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. QCD and Chiral Perturbation Theory

QCD simulations in the δ-regime

IV. Topological summation and density correlation

approach to a problem ahead of us

V. Prospects for Quantum Simulations ?

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

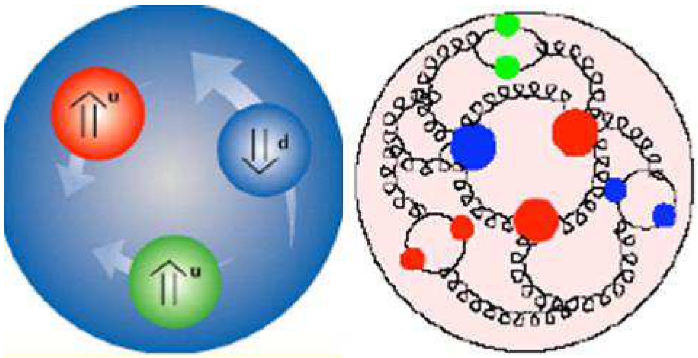
mesons ("consisting of a quarks-antiquark pair (q $\bar{\mathrm{q}}$)") such as pions.

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

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

$\Rightarrow$ 3 valence quarks together account for $\approx 1\ \%$ of the nucleon masses $M_{\mathrm{p,\,n}} \simeq 939\ \mathrm{MeV}$

$99\ \%$ of the masses of macroscopic objects *binding energy*, a *mess of gluons and sea-quarks* inside the nucleons.



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 fields, $\hbar = 1$)
- Vacuum Expectation Value of an 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 for field 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 on lattice sites x

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

Idea of Lattice Simulations :

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

Summation over this set $\rightarrow$ measure observables (n-point functions) up to

- statistical errors (finite set), can be estimated and reduced with enlarged statistics
- systematic errors (finite a, finite volume $\ldots$), can be varied and extrapolated, estimate error in physical limit (continuum, $V \rightarrow \infty \ldots$)

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

Monte Carlo Simulation and Numerical Measurement

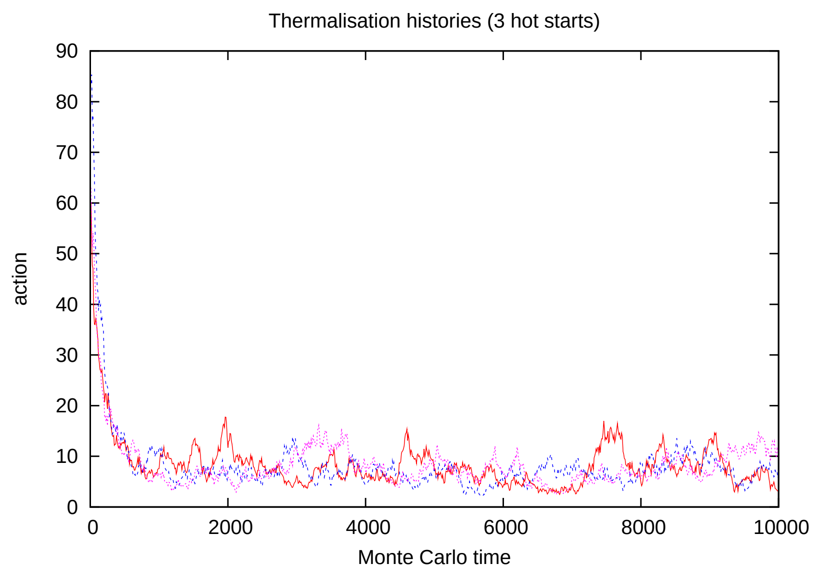
Start sequence of conf's $[\Phi] \to [\Phi'] \to [\Phi''] \ldots$ *e.g.* from a random conf. ("hot start")

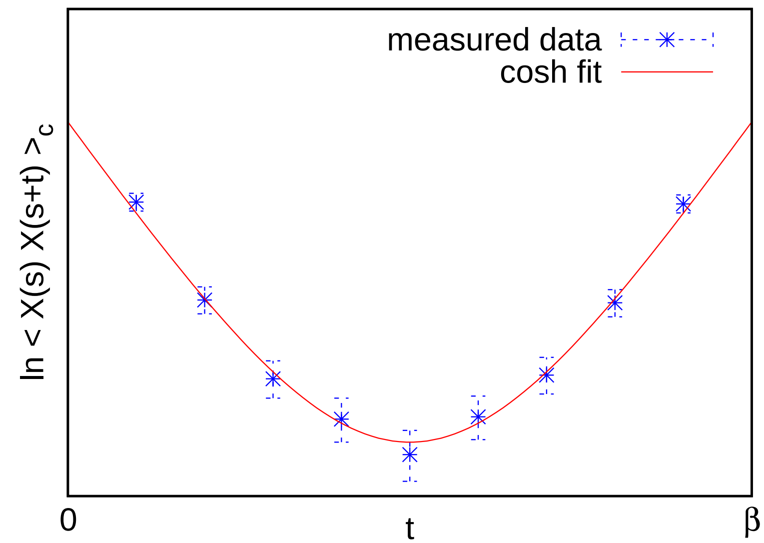
Condition: "Detailed Balance" for transition between confs. $\Phi_1 \longleftrightarrow \Phi_2$:

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

after many steps correct statistical distribution $\propto p[\Phi]$

First discard many steps, until the right regime is attained (“thermalisation”).
Then pick well separated (“de-correlated”) confs to measure observables.





With this set, measure *e.g.* connected correlation function

$$\langle X(\vec{x}, s) X(\vec{x}, s+t) \rangle_c \; \propto \; \cosh(M(t - \beta/2))$$

X : (product of) fields, separated by Euclidean time t (periodic boundary conditions).

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

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

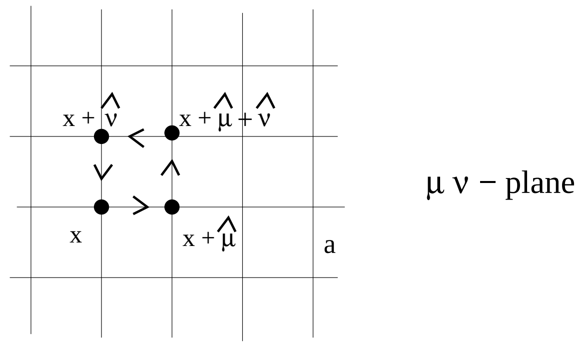
$$\Phi_x^* \Phi_{x+\hat{\mu}} \to \Phi_x^* U_{x,\mu} \Phi_{x+\hat{\mu}} \ , \qquad U_{x,\mu} \in \mathrm{U}(1)$$

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

Discrete covariant derivative, **regularised system is gauge invariant.**
Deal with "compact link variables" $\in$ gauge group, also 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 $\to$ gauge invariant

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

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 $\to$ lattice sites
- internal degrees of freedom (spinor index, ev. flavour and 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.

Components $\bar{\psi}_i$, ψ_j anti-commute,

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

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

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 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, in QCD: quarks cost $O(100)$ 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 $P = \bar{\Psi}\gamma_5\Psi$

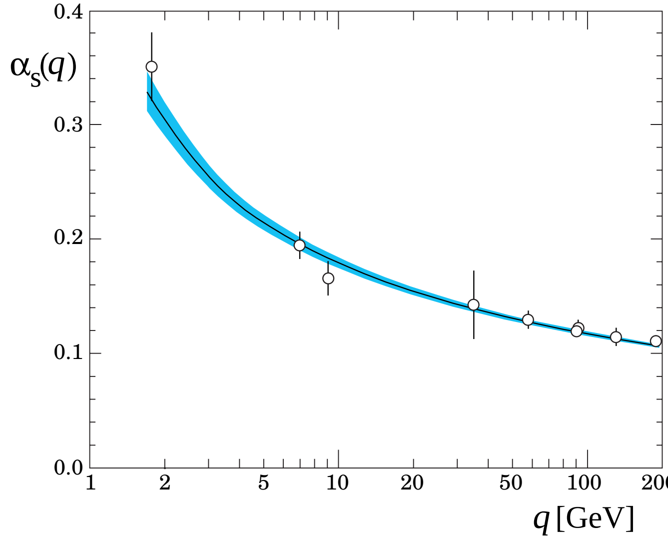
$\langle P_x \, P_y \rangle_c \propto \exp(-M_\pi |x - y|) \;\Rightarrow\;$ pion mass M_π

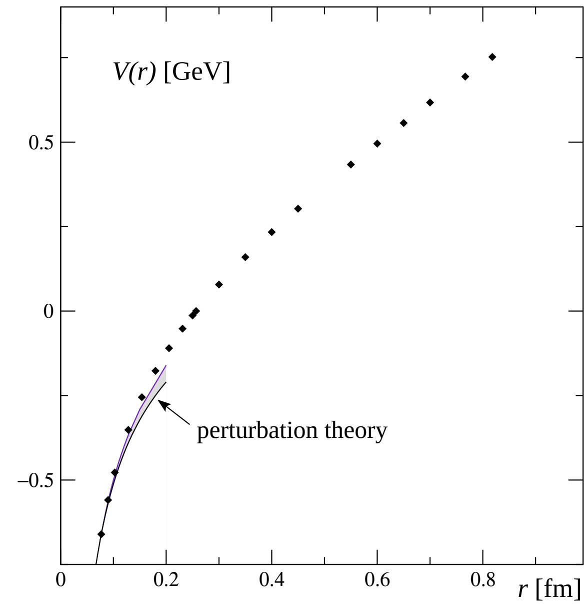
$\Rightarrow$ Explicit results for hadron masses, matrix elements, critical temperature for transition: confinement $\leftrightarrow$ de-confinement, decay constants, topological susceptibility, etc.

REALLY based on QCD.

Method also applies to other quantum field theories, like

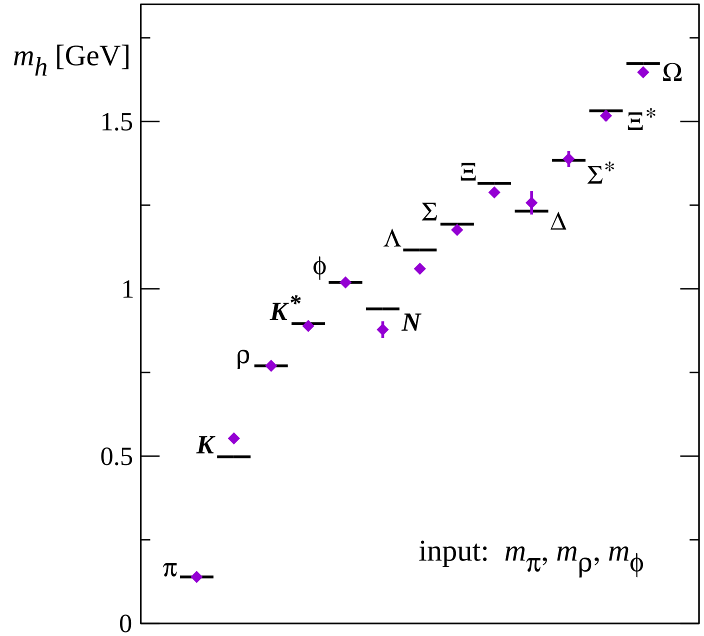
QED, Higgs theory, models for condensed matter . . .





- Left: strong coupling $\alpha_s(q) = g_s^2(q)/4\pi$ at transfer momentum q.
  Fit: $\alpha_s(q) \propto 1/\ln(q/\Lambda_{QCD})$ $\quad (\Lambda_{QCD} \approx 250 \text{ MeV})$

- Right: the potential between static quarks;
  numerical results confirm confinement. $\quad (0.2 \text{ fm} \simeq (1 \text{ GeV})^{-1})$



Hadron Masses :

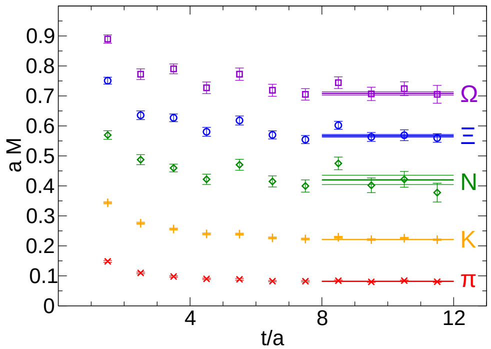
Status: year 2002 (CP-PACS Collaboration), "quenched" simulations (generate conf's with $\det M = 1$, corresponds to $N_f = 0$)

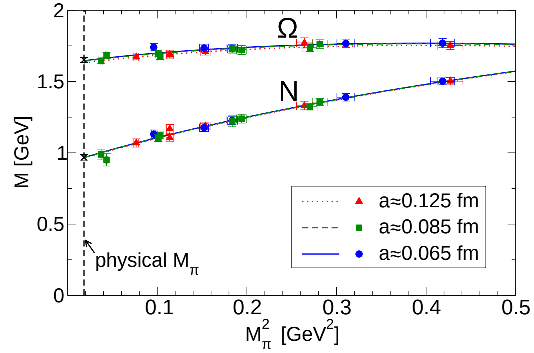
Simulation much faster, but uncontrolled systematic error (no sea quarks).

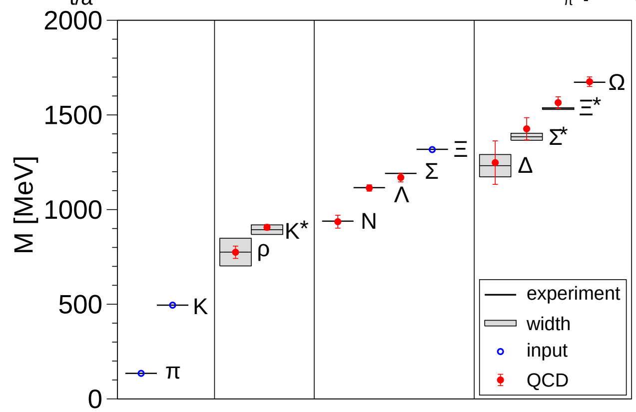
Compared to experiment: agreement up to $\approx 10\% \ldots 15\%$

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 ≈ 190 MeV. System size $L \simeq 4/m_\pi$ *i.e.* up to 4 fm : finite size effects under control. Continuum extrapolation based on lattice spacings $a = 0.125$ fm, 0.085 fm, 0.065 fm.

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

New 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,

[*Phys. Lett. B 690 (2010) 436* and *Phys. Rev. D 84 (2011) 054509*]

Traditional treatment of $2+1$ flavours:

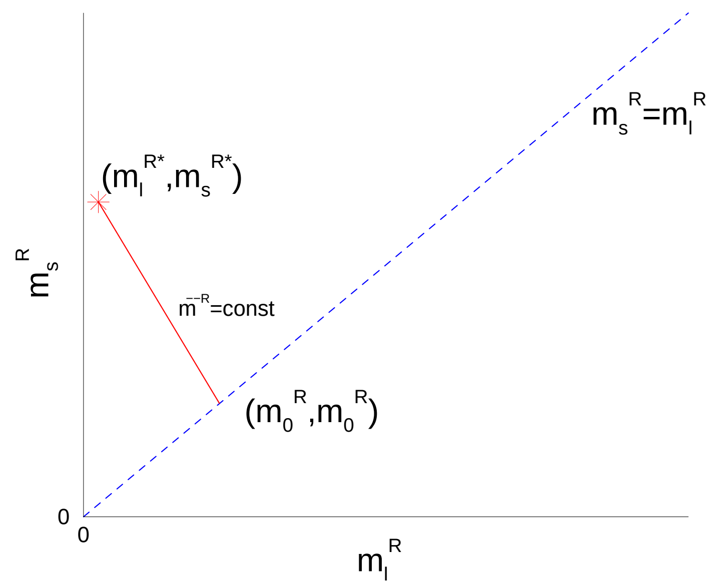
1. Get kaon mass M_K (resp. renormalised s-quark mass) $\approx$ right
2. Push for lighter pions, keeping $M_K \approx \mathrm{const.}$

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)

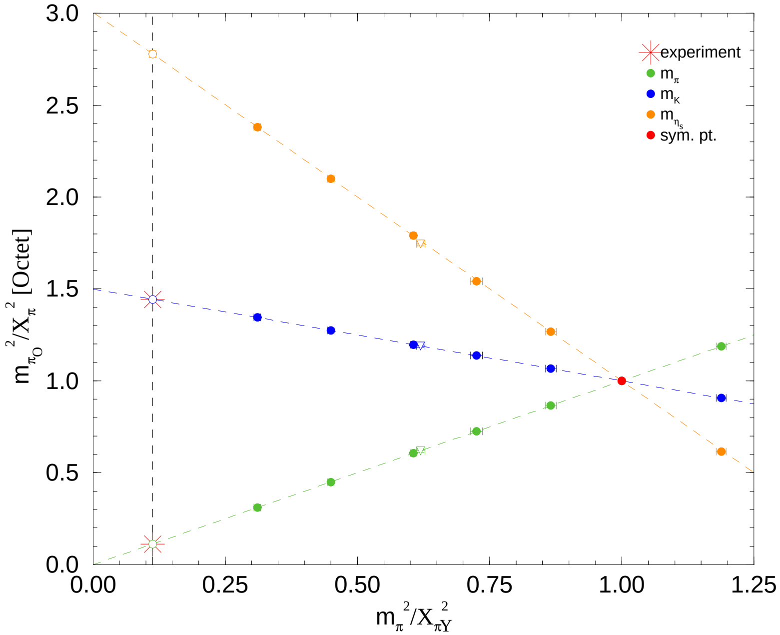
   M_π down, M_K up; χPT safe guide in extrapolation

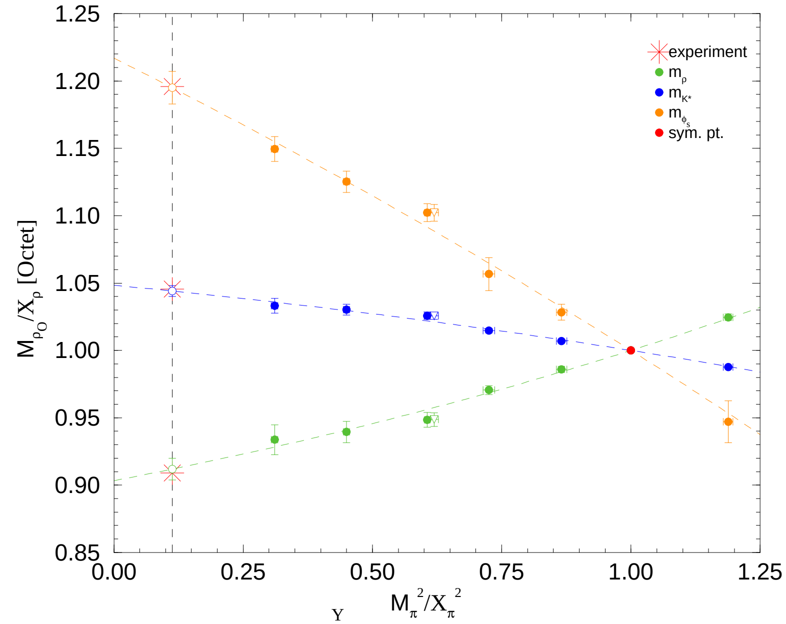


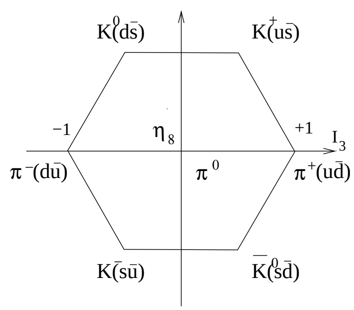
• Virtue: trajectory towards physical point $(m_l^{R\,*},\, m_s^{R\,*})$ is constrained and stable. Any flavour singlet quantity $X_S(\bar{m}_0^R)$ $(\bar{m}_0^R = m_l^R = m_s^R)$ obeys under quark mass variations

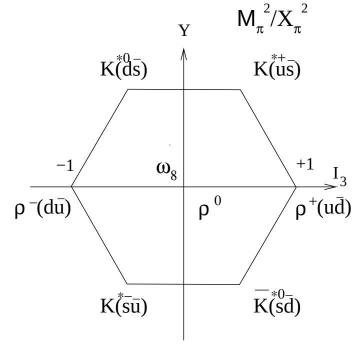
$$X_S(\bar{m}_0^R + \delta m_l^R, \bar{m}_0^R + \delta m_s^R)\Big|_{2\delta m_l^R + \delta m_s^R = 0} = X_S(\bar{m}_0^R, \bar{m}_0^R) + \underline{O\Big((\delta m^R)^2\Big)}$$

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





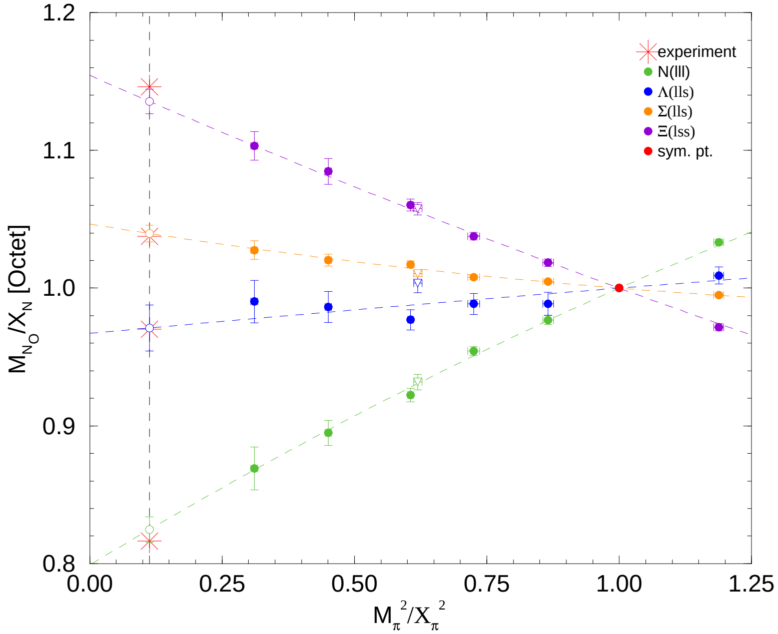


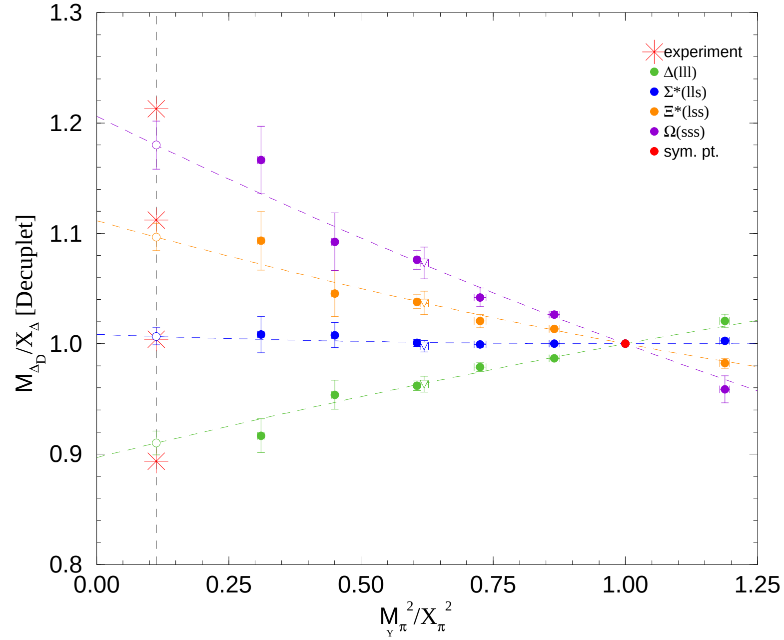


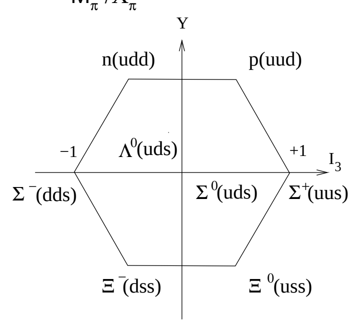
pseudo-scalars π, K, η_s

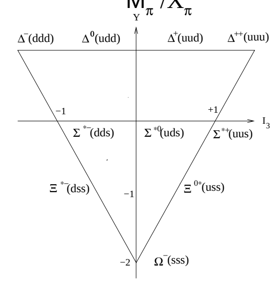
vector mesons ρ, K^*, ϕ

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



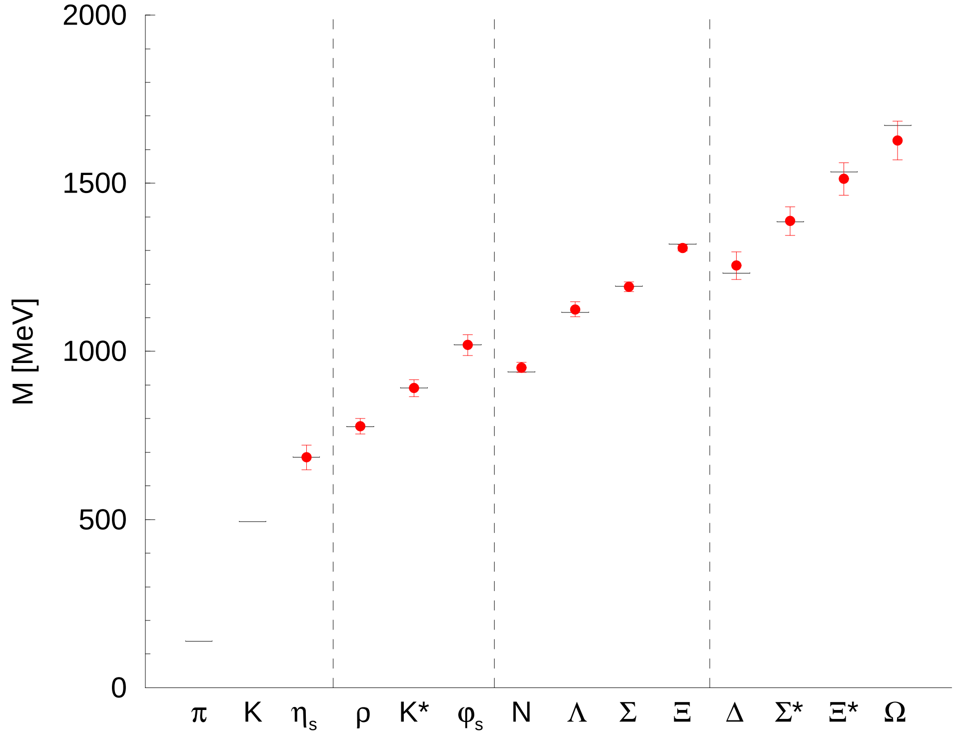






Nucleon (lll), Λ (lls), Σ (lls), Ξ (lss) Δ (lll), Σ^* (lls), Ξ^* (lss), Ω (sss)

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 Report, arXiv:1310.8555 [hep-lat]

III. QCD and Chiral Perturbation Theory (χPT)

QCD with massless quarks : L, R spinor components decouple

$$\mathcal{L}_{\rm QCD} = \bar\Psi_L D\Psi_L + \bar\Psi_R D\Psi_R + \mathcal{L}_{\rm gauge}$$

With N_f flavours: global symmetry

$$\mathrm{U}(N_f)_L \otimes \mathrm{U}(N_f)_R = \underbrace{\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R}_{\text{chiral flavour sym.}} \otimes \underbrace{\mathrm{U}(1)_{L=R}}_{\text{baryon number}} \otimes \underbrace{\mathrm{U}(1)_{\rm axial}}_{\text{anomalous}}$$

Chiral flavour symmetry breaks spontaneously

$$\mathrm{SU}(N_f)_L \otimes \mathrm{SU}(N_f)_R \;\rightarrow\; \mathrm{SU}(N_f)_{L+R}$$

χPT : eff. Lagrangian with field $U(x) \in \mathrm{SU}(N_f) \equiv$ coset space $\qquad m_q \gtrsim 0$:

$N_f^2 - 1$ quasi Nambu-Goldstone bosons $\sim$ light mesons

(Weinberg '79, Gasser/Leutwyler '82 . . . '88)

Consider $N_f = 2$; $\mathbf{m_q}$: mass for (degenerate) u and d quark
U captures $\pi^0, \ \pi^\pm$. Leading terms in effective low energy Lagrangian:

$$
\begin{aligned}
\mathcal{L}_{\text{eff}}[U] = & \frac{\mathbf{F_\pi^2}}{4} \mathrm{Tr}[\partial_\mu U^\dagger \partial_\mu U] + \frac{\mathbf{\Sigma \, m_q}}{2} \mathrm{Tr}[U + U^\dagger] \\
& - l_1 \frac{1}{4} \left(\mathrm{Tr}[\partial_\mu U^\dagger \partial_\mu U]\right)^2 - \ l_2 \frac{1}{4} \left(\mathrm{Tr}[\partial_\mu U^\dagger \partial_\nu U]\right)^2 \\
& -(l_3 + l_4) \Big(\frac{\Sigma m_q}{2F_\pi}\Big)^2 \left(\mathrm{Tr}[U^\dagger + U]\right)^2 + l_4 \frac{\Sigma m_q}{4F_\pi} \mathrm{Tr}[\partial_\mu U^\dagger \partial_\mu U] \ \mathrm{Tr}[U^\dagger + U] + \dots
\end{aligned}
$$

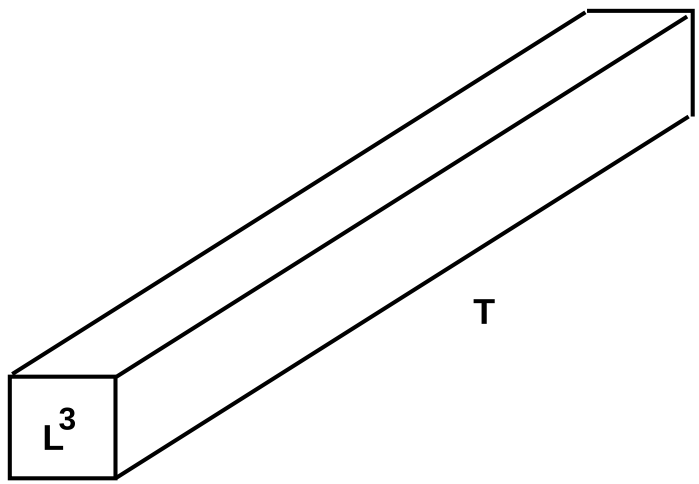
$\mathbf{F_\pi}$	:	pion decay constant	Low Energy Constants
$\mathbf{\Sigma}$	:	chiral condensate	
$l_1, \ l_2, \dots$			

LECs : Free parameters in χPT,
evaluation only from **fundamental theory**, *i.e.* **QCD**

Challenge : **Non-perturbative QCD results for LECs from lattice simulations**

- **δ-Regime of QCD** (H. Leutwyler '87)

Small spatial volume, say $L^3 \times T$, $L \lesssim \xi \ll T$ (opposite to finite temperature)

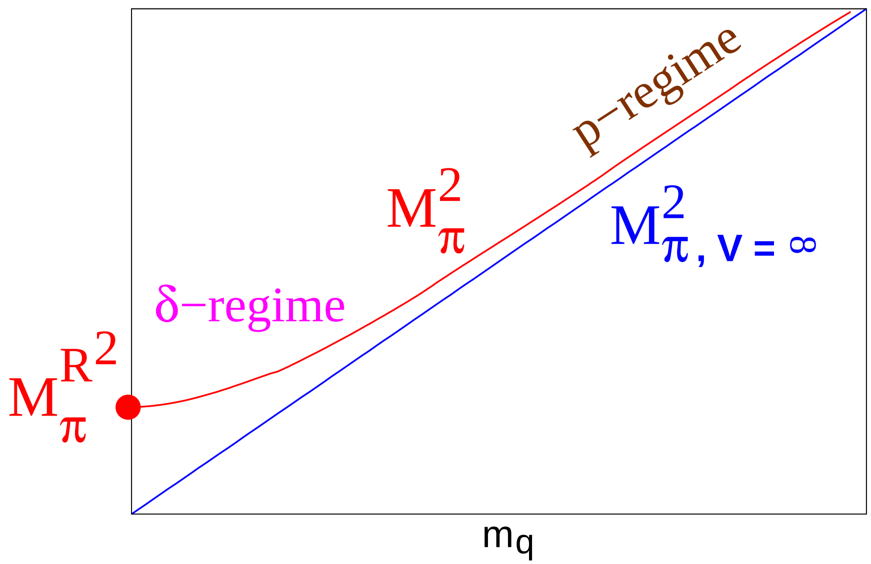


Analytical treatment ≈ quantum rotator, 1d O(4) ∼ SU(2)⊗SU(2) model

Experimentally not accessible, but simulations are possible, determine LECs (same as in $V = \infty$)

Finite volume $\longrightarrow$ no spont. sym. breaking. In the chiral limit $m_q \to 0$:

Residual pion mass M_π^R Schematically:



Fixed spatial box :

- Large m_q : behaviour of p-regime: $M_\pi^2 \propto m_q$ (Gell-Mann/Oakes/Renner relation)
- Small m_q : strong finite size effects, behaviour of δ-regime

Result of δ-expansion : mass gap for rotator spectrum $E_\ell = \ell(\ell+2)/(2\Theta)$

$$M_\pi^R = \frac{3}{2F_\pi^2 L^3(1+\Delta)}$$

$$\Delta = \frac{0.452}{F_\pi^2 L^2} + \frac{0.0884}{F_\pi^4 L^4}\left[1 - 0.160\Big(\ln(\Lambda_1 L) + 4\ln(\Lambda_2 L)\Big)\right]\ldots$$

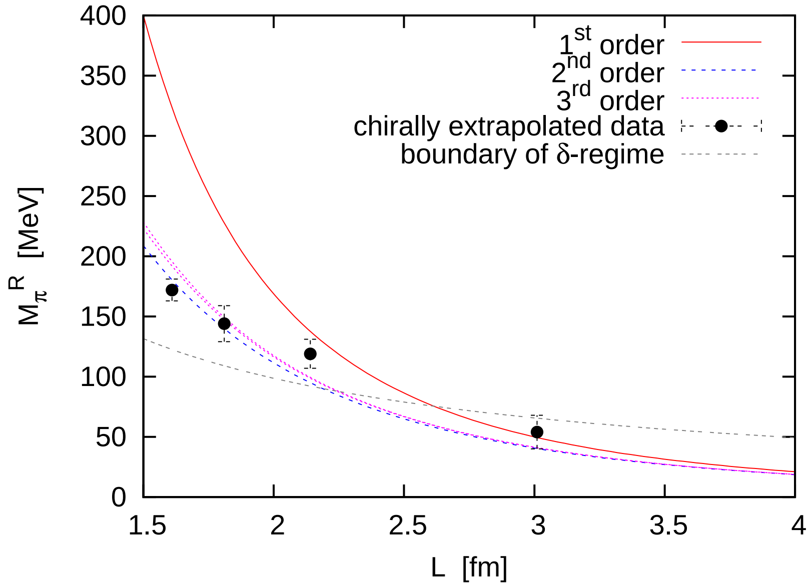
Λ_i : scale parameters for renormalised sub-leading LECs, $\bar{l}_i = \ln\left(\frac{\Lambda_i}{M_\pi^{\rm phys}}\right)^2$

$1^{\rm st}$ order : Leutwyler '87 $(\Theta \approx F_\pi^2 L^3 \;\rightarrow\; \Delta = 0)$
$2^{\rm nd}$ order : Hasenfratz/Niedermayer '93
$3^{\rm rd}$ order : Hasenfratz '10

Goal: measure M_π^R based on numerical simulations

$\rightarrow$ Test δ-regime predictions, determine LECs from first principles of QCD

Simulation results near transition zone and in δ-regime



Data down to $M_\pi^R < M_\pi^{\rm phys} \simeq 138 \ {\rm MeV}$, and in δ-regime $(M_\pi^R L \leq 1)$.

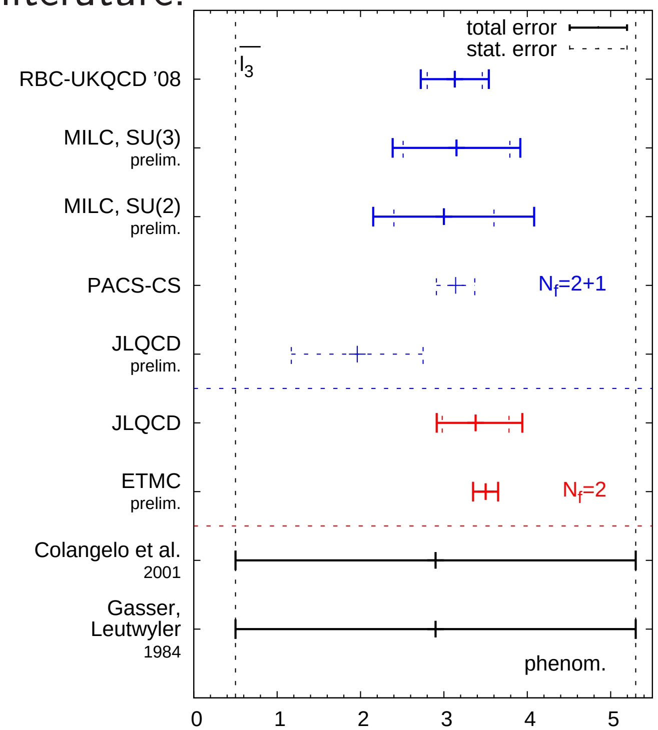
Good agreement with χPT prediction !

W.B., M. Göckeler, R. Horsley, Y. Nakamura, D. Pleiter, P.E.L. Rakow, G. Schierholz and J.M. Zanotti, Phys. Lett. B687 (2010) 410

Moreover, fits yield (with phen. values for F_π, $\bar{l}_1$, $\bar{l}_2$, $\bar{l}_4$)

$$\bar{l}_3 \;=\; 4.2(2)$$

In upper range compared to literature: (plot by E. Scholz)



World average according to FLAG Working Group : $\bar{l}_3 = 3.3 \pm 0.7$

IV. Topological Summation and density correlation

Motivation: Status of Lattice QCD

• For the light hadron spectrum, low energy QCD is now tested from 1^{st} principles and confirmed to ≈ 1 %. { K. Wilson's pessimism in 1989: will take > 30 years . . . }

⋆ 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.

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

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

Remedy: open boundary conditions (Lüscher) or top. summation (last subject of this talk)

- **Top. sectors for configurations in Quantum Field Theory**

  in space with periodic boundary conditions (torus).

  Examples:

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

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

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

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

Functional integral splits into separate integrals for each $Q \in \mathbb{Z}$.

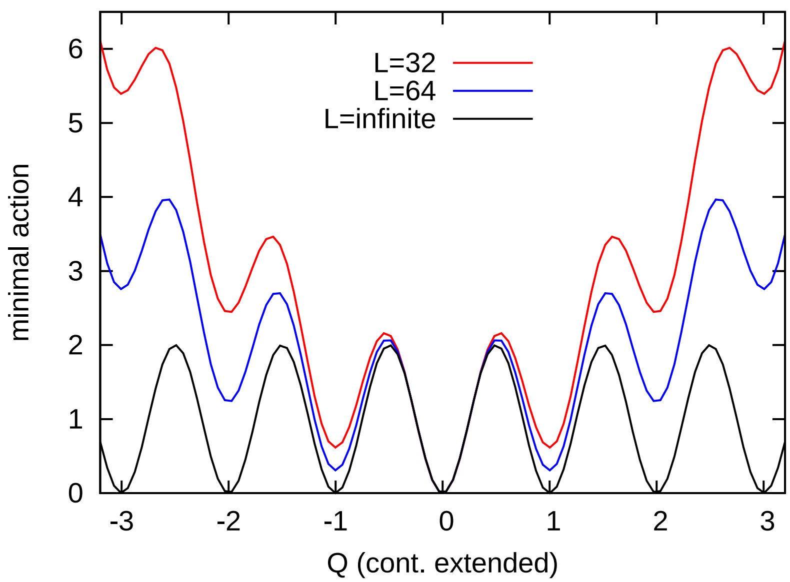
Example on the **lattice:** 2d U(1) lattice gauge theory

$Q = \frac{1}{2\pi} \sum_x \epsilon_{\mu\nu} U_{x,\mu\nu}$ (plaquette variable $U_{x,\mu\nu} = U^*_{x,\nu} U^*_{x+\hat\nu,\mu} U_{x+\hat\mu,\nu} U_{x,\mu}$)

Action minimum at fixed Q on $L \times L$ lattice (Sinclair '90)

$$S_{\min} = L - (L-1)\cos(2\pi Q/L) - \cos(2\pi Q(L-1)/L)$$

Interpolation to $Q \in \mathbb{R}$:



Monte Carlo Simulation

Generate a set of lattice configurations $[\Phi]$ with probability

$$p[\Phi] = \frac{1}{Z} \exp\{-S[\Phi]\}$$

Sum over this set to **compute expectation values** $\langle \dots \rangle$ of observables

Most popular algorithms to generate confs perform a sequence of **small update steps** *(Markov chain)*, 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.

Problem: local updates rarely change the top. sector

• 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.

⇒ Monte Carlo history tends to be **trapped** for a very long (computing) time (many, many update steps) in **one top. sector**.

Extremely long topological auto-correlation time.

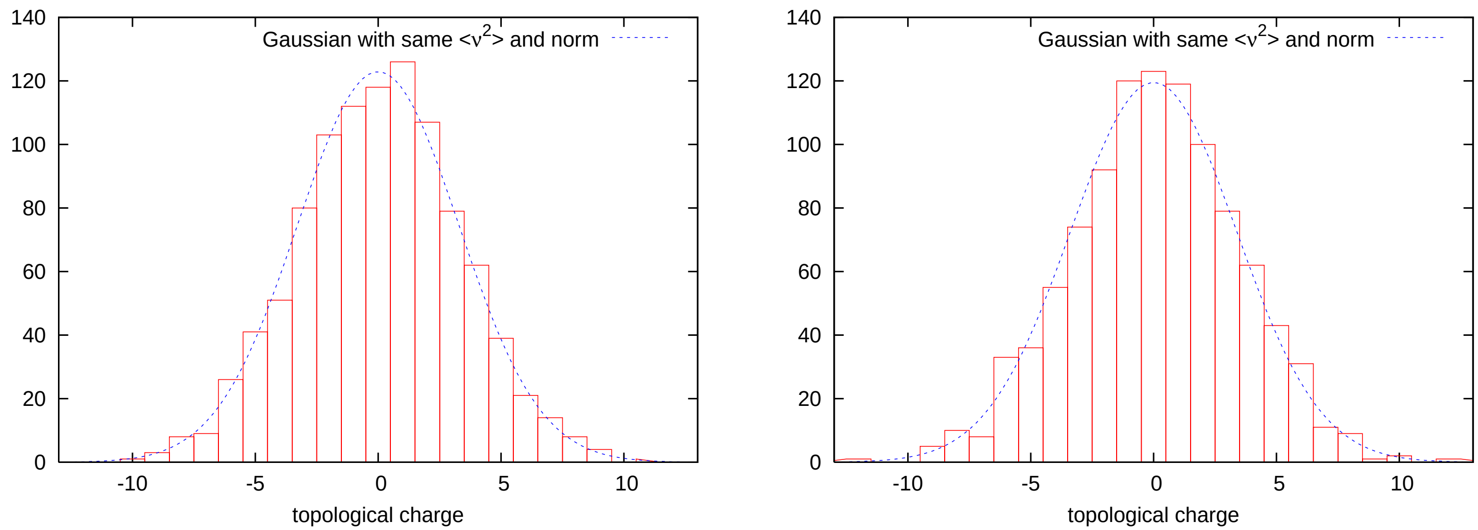
So how can we measure n-point functions, or the top. susceptibility

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

Should be summed over all sectors, with suitable statistical weight. . .

Easier in quenched QCD, results by W.B./Shcheredin '06

Charge histograms for overlap-HF (left) , and standard overlap (right)

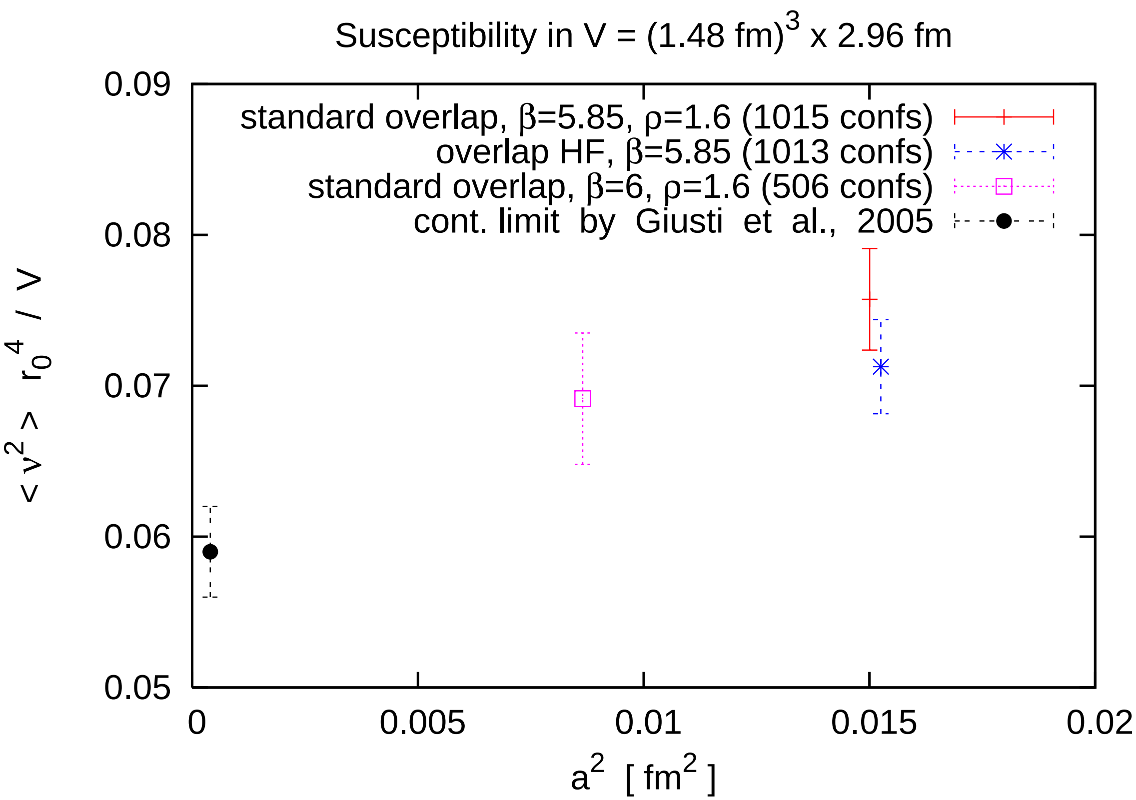


$\approx$ Gauss distribution (1013 conf's)

Peak profile $\sim$ **parity:** spontaneous breaking is not fully ruled out (Azcoiti/Galante '99)
No evidence for spontaneous parity breaking, nor kurtosis $\frac{1}{V}(3\langle Q^2\rangle^2 - \langle Q^4\rangle)$

[Consistent with Alles/D'Elia/DiGiacomo '05, Dürr/Fodor/Hoelbling/Kurth '07]

Topological susceptibility $\chi_t = \frac{1}{V}\langle Q^2 \rangle$



Witten, Veneziano '79: (leading order in $1/N_c$) $\mathbf{m}^2_{\eta'} = \frac{2N_f}{F_\pi^2}\chi_t$ (quenched χ_t)

result supports WV scenario; $m_{\eta'} \approx 1$ GeV $\pm$ 60 MeV (compatible with 958 MeV)

Back to the problem of topological transitions in presence of dynamical quarks:

- Lüscher '10, Lüscher/Schaefer '11 :

  suggest the use of open boundary conditions $\to Q \in \mathbb{R}$ changes gradually.

  May solve the problem in some sense, but *e.g.* to check predictions in the ϵ-regime, and extract Low Energy Constants, integer Q are useful

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

Studies in

- 2d O(3) non-linear σ-model (Heisenberg model) with *cluster algorithm*
- 2-flavour Schwinger model (QED_2) with dynamical chiral fermions
- 4d SU(2) YM theory,

as toy models for QCD

Summation Formula for Observables

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

Brower/Chandrasekharan/Negele/Wiese '03
Approximation formula for pion mass in QCD. Generalisation:

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

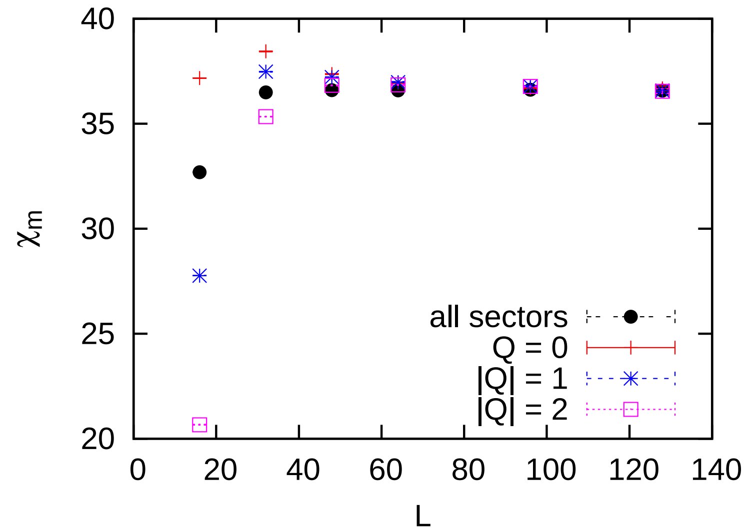
Measure left-hand-side for several $|Q|$ and V, 3-parameter fit $\Rightarrow$ $\langle \Omega \rangle$, χ_{t}, (c)

