The Phase Diagram of Strong Interactions from Lattice QCD Simulations

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A full comprehension of strong interactions represents a long standing issue. Perturbative QCD works well at high energies (asymptotic freedom), while the low energy regime is non-perturbative.

Various analytic approaches try to attack the problem

One possibility is to compute the theory numerically: Lattice QCD simulations

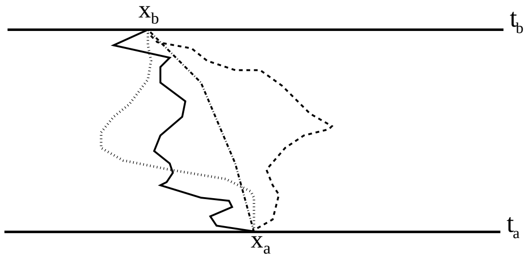
What I would like to do in my talk:

- Discuss the computational difficulty of such a task and its feasibility today

- Discuss a couple of issues where standard computations meet difficulties or fail:
  - The QCD phase diagram at finite T and baryon density
  - The study of topological properties in the high T phase and its connection to axion phenomenology

LATTICE QCD IN BRIEF

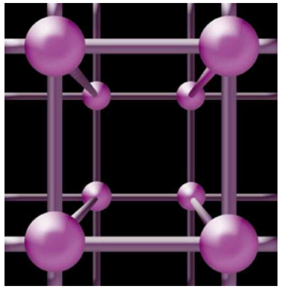
The starting point is the path-integral approach to Quantum Mechanics and Quantum Field Theory, opened by R. Feynman in 1948.



$$\longrightarrow \langle 0|O|0\rangle \Rightarrow \int \mathcal{D}\varphi e^{-S[\varphi]} O[\varphi]$$

The QCD path integral is discretized on a finite space-time lattice

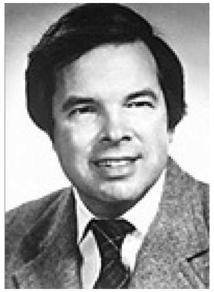
$\Longrightarrow$ **finite number of integration variables**

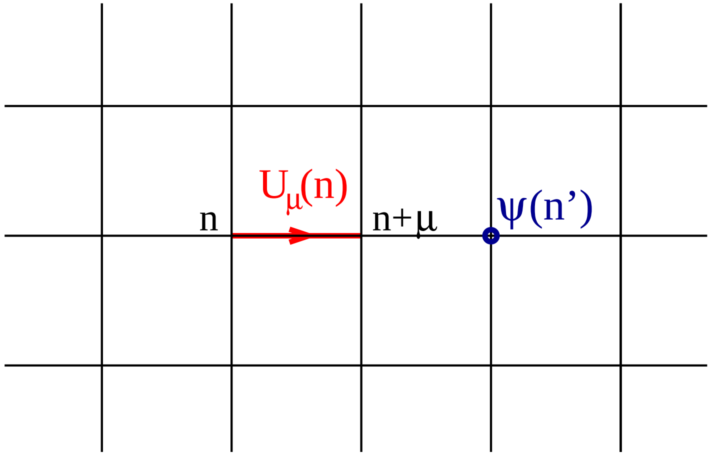


The path-integral is then computed by Monte-Carlo algorithms which sample field configurations proportionally to $e^{-S[U]}$

$$\langle O\rangle = \frac{1}{Z}\int \mathcal{D}U e^{-S[U]} O[U] \quad \simeq \quad \bar{O} = \frac{1}{M}\sum_{i=1}^{M} O[U^{\{i\}}]$$

An elegant gauge invariant regularization is given in terms of elementary parallel transports: non-Abelian phases picked up by quarks moving from one lattice site to the other (K. G. Wilson 1974)





Gauge fields are 3×3 unitary complex matrixes living on lattice links (link variables)

$$U_\mu(n) \simeq \mathcal{P}\exp\left(ig\int_n^{n+\mu} A_\mu dx_\mu\right)$$

Fermion fields are Grassman variable living on lattice sites. Best way to deal with them is to integrate them out.

$\int d^4x G^a_{\mu\nu} G^{\mu\nu}_a \Rightarrow S_G$ $\int d^4x \bar\psi^f_i \left(D^\mu_{ij}\gamma^E_\mu + m_f\delta_{ij}\right)\psi^f_j \Rightarrow S_F = \bar\psi_n M[U]_{n,m}\psi_m$

$$Z = \int \mathcal{D}U\mathcal{D}\psi\mathcal{D}\bar\psi e^{-(S_G[U]+\bar\psi M[U]\psi)} = \int \mathcal{D}U e^{-S_G[U]}\det M[U]$$

- **As long as $\mathcal{D}U e^{-S_G}\det M[U]$ is positive, a probabilistic interpretation is viable**
- **Sampling $\det M$ is the most challenging part. Numerically inconceivable in 1974**

