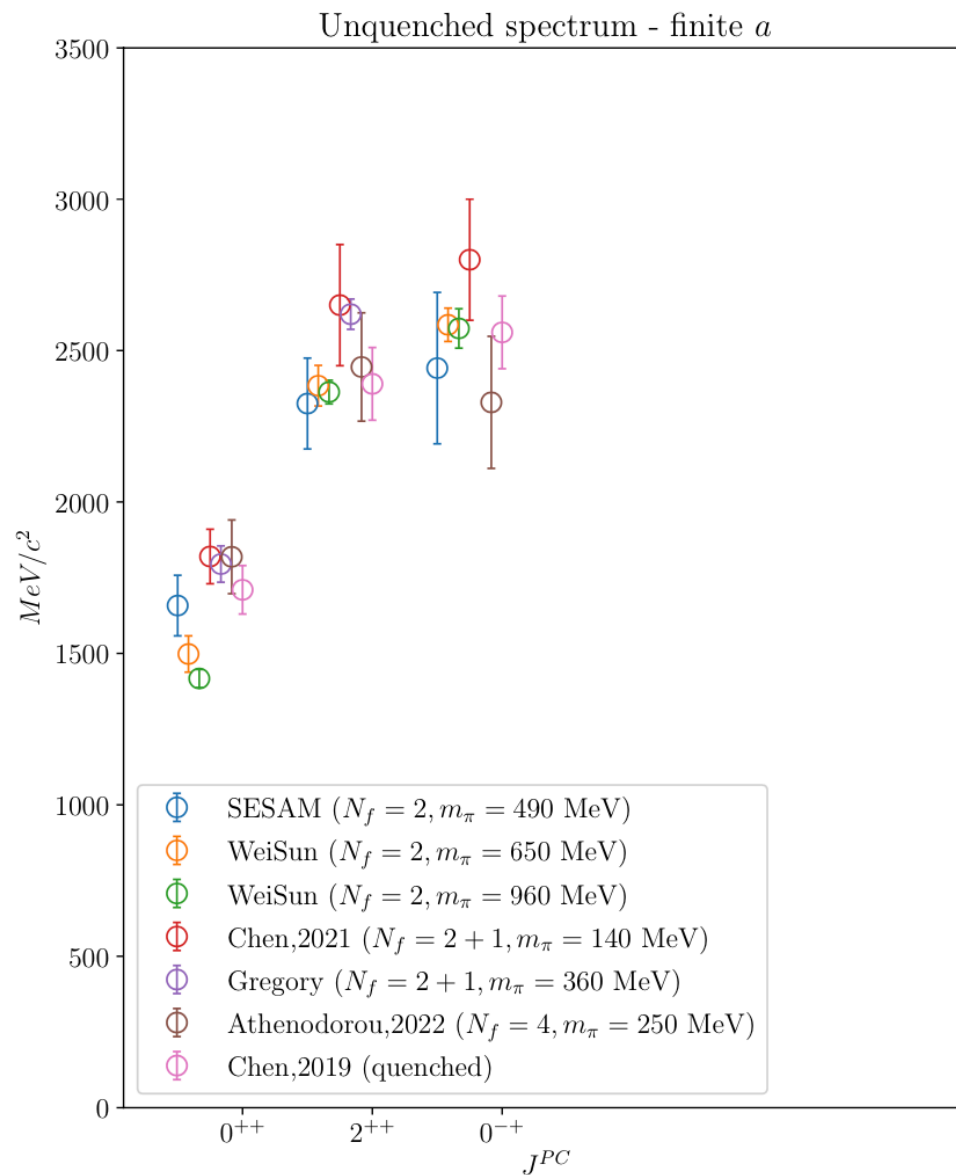


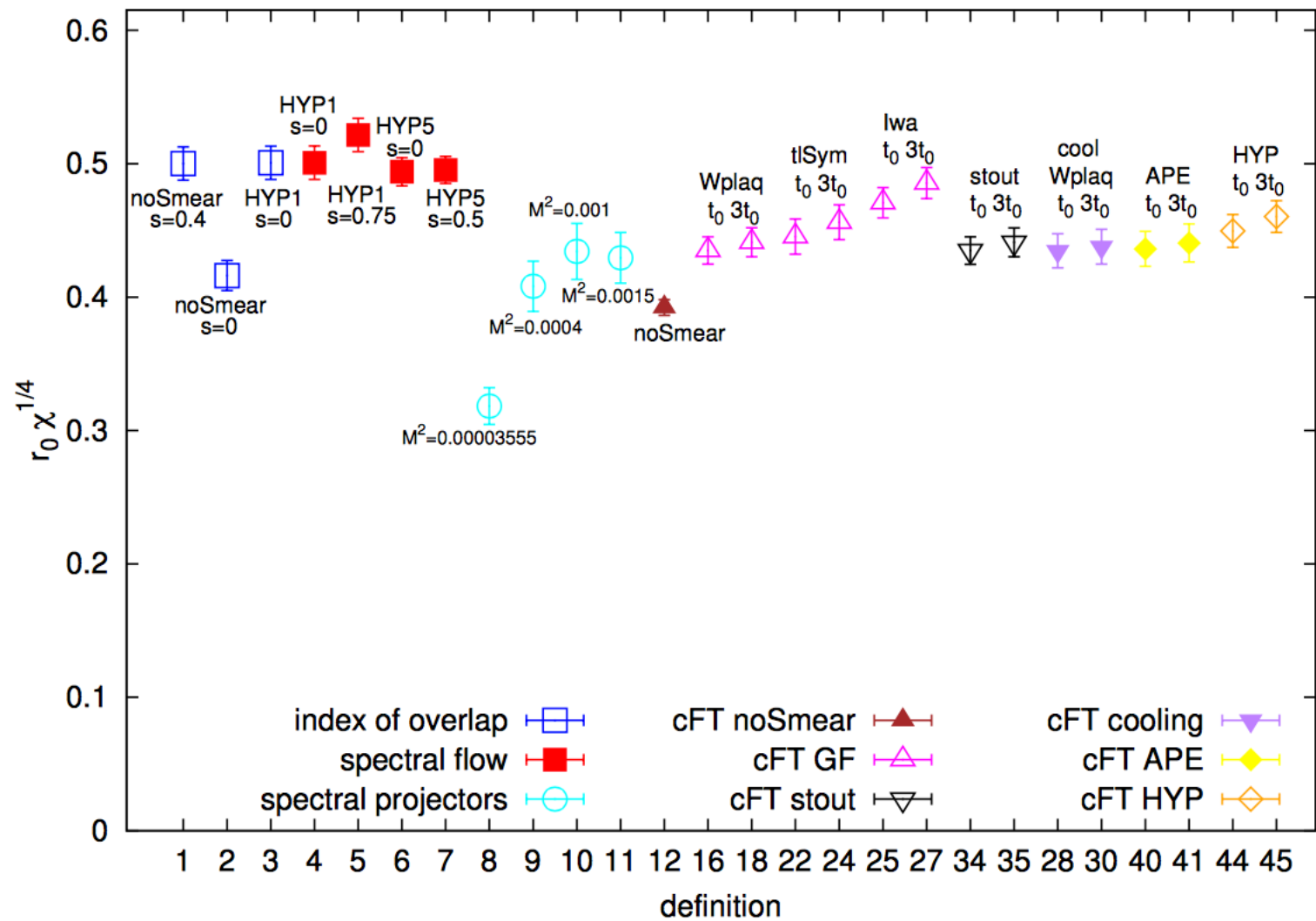


2006 data, From PDG 2022

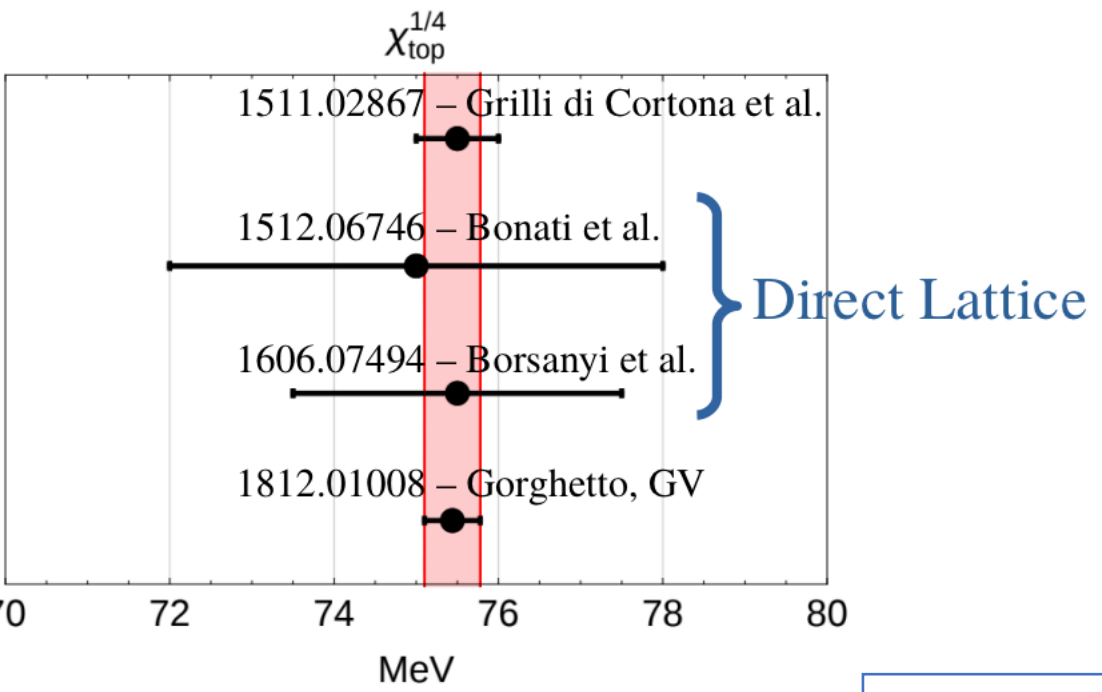


2022 compilation, Vadamchino@lat22

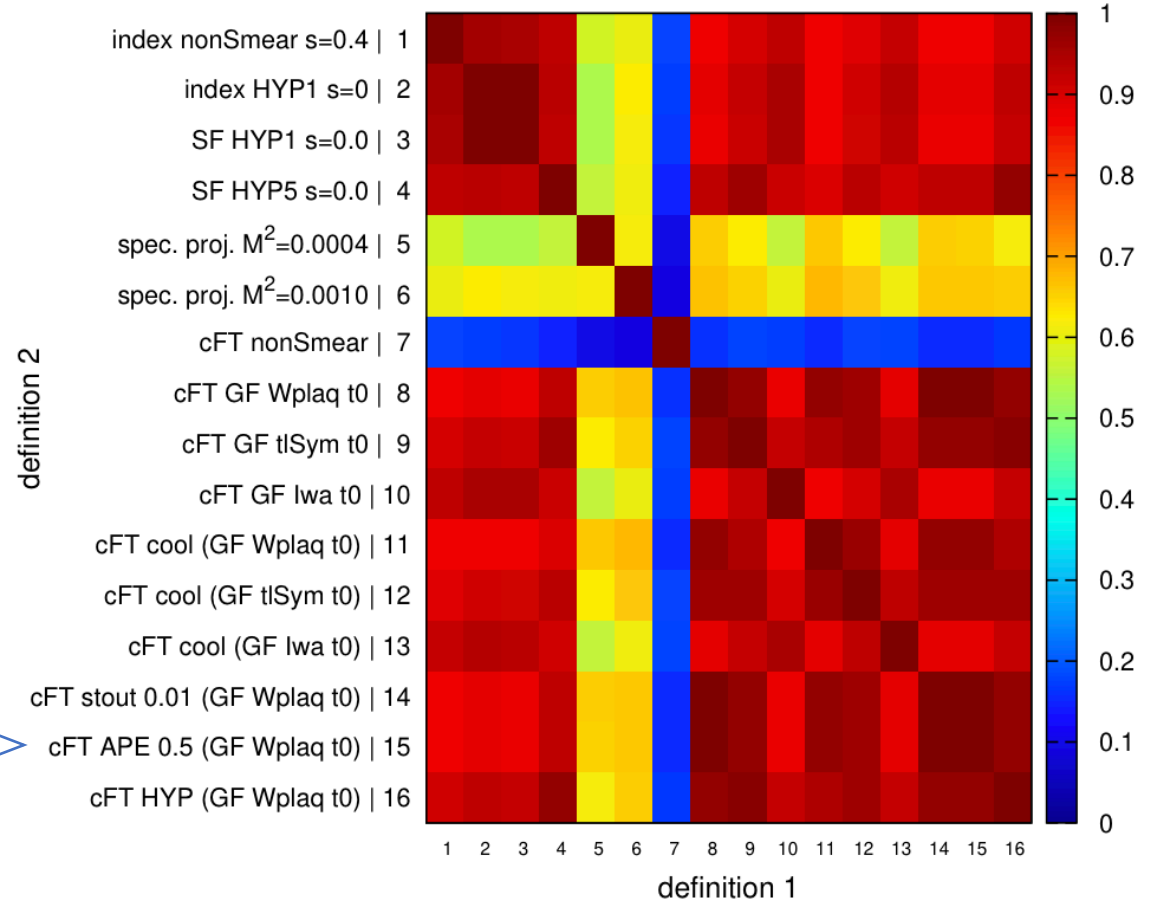
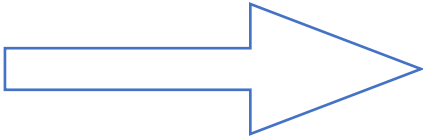




Many varieties of methods and smearing/smoothing/flowing/cooling.. good agreement at T=0



Plot by G. Villadoro



ETMC collaboration, 2017

Rather than a summary:

More on Euclidean formulation

Light quarks - chiral symmetry (and confinement)

Theta term, strong CP problem, topology, axion (brief recap)

Topology

Heavy quarks

Lattice QCD and axion cosmology