Towards the continuum limit in Lattice QCD: Physics on CLS ensembles

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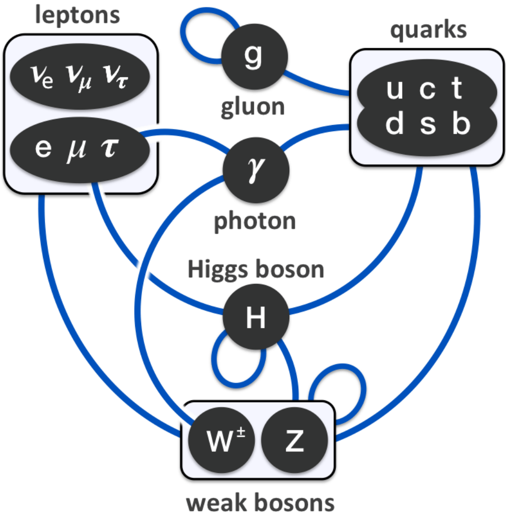
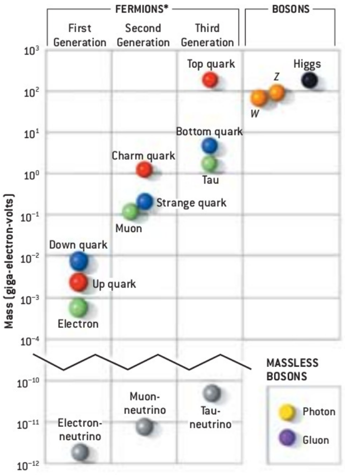
Outline

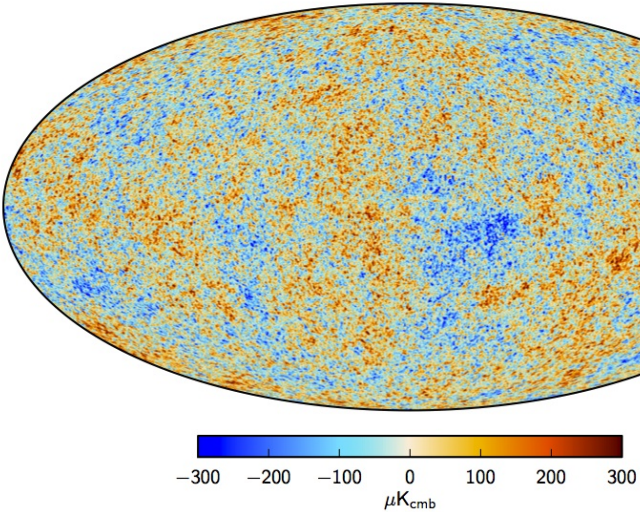
- Prologue: motivation for precision physics
- Lattice QCD
- The continuum limit: CLS simulations
- Baryon masses and scale setting
- D and D_s meson decay constants
- The axial charge of the nucleon g_A
- Summary
- Epilogue: What else are Lattice QFT simulations good for?

The standard model of particle physics





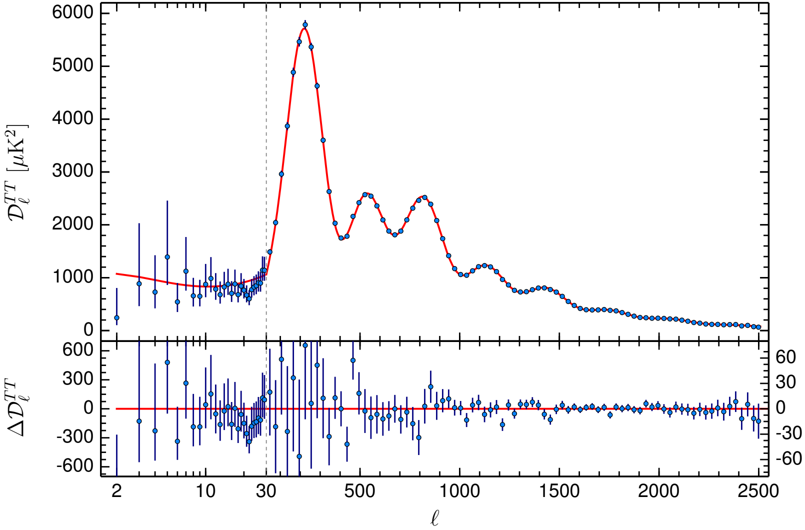
Cosmic microwave background



Planck 2015 arXiv:1502.01582: $2.7247\,\mathrm{K} < T < 2.7253\,\mathrm{K}$

(3000 K at 380000 years ⇒ 2.725 K at $13.7 \cdot 10^9$ years.)

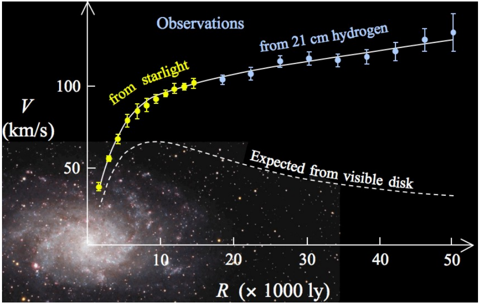
Comparison with cosmological Λ-CDM "standard model"



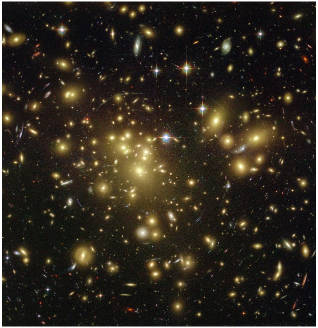
Cold dark matter is needed! You can play around yourself:

http://wmap.gsfc.nasa.gov/resources/camb_tool/index.html

Dark matter really exists



Rotational curve of M33 galaxy.



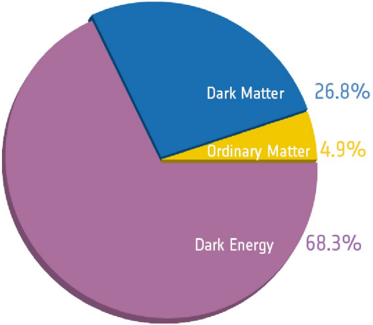
Hubble Deep Space mission: gravitational lensing.

... and is distributed differently from known matter.

Can only interact very weakly since it failed to radiate away angular momentum, forming disks and clump.

No credible dark matter candidates exist within the Standard Model.

- Almost all **known mass** of the universe is due to nucleons (protons and neutrons) ("baryonic matter").
- Most baryonic mass is "generated" by QCD via the spontaneous breaking of an (approximate) chiral global symmetry.
- The small remainder, i.e. the masses of the quarks and of leptons (electron, muon, tau, neutrinos), can be attributed to the Higgs mechanism.

