High Precision Results from Numerical Simulations of Quantum Chromodynamics

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The Standard Model

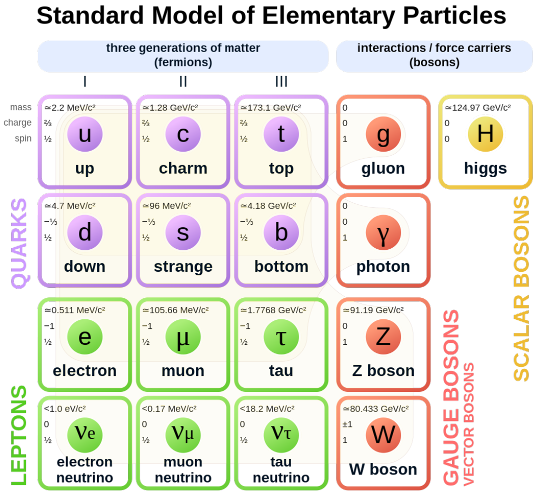


Fig.: [Wiki]

The Standard Model

Matter particles (spin $S = 1/2\hbar \rightarrow$ fermions)

- quarks: "up" (u), "charm" (c) und "top" (t), "down" (d), "strange" (s), "bottom" (b)
  $\rightarrow$ masses: $m_u = 2.3 MeV/c^2$ (up quark), ..., $m_t = 173 GeV/c^2$ (top quark)
- leptons: electron (e^-), muon (μ^-), tau (τ^-), electron neutrino (ν_e), muon neutrino (ν_μ), tau neutrino (ν_τ)

Interaction particles (spin $S = 1\hbar \rightarrow$ bosons)

- there are (only) 4 fundamental forces (with associated interaction particles):
  - electromagnetic force (photon γ)
  - strong force (gluons g)
  - weak force ($W^\pm$, Z^0 bosons)
  - gravitational force (graviton G (?)) $\leftarrow$ not included in the Standard Model

Bound states

Quarks can form bound states (due to the strong force)

- baryons (consist of 3 quarks: $q_1 q_2 q_3$):
  proton p (uud), neutron n (udd), lambda Λ (uds), sigma Σ^+ (uus), xi Ξ^- (dss), omega Ω (sss),...
- mesons (consist of quark and anti-quark: $q_1 \bar{q}_2$): pion π^+ ($u\bar{d}$), kaon K^+ ($u\bar{s}$)
- ...

$\Rightarrow$ masses can be calculated numerically $\leftarrow$ part of this project (focus on strong force + light quarks (up, down, strange, charm))

Physics of the Standard Model

Physics of the Standard Model

- (almost too) perfect agreement of experimental results and theoretical predictions within the Standard Model
- BUT, there are good reasons to believe that the Standard Model is incomplete
  $\rightarrow$ e.g., it is not known how to include gravity in the Standard Model consistently

$\rightarrow$ ongoing search for little deviations from experiment results and theoretical predictions

$\rightarrow$ such deviations may hint how to extend the Standard Model

$\Rightarrow$ high precision is needed in both experiments and theoretical predictions

At Regensburg: focus on physics related to the strong force

$\rightarrow$ theoretical calculations at Regensburg performed both numerically and analytically

$\rightarrow$ numerical projects at Regensburg:

- light baryon spectrum/scale setting
- heavy baryon spectrum
- pseudoscalar decay constants (+ charm), charmonium resonances
- quark masses (+ charm)
- η/η'-mixing
- hadron structure: baryon charges, form factors, TMD, MDA/BDA, DPD, LECs

$\Rightarrow$ goal: high precision results from numerical calculations

Remark: numerical simulations are also very important for quantities where accessibility w.r.t. other methods is limited

Numerical Simulations of the Strong Force

Theory of the Strong Force = Quantum Chromodynamics (QCD)

- QCD is a non-linear theory
  $\rightarrow$ many important quantities can only be calculated numerically
- only ab-initio framework known for numerical simulations of QCD $\rightarrow$ Lattice QCD

Lattice QCD

Algorithm: Hybrid Monte Carlo (HMC)

- Generate ensembles by a Langevin-type algorithm (stochastic differential equation)
- evolve along classical trajectory:
  $\rightarrow$ integration along extra dimension (simulation time)
- solve equation of motion of 5-dim. Hamiltonian