Sampling strategy

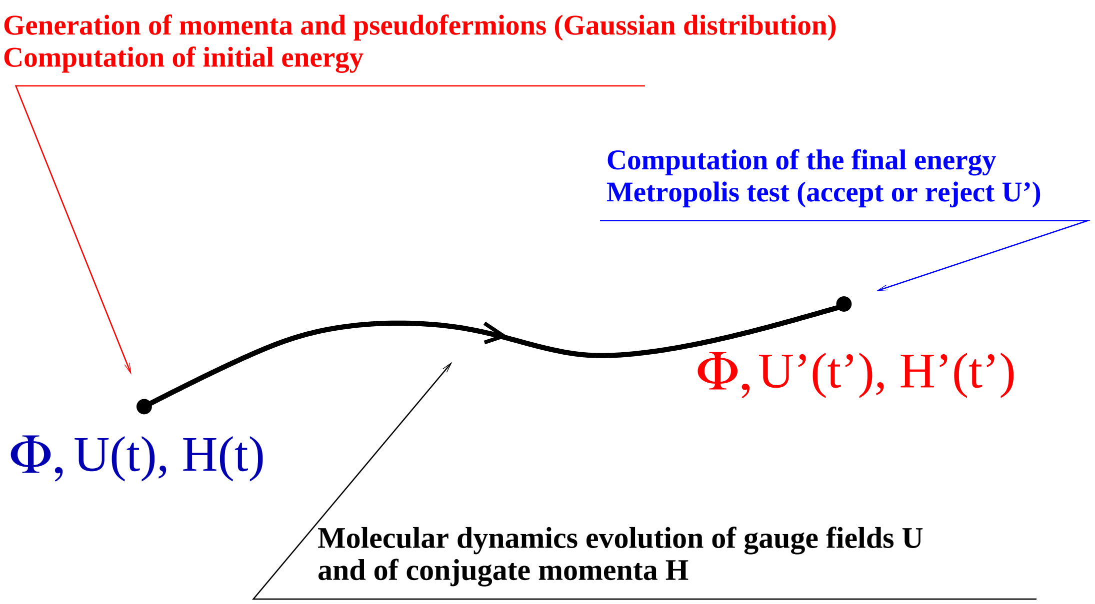
Hybrid Monte-Carlo algorithm

$$\int \mathcal{D}U e^{-S_G[U]} (\det M[U])^2 = \int \mathcal{D}H \mathcal{D}\Phi^\dagger \mathcal{D}\Phi \mathcal{D}U e^{-S_G[U]} e^{-\frac{1}{2}H^2} e^{-\Phi^\dagger (MM^\dagger)^{-1}\Phi}$$

- **Introduce auxiliary fields $\Phi, \Phi^\dagger$ to bosonize the determinant**
- **Introduce auxiliary conjugate momenta $H_\mu(n) \in su(3)$**
- **Perform a dynamical Monte-Carlo (Markov chain)**

Scheme of the elementary dynamical Monte-Carlo step

The most expensive part is the repeated computation of $(MM^\dagger)^{-1}\Phi$, needed during Molecular Dynamics.



Computational Complexity 1

How big and how ill-conditioned is the fermion matrix M

M **is roughly a** $(L/a)^4 \times (L/a)^4$ **sparse matrix** (plus color-flavor indexes)

What are acceptable values for L and a to get reliable computations?

- $L \gg$ **largest length** $m_\pi^{-1} \sim 10^{-15}$ **m = 1 fm**
- $a \ll$ **shortest length** $\sim 10^{-16}$ **m or shorter**

$\Longrightarrow$ **ideally** $L/a \sim O(100) \Longrightarrow M \sim 10^8 \times 10^8$ **matrix.**

$$M \sim \left(D^{\mu}_{ij}\gamma^{E}_{\mu} + m_f \delta_{ij}\right) \quad \Longrightarrow \quad M = am_f \,\mathrm{Id} + K$$

Chiral symmetry breaking $\Longrightarrow$ **small imaginary eigenvalues for K (anti-hermitean)**

$\Longrightarrow$ **for** $MM^\dagger$ **we have** $\lambda_{min} \sim (am_f)^2$ **and** $\lambda_{max} \sim O(10)$

The problem becomes more and more challeging as we try to reach small, physical quark masses and as we try to reach the continuum limit:

$$m_{u/d}/\Lambda_{QCD} \sim 10^{-2} \text{ and } a \ll \Lambda_{QCD}^{-1} \quad \Longrightarrow \quad am_f \lesssim 10^{-3}$$

Computational Complexity 2

Fighting by thinking about new algorithms

2001 estimate of the numerical cost of Lattice QCD (A. Ukawa, Lattice2001)

$$3.10 \left(\frac{L_s}{3\text{ fm}}\right)^5 \left(\frac{L_s}{2L_t}\right) \left(\frac{0.2}{\hat{m}/m_s}\right)^3 \left(\frac{0.1\text{ fm}}{a}\right)^7 \text{TFlops} \cdot \text{year}$$

This is the time to get a sample of 100 well decorrelated field configurations.

$m_s \sim 28 m_u$, $L_s \sim 6$ **fm,** $a \sim 0.04$ **fm)** $\Longrightarrow \sim 10^7\ \text{TFlops} \cdot \text{year} \sim 10^{26}$ **ops**

WHERE WE CAN ACT (some significant examples):

- **Higher order symplectic and multiple step integrators for MD**
- **Preconditioning by rewriting the determinant (Hasenbusch trick):**

$$\det(MM^\dagger) = \frac{\det(MM^\dagger)}{\det(MM^\dagger + \mu_1^2)} \frac{\det(MM^\dagger + \mu_1^2)}{\det(MM^\dagger + \mu_2^2)} \cdots \det(MM^\dagger + \mu_N^2)$$

- **Preconditioning by deflation**

  compute the first N eigenvectors exactly and factorize them out

SITUATION TEN YEARS LATER (S. Schaefer, Lattice2012):

same estimate as above goes down to $\sim 10^3\ \text{TFlops} \cdot \text{year} \sim 10^{22}$ **ops**

Computational Complexity 3

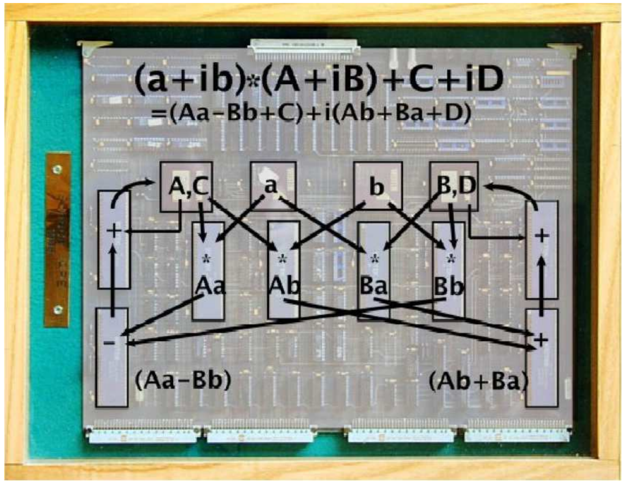
Fighting by thinking/hoping for new machines

After Wilson's dream (1974), M. Creutz started LQCD on a 10 Mflops machine (1979)

pure gauge theory (no dynamical quarks) with gauge group $SU(2)$ on a 10^4 lattice

Computer power has grown a lot since then. LQCD simulations have been a major stimulus for the development of High Performance Computing resources.

An example is the series of APE machines "made in INFN" (N. Cabibbo *et al*)



APE project, 1988, 250 Mflops

first

APEnext, 2006, 10 Tflops

or the series of BlueGene machines developed by IBM

Computational Complexity 4

Do we rely more on better algorithms or on better machines?