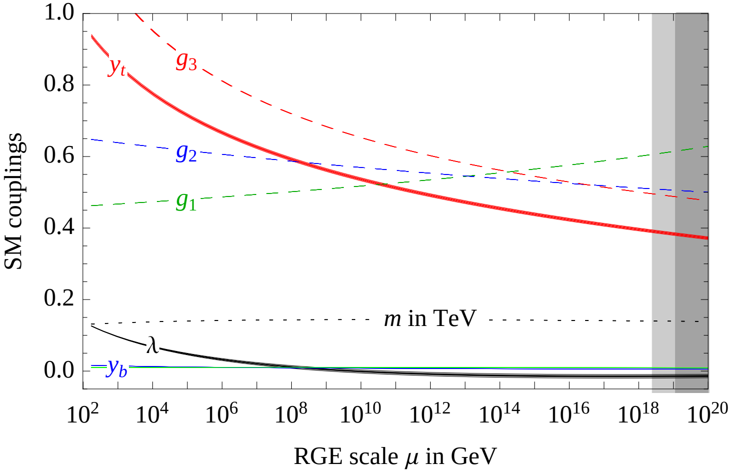


Problems of the Standard Model

- ★ Aesthetics, e.g., $14 + 3 + 4 + 4(6) + 1 = 25(27)$ parameters.
  - Masses: $q \in \{u, d, s, c, b, t\}$, $\ell \in \{e, \mu, \tau\}$, $\nu \in \{\nu_e, \nu_\mu, \nu_\tau\}$, W, h (cover 14 orders of magnitude).
  - Couplings: α_s, α_w, α_{em}
  - Quark mixing: 3 angles, 1 CP violating phase
  - Neutrino mixing: 3 angles, 1 (Dirac) or 3 (Majorana) phase(s)
  - Strong CP angle: θ
- ★ Why the $SU(3) \otimes SU(2) \otimes U(1)$ gauge group?
- ★ Why 3 families?
- ★ Why was there more matter than anti-matter in the early universe?
- ★ Dark matter?
- ★ Inconsistent, due to Landau pole(s) $\Rightarrow$ cut-off, e.g., Planck mass.
- ★ Does gravity have to be included? UV completion of gravity?
- ★ ...

Running of Standard Model couplings with the scale

g_3: QCD coupling, g_1, g_2: Electroweak U(1), SU(2) couplings,
λ: quartic Higgs coupling. Only SU(N) can be "fundamental".



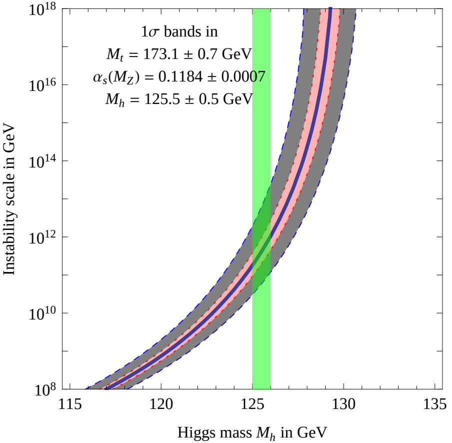
D Buttazzo et al, 1305.3536 Planck mass: $1/\sqrt{G_N} \approx 1.2 \cdot 10^{19}$ GeV

Should we sleep well at night? Precision is required.

stable: $\lambda > 0$

not so stable: $\lambda \lesssim 0$

quartic Higgs potential: $\frac{1}{4}\lambda(h)\,h^4$



D Buttazzo et al, 1305.3536

A Datta, S Raychaudhuri, 1207.0476

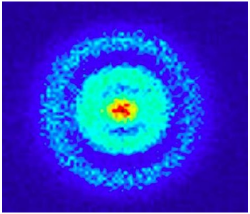
This also depends on $\alpha_s = g_3^2/(4\pi)$!

Fascinating SU(3): hydrogen and proton

mass of the hydrogen atom:

$$\underbrace{938.29\,\text{MeV}}_{\text{proton}} + \underbrace{0.51\,\text{MeV}}_{\text{electron}} - \underbrace{0.0000136\,\text{MeV}}_{\text{binding energy:}\,\frac{m_e\alpha_{em}^2}{2}}$$

RMS radius $\approx 0.92 \cdot 10^{-10}\text{m} = 0.092$ nm

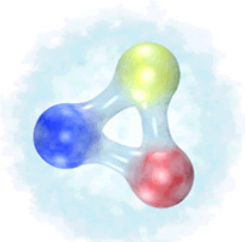


AS Stodolna et al, PRL (13) 213001

mass of the proton m_p:

$$\underbrace{2 \cdot 2.2\,\text{MeV}}_{\text{up quarks}} + \underbrace{4.7\,\text{MeV}}_{\text{down quark}} \underbrace{+}_{!!!} \underbrace{929.2\,\text{MeV}}_{???}$$

RMS charge radius $\approx 0.84 \cdot 10^{-15}\text{m} = 0.84$ fm



artist's impression

$$\text{Hydrogen:}\quad |E|\langle r_H^2\rangle^{1/2} = \sqrt{3}\underbrace{(m_e\alpha_{em})^{-1}}_{a_{\rm B}\approx 0.053\,\mathrm{fm}}|E| = \frac{\sqrt{3}}{2}\alpha_{em} \approx 0.006$$

$$\text{Proton:}\quad m_p\langle r_p^2\rangle^{1/2} \approx 4 = \mathcal{O}(1)$$

Solving a strongly coupled, non-linear, relativistic four-dimensional quantum system is not so easy
$\Longrightarrow$ numerical simulation.

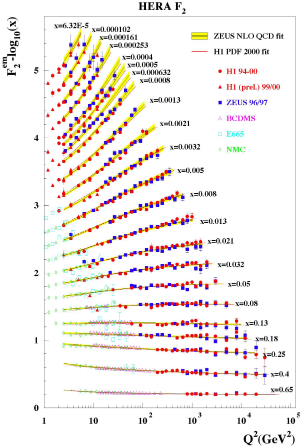
Lattice spacing $a < 1/m_p$, i.e. $a\Lambda_{\rm QCD} \ll 1$, for polynomial cut-off effects.
$\Longrightarrow a^{-1} \gtrsim 2\,\mathrm{GeV}$

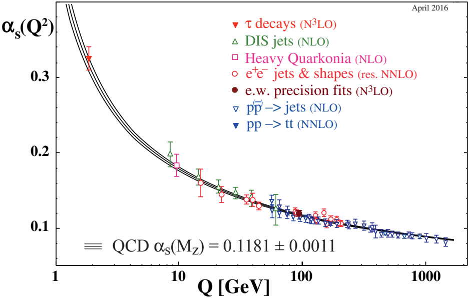
Lattice extent $L \gg r_p$. Actually, finite size effects $\propto e^{-M_\pi L}$.
$\Longrightarrow L \gtrsim 4/M_\pi$
$\Longrightarrow L \gtrsim 5.8\,\mathrm{fm}$ for physical pion mass.