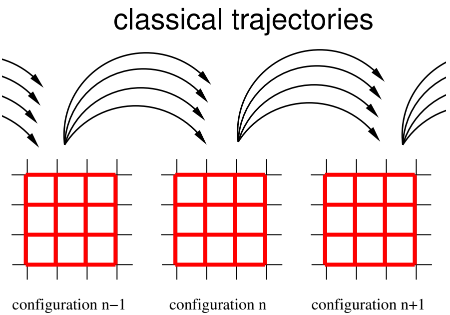
Ensembles $\leftarrow$ calculation of observables

$\Rightarrow$ each ensemble consists of several configurations

$\Rightarrow$ single config. = 4d lattice grid (with lattice spacing a)

$\rightarrow$ on each site: 4×9 complex numbers

$\rightarrow$ 4d = 3 spatial + 1 temp. directions (volume = $L^3 \times T$)



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Simulation Overview

Simulation details

- due to computational costs → simulations are performed mostly at
  - larger quark than physical quark masses
  - rather coarse lattice spacing
  - not too large finite volume
- in addition approximation are made: light quark mass $m_\ell = m_{up} \approx m_{down}$, heavier quarks (charm and heavier) are not simulated, no electromagnetic contributions included (also weak force neglected)
  → reasonable assumptions w.r.t. precision reached at state of the art lattice QCD simulations

⇒ however, we need to take the following limits to obtain physical results
  - chiral extrapolation: light and strange quark mass $m_\ell \to m_{\ell,physical}$ $m_s \to m_{s,physical}$
  - continuum extrapolation: lattice spacing $a \to 0$
  - (spatial) volume $V_s \to \infty$

CLS $2+1$f simulation program

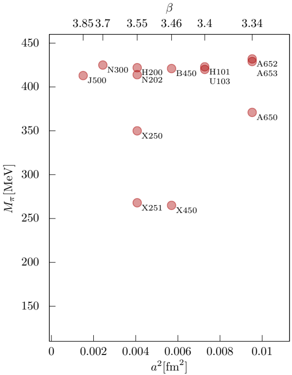
→ see https://www-zeuthen.desy.de/alpha/public-cls-nf21/

Such simulations are a large scale project → ongoing for more than 10 years now

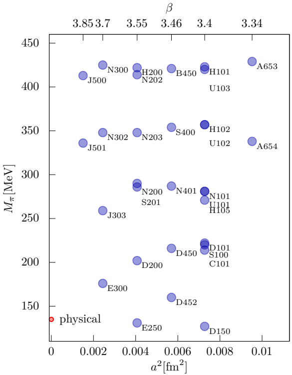
- large collaboration → CLS (Coordinated Lattice Simulations): HU Berlin, CERN, TC Dublin, Krakow, UA Madrid, Mainz, Milano Bicocca, Münster, Odense/CP3-Origins, Regensburg, Roma I, Roma II, Wuppertal, DESY Zeuthen

⇒ main focus of this large scale project: performing a well controlled continuum limit

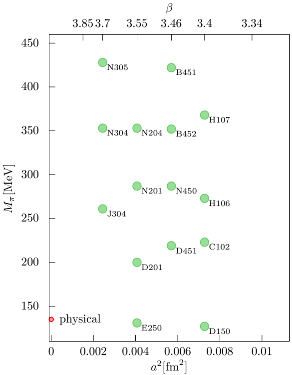
Ensemble Overview



$m_s = m_\ell$



$m_s + 2m_\ell \approx$ phys.



$\widehat{m}_s \approx$ phys.

- simulations are performed at unphysical light and strange quark masses m_ℓ, m_s and at finite lattice spacing a
  $\rightarrow$ extrapolation to physical quark masses and zero lattice spacing necessary!
  $\rightarrow$ computational costs increase drastically along these limits!
- 6 different lattice spacings ($a \approx 0.098 - 0.039$ fm), 2 ensembles at the physical point
- geometries range from 48×24^3 to 192×96^3

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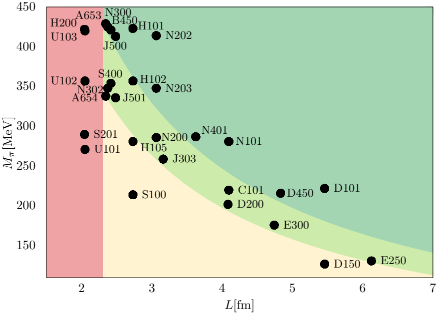
Finite volume effects ← this project

$m_s + 2m_\ell \approx$ phys.