Let us look at improvements on both sides in a well defined period:

2001 $\longrightarrow$ 2012

Computational effort for 100 independent confs ($L \sim 6$ fm, $a \sim 0.04$ fm) goes from 10^7 to 10^3 Tflops · year

$\downarrow$

Factor 10^4 improvement

Peak performance of the most powerful parallel machine on Earth goes from 10 Teraflop to 10^4 Teraflop

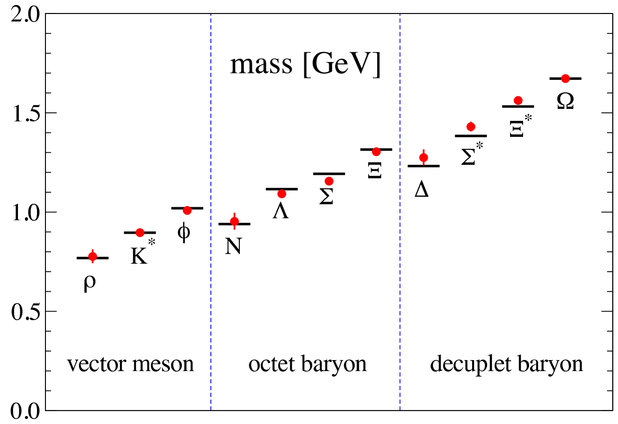
$\downarrow$

Factor 10^3 improvement

Both machine and algorithmic improvements have been essential, with slightly more success from the algorithmic side

We have reached the possibility of performing realistic computations for several aspects of strong interactions

For instance, we can compute the hadron spectrum at the 1% precision level



Aoki et al. Phys.Rev. D81, 074503, 2010

In the following I will focus on aspects regarding strong interactions under extreme conditions (temperature, baryon density, ...).

Those are fundamental for various fields, including astrophysics cosmology, and heavy ion collision experiments.

Lattice QCD at finite temperature

The thermal QCD partition function is naturally rewritten in terms of an Euclidean path integral with a compactified temporal extension

$$T = \frac{1}{\tau} = \frac{1}{N_t a(\beta, m)}$$

τ **is the extension of the compactified time**

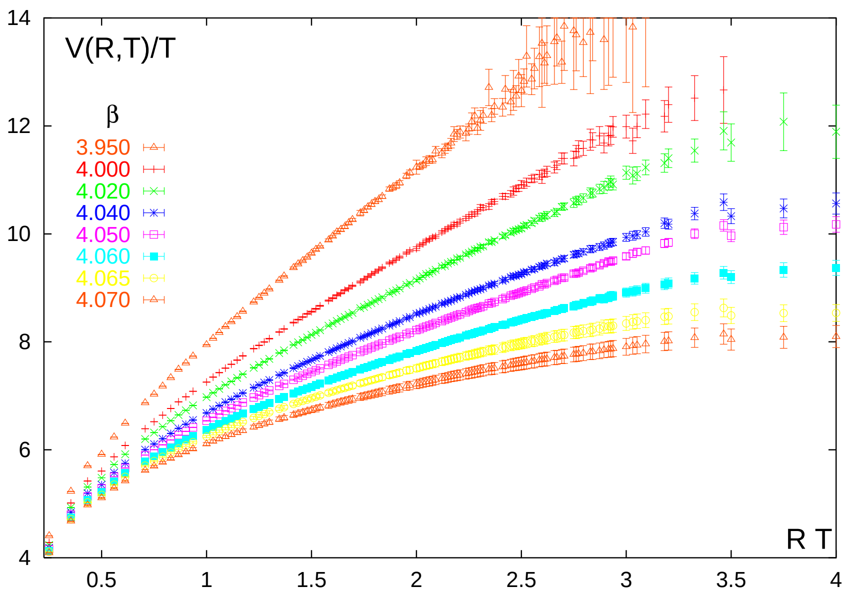
Sample averages give access to equilibrium properties (energy density, specific heat, etc.)

To understand the nature of phase transitions, we study different growing spatial sizes and look for possible singularities in the infinite volume limit: finite size scaling

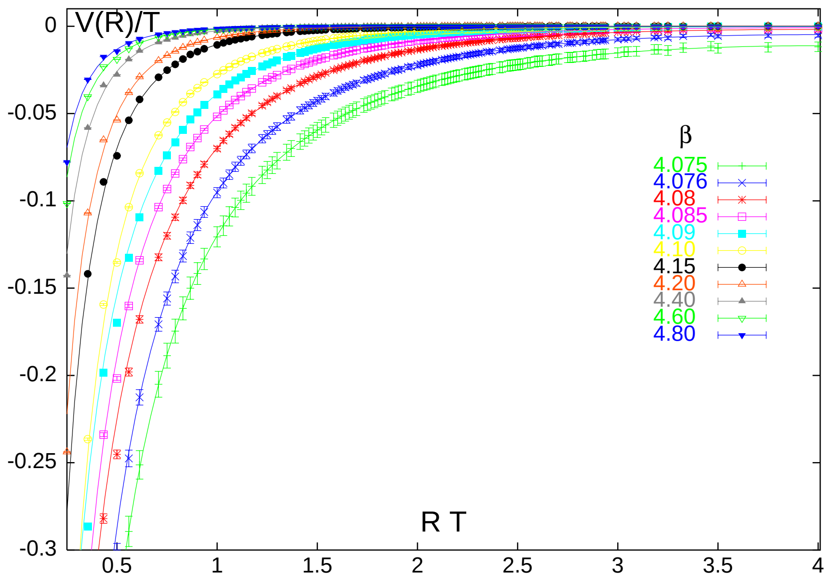
The computation of out-of-equilibrium or transport properties is far less trivial

Finite T transition

Clear evidence for deconfinement is obtained both in the pure gauge theory (quenched approximation) and in presence of dynamical fermions



low T



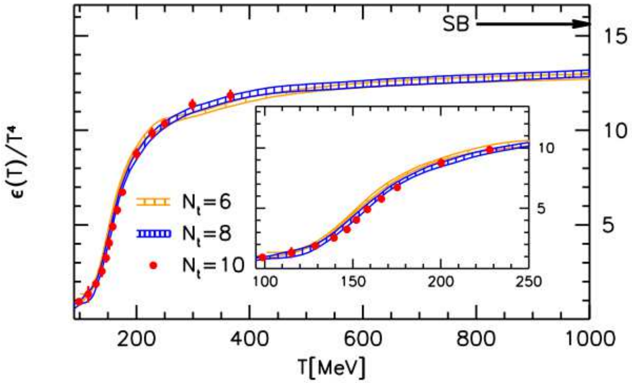
high T

Taken from O. Kaczmarek, F. Karsch, E. Laermann and M. Lutgemeier, Phys. Rev. D 62, 034021 (2000)

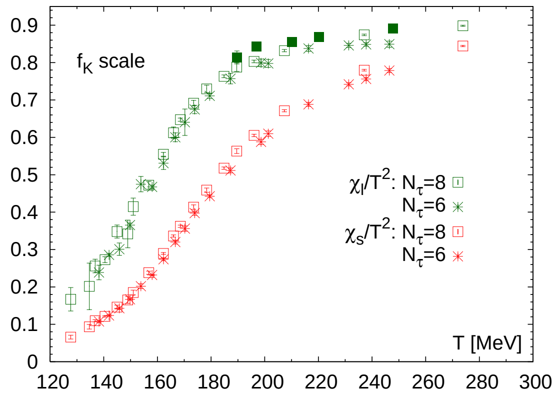
The confining potential between static color sources, which is present at low T, disappears at high T

The liberation of color degrees of freedom is clearly visible in thermodynamical quantities and coincides with chiral symmetry restoration.

energy density — **u/d and s number fluctuations** — **chiral condensate**



arXiv:1007.2580



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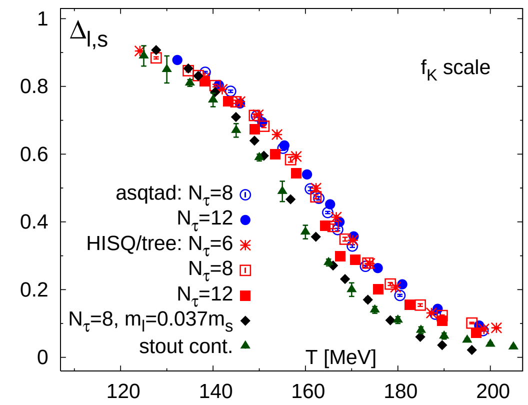


arXiv:1111.1710

Temperature of the transition (from the chiral condensate)

S. Borsanyi *et al.* **JHEP 1009, 073 (2010)** $T_c = 155(6)$ **MeV** (stout link stag. discretization, $a_{min} \simeq 0.08$ fm)

A. Bazavov *et al.*, **PRD 85, 054503 (2012)** $T_c = 154(9)$ **MeV** (HISQ/tree stag. discretization, $a_{min} \simeq 0.1$ fm)

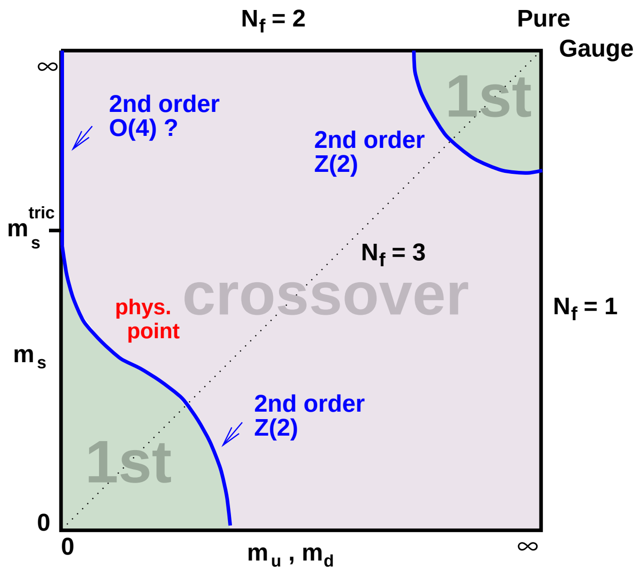
Nature of the transition

No exact symmetries are known for QCD with physical masses. Then, it is not granted that a true transition takes place

Indeed, the physical point (simulations with physical quark masses) is consistent with a crossover (no discontinuity or divergence)

(Aoki et al., Nature 443, 675 (2006))

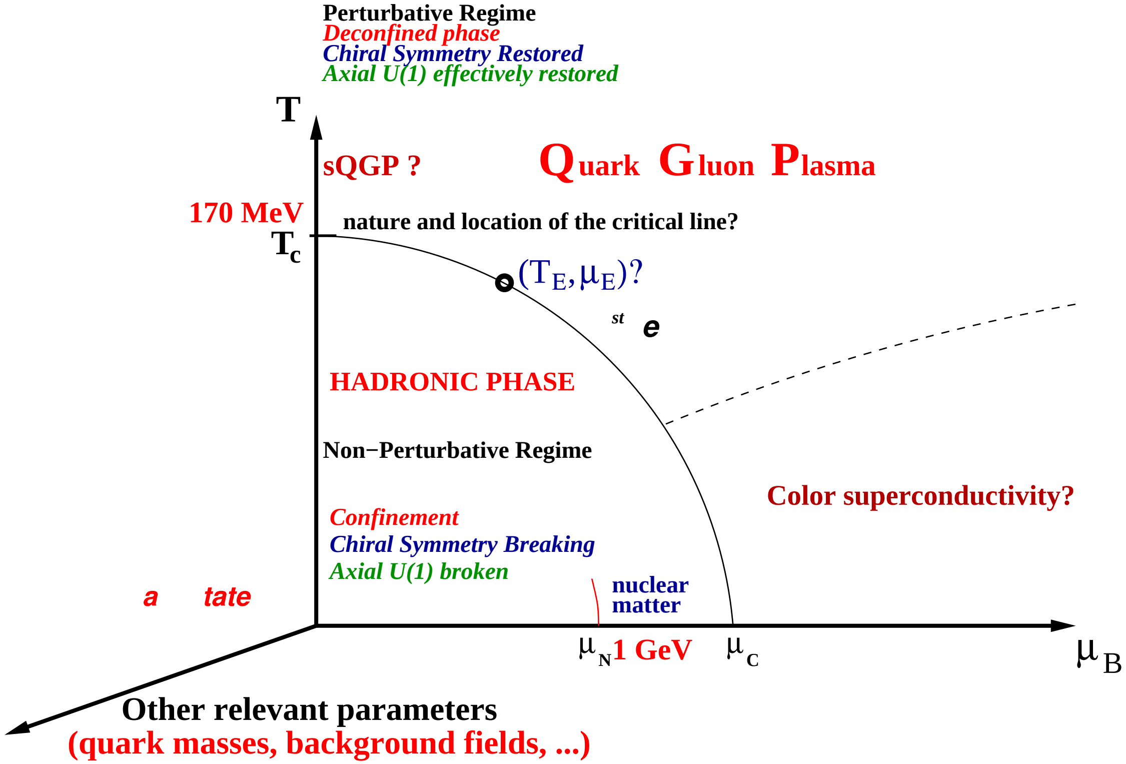
However, one can thus study the nature of the transition as a function of u/d, s quark masses



$\Longleftarrow$ **COLUMBIA PLOT**

A true, first order transition is present for very light or very heavy quark masses

The QCD phase diagram: not just temperature ...



What we would like to know:

- Location and nature of deconfinement/chiral symmetry restoration as a function of other external parameters (μ_B, external fields, ...)
- Properties of the various phases of strongly interacting matter
- Critical endpoint at finite μ_B?

Problems in lattice QCD at $\mu_B \neq 0$

$$Z(\mu_B, T) = \mathrm{Tr}\left(e^{-\frac{H_{\mathrm{QCD}} - \mu_B N_B}{T}}\right) = \int \mathcal{D}U e^{-S_G[U]} \det M[U, \mu_B]$$

$\det M[\mu_B]$ **complex** $\Longrightarrow$ **Monte Carlo simulations are not feasibile.**

This is usually known as the sign problem

By now, we can rely on a few approximate methods, viable only for small μ_B/T, like

- **Taylor expansion of physical quantities around $\mu = 0$**

  Bielefeld-Swansea collaboration 2002; R. Gavai, S. Gupta 2003

- **Reweighting (complex phase moved from the measure to observables)**

  Barbour et al. 1998; Z. Fodor and S, Katz, 2002

- **Simulations at imaginary chemical potentials (plus analytic continuation)**

  Alford, Kapustin, Wilczek, 1999; de Forcrand, Philipsen, 2002; M.D'E., Lombardo 2003.

Others are being developed but still not fully operative

(Langevin simulations, density of states method, Lefschetz thimble simulations, rewriting the partition function in terms of dual variables, ...)

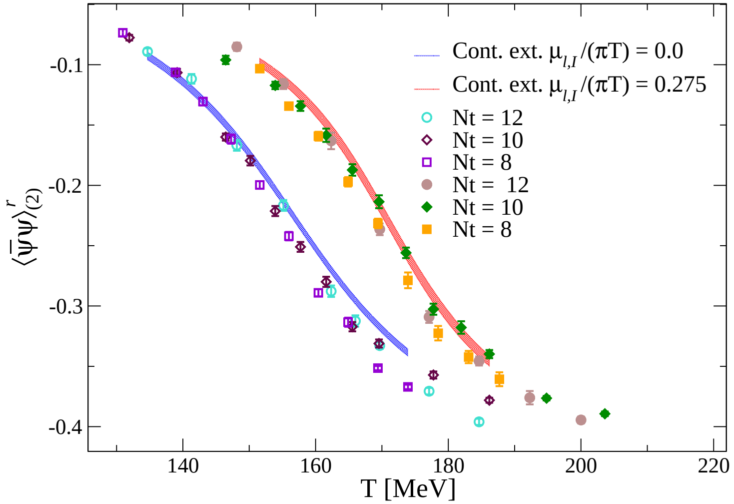
As a consequence, most present reliable results regards the physics at small chemical potential. **An example is the dependence of T_c on μ_B:**

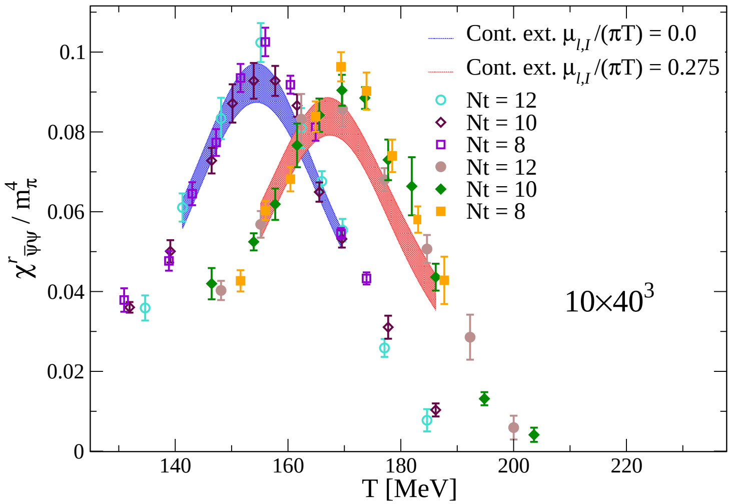
$$\frac{T(\mu_B)}{T_c} \simeq 1 - \kappa \left(\frac{\mu_B}{T(\mu_B)} \right)^2 = 1 - 9\kappa \left(\frac{\mu}{T(\mu)} \right)^2$$

μ is the quark chemical potential, κ is the curvature of the pseudo-critical line at $\mu_B = 0$ and can be obtained either by Taylor expansion technique or by numerical simulations at imaginary μ_B, assuming analyticity around $\mu_B = 0$:

$$\frac{T(\mu_I)}{T_c} \simeq 1 + 9\kappa \left(\frac{\mu_I}{T(\mu_I)} \right)^2$$

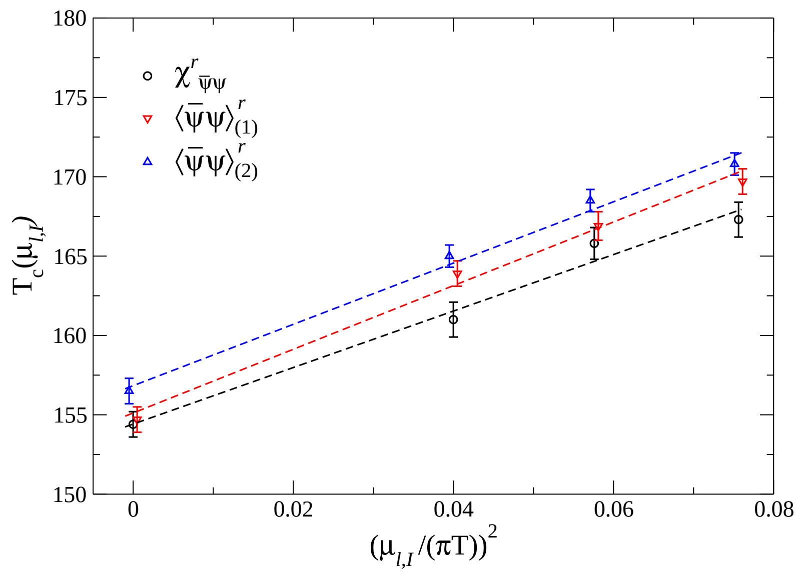
In the imaginary chemical potential approach, T_c is computed as a function of μ_I from various quantities (from Bonati et al., arXiv:1507.03571) **:**



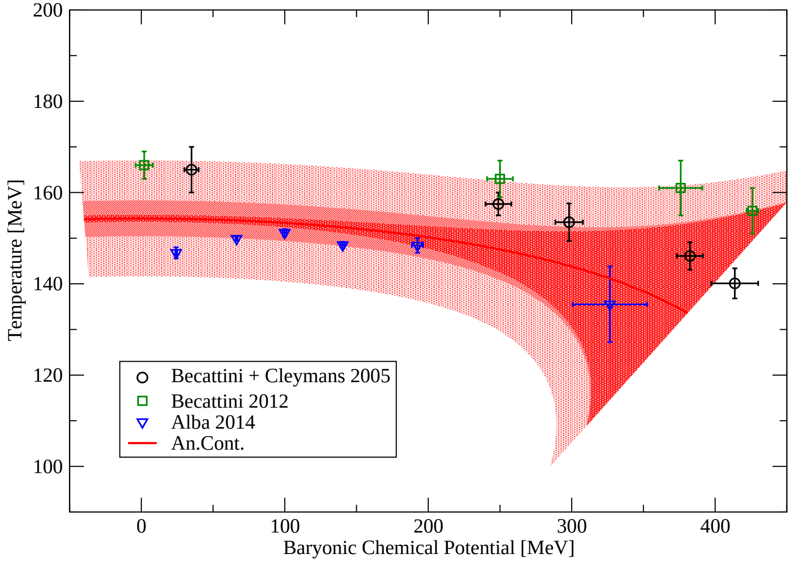


chiral condensate **chiral susceptibility**

then, assuming analyticity, κ is extracted by fitting a linear dependence in μ_I^2 for small μ_I.

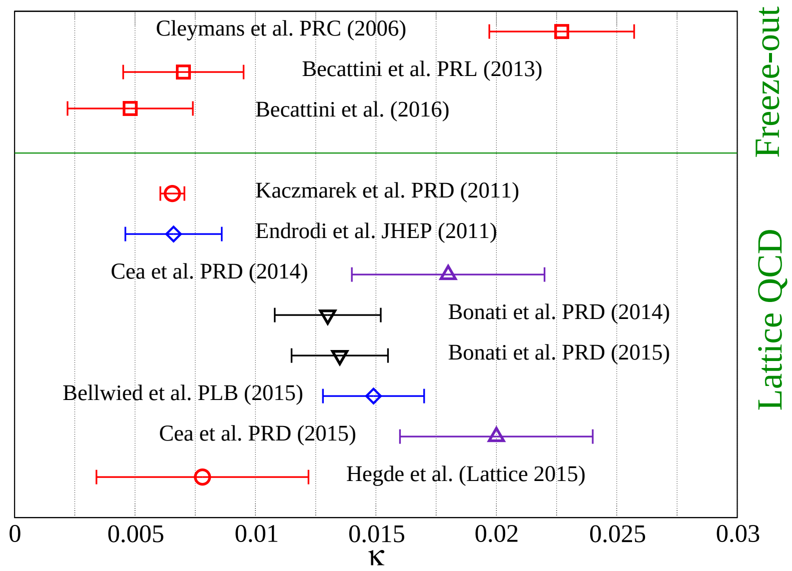


The pseudo-critical line from analytic continuation, compared with determinations of the freeze-out line from heavy ion experiments



The curvature of the pseudo-critical line: various lattice determinations and comparison with freeze-out

Convergence of most recent results indicates good control over possible systematic effects.



Unfortunately the determination of the critical endpoint is still far from that

QCD and θ-dependence: standard model and beyond

Gauge field configurations relevant to the QCD path integral divide in homotopy classes, characterized by a winding number $Q = \int d^4x\, q(x)$

$$q(x) = \frac{g^2}{64\pi^2} G^a_{\mu\nu}(x)\tilde{G}^a_{\mu\nu}(x) = \frac{g^2}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}G^a_{\mu\nu}(x)G^a_{\rho\sigma}(x) \qquad G\tilde{G} \propto \vec{E}^a \cdot \vec{B}^a \ \text{CPodd quantity}$$

The QCD action can be modified by introducing a θ-parameter coupled to Q:

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

The theory at $\theta \neq 0$ is renormalizable and presents explicit CP-breaking

The euclidean path integral measure is complex (sign problem for numerical simulations)

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

$$\chi = \frac{1}{V_4}\langle Q^2\rangle_0 = F^{(2)} \qquad b_2 = -\frac{\langle Q^4\rangle_0 - 3\langle Q^2\rangle_0^2}{12\langle Q^2\rangle_0} \qquad b_4 = \frac{\langle Q^6\rangle_0 - 15\langle Q^2\rangle_0\langle Q^4\rangle_0 + 30\langle Q^2\rangle_0^3}{360\langle Q^2\rangle_0}$$

The probability distribution $P(Q)$ is a non-perturbative property of QCD

Predictions about θ-dependence

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

One can integrate quantum fluctuations around classical solutions with non-trivial winding around the gauge group: instantons. Effective action known only perturbatively

$$1-\mathrm{loop} \qquad \exp\left(-8\pi^2/g^2(\rho)\right)$$

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

Breaks down for large instantons ($1/\rho \lesssim \Lambda_{QCD}$), which however are suppressed by thermal fluctuations at high T (in particular for $\rho \gg 1/T$), where instantons of effective perturbative action $8\pi/g^2(T)$ dominate.