Assumptions:

large $\langle Q^2 \rangle \equiv V \chi_{\mathrm{t}}$, 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 $\chi_\mathrm{m} = \langle \vec{M}^2 \rangle / V$ $\quad (\vec{M} = \sum_x \vec{e}_x \, , \ \langle \vec{M} \rangle = \vec{0})$



fitting range for L	$48 - 64$	$48 - 96$	$48 - 128$	directly measured in all sectors at $L = 128$
χ_m	36.56(4)	36.58(3)	36.57(2)	36.57(2)
χ_t	0.00262(17)	0.00256(16)	0.00259(14)	0.002790(5)

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

Application to the "pion mass" M_π in the 2-flavour Schwinger model

Degenerate fermion mass

- $\mathbf{m = 0.01}$

$$\left.\begin{array}{lcc} & M_{\pi,0} & M_{\pi,1} \\ L = 28: & & 0.146(4) \\ L = 32: & 0.05(1) & 0.160(8) \end{array}\right\} \overset{\text{fit}}{\longrightarrow} \mathbf{M_\pi = 0.073(25)}$$

Matches well theoretical prediction (Smilga '97): $\mathbf{M_\pi = 2.008 \cdot m^{2/3} \beta^{1/6} = 0.071}$
(though with large error)

- $\mathbf{m = 0.06}$

$$\left.\begin{array}{lcc} & M_{\pi,0} & M_{\pi,1} \\ L = 16: & 0.041(1) & 0.271(4) \\ L = 32: & 0.23(1) & 0.232(7) \end{array}\right\} \overset{\text{fit}}{\longrightarrow} \mathbf{M_\pi = 0.232(8)}$$

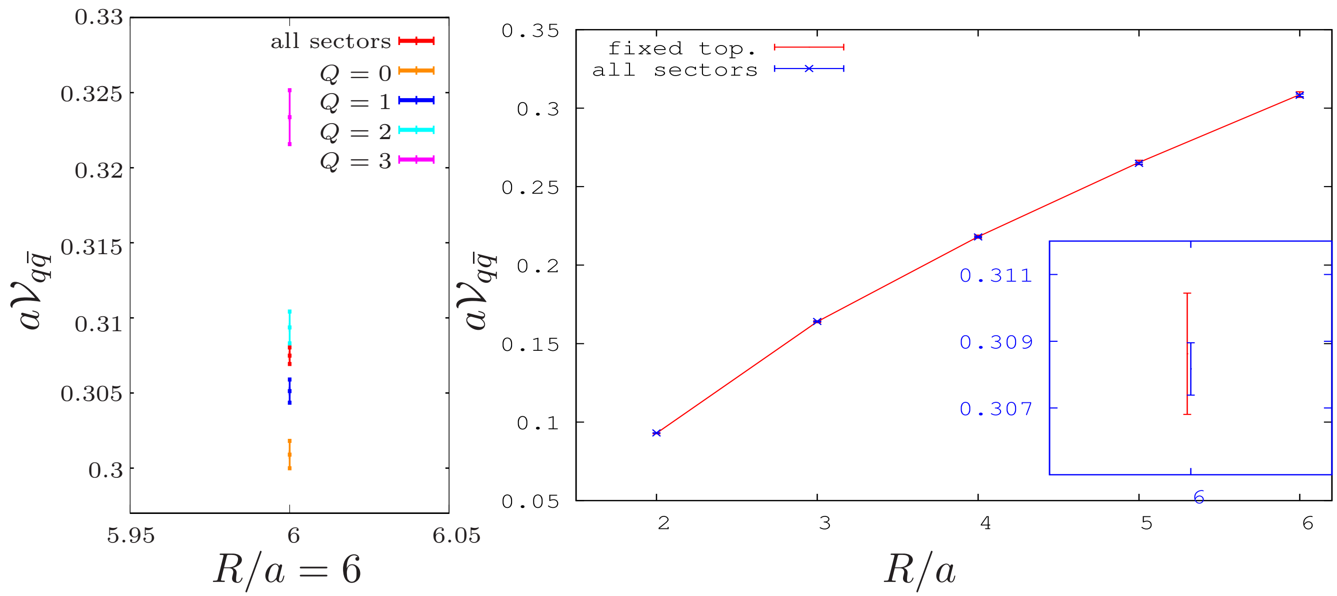
$$\text{Theory}: \mathbf{M_\pi = 0.235}$$

W.B./Hip/Shcheredin/Volkholz '12

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: so far problems with $\chi_{\rm t}$, study is ongoing.



Dromard/W.B./Gerber/Mejía-Díaz/Wagner '15

Summary of the last project

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.

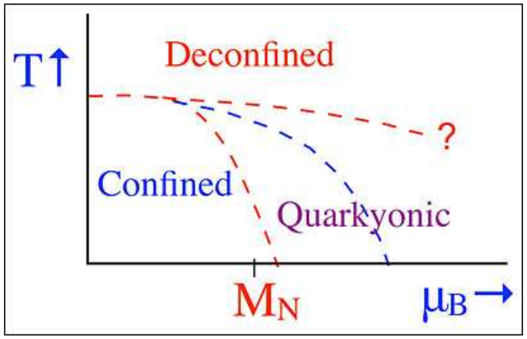
Can we obtain physical results despite top. restriction ?

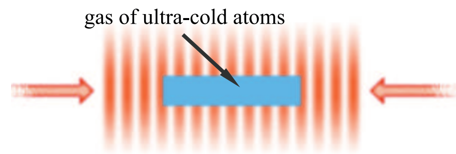
Top. summation works for observables, in suitable regime also for $\chi_{\rm t}$.

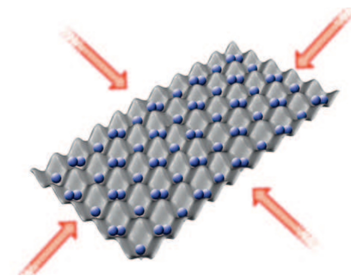
Conditions: $\langle Q^2 \rangle \gtrsim 1.5$, $|Q| \leq 2$

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

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







High density requires chemical potential $\Rightarrow$ Euclidean QCD action $\in \mathbb{C}$

$p[U] = \exp(-S_{\text{QCD}}[U])/Z \notin \mathbb{R}$, 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 CP(2) model (topology, asympt. freedom, dyn. mass gap $\sim$ QCD):
ultra-cold (nK) Alkaline Earth Atoms trapped in an optical lattice: nuclear spin as SU(3) field, SSB SU(3) $\rightarrow$ U(2), low energy action for Nambu-Goldstone bosons $\stackrel{!}{=}$ CP(2) model

Laflamme/Evans/Dalmonte/Gerber/Mejía-Díaz/W.B./Wiese/Zoller '15; to be implemented in Innsbruck