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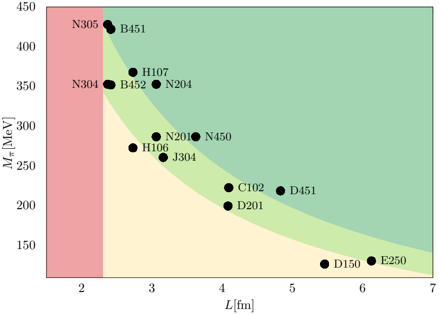
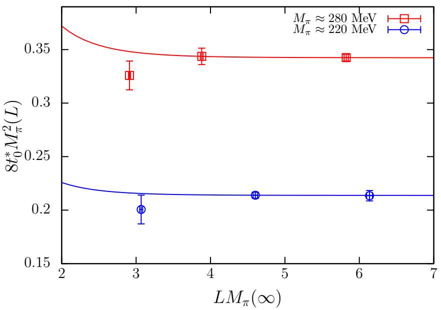


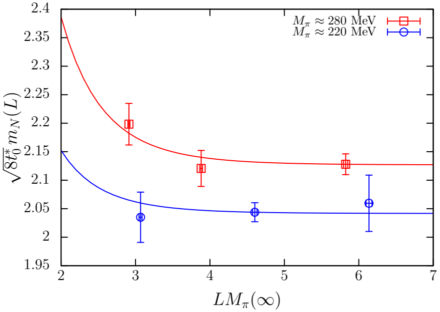
Finite volume effects in Lattice QCD

- remove finite volume effects → take the limit of infinite spatial volume $V_s = L^3$ ($L \to \infty$)
- finite volume effects are dictated by pion mass M_π and L
- yellow area: $M_\pi L \leq 4$
  light green area: $4 < M_\pi L \leq 5$
  green area: $5 < M_\pi L$
- almost all ensembles are within light green or green area (and also $L \gtrsim 2.3$ fm)
  → small finite volume effects

Finite volume effects ← this project



pion mass



nucleon mass

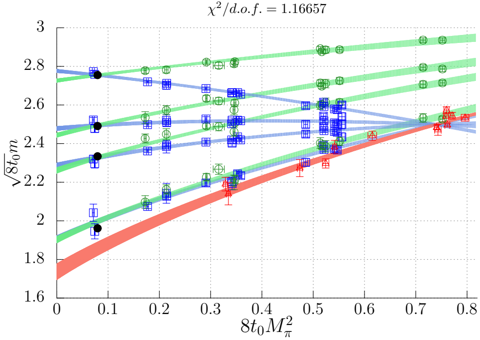
Dedicated ensembles with small/large volumes ← additional ensembles currently generated within this project

→ small finite volume effects for $m_\pi L > 4$

→ given the large number of ensembles, small effects add up!
→ include finite volume effects for baryons in fits: quality of fits increases significantly ($\chi^2/dof \sim 1.4 \to 1.2$)
→ finite volume effects are relevant and a good understanding of these effects is needed

⇒ detailed investigation of finite volume effects needed ← this project (results in progress)

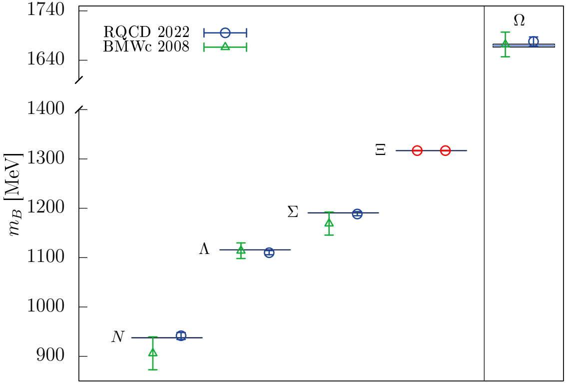
Chiral and Continuum Extrapolation Baryon Spectrum



Extrapolation in lattice spacing a (continuