Hadrons Physics from Lattice QCD

I. Concepts of lattice field theory

regularisation, simulation, numerical measurements

II. Results for the hadron spectrum

from quenched to dynamical quarks, results to %-level

III. Topological summation

IV. Topological susceptibility from a fixed sector

V. Prospects for quantum simulations

Roughly following *Int. J. Mod. Phys. E25 (2016) 1642008*

Motivation : QCD : assumed to be the fundamental theory behind nuclear physics, formulated in terms of quark– and gluon–fields.

But what we perceive are **hadrons**:

baryons ("consisting of 3 quarks (qqq)"), such as protons and neutrons

mesons ("consisting of a quarks-antiquark pair $(\mathrm{q\bar{q}})$"), such as pions and kaons.

However, consider nucleons: proton (uud) and neutron (udd)

masses (from Higgs mechanism) $m_u \simeq m_d \approx 3 \dots 5\ \mathrm{MeV}$

$\Rightarrow$ 3 valence quarks together account for $\mathcal{O}(1)\ \%$ of $M_{\mathrm{nucleon}} \simeq 939\ \mathrm{MeV}$

Masses of macroscopic objects mostly due to *mess of gluons (and sea-quarks)* inside the nucleons. $\approx 95\ \%$ energy of (massless) gluons, *not* from the celebrated Higgs mechanism

Is this in agreement with the Standard Model, and in particular with QCD?

Answered only recently, by lattice simulations.
We summarise its concepts, some results and prospects for open questions.

I. Concepts of Lattice QCD

Functional integral formulation of Quantum Field Theory in Euclidean space

- Partition function : $Z = \int \mathcal{D}\Phi \, e^{-S_{\mathrm{E}}[\Phi]}$ ($\Phi(x)$: some field, $\hbar = 1$)

- n-point function:

$$\langle 0 | \mathrm{T} \, \hat{\Phi}(x_1) \ldots \hat{\Phi}(x_n) | 0 \rangle \; = \; \frac{1}{Z} \int \mathcal{D}\Phi \; \Phi(x_1) \ldots \Phi(x_n) \, e^{-S_{\mathrm{E}}[\Phi]}$$

- Interpretation as a statistical system:

$p[\Phi] = e^{-S_{\mathrm{E}}[\Phi]}/Z \overset{!}{=}$ probability of configuration $[\Phi]$ (*if* $S_{\mathrm{E}}[\Phi] \in \mathbb{R}_+$)

- Lattice regularisation:
  discrete Euclidean space-time, lattice spacing a implies UV cutoff π/a

Reduces $\Phi(x)$ to Φ_x, field variables defined only at lattice sites x

$\int \mathcal{D}\Phi \to \prod_x \int d\Phi_x$ is well-defined

Idea of Lattice Simulations :

Generate a large set of field configurations, independent and distributed with probability $p[\Phi] \propto \exp(-S_{\mathrm{E}}[\Phi])$.

Summation over this set → measure observables (n-point functions) up to:

- statistical errors (finite set), to be estimated, $\propto 1/\sqrt{\mathrm{statistics}}$
- systematic errors (finite a, finite volume, (heavy M_π)), can be varied and extrapolated, estimate error in physical limit (continuum, . . .)

Truly **non-perturbative !** Results at finite coupling strength.
No problem with strong coupling, in particular: QCD at low energy!

Monte Carlo Simulation and Numerical Measurement

Markov chain of confs $[\Phi] \to [\Phi'] \to [\Phi''] \dots$ *e.g.* from a "hot start" (random conf.)

Condition: Detailed Balance for transition between confs. $\Phi_1 \leftrightarrow \Phi_2$:

$$\frac{p[\Phi_1 \to \Phi_2]}{p[\Phi_2 \to \Phi_1]} \stackrel{!}{=} \frac{p[\Phi_2]}{p[\Phi_1]} = \exp(S[\Phi_1] - S[\Phi_2])$$

and ergodicity (no restriction) $\Rightarrow$ after many steps: correct stat. distribution $\propto p[\Phi]$

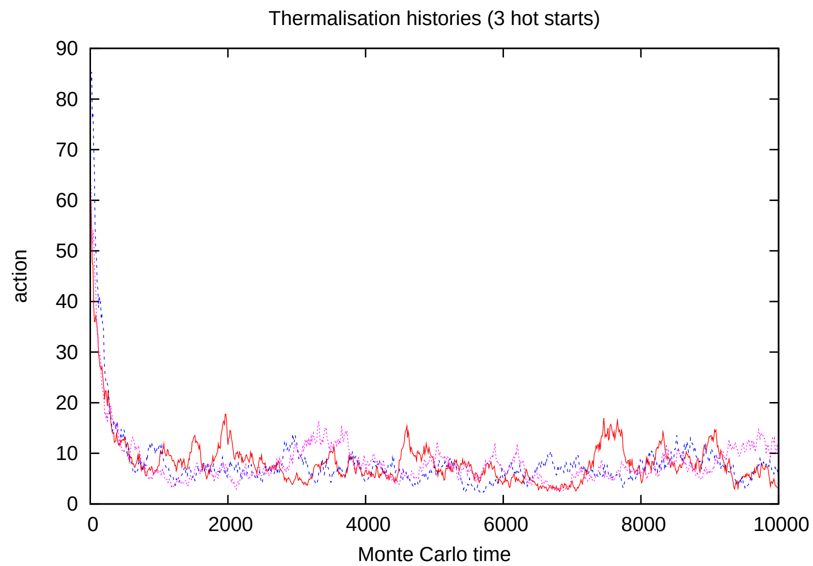
Simple algorithm: Metropolis

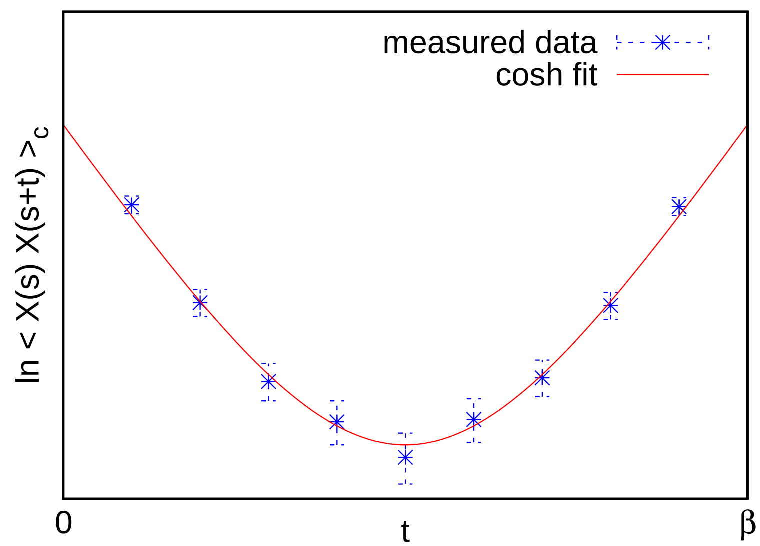
Start from current conf. $[\Phi]$, suggest a new (modified) conf. $[\Phi']$

- IF $S[\Phi'] \leq S[\Phi]$: accept !
- OTHERWISE : accept with probability $\exp(S[\Phi] - S[\Phi'])$.

If accepted (rejected), continue with $[\Phi']$ $([\Phi])$ $\Rightarrow$ *Detailed Balance is implemented*

First discard many steps, until equilibrium is attained ("thermalisation").
Then pick well separated ("de-autocorrelated") confs to measure observables.





Measure *e.g.* connected correlation function of $X(t) = \sum_{\vec{x}} \Phi(\vec{x}, t)$

$\langle X(s)X(s+t)\rangle_c = \langle X(s)X(s+t)\rangle - \langle X(s)\rangle \langle X(s+t)\rangle \propto \underline{\cosh(M(t-\beta/2))}$

$X(t)$: field (product) in layer at Euclidean time t (periodic boundary conditions).

Fit yields *energy gap* $M = E_1 - E_0 = \{\text{Mass of particle described by } X\} = 1/\xi$

2nd order phase transition: correlation length $\xi/a \to \infty$: cont. limit $\sim$ critical point

Lattice Gauge Theory

Consider a scalar field $\Phi_x \in \mathbb{C}$ with some action like

$$S[\Phi] = \frac{a^2}{2} \sum_{x,y} \Phi_x^* M_{xy} \Phi_y + \frac{\lambda}{4!} a^4 \sum_x |\Phi_x|^4$$

$$M_{xy} = \sum_{\mu=1}^{4} (-\delta_{x+\hat{\mu},y} - \delta_{x-\hat{\mu},y} + 2\delta_{x,y}) + (ma)^2 \delta_{x,y}$$

$|\hat{\mu}| = a$, vector in μ-direction

Global symmetry $\Phi_y \to \exp(\mathrm{i}g\varphi)\, \Phi_y$

is promoted to local symmetry $\Phi_y \to \exp(\mathrm{i}g\varphi_y)\Phi_y$

by replacing the δ-links as

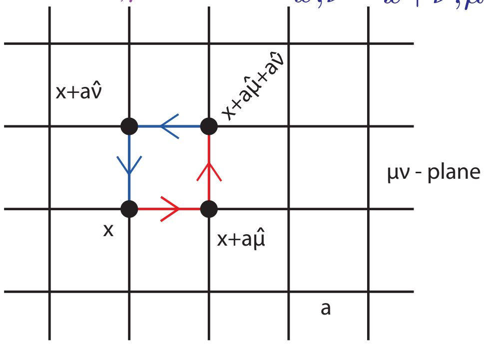
$$\Phi_x^* \Phi_{x+\hat{\mu}} \to \Phi_x^* U_{x,\mu} \Phi_{x+\hat{\mu}} \, , \qquad U_{x,\mu} \in \mathrm{U}(1)$$

$U_{x,\mu}$: gauge link variable, $U_{x,\mu} = e^{\mathrm{i}gaA_{x,\mu}} \to \exp(\mathrm{i}g\varphi_x)\, U_{x,\mu}\, \exp(-\mathrm{i}g\varphi_{x+\hat{\mu}})$

Discrete covariant derivative, **regularised system is gauge invariant.**
Deal with *compact link variables* $\in$ gauge group, also $\mathrm{SU}(N)$
No gauge fixing needed !