$\Longrightarrow$ **instantons-antiinstantons form a dilute non interacting gas**

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

At low T, instead, chiral perturbation theory gives reliable estimates:

$\chi(T=0) \simeq (78\,\mathrm{MeV})^4$

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 about 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:

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

- 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

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

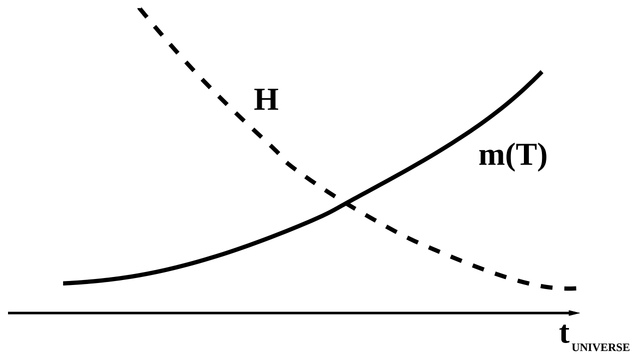
$$\ddot{a}(t) + 3H(t)\dot{a}(t) + m_a^2(T)a(t) = 0 \ ; \quad m_a^2 = \chi(T)/f_a^2$$

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

$m_a \gtrsim H$ oscillations start $\implies$ 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 $\implies$ oscill. time anticipated $\implies$ less axions $\implies$ require larger f_a to maintain N_a

On the other hand, larger f_a means smaller m_a today

Numerical Results from Lattice QCD

Direct simulations at $\theta \neq 0$ face a sign problem again, however lattice QCD represents the ideal tool to sample the topological charge distribution $P(Q)$ at $\theta = 0$.

main technical and numerical issues

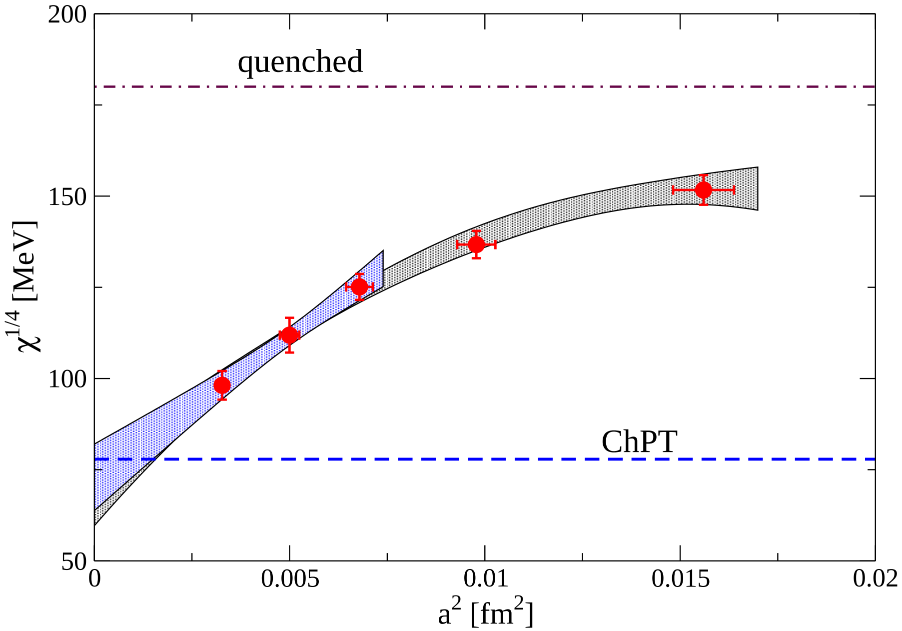
- topological charge renormalizes, naive lattice discretizations are non-integer valued. Various methods devised leading to consistent results
  - field theoretic compute renormalization constants and subtract
  - fermionic definitions use the index theorem to deduce Q from fermionic zero modes
  - smoothing 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, Alexandrou, Athenodorou, Jansen, 1509.04259)

- Freezing of topological modes in the continuum:
  configurations with different Q related by discontinuous field transformations;
  tunneling probability by standard local algorithms decreases exponentially as the continuum limit is approached

Some recent numerical results

from C. Bonati, M.D., M. Mariti, G. Martinelli, M. Mesiti, F. Negro, F. Sanfilippo and G. Villadoro, 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)



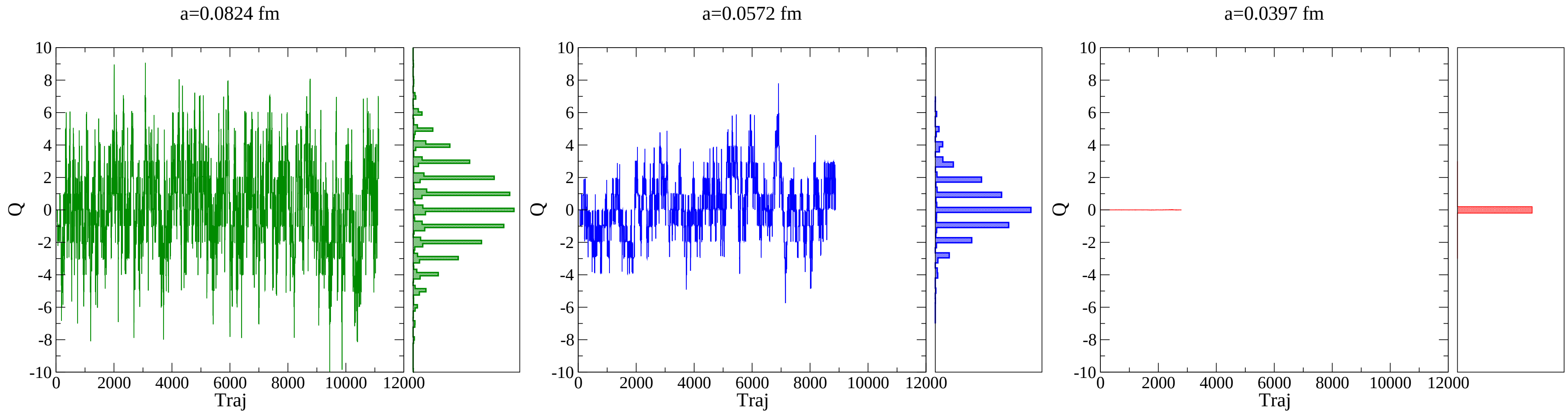
At zero temperature, we compare with predictions from chiral perturbation theory