This means $N = L/a > 5.8\,\mathrm{fm} \cdot 2\,\mathrm{GeV} \approx 60$.

We are lucky: $m_p/M_\pi \ll 60 \ll M_W/\Lambda_{\rm QCD} \ll M_{\rm Planck}/M_W$.
(Impossible to put electroweak theory and QCD on the same lattice, effective field theories/operator product expansion needed for this!)

Successes of perturbative QCD



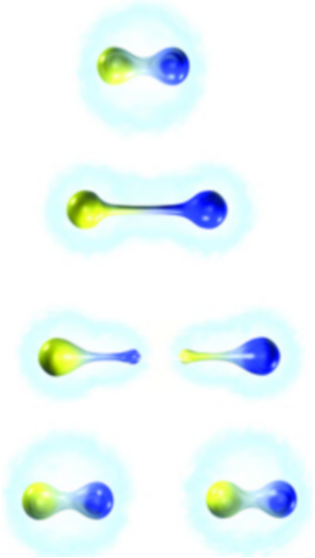


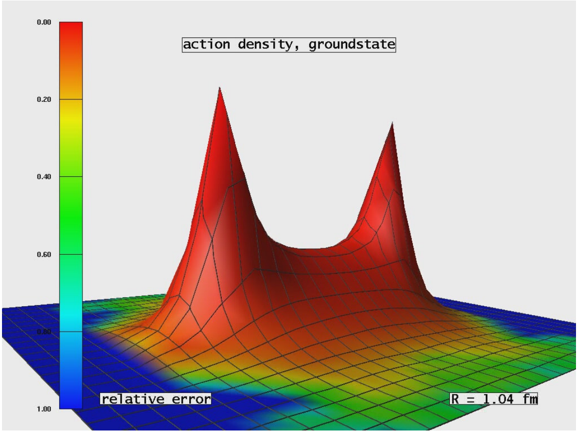
Above: Running coupling parameter (Higgs stability plot was for 0.1184(7))

Left: structure function F_2 of the proton

The QCD "String" from numerical simulation

$m_p > 2m_u + m_d$: why does the proton not decay? Confinement!

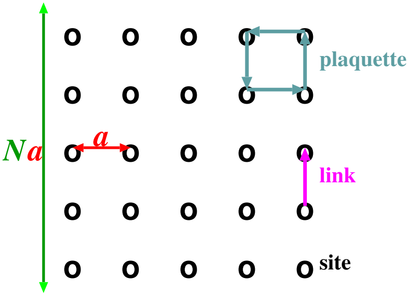




GB et al, hep-lat/0505012,0512018

string tension: 1 GeV/fm ≈ 160 kN

Lattice QCD



typical values:

$a^{-1} = 2$–5 GeV, $Na = 2$–7 fm

continuum limit: $a \to 0$, Na fixed

infinite volume: $Na \to \infty$

$$\langle O \rangle = \frac{1}{Z} \int [dU]\,[d\psi][d\bar{\psi}]\; O[U] e^{-S[U,\psi,\bar{\psi}]}$$

"Measurement": average over a representative ensemble of gluon configurations $\{U_i\}$ with probability $P(U_i) \propto \int [d\psi][d\bar{\psi}] e^{-S[U,\psi,\bar{\psi}]}$

$$\langle O \rangle = \frac{1}{n} \sum_{i=1}^{n} O(U_i) + \Delta O \qquad\qquad \Delta O \propto \frac{1}{\sqrt{n}} \stackrel{n\to\infty}{\longrightarrow} 0$$

Input: discretized $\mathscr{L}_{QCD} = \frac{1}{16\pi\alpha_s(a)} FF + \sum_f \bar{q}_f(\not{D} + m_f(a))q_f$

$$m_{\Xi}^{\text{latt}} = m_{\Xi}^{\text{phys}} \quad \longrightarrow \quad a$$
$$M_{\pi}^{\text{latt}}/m_{\Xi}^{\text{latt}} = M_{\pi}^{\text{phys}}/m_{\Xi}^{\text{phys}} \quad \longrightarrow \quad m_u(a) \approx m_d(a)$$
$$\cdots$$

Output: hadron masses, matrix elements, decay constants, etc...

Required:

1. $L = Na \to \infty$: FSE suppressed with $\exp(-LM_\pi) \Rightarrow LM_\pi \gtrsim 4$.
2. $m_q^{\text{latt}} \to m_q^{\text{phys}}$: chiral perturbation theory (χPT) helps for m_{ud} but m_{ud}^{latt} must be sufficiently small to start with ($M_\pi \lesssim 200\,\text{MeV}$?).
3. $a \to 0$: functional form known: $\mathcal{O}(a^2), \mathcal{O}(\alpha_s a) \Rightarrow \approx 4$ lattice spacings.

Only in very few calculations (almost) all the above is done as yet, e.g., light hadron spectrum, meson decay constants, α_s, $m_{u,d,s,c}$.

Computational challenges

Cost of simulation is proportional to

- number of points: $(L/a)^4$
- condition number of the linear system: $1/M_\pi^2$
- $L^{1/2}/M_\pi$ in (Omelyan) time integration within hybrid Monte Carlo
- $1/a^{\geq 2}$ critical slowing down (autocorrelations)

Adjusting $L \propto 1/M_\pi$, this means:

$$\mathrm{cost} \propto \frac{1}{a^{\geq 6}\, M_\pi^{7.5}}$$

NB: for baryonic observables at small M_π additional noise/signal problems.

State of the art: $192 \cdot 64^3$ sites, corresponding to $\approx (6 \cdot 10^9)^2$ (sparse) complex matrices.

Tremendous progress in Hybrid Monte Carlo, solver, noise reduction.

Less improvement recently in compute power: The power wall.