Gauge Action

Plaquette variable : $U_{x,\mu\nu} := U^\dagger_{x,\nu} U^\dagger_{x+\hat{\nu},\mu} U_{x+\hat{\mu},\nu} U_{x,\mu} \in \mathrm{SU}(N)$



minimal lattice Wilson loop, closed $\rightarrow$ gauge invariant

$$S_{\mathrm{gauge}}[U] = \frac{1}{4a^2 g^2} \sum_{x,\mu<\nu} \left(2N - \mathrm{Tr}[U_{x,\mu\nu} + U^\dagger_{x,\mu\nu}]\right)$$

$$\overset{a\to 0}{\longrightarrow} \quad \frac{1}{4} \sum_{x,\mu,\nu} \mathrm{Tr} F_{x,\mu\nu} F_{x,\mu\nu} + \mathcal{O}(a^2)$$

Fermion fields : $\bar{\Psi}_x$, Ψ_y

$$Z = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \ \exp(-\bar{\psi}_i M_{ij} \psi_j)$$

i, j run over :

- space-time points $\rightarrow$ lattice sites
- internal degrees of freedom (spinor index, possibly flavour, color)

M contains for each spinor a (discrete, Euclidean) Dirac operator.

Variety of formulations is used, but differences are irrelevant (in the RG sense).

With gauge interaction: covariant derivative.

Pauli Principle: components $\bar{\psi}_i$, ψ_j anti-commute,

representation by Grassmann variables : $\eta_1, \ \eta_2, \ \eta_3, \ldots$ (Berezin '66)

$$\{\eta_i, \eta_j\} = 0 \ \ , \quad \frac{\partial}{\partial_{\eta_i}} \eta_j = \delta_{ij} = \int d\eta_i \ \eta_j \qquad \text{(no bounds)}$$

General results: fermion determinant and chiral condensate

$$\int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi \ \exp(-\bar{\Psi} M \Psi) = \det M \quad , \qquad \langle \bar{\Psi}_i \Psi_j \rangle = -(M^{-1})_{ij}$$

$\Rightarrow$ Computer never deals with Grassmann variables, "just" needs $\det M$, M^{-1} (though typically millions of components . . .) Bottleneck in simulations !

Optimal algorithm (HMC) circumvents computation of $\det M$ by updating an auxiliary boson field $\vec{\Phi} \in \mathbb{C}^N$

$$\det M[U] = \int D\Phi \ \exp(-\vec{\Phi}^\dagger M[U]^{-1} \vec{\Phi})$$

Still requires $M[U]^{-1}$

Gauge action: shift for local update $[U] \to [U']$ can be computed locally $\to$ fast

With fermions tedious, QCD: dynamical quarks cost $\mathcal{O}(100)$ times more compute time.

Lattice QCD

- Gauge configuration $[U]$: set of compact link variables $U_{x,\mu} \in \mathrm{SU}(3)$.
- Gauge action: sum over plaquette variables $U_{x,\mu\nu}$.
- Quark fields $\bar{\Psi}$, Ψ on lattice sites $\longrightarrow$ fermion determinant

$$Z = \int \mathcal{D}U \underbrace{\det M[U] \exp(-S_{\mathrm{gauge}}[U])}_{\text{statistical weight of conf. } [U] \,\to\, \textit{Monte Carlo}}$$

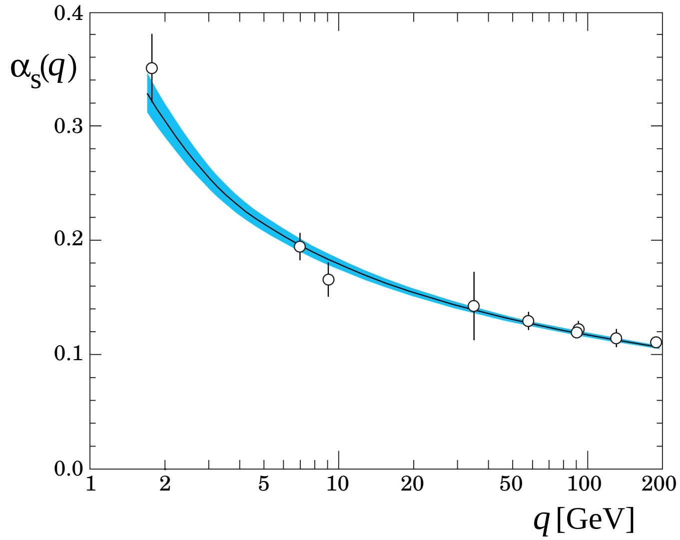
Measure correlation functions, $e.g.$ of pseudoscalar density $P_x = \bar{\Psi}_x \gamma_5 \Psi_x$, $P_t = \sum_{\vec{x}} P_x$

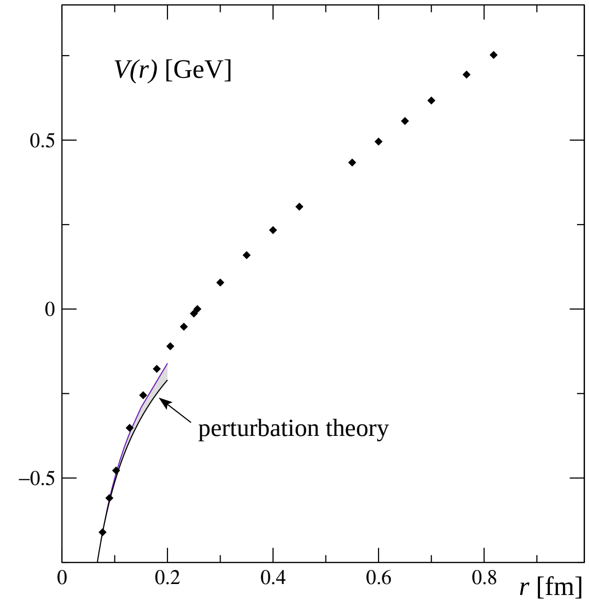
$\langle\, P_s\, P_{s+t} \,\rangle_{\mathrm{c}} \propto \exp(-M_\pi |t|) \;\Rightarrow\;$ pion mass M_π

$\Rightarrow$ Explicit results for hadron masses, matrix elements, susceptibilities, critical or crossover temperature $e.g.$ for transition: confinement $\leftrightarrow$ de-confinement, decay constants, etc.

REALLY based on QCD

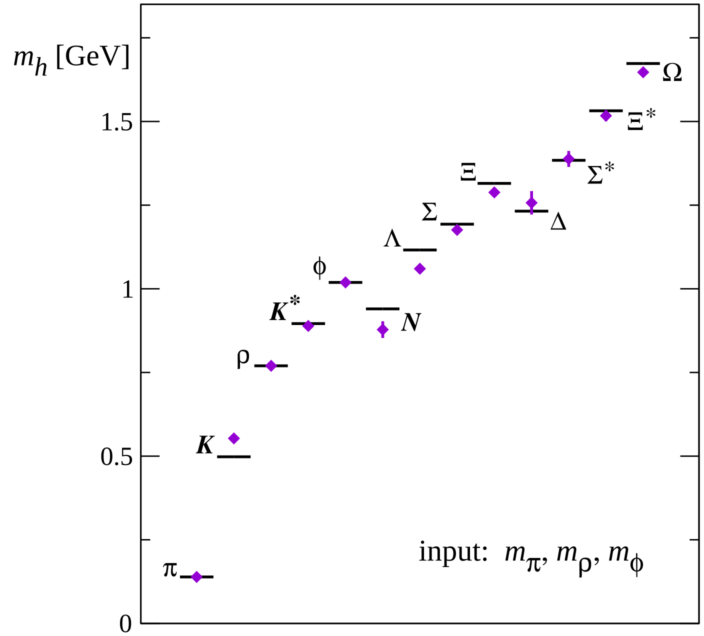
Method also applies to other quantum field theories, like
QED, Higgs model, spin models, condensed matter theories . . .





- Left: strong coupling $\alpha_s(q) = g_s^2(q)/4\pi$ at transfer momentum q.
  Fit: $\alpha_s(q) \propto 1/\ln(q/\Lambda_{QCD})$ $\quad (\Lambda_{QCD} \approx 300\,\text{MeV} \ll v_{Higgs} = 246\,\text{GeV})$

- Right: potential between static quarks;
  numerical results confirm confinement. $\quad (0.2\ \text{fm} \simeq (1\ \text{GeV})^{-1})$
  With dynamical quarks more involved: "string breaking" . . .



Hadron Masses :

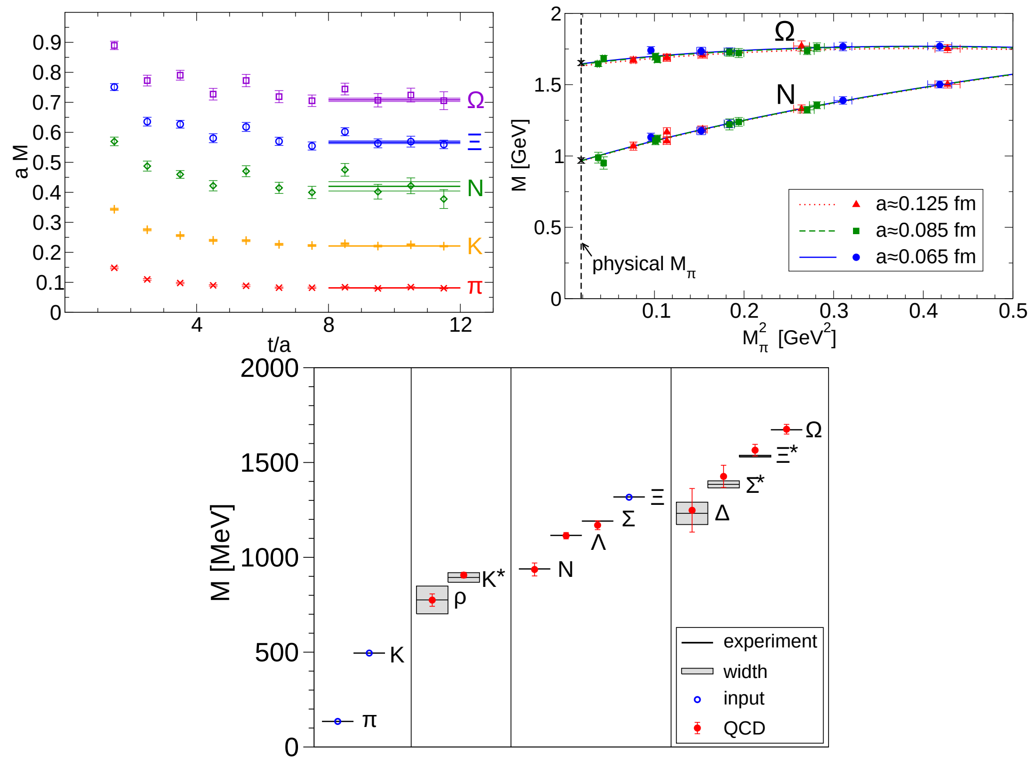
Status in 2002, CP-PACS Collaboration, “quenched” simulations
(generate confs with $\det M = 1$, corresponds to $N_f = 0$, or $m_{\text{quark}} \to \infty$)

Simulation much faster, but uncontrolled systematic error (no sea quarks).

Compared to experiment: agreement up to $\mathcal{O}(10)$ %

Moreover: 20$^{\text{th}}$ century: $M_\pi \gtrsim 600\,\text{MeV}$, required risky “chiral extrapolation”.

Dynamical quarks (det M included), *e.g.* Budapest-Marseille-Wuppertal Collab. (2008)



Now M_π down to $\approx 190\,\mathrm{MeV}$. System size $L \simeq 4/m_\pi$ *i.e.* up to $4\,\mathrm{fm}$: finite size effects mild.
Continuum extrapolation based on lattice spacings $a = 0.125\,\mathrm{fm},\ 0.085\,\mathrm{fm},\ 0.065\,\mathrm{fm}$.

Above: evaluation from exp. decay, and chiral extrapolation $M_\pi \to 135\,\mathrm{MeV}$. *Below:* **hadron spectrum,** in particular $\mathbf{M_{Nucleon} = 936(25)(22)\,MeV}$ vs. $939\,\mathrm{MeV}$ in Nature (statistical) (systematic) error.

Alternative Approach by **QCDSF Collaboration**

W.B., V. Bornyakov, N. Cundy, M. Göckeler, R. Horsley, A. Kennedy, W. Lockhart, Y. Nakamura, H. Perlt, D. Pleiter, P. Rakow, A. Schäfer, G. Schierholz, A. Schiller, T. Streuer, H. Stüben, F. Winter, J. Zanotti, since 2011

Traditional treatment of $2+1$ flavours:

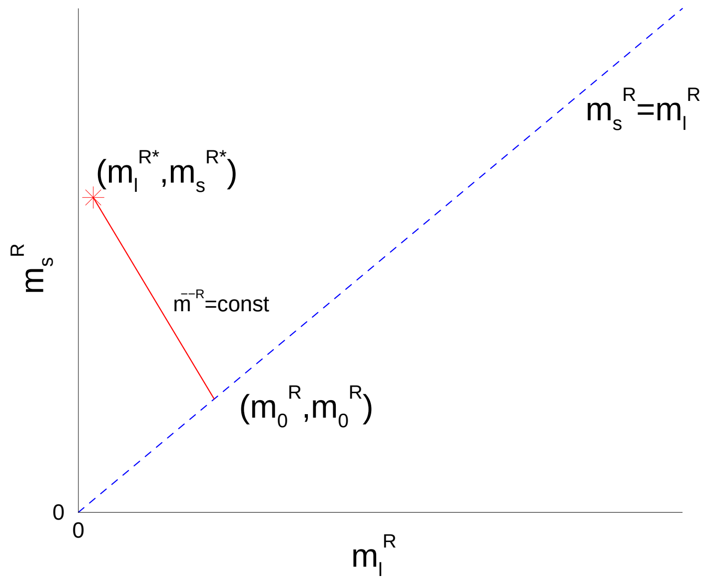
1. Get kaon mass M_K (resp. renormalised s-quark mass) $\approx$ right
2. Push for lighter pions, keeping $M_K \approx \mathrm{const.}$

New Strategy:

1. Start from a SU(3)$_{\mathrm{flavour}}$ symmetric point: $m_u^R = m_d^R = m_s^R$, $M_\pi = M_K$
2. Approach physical point with $m_s^R - m_l^R$ splitting while keeping

   $X_\pi^2 := \frac{1}{3}(M_\pi^2 + 2M_K^2) \approx \mathrm{const.}$ (centre of mass^2 in meson octet)

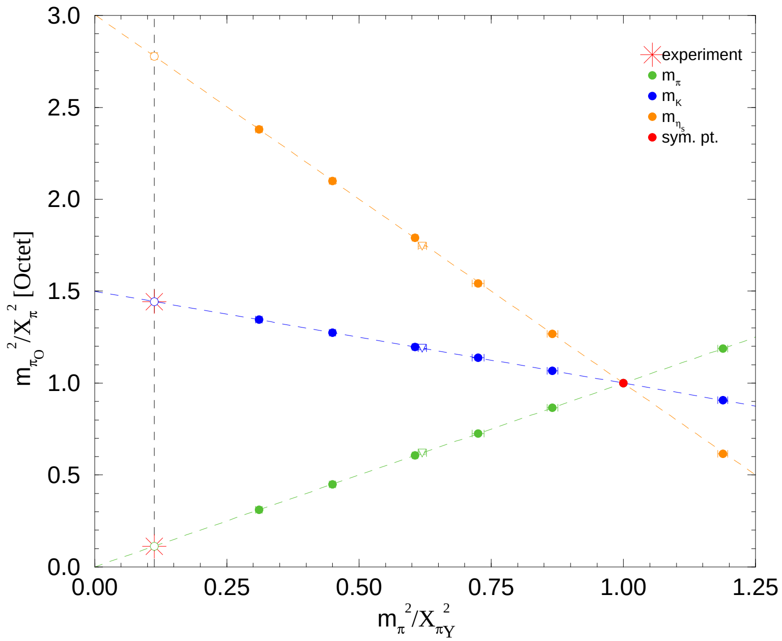
   M_π down, M_K up; extrapolation guided by Chiral Perturbation Theory

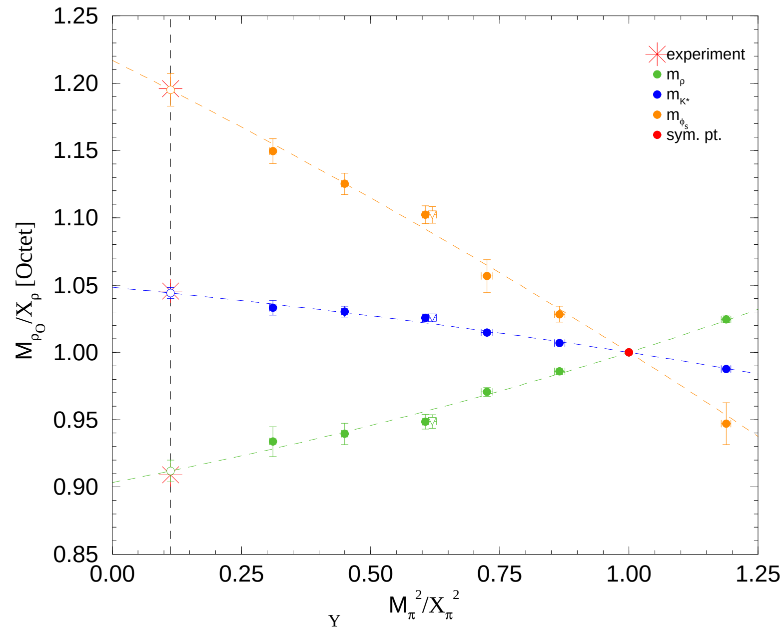


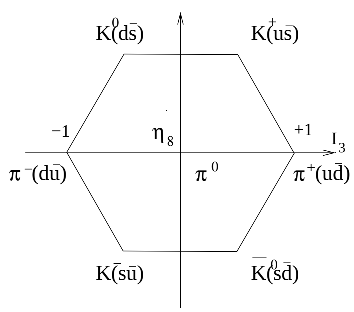
• Virtue: trajectory towards physical point $(m_l^{R*},\, m_s^{R*})$ is constrained and stable. Any flavour singlet quantity $X_S(\bar{m}_0^R)$ $(\bar{m}_0^R = m_l^R = m_s^R)$ obeys under quark mass variations

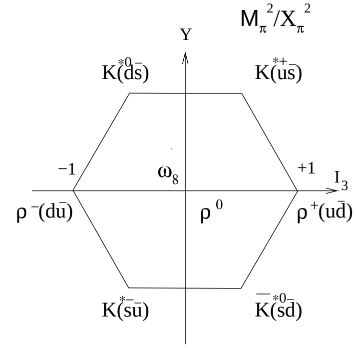
$$X_S(\bar{m}_0^R + \delta m_l^R, \bar{m}_0^R + \delta m_s^R)\Big|_{2\delta m_l^R + \delta m_s^R = 0} = X_S(\bar{m}_0^R, \bar{m}_0^R) + \underline{\mathcal{O}\Big((\delta m^R)^2\Big)}$$

Fan Plots for Meson Spectrum [$V = 24^3 \times 48$ and $32^3 \times 64$, $a = 0.0765(15)$ fm]