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

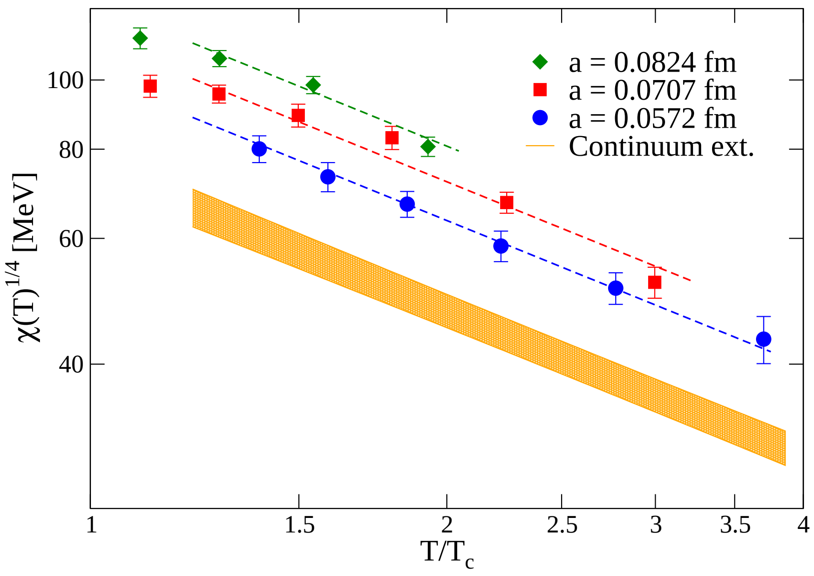
As we approach the continuum limit, standard LQCD algorithms (Rational Hybrid Monte Carlo in this case) face strong ergodicity problems: tunneling between different topological sectors are strongly suppressed and a correct sampling of $P(Q)$ becomes a hard theoretical task



That sets a limit for high T simulations as well. $T = 1/(N_t a)$ can be increased by diminishing either a or N_t :

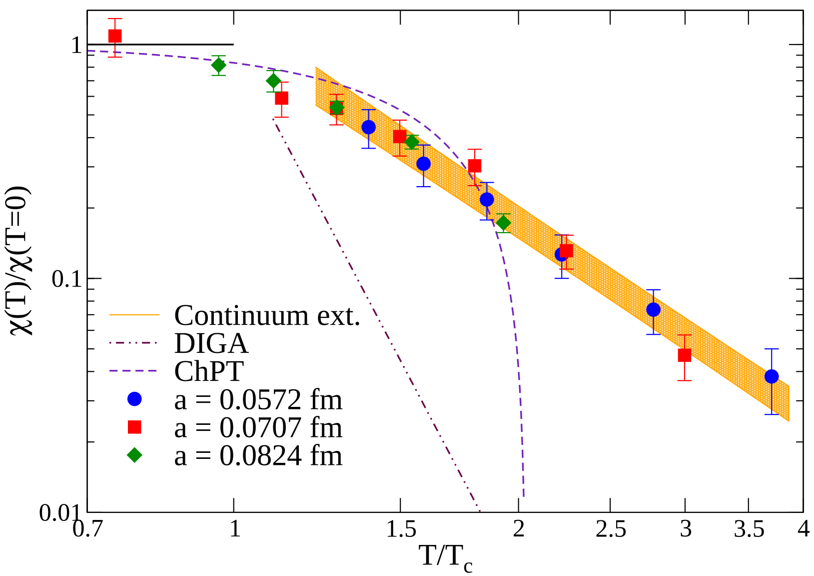
a ~ 0.05 fm and $N_t = 6$ $\Longrightarrow$ $T \sim 6 - 700$ **MeV** $\sim 4\,T_c$

Finite T results provide some surprises



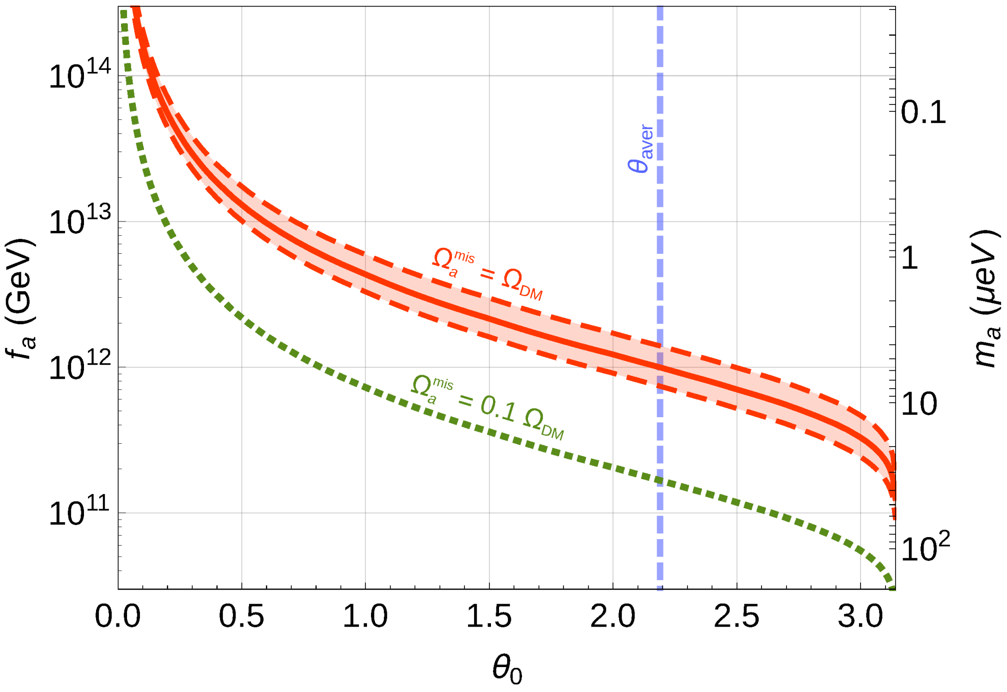
Drop of $\chi(T)$ much smoother than perturbative estimate: $\chi(T) \propto 1/T^b$ with $b = 2.90(65)$ (DIGA prediction: $b = 7.66 \div 8$)

That would move the oscillation point to higher T (few GeVs), however our continuum limit reliable just for $T \lesssim 2\, T_c$ where we have data from three different lattice spacings



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

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



order of magnitude prediction for present $m_a \sim 10\ \mu\mathrm{eV}$

Other recent lattice studies report results more in line with DIGA at higher T

P. Petreczky, H.P. Schadler, S. Sharma, arXiv:1606.0315; Sz. Borsanyi et al, arXiv:1606.07494)

and lead to higher values of $m_a \sim 100\ \mu\mathrm{eV}$

the difference is fundamental (detectable or not detectable) for experiments trying to detect axions

New algorithms are needed! Capable of correctly sampling topological modes in the continuum limit

(Resampling methods? Metadynamics? ... work in progress)

CONCLUSIONS

- Numerical simulations of strong interactions are a computational challenge since a few decades Progress is obtained both by developments in HPC architectures and by advancements in numerical methods

- We have reached a mature era, where precise QCD predictions can be made for several aspects of strong interaction physics (hadron masses, flavor physics, ...)

- Some hot issues however still need progress.
  Not just algorithmic improvements, but breakthroughs, either in algorithms or in the computational approach