The "Power Wall" (example: NSA data centre)

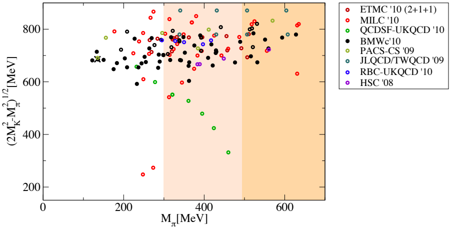
90 MWatt $\Rightarrow > 5 \cdot 10^7$ US$/year in Fort Meade, Maryland, USA

Fastest supercomputer: ShenWei TaihuLight at NSC Wuxi, Jiangsu, China: 15+5 MWatt, 93 PetaFLOP/s LINPACK.

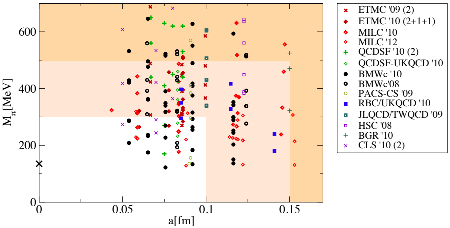
MAHAGENCO: 1 kWh at ₹ 9 vs € 0.2 $\approx$ ₹ 14 ! (production cost 3 vs 10)

Landscape of (not so) recent lattice simulations

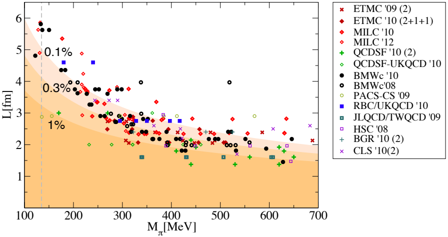
$M_{ss} \propto m_s$ vs. M_π



M_π vs. a



L vs. M_π

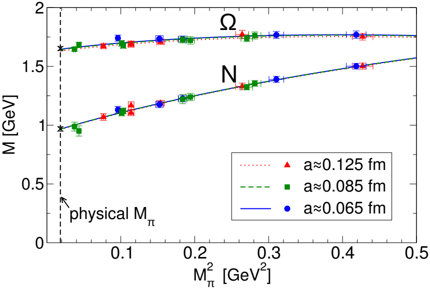


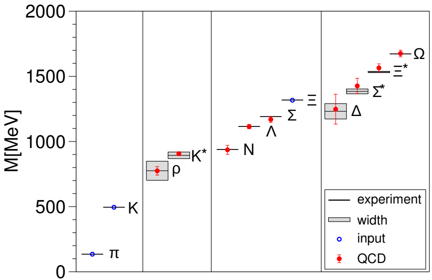
Figures taken from

C Hoelbling, arXiv:1410.3403

Typically: Coarse a, small statistics at small M_π!

The light hadron spectrum





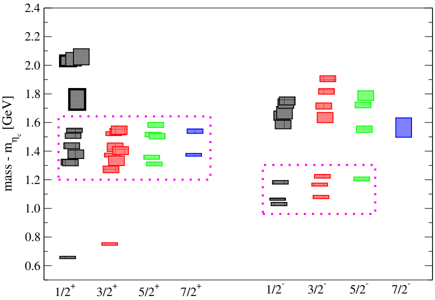
BMW-c: S Dürr et al, arXiv:0906.3599

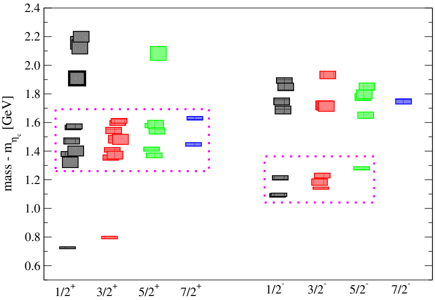
Joint chiral and continuum limit.

Doubly charmed baryons

One can also predict what has not yet been discovered:

$\Xi_{cc} \sim ccu$ baryons $\qquad$ $\Omega_{cc} \sim ccs$ baryons





M Padmanath, R Edwards, N Mathur & M Peardon, 1502.01841

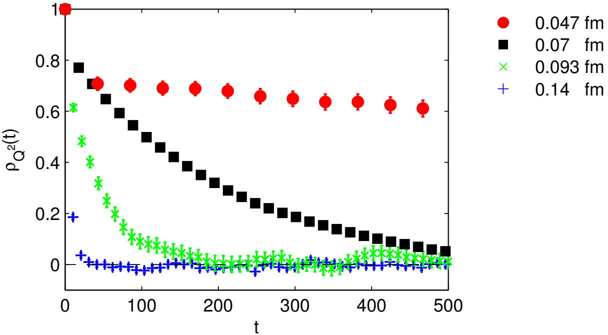
Symanzik improvement and the continuum limit

$$S_{\text{lattice}} = S_{\text{continuum}} + aS_1 + a^2 S_2 + \ldots$$

We add non-perturbative $\mathcal{O}(a)$ improvement terms to the action and to local operators, cancelling S_1 type terms.

S_2 is new physics(!) at the scale a^{-1}. $a \to 0$: Effect of S_2 is suppressed.

Problem: Critical slowing down of local updating algorithms:



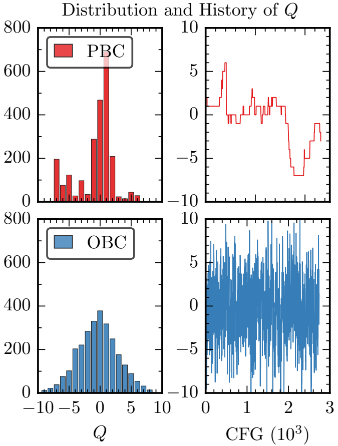
Autocorrelation function for the squared topological charge $Q \propto \int d^4x\, F\widetilde{F}$ versus Monte Carlo time.

$0.1\,\text{fm} \approx (2\,\text{GeV})^{-1}$

S Schaefer, R Sommer, F Virotta, 1009.5228

Open boundary conditions in time

OBC in time [S Schaefer, M Lüscher, 1105.4749] allow the flow of topological objects (instantons) into and out of the lattice.



SU(7) gauge theory.

$a \approx 0.094$ fm.

Problem becomes worse at large N_c:

Instanton action: $8\pi^2 N_c/\lambda$.

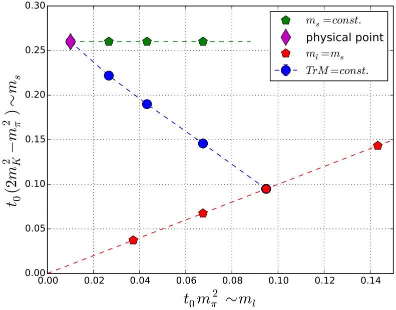
Higher cost to create an (anti)instanton!