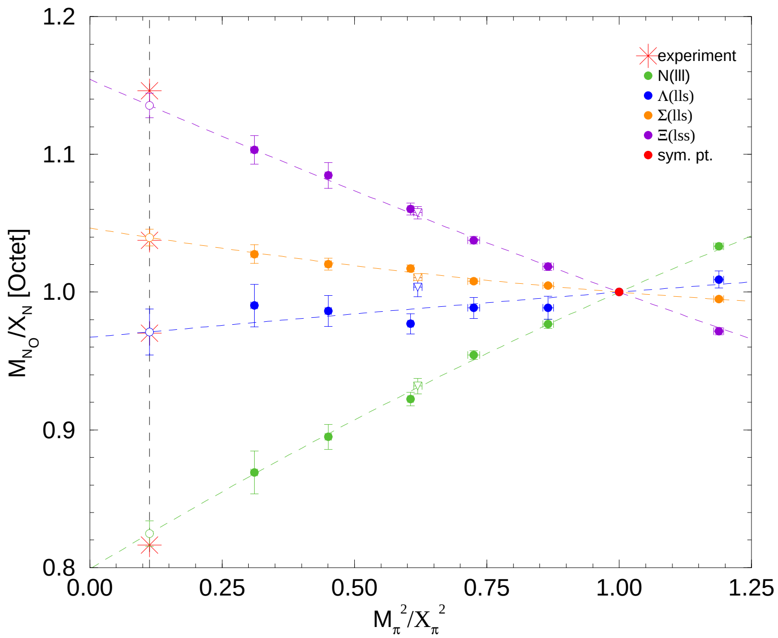


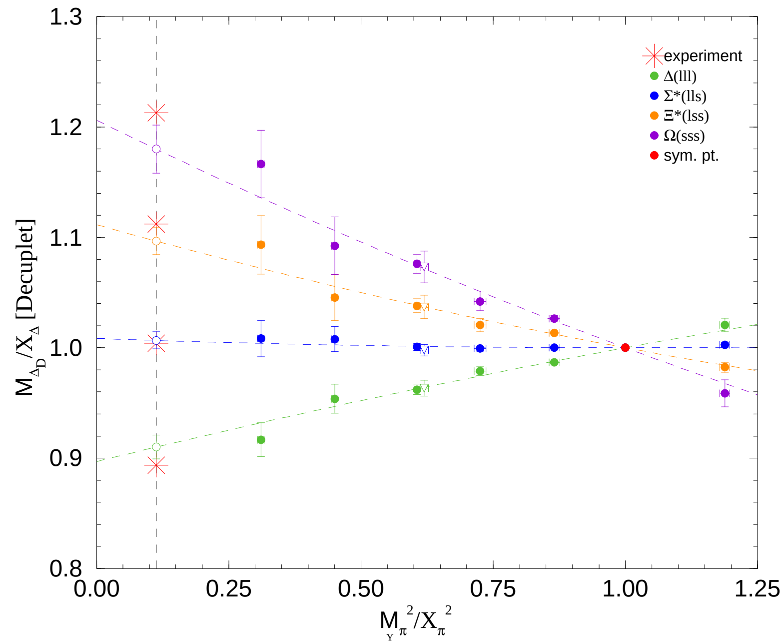


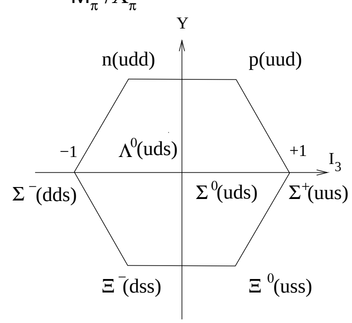
pseudo-scalars π, K (input), η_s

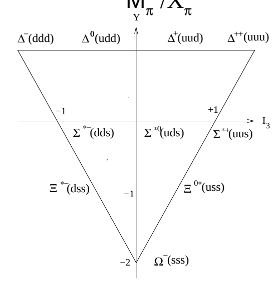
vector mesons ρ, K^*, ϕ

Fan Plots for Baryon Octet (spin-1/2) and Decuplet (spin-3/2)



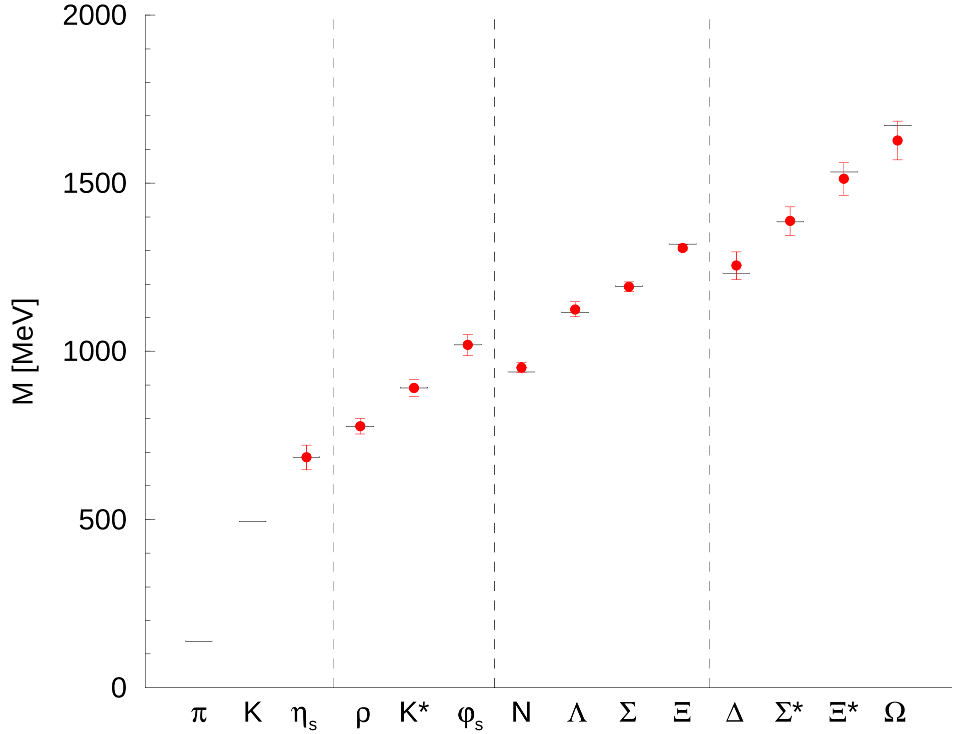






Nucleon (lll), Λ (lls), Σ (lls), Ξ (lss) Δ (lll), Σ^* (lls), Ξ^* (lss), Ω (sss)

Results for the Hadron Spectrum

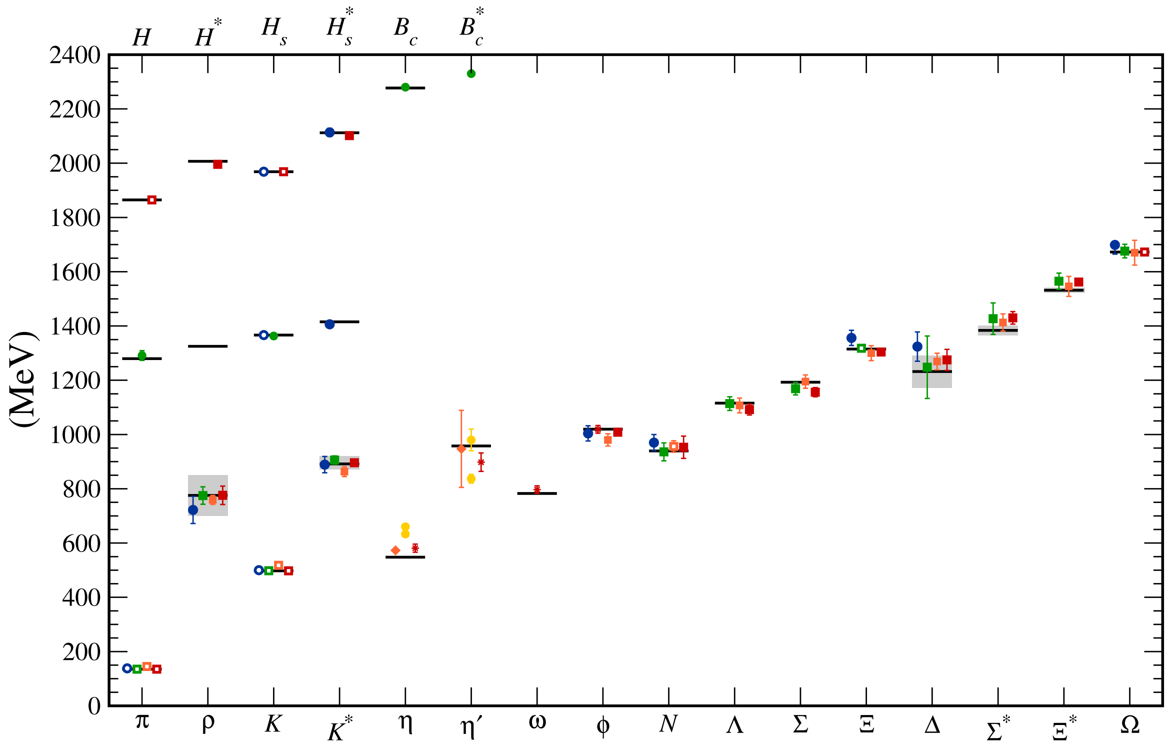


Phenomenology vs. (extrapolated) **numerical results**

Input: M_π, M_K and scale based on flavor symmetric point of the multiplet.

World data: FLAG Review 2019, Flavour Lattice Averaging Group, arXiv:1902.08191 [hep-lat]

Overview by A. Kronfeld, '12



Compilation of results by the collaborations MILC (USA), PACS-CS (Japan), BMW (Germany/Ungary/France), QCDSF (Germany/UK/Russia/Japan/Australia/Mexico), RBC (USA/Irland), UKQCD (UK), HPQCD (USA), Mohler and Woloshyn (Canada)

Status of Lattice QCD

- For the light hadron spectrum, low energy QCD is now tested from 1$^{\rm st}$ principles and confirmed to $\approx 1\,\%$. {despite K. Wilson's pessimism in 1989: will take forever . . . }

  ⋆ Sub-% level: QED effects; m_u, m_d splitting $\to M_n - M_p$ (Borsanyi et al. '15)

- Outstanding challenges: *e.g.* precision data for excited states (Roper resonance!).
  Generally: Step from post-dictions to pre-dictions

  ⋆ M_{Bc} *predicted* by HPQCD (2005): $6.82(8)$ GeV; CDF (2006): $6.78(7)$ GeV.
  ⋆ F_{Ds} *Puzzle:* 2008: Lattice $241(3)$ MeV vs. CLEO, Belle: $270(8)$ MeV.
  2010: Lattice (MILC) $253(8)$ MeV vs. CLEO-c, Belle: $261(7)$ MeV.
  ($B_c^+ \sim (c\bar{b})$, $D_s^+ \sim (c\bar{s})$)

- Everything looks smooth, but conceptual worry expressed by Lüscher '10:

At tiny $a \lesssim 0.05\,\mathrm{fm}$ the Markov chains of most algorithms — such as Hybrid Monte Carlo — get stuck in one topological sector; not ergodic, wrong results . . .

Remedy: open boundary conditions (Lüscher), or summation of fixed topology results

- **Topological sectors for configurations in Quantum Field Theory**

  in volume V with periodic boundary conditions (torus), or $V = \infty$ and S finite

  Examples:

  - O(N) models in $d = N - 1$ dimensions, spin $\vec{e}(x) \in S^{N-1}$
  - 2d $\mathbb{C}$P($N-1$) models, $\vec{c}(x) \in \mathbb{C}^N, \ |\vec{c}(x)| = 1, \quad N = 2, 3, 4, \dots$
  - Gauge theories (may include fermions):

$$\text{2d U(1)} : \quad Q = \frac{1}{2\pi} \int d^2x \, \epsilon_{\mu\nu} F_{\mu\nu} \in \mathbb{Z}$$

$$\text{4d SU}(N \geq 2) : \quad Q = \frac{1}{32\pi^2} \mathrm{Tr} \int d^4x \, F_{\mu\nu} \tilde{F}_{\mu\nu} \in \mathbb{Z} \qquad (\tilde{F}_{\mu\nu} = \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma})$$

Confs can be continuously deformed only within a fixed top. sector.

Functional integral splits into separate integrals for each $Q \in \mathbb{Z}$.
Lattice: for usual actions, no strict separation, but "potential walls" between top. sectors

Monte Carlo Simulation

Almost all applicable algorithms to generate confs perform a sequence of **small update steps,** until a new (quasi-)independent conf. emerges,

$$[\Phi] \to [\Phi'] \to [\Phi''] \to [\Phi'''] \to \dots$$

In particular: Hybrid Monte Carlo algorithm for QCD with dynamical quarks.