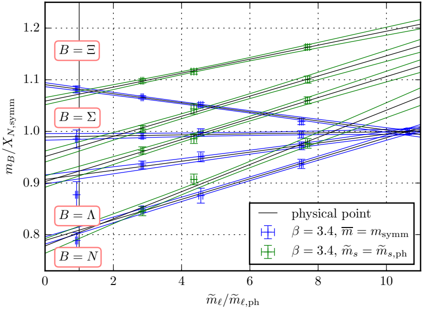
A Amato, G Bali, B Lucini, 1512.00806

Disadvantage: Breaking of translational invariance in time near the boundaries. $\Rightarrow$ Discard part of the simulated volume.

New simulation strategy

RQCD: G Bali et al, 1606.09039; 1702.01035: Simulate along $m_s + 2m_\ell = \text{const}$ **and** $m_s = \text{const}$ mass-plane trajectories, enabling combined SU(2) χPT and Gell-Mann–Okubo/SU(3) extrapolations.





(Only linear unconstrained baryon mass fits are shown.)

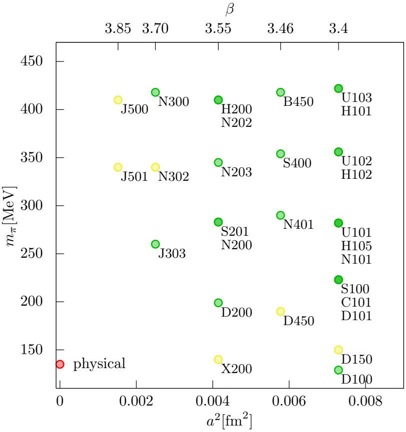
Coordinated Lattice Simulations (CLS)

CLS members/groups at

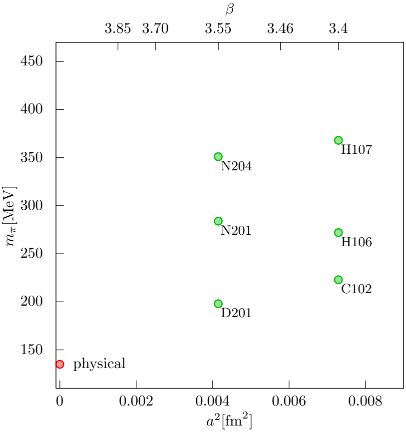
- HU Berlin
- CERN
- Jena
- Ljubljana
- Mainz
- UA Madrid
- Milano Bicocca
- Münster
- Odense/CP3 Origins
- Regensburg
- Roma I + II
- Wuppertal
- DESY/Zeithen

Coordinated generation of gauge ensembles using openQCD
https://luscher.web.cern.ch/luscher/openQCD/

Ensemble overview



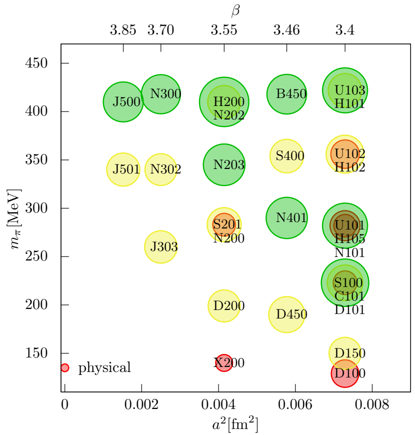
$\mathrm{tr}\,m = \mathrm{const}$



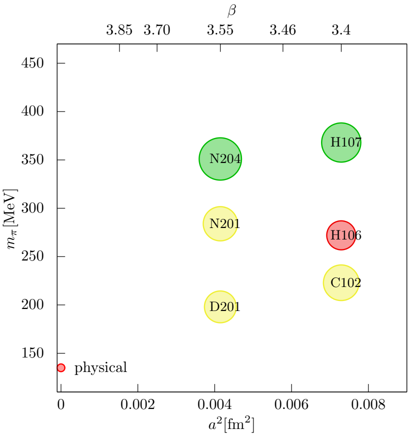
$\widetilde{m}_s = \mathrm{const}$

J: $192 \cdot 64^3$, D: $128 \cdot 64^3$, N: $128 \cdot 48^3$, C: $96 \cdot 48^3$,
X: $64 \cdot 48^3$ (to be increased to $192 \cdot 96^3$),
S: $128 \cdot 32^3$, H: $96 \cdot 32^3$, B: $64 \cdot 32^3$, U: $128 \cdot 24^3$.

Volumes



$$\mathrm{tr}\, m = \mathrm{const}$$

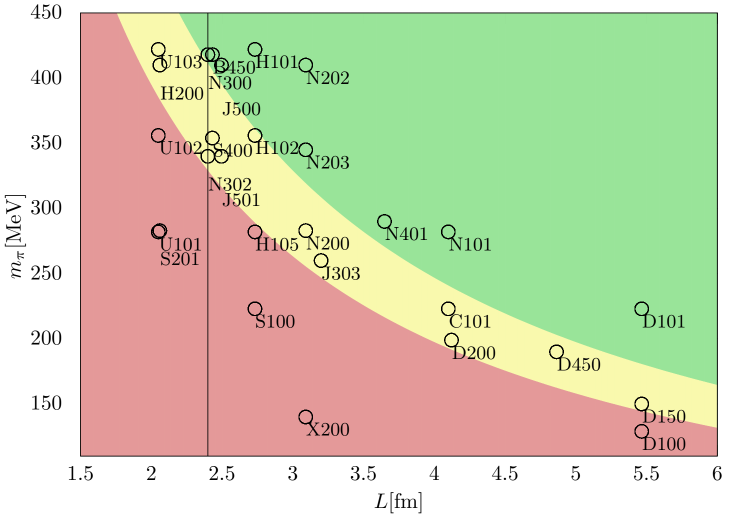


$$\widetilde{m}_s = \mathrm{const}$$

$M_\pi L < 4$, $4 \leq M_\pi L < 5$, $M_\pi L \geq 5$.

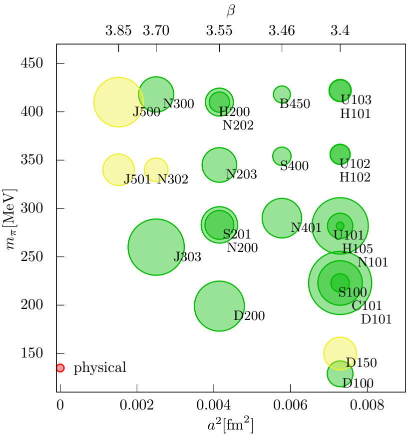
Radius $\propto M_\pi L$.

Volumes II

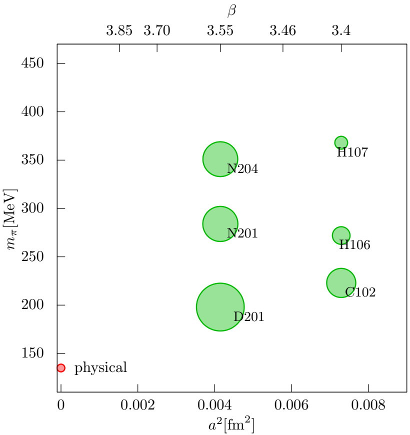


$M_\pi L < 4$, $4 \leq M_\pi L < 5$, $M_\pi L \geq 5$.

Cost so far



$\mathrm{tr}\, m = \mathrm{const}$



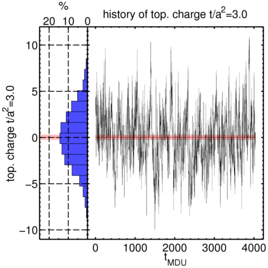
$\widetilde{m}_s = \mathrm{const}$

Area $\propto$ core hours spent, normalized to Xeon E5-2697 (2.6 GHz Haswell)

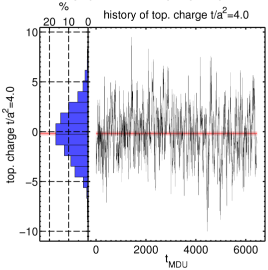
$>$ 320 TB configurations redundantly stored at Regensburg and Zeuthen.

History of the topological charge

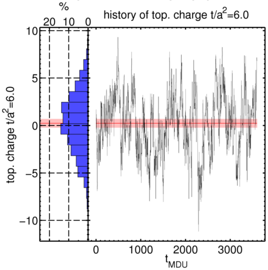
H101 $a = 0.085\,\mathrm{fm}$



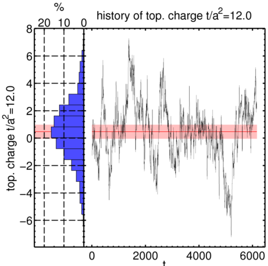
B450 $a = 0.076\,\mathrm{fm}$



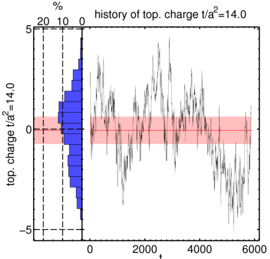
N202 $a = 0.064\,\mathrm{fm}$



N300 $a = 0.050\,\mathrm{fm}$



J500 $a = 0.039\,\mathrm{fm}$



$\langle Q^2 \rangle \propto V$ is violated in plots:

-Physical flow time varies.

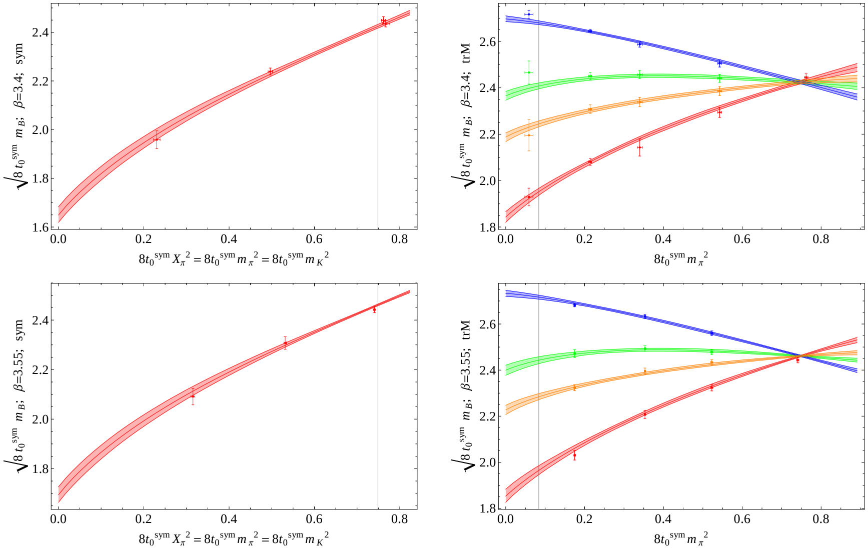
-Time range of average varies.

-Physical V varies.

-Lattice spacing effects.

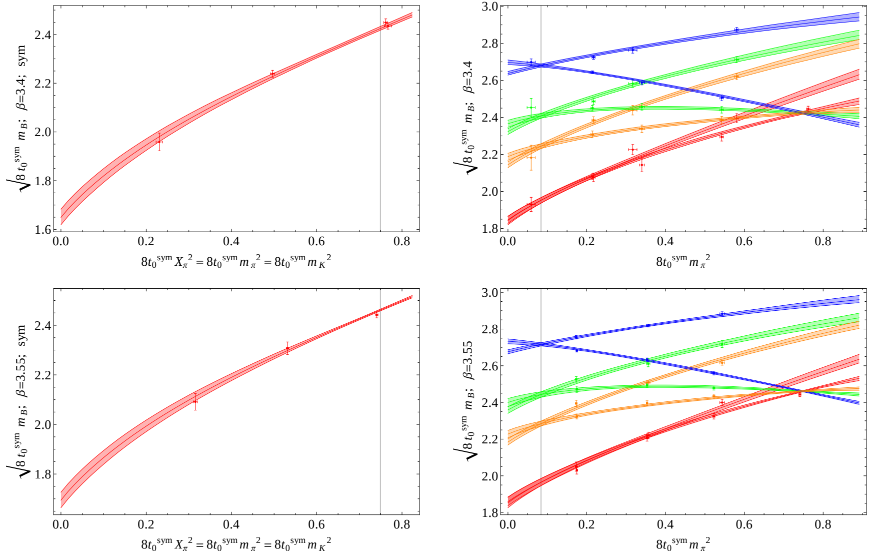
Preliminary: NNLO χPT fit at $a \approx 0.085\,\text{fm}, 0.064\,\text{fm}$

$\sqrt{8t_0^*} \approx 0.414\,\text{fm}$, Ξ: $ss\ell$, Σ/Λ: $s\ell\ell$, N: $\ell\ell\ell$.