(Uncontrolled) large jumps tend to drastically increase S, rejected

Problem: small updates rarely change the top. sector

Sequence has to pass through stat. suppressed regime ("potential walls")

between top. sectors, hight $\overbrace{\longrightarrow}^{a \to 0} \infty$

• Striking for QCD with chiral quarks

E.g. JLQCD '07; Wuppertal Collab. '15 :

HMC trajectory permanently confined in $Q = 0$

• Non-chiral lattice quarks (*e.g.* Wilson fermions): problem less severe so far, *i.e.* for $0.05 \text{ fm} \lesssim a \lesssim 0.15 \text{ fm}$. But: *will* show up on even finer lattices; continuum-like.

$\Rightarrow$ Monte Carlo history tends to be **trapped** for a very long (computing) time, huge number of update steps in **one top. sector**.

Extremely long topological autocorrelation time.

So how can we measure n-point functions, or the top. susceptibility

$$\chi_{\rm t} = (\langle \mathbf{Q^2} \rangle - \langle \mathbf{Q} \rangle^2)/\mathbf{V} \qquad ?$$

By default, we should all sectors, with suitable statistical weight...

Lack of topological transitions in presence of dynamical quarks:

• Lüscher '10, Lüscher/Schaefer '11 :

suggest open boundary conditions in t-direction $\to Q \in \mathbb{R}$ changes gradually.

Avoids *top. freezing*, but breaks (discrete) time translation invariance, and $Q \in \mathbb{Z}$ is useful $e.g.$ to check predictions in the ϵ-regime and extract Low Energy Constants

• **Here: approach with periodic b.c.** $\to$ **maintains** $Q \in \mathbb{Z}$

Studies in toy models for QCD:

• 2d O(3) non-linear σ-model (Heisenberg model)
with *cluster algorithm* (Wolff '89): *non-local updates*

• 4d SU(2) YM theory
with *heatbath algorithm* (considers all options for local updates)

Summation Formula for Observables

Goal: compute an observable $\langle \Omega \rangle$, only with input of some measurements $\langle \Omega \rangle_{|Q|}$ at fixed $|Q|$, in several volumes.

Brower/Chandrasekharan/Negele/Wiese (BCNW) '03

expansion in vacuum angle θ, $S[\Phi] = S_0[\Phi] + \mathrm{i}\theta Q[\Phi] \rightarrow$

Approximation formula for pion mass in QCD. Generalisation:

$$\langle \Omega \rangle_{|Q|} \approx \langle \Omega \rangle + \frac{c}{V \chi_{\mathrm{t}}} \Big(1 - \frac{Q^2}{V \chi_{\mathrm{t}}} \Big)$$

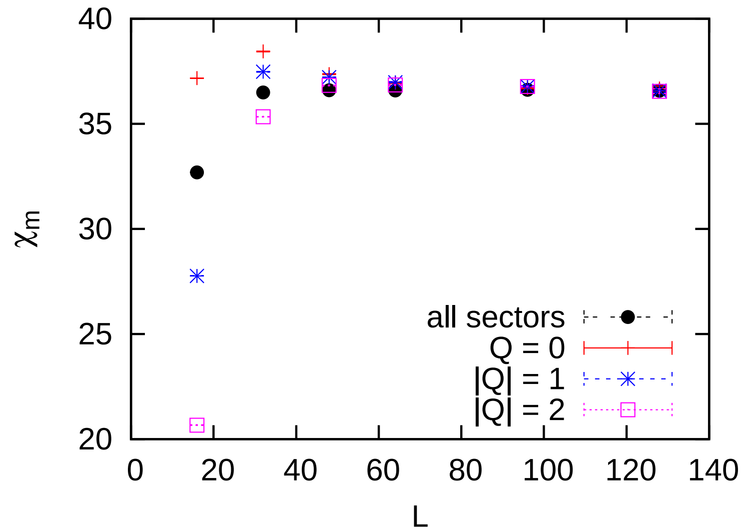
Measure left-hand side for several $|Q|$ and V, 3-parameter fit $\Rightarrow$ $\langle \Omega \rangle$, χ_{t}, (c)

Assumptions:

large $\langle Q^2 \rangle := V \chi_{\mathrm{t}}$, small $|Q| / \langle Q^2 \rangle$ $\Rightarrow$ work at small $|Q|$

2d O(3) model, $L \times L$ lattices, $L = 16 \ldots 128$, $\xi \simeq 3.6$

Magnetic susceptibility $\chi_{\rm m} = \langle \vec{M}^2 \rangle / V \qquad (\ \vec{M} = \sum_x \vec{e}_x \ , \ \langle \vec{M} \rangle = \vec{0} \ )$



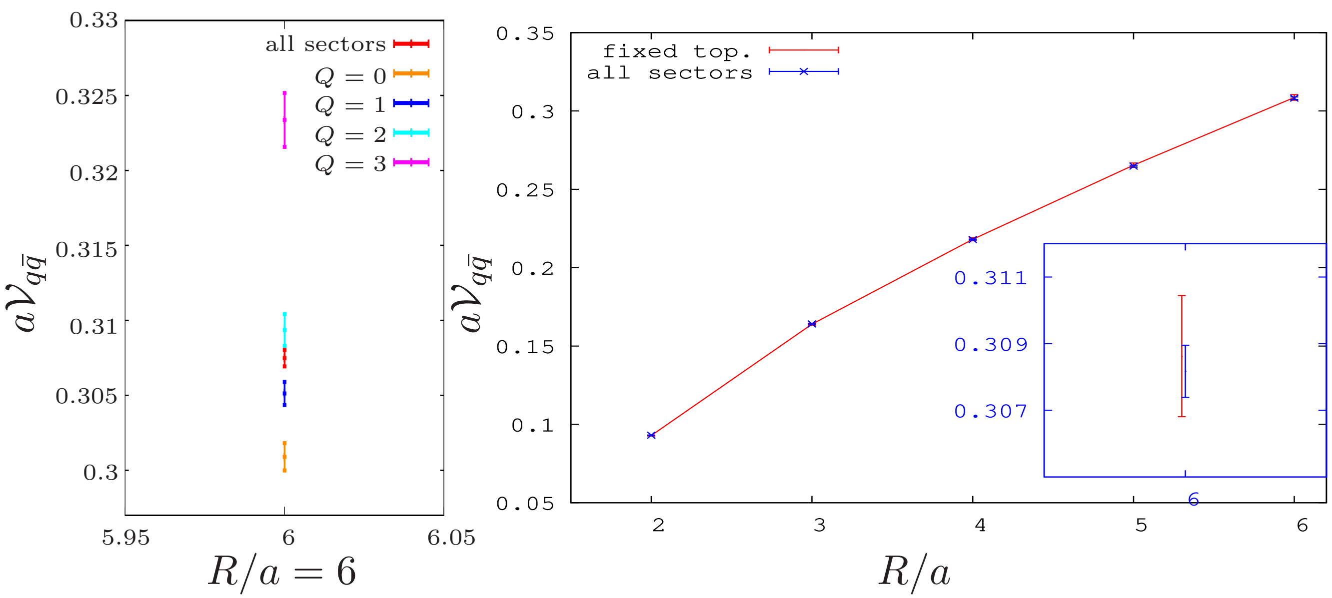
fitting range for L	$48 \ - \ 64$	$48 \ - \ 96$	$48 \ - \ 128$	directly measured in all sectors at $L = 128$
$\chi_{\rm m}$	36.56(4)	36.58(3)	36.57(2)	36.57(2)
$\chi_{\rm t}$	0.00262(17)	0.00256(16)	0.00259(14)	0.002790(5)

Bautista/W.B./Gerber/Hofmann/Mejía-Díaz/Prado '14

4d SU(2) Yang-Mills gauge theory

Identify Q by "cooling" on a 16^4 lattice ($a \simeq 0.076$ fm)
measure static "quark–anti-quark potential" $\mathcal{V}_{q\bar{q}}(R)$ over distances $R/a = 2 \ldots 6$

Values for $\mathcal{V}_{q\bar{q}}(r)$ à la BCNW, and reproduce accurately the potential from all sectors.
However: results for χ_t plagued by large uncertainties.



W.B./Czaban/Dromard/Gerber/Hofmann/Mejía-Díaz/Wagner '16

Summary

For local update algorithms, Monte Carlo histories can be trapped in **one** top. sector over a **long** (simulation) time.

Very large volume overcomes this problem ($\langle \Omega \rangle_Q \equiv \langle \Omega \rangle$, the same $\forall\, Q$), but in general — *e.g.* in QCD simulations — not accessible.

Can we obtain physical results despite top. restriction ?

Top. summation works for observables, in suitable regime also for $\chi_{\rm t}$.

Conditions: $\langle Q^2 \rangle \gtrsim 1.5$, $|Q| \leq 2$

Prospects for application to QCD; typically $\langle Q^2 \rangle = \mathcal{O}(10)$.

Measuring the top. susceptibility

W.B., K. Cichy, P. de Forcrand, A. Dromard, U. Gerber, H. Mejía-Díaz, I.O. Sandoval
JHEP 12(2015)070, EPJ Web Conf. 175 (2018) 11024, Phys. Rev. D 98 (2018) 114501

Continuum (lattice) : continuous deformations of a conf. (at finite action) can never (only painfully) alter Q.

Top. susceptibility

$$\chi_{\rm t} = \frac{1}{V}\Big(\langle Q^2 \rangle - \langle Q \rangle^2 \Big) \ , \quad \text{here} : \ \langle Q \rangle = 0 \quad (\text{P invariance})$$

Non-trivial sectors are exp. suppressed $\Rightarrow$ pert. theory "topology blind"

Non-perturbative quantity $\Rightarrow$ *issue for lattice simulations*

- Quantitative solution to the U(1) problem [Witten, Veneziano '79]

  Re-scale strong coupling as $g^2 = g_\mathrm{s}^2 N_\mathrm{c}$, large N_c , small g_s ['t Hooft]

  - N_f massless quark flavours

    $$M_{\eta'}^2 \propto 1/N_\mathrm{c} \quad (\,\mathrm{NGB\ at\ } N_\mathrm{c} \to \infty, \quad \mathrm{SSB\ of\ U}(N_f)_L \times \mathrm{U}(N_f)_R\,)$$

  $1/N_\mathrm{c}$-correction $\Rightarrow$ $\underline{\chi_\mathrm{t}^{\mathrm{quenched}} \simeq \frac{F_\pi^2 M_{\eta'}^2}{2N_\mathrm{f}}}$ no U(1) SSB at finite N_c

  - For $m_u = m_d = 0$, $m_s > 0$:

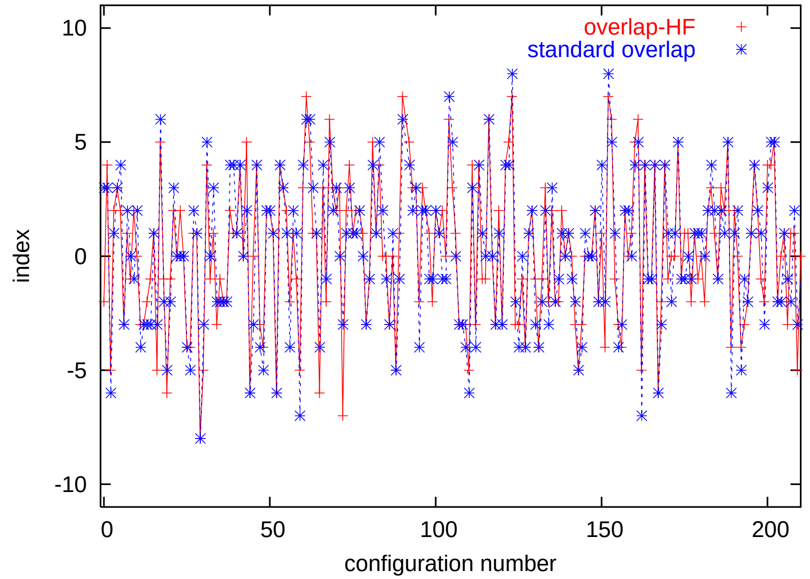
    $$\chi_\mathrm{t}^{\mathrm{quenched}} \simeq \frac{F_\pi^2}{6}\left(M_{\eta'}^2 + M_\eta^2 - 2M_K^2\right)$$

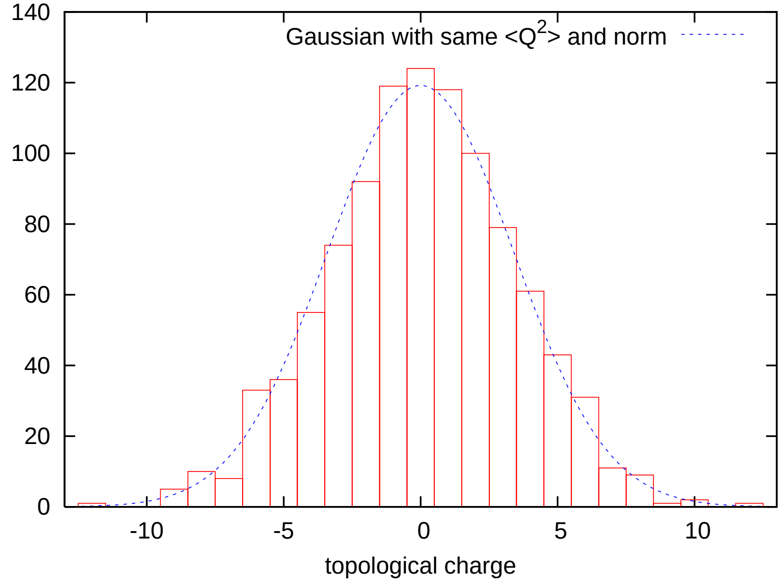
- QCD with dynamical quarks plus <u>axion</u>: $\chi_\mathrm{t} \simeq F_{\mathrm{axion}}^2 M_{\mathrm{axion}}^2$

  Dark Matter candidate ? [Lattice studies: Petreczky et al. '16, Borsanyi et al. '16 . . .]

Example for a direct measurement of $\langle Q^2 \rangle$ in quenched QCD [W.B./Shcheredin '06]

$Q :=$ index of $D_{\rm chiral}$ $(V = 12^3 \times 24,\ \beta = 5.85 \ \Rightarrow \ a \simeq 0.123\,{\rm fm})$

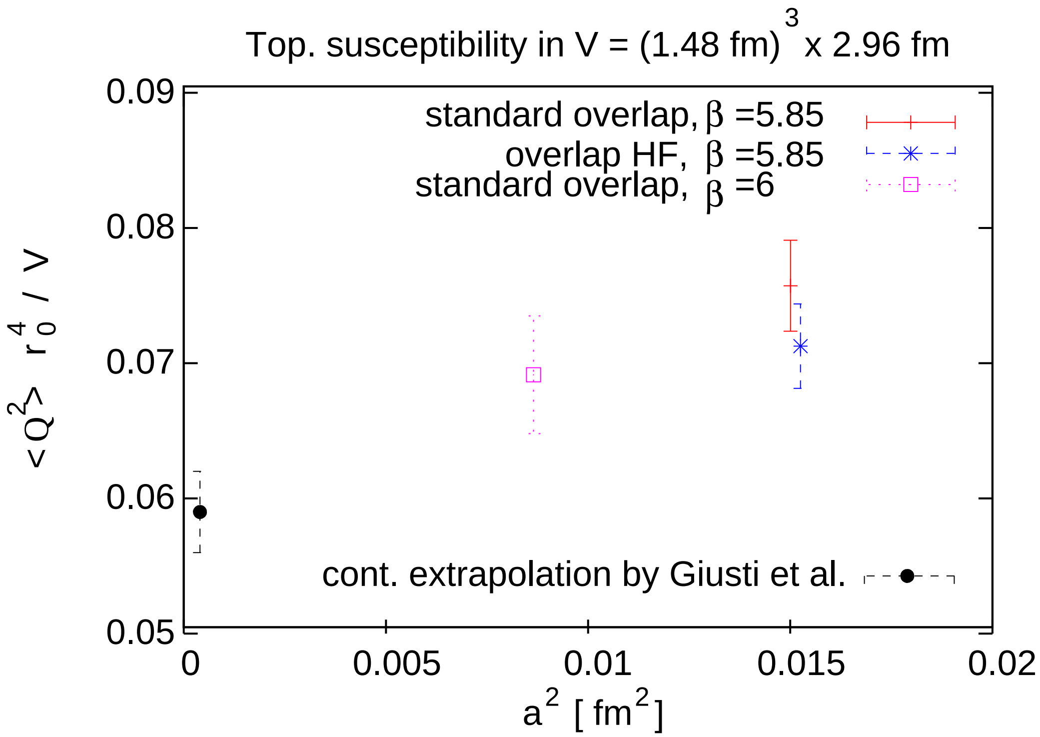




History well de-correlated

histograms for standard overlap and overlap hypercube $\approx$ Gaussian

width $\Leftrightarrow$ $\chi_{\rm t}$



$$M_{\eta'} \simeq 1\,\mathrm{GeV} \pm 60\,\mathrm{MeV}$$

Compatible with Witten-Veneziano formula at $M_{\eta'} = 958\,\mathrm{MeV}$

High statistics and cont. extrapolation: Del Debbio et al. '05, Dürr et al. '07 . . .

Fine lattices: top. sectors separated by high potential walls

Markov chain with small updates: confined to one sector over a LONG computation time.

QCD: autocorrelation time with respect to Q at least $\propto a^{-10}$
lattice spacing $a \lesssim 0.05\,\mathrm{fm}$ intractable (?) [Schaefer/Sommer/Virotta '11]
Main source of systematic errors: further suppression not straightforward

Can we still measure $\chi_{\rm t}$? Yes, by indirect methods !

• BCNW formula:
Works quite well to determine $\langle \mathcal{O} \rangle$ from $\langle \mathcal{O} \rangle|_{|Q|}$, but large uncertainties for $\chi_{\rm t}$

• Aoki-Fukaya-Hashimoto-Onogi (AFHO) '07: formula exclusively for $\chi_{\rm t}$

$$\langle q_0 \, q_x \rangle|_{|Q|,\,\mathrm{large}\,|x|} \approx -\frac{\chi_{\rm t}}{V} + \frac{Q^2}{V^2}$$

q_x: top. charge density, plateau value of correlation $\Rightarrow$ $\chi_{\rm t}$

Successful in some regime, similar to BCNW (small $|Q|$, $\langle Q^2 \rangle \gtrsim 1.5$);
large V $\to$ tiny signal, to be extracted by all-to-all correlations [Bautista et al., '15]

Slab Method

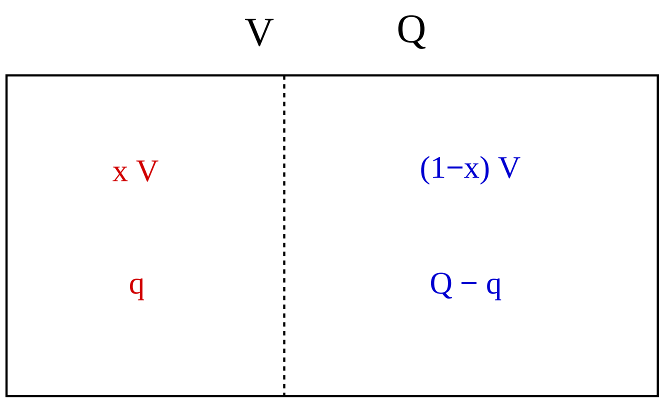
[W.B./de Forcrand/Gerber '15]

Assume Gaussian distribution of top. charges,

$$p(Q) \propto e^{-Q^2/(2\chi_t V)}$$

usually well approximated.

Split volume V into sub-volumes := **slabs** of sizes xV, $(1-x)V$ $\quad (0 < x < 1)$



Total charge $Q \Rightarrow$ slab charges $\sum_y q_y$: q, $Q-q \in \mathbb{R}$ (face between slabs non-periodic)

Probability distribution (at fixed V, x, Q):

$$p_1(q)\, p_2(Q-q) \quad \propto \quad \exp\left(-\frac{q^2}{2\chi_t V x}\right) \cdot \exp\left(-\frac{(Q-q)^2}{2\chi_t V(1-x)}\right)$$

$$\propto \quad \exp\left(-\frac{1}{2\chi_t V}\,\frac{q'^{\,2}}{x(1-x)}\right), \qquad q' := q - xQ$$

$$\langle q \rangle = xQ \quad \Rightarrow \quad \langle q'^{\,2} \rangle = \langle q^{\,2} \rangle - x^2 Q^2$$

Measure $\langle q^{\,2} \rangle \;\Rightarrow\; \langle q'^{\,2} \rangle$ at fixed Q, V and varying x (same confs)

fit to parabola $\chi_t V\, x(1-x) \quad \Rightarrow \quad \chi_t$

The 2d O(3) Model (Heisenberg model)

Popular in **solid state physics**: model for ferromagnets. **Particle physics**: toy model for QCD: **asymptotically free, dyn. generated mass gap, top. sectors**

Continuum $\vec{e}(x) \in S^2$ (periodic boundary conditions)

$$S[\vec{e}] = \frac{\beta}{2} \int d^2x \; \partial_\mu \vec{e} \cdot \partial_\mu \vec{e} \; , \quad Q[\vec{e}] = \frac{1}{8\pi} \int d^2x \; \epsilon_{\mu\nu} \, \vec{e} \cdot (\partial_\mu \vec{e} \times \partial_\nu \vec{e}) \in \mathbb{Z}$$

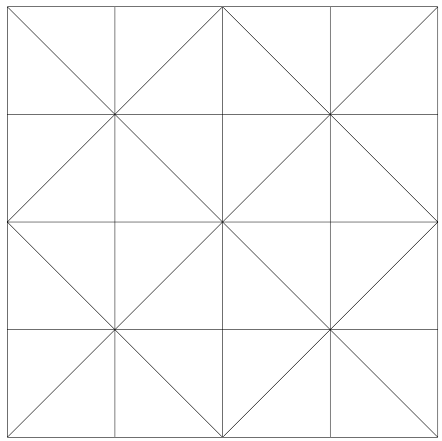
Lattice actions $\vec{e}_x \in S^2$ i.e. $|\vec{e}_x| = 1 \; \forall x$, lattice units: $a = 1$, $|\hat{\mu}| = 1$

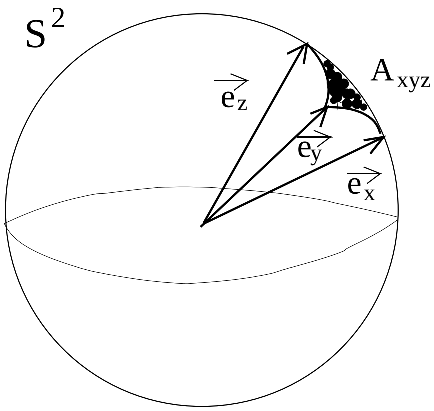
Standard $S[\vec{e}] \; = \; \frac{\beta}{2} \sum_{x,\mu} (\vec{e}_{x+\hat{\mu}} - \vec{e}_x)^2 = \beta \sum_{x,\mu} (1 - \vec{e}_x \cdot \vec{e}_{x+\hat{\mu}})$

Manton $S[\vec{e}] \; = \; \frac{\beta}{2} \sum_{x,\mu} \mathrm{arccos}^2 (\vec{e}_x \cdot \vec{e}_{x+\hat{\mu}})$

Constraint $S[\vec{e}] \; = \; \sum_{x,\mu} s(\vec{e}_x, \vec{e}_{x+\hat{\mu}}), \;\; s(\vec{e}_x, \vec{e}_{x+\hat{\mu}}) = \begin{cases} 0 & \vec{e}_x \cdot \vec{e}_{x+\hat{\mu}} > \cos\delta \\ +\infty & \text{otherwise} \end{cases}$

Lattice: Geometric def. of Q Triangle decomposition of each plaquette, $\langle xyz \rangle$



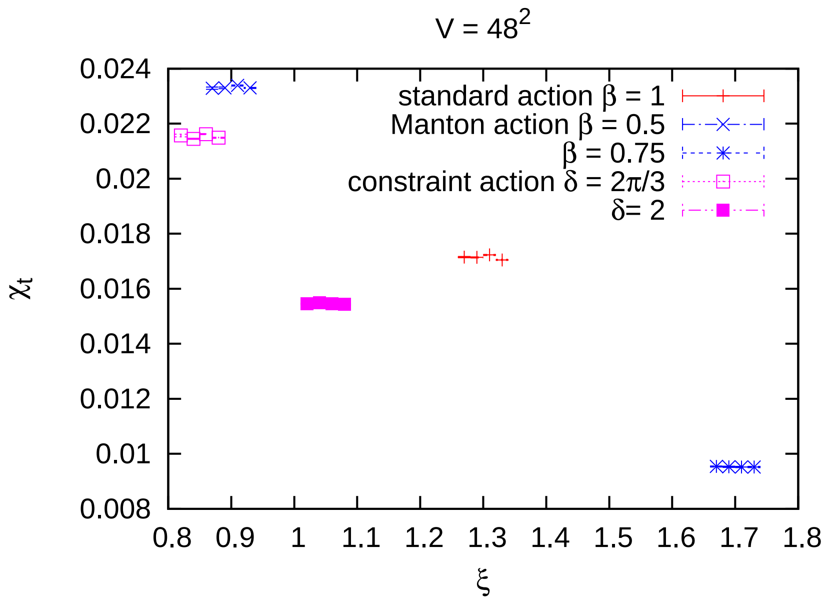


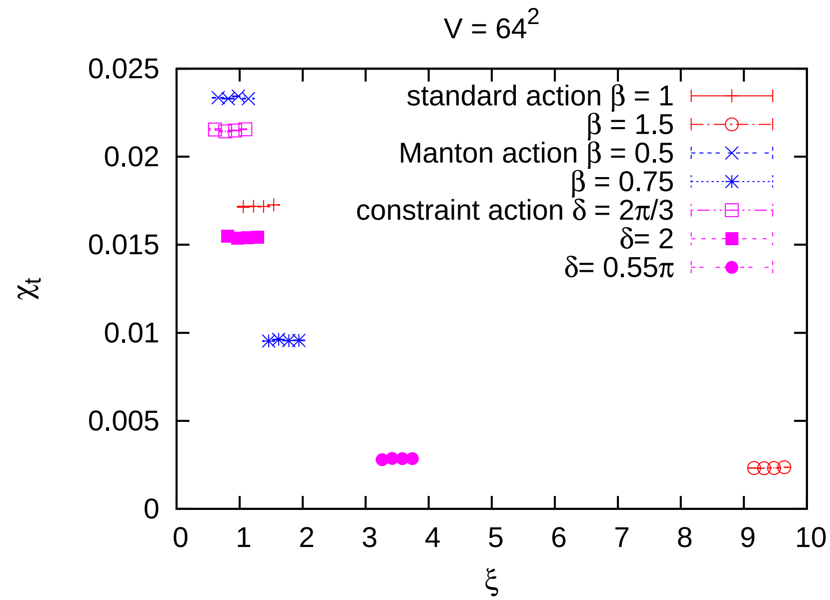
A_{xyz} : (minimal) oriented solid angle spanned by $\vec{e}_x, \ \vec{e}_y, \ \vec{e}_z$

$$Q[\vec{e}] = \frac{1}{4\pi} \sum_{\langle x,y,z \rangle} A_{xyz}$$

Periodic b.c.: sum covers S^2 just $Q \in \mathbb{Z}$ times

Geometric formulation of Q, three lattice actions



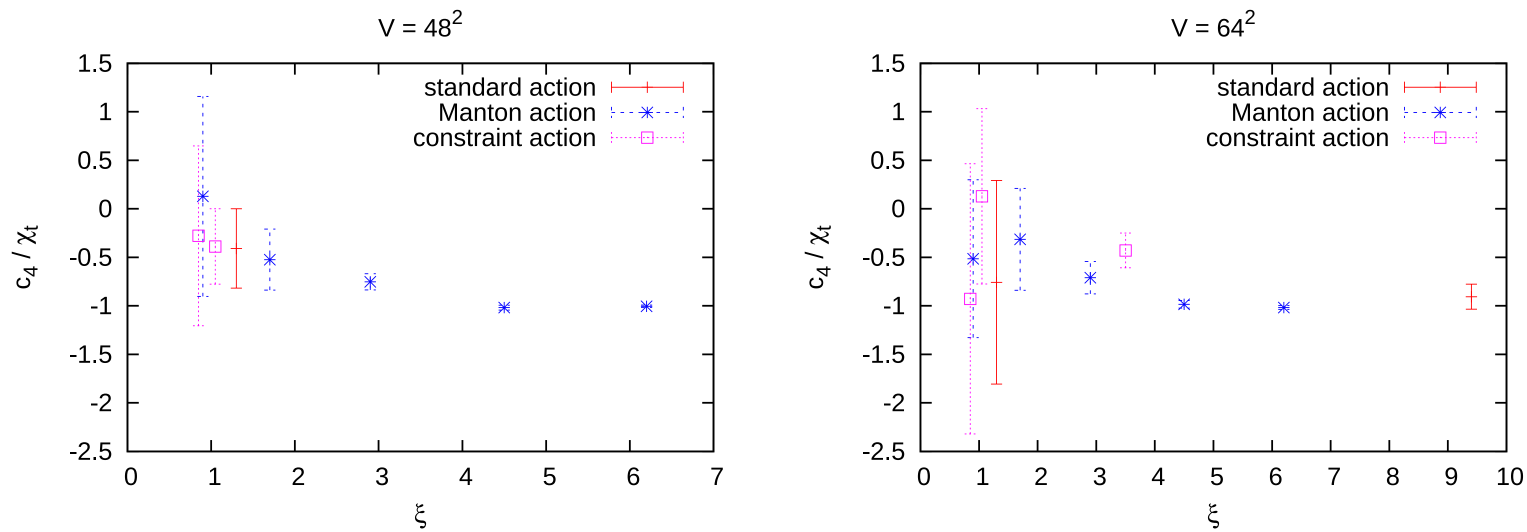


Each quadruplet of points shows (from left to right): χ_t directly measured (feasible with cluster algorithm), and with slab method at $|Q| = 0,\, 1,\, 2$

Kurtosis

$$c_4 = \frac{1}{V}\Big(3\langle Q^2\rangle^2 - \langle Q^4\rangle\Big) = -\frac{1}{V}\langle Q^4\rangle_{\rm connected}$$

measures deviation from a Gauss distribution (Gaussian: $c_4 = 0$)



Cont. limit $\xi \to \infty$: $c_4/\chi_{\rm t} \approx -1$ (stable in V) Value of a dilute instanton gas !

- 4d SU(3) YM theory: $c_4/\chi_{\rm t} \approx -0.26$

  [Panagopoulos/Vicari '11, Cè et al. '15, Bonati/D'Elia/Scapellato '16]

2-Flavour QCD

- Wilson gauge action, q_x from lattice discretised $F_{\mu\nu}\tilde{F}_{\mu\nu}$

  after smoothing, $\sum_x q_x$ is rounded to $Q \in \mathbb{Z}$

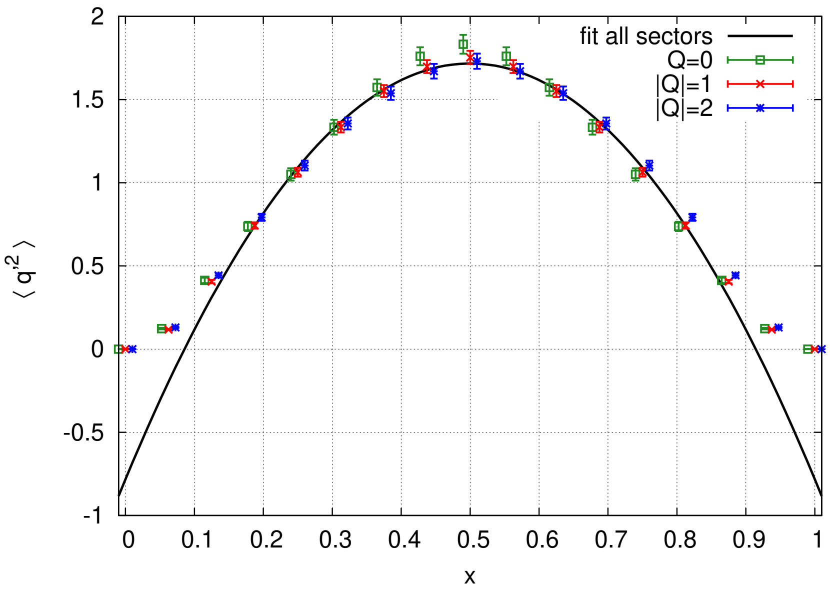
- Twisted mass quarks, $M_\pi \simeq 650\,\mathrm{MeV}$

- $20\,000$ confs, $V = 16^3 \times 32$, $\beta = 3.9 \;\Rightarrow\; a \simeq 0.079\,\mathrm{fm}$

Gradient flow: smoothing of the confs,
corresponds to RG transformation [Lüscher '10]

Lüscher's reference scale $\langle E \rangle\, t_0^2 = 0.3$, here: $t_0/a^2 = 2.42$

Slabs: $16^3 \times 32x$ and $16^3 \times 32(1-x)$



$\langle {q'}^2 \rangle(x)$ for $|Q| = 0,\ 1,\ 2$ at $t = 5t_0$

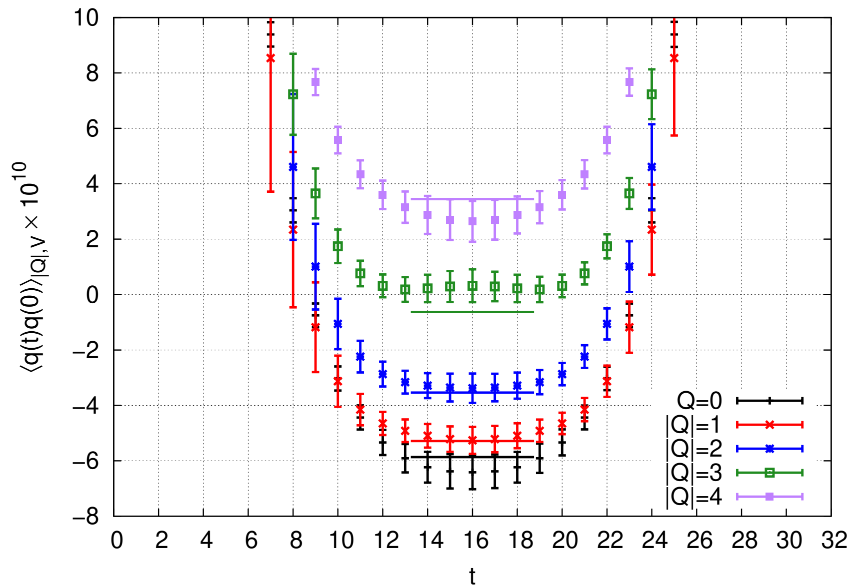
$x \gtrsim 0$ and $x \lesssim 1$: thin slabs involved, do not follow parabola

For $0.2 \lesssim x \lesssim 0.8$ matches well (joint) fit to:

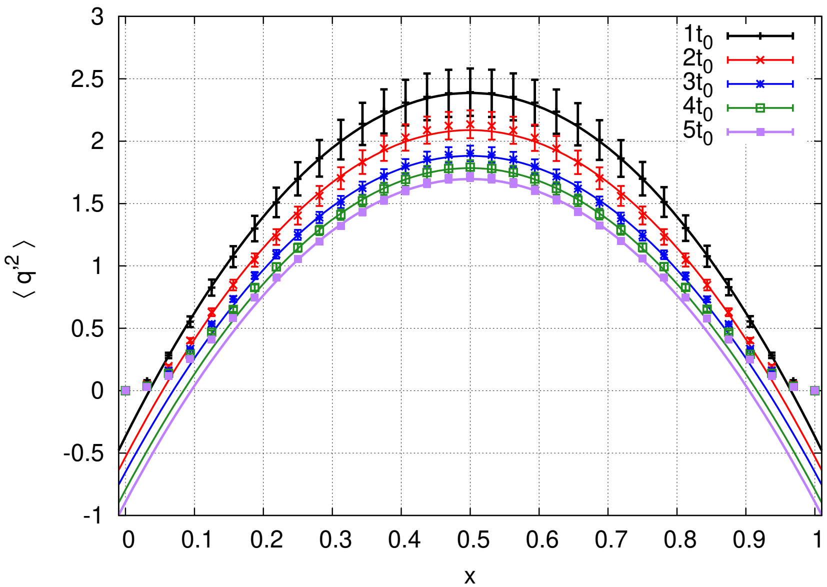
$$\langle {q'}^2 \rangle(x) = \chi_{\rm t} V x(1-x) + \text{const}$$

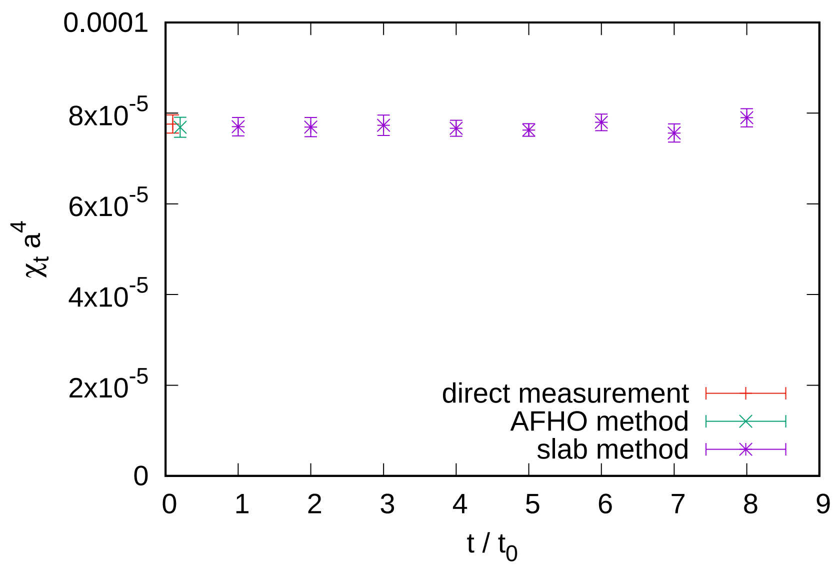
Perfect agreement with other methods:

$$\chi_t\, a^4 = \begin{cases} 7.76(20)\cdot 10^{-5} & \text{direct} \\ 7.63(14)\cdot 10^{-5} & \text{slab method for } |Q| \le 2 \\ 7.69(22)\cdot 10^{-5} & \text{AFHO method for } |Q| \le 2 \end{cases}$$



Data for $\langle q_0\, q_t\rangle|_{|Q|} \simeq -\frac{\chi_t}{V} + \frac{Q^2}{V^2}$ at flow time $6t_0$





Left: $\langle {q'}^2 \rangle(x)$ in the sector $|Q| = 1$, at $t = t_0 \ldots 5t_0$

Long flow time: reduces stat. errors, enhances deviations at extreme x

Right: $\chi_t \, a^4 \cdot 10^5 \simeq 7.7(2)$ **is stable under Gradient Flow**

Subtractive constant $\propto \sqrt{t}$ (like diffusion range)

Conclusions about the Slab Method

Simple approach to measure $\chi_{\rm t}$ within a fixed top. sector, hardly any computational cost

Only assumption: Gauss-distribution of top. charges (works well)

[Generalisation to $p(Q) \propto \exp(-a_1 Q^2 - a_2 Q^4)$ is feasible, determines also c_4]

Precision best for small $|Q|$, not affected by "topological slowing down",
but persistent finite-size effects (polynomial at fixed topology)

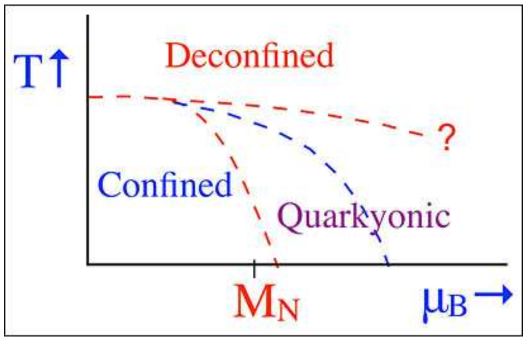
Successful tests in

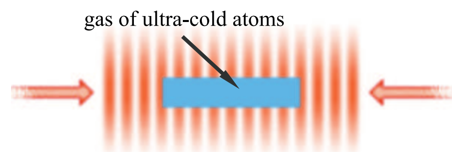
- non-linear σ-models: straight application

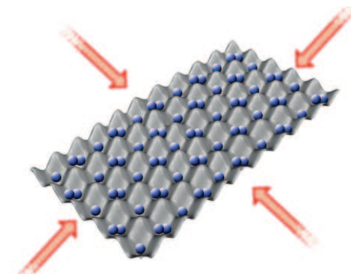
  1d O(2) model: ‰-level precision, 2d O(3): %-level

- 2-flavour QCD: %-level, stable within gradient flow time $t_0 \dots 8t_0$

Outlook: Millennium problem: **QCD phase diagram at high baryon density**







$T_{\text{crossover}} \approx 155\,\text{MeV}$, but finite density needs chemical potential $\Rightarrow$ Euclidean QCD action $\in \mathbb{C}$, $p[U] = \frac{1}{Z}\exp(-S_{\text{QCD}}[U]) \notin \mathbb{R}$, not a probability
straight Monte Carlo fails (re-weighting requires statistics $\propto \exp(c\,V)$, "sign problem")

Possible solution: (analog) quantum computing, complex phase is included.

Proposal for 2d $\mathbb{C}$P(2) model (topology, asympt. freedom, dyn. mass gap $\sim$ QCD):
ultra-cold (nK) Alkaline Earth Atoms trapped in optical lattice: nuclear spin as SU(3) field,
SSB SU(3) $\rightarrow$ U(2), low energy action for Nambu-Goldstone bosons $\stackrel{!}{=}$ $\mathbb{C}$P(2) model

Laflamme/Evans/Dalmonte/Gerber/Mejía-Díaz/W.B./Wiese/Zoller '16; to be implemented in Trieste