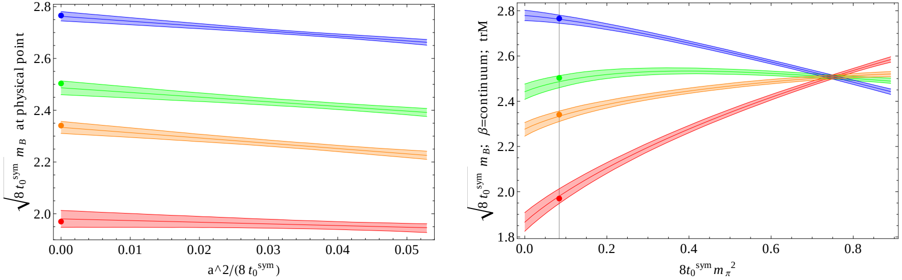
Preliminary: NNLO χPT fit at $a \approx 0.085\,\text{fm}, 0.064\,\text{fm}$

$\sqrt{8t_0^*} \approx 0.414\,\text{fm}$, Ξ: $ss\ell$, Σ/Λ: $s\ell\ell$, N: $\ell\ell\ell$.



Preliminary: Continuum limit and setting the scale

Projections of the global fit onto the a^2 and the M_π^2 axes:



Experimental points correspond to $\sqrt{8t_0^*} = 0.414\,\mathrm{fm}$.

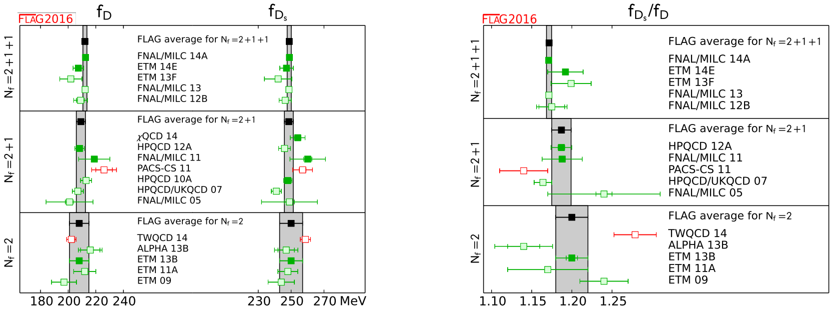
Coarsest lattice has $a^2/(8t_0^*) \approx 0.043$, finest $a^2/(8t_0^*) \approx 0.009$.

RQCD: G Bali, S Collins, F Hutzler, A Schäfer, E Scholz, J Simeth, W Söldner, P Wein, 1702.01035 and in preparation

High precion QCD: D and D_s decay constants

f_{D_s}/f_{D^+} & leptonic decay width $\Rightarrow$ $|V_{cs}/V_{cd}|$.

FLAG 3 report: [FLAG: S Aoki et al, 1607.00299]



$$N_f = 2+1: \quad f_{D_s} = 249.8(2.3)\,\text{MeV}, \; f_{D_s}/f_{D^+} = 1.187(12)$$
$$N_f = 2+1+1: \; f_{D_s} = 248.8(1.3)\,\text{MeV}, \; f_{D_s}/f_{D^+} = 1.172(3)$$

Latest http://ckmfitter.in2p3.fr/ (also http://utfit.org):

f_{D_s}

Reference	Article	N_f	Mean	Stat	Syst
ETM13	[51]	2	250	5	5
HPQCD10	[52]	2+1	248.0	1.4	4.5
FNAL-MILC11	[53]	2+1	260.1	8.9	16.2
ChiQCD14	[54]	2+1	254	2.2	10.2
FNAL-MILC14	[50]	2+1+1	249.0	0.3	${}^{+1.7}_{-2.1}$
ETM14	[48]	2+1+1	247.2	3.9	2.2
Our average			248.2	0.3	1.9

f_{D_s}/f_D

Reference	Article	N_f	Mean	Stat	Syst
ETM13	[51]	2	1.201	0.007	0.020
FNAL-MILC11	[53]	2+1	1.188	0.014	0.054
HPQCD12	[55]	2+1	1.187	0.004	0.023
FNAL-MILC14	[50]	2+1+1	1.1712	0.0010	${}^{+0.0037}_{-0.0040}$
ETM14	[48]	2+1+1	1.192	0.019	0.017
Our average			1.175	0.001	0.004

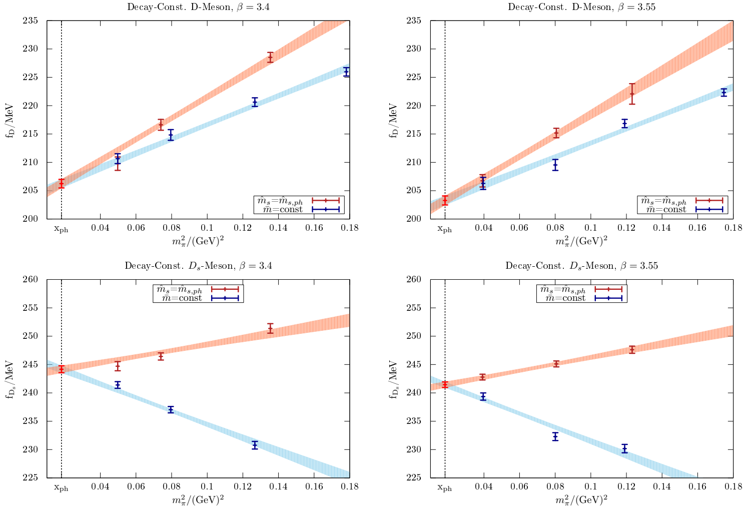
Dangerous: [50] dominates. [53,55] are not really independent studies.

Difference f_{D^+} vs f_{D^0}? How are f_{D^+}, f_{D_s} defined?

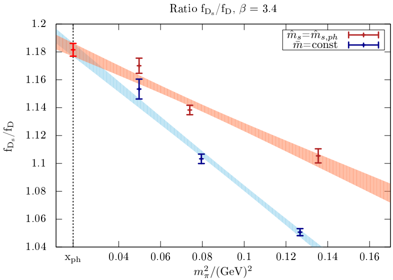
Electromagnetic corrections, e.g., [N Carrasco et al, 1502.00257]!

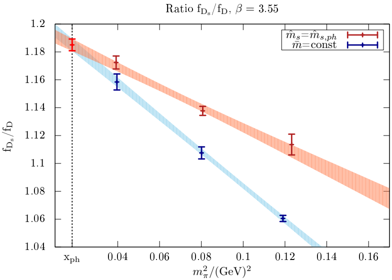
$D_{(s)}$ meson decay constants on CLS ensembles I

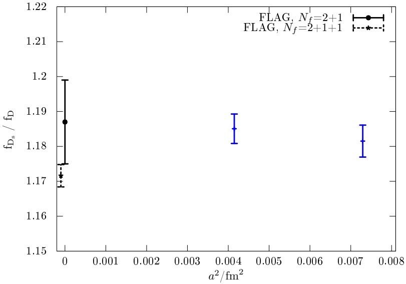
RQCD+ALPHA: S Collins, K Eckert, J Heitger, S Hofmann, W Söldner, 1701.05502



$D_{(s)}$ meson decay constants on CLS ensembles II







PRELIMINARY!

Order a improvement [P Korcyl, GB, 1607.07090 + in preparation; ALPHA: J Bulava et al, 1502.04999] has not been fully implemented as yet.

Also 3 more lattice spacings to come!

The axial charge of the nucleon g_A

g_A enters $n \to p + \bar{\nu}_e + e^-$

$$g_A = -\frac{s_\mu}{m_N}\langle p, s|\bar{u}\gamma_\mu\gamma_5 d|n, s\rangle = -\frac{s_\mu}{m_N}\langle p, s|\bar{u}\gamma_\mu\gamma_5 u - \bar{d}\gamma_\mu\gamma_5 d|p, s\rangle$$

Most lattice simulations obtain an axial charge that is too small.

Most likely reason: Finite volume effects. [RQCD: GB et al, 1412.7336]

But all systematics need to be investigated!

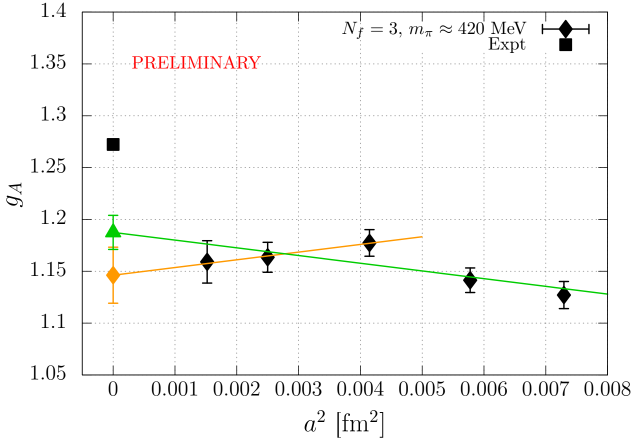
Differences from β decay measurements could also mean new physics.

g_T and g_S are being determined too: If BSM β decay was found, these couplings would constrain parameters of the effective BSM Lagrangian.

Remark: The axial form factor is needed for terrestrial long-baseline neutrino oscillation experiments.

The continuum limit of g_A

RQCD: G Bali, S Collins, M Göckeler, A Schäfer, J Simeth, W Söldner, A Sternbeck, T Wurm, 1702.01035 and in preparation

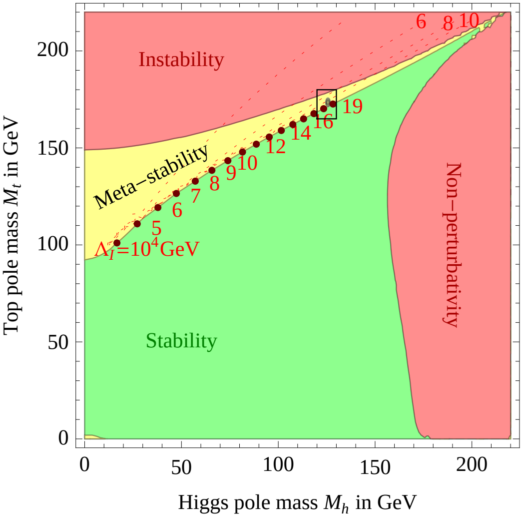


Misses experiment but experiment is at $M_\pi \approx 135\,\text{MeV} < 420\text{MeV}$.

Next step: quark mass extrapolation.

Summary

- Certain limits need to be taken in Lattice QCD:
  $t \to \infty$, $m_q \to m_q^{\text{phys}}$, $V = a^4 N_t N_s^3 \to \infty$, $a \to 0$.
- Wilson fermions are theoretically clean (unlike staggered).
- Chiral symmetry will be restored in the continuum limit.
  Drawback: More involved operator mixing and order a improvement than for overlap fermions that have a chiral symmetry at $a > 0$.
- Within CLS we implement full order a improvement and vary a^2 by a factor > 5. This is possible using open boundary conditions in time.
- At $a \lesssim 0.05\,\text{fm}$ the physical point will require $N_s = 128$. This is too expensive. Instead, we perform joint extrapolations along two quark mass trajectories.
- First results exist on α_s and pion/kaon decay constants (ALPHA), on distribution amplitudes and the baryon spectrum (RQCD) and on f_D, f_{D_s} (RQCD+ALPHA).
- Soon: Quark masses, charmed and light hadron spectroscopy, nucleon structure observables, semileptonic decay form factors.



(Almost) anything non-perturbative !!!

Unfortunately, the SM Higgs is too light for that but maybe it is not elementary?

QCD is too nice to remain single.

It calls for non-perturbative partner theories:

What happens once is bound to happen twice.

Some applications of Lattice QFT

- Non-perturbative dynamics beyond the standard model: mostly technicolour. Recently axions: topological susceptibility $\chi_t = f_a^2 m_a^2$ at high temperatures of interest. [E Berkowitz et al, 1505.07455, R Kitano, N. Yamada, 1506.00370, S Borsanyi et al, 1508.06917]
- Fundamental quantum field theory questions: orbifold equivalence, SUSY QCD, Large N QCD, phase diagrams etc.
- QCD at high temperatures: transition temperature T_c to the QGP, hadron modifications at high T, Debye screening lengths, fluctuations of conserved charges, freezeout curve, equation of state, conductivity, **role of magnetic fields** etc.
- Low energy standard model tests: matrix elements relevant for (B)SM β-decay, $(g-2)_\mu$, dark matter couplings, K physics ($K \to \pi\pi$, ϵ'/ϵ [T Blum et al, 1502.00263; I Ishizuka et al, 1505.05289; C Lehner et al 1508.01801]).

Applications of Lattice QCD II

- Fundamental parameters: connect experiment to m_u, m_d, m_s, m_c, m_b, V_{cs}, V_{cd}, V_{cb}, V_{ub} (through computation of $f_B, f_{B_s}, f_D, f_{D_s}$ and electroweak formfactors), α_s, running of α_{em} and of weak charge.
- Light hadron spectroscopy, decay constants and distribution amplitudes: BES III, JLAB, Belle 2, LHCb etc.
- Spectroscopy of mesons and baryons with open and closed charm and bottom (LHC by-products, BES III, Belle 2) and some of their properties.
- Hadron/proton structure: moments of PDFs, Generalized formfactors (i.e. moments of GPDs), transverse momentum distributions (TMDs), double parton distributions (DPDs), also distribution amplitudes for particle production etc., relevant for LHC, COMPASS 2, JLAB, BNL, MAMI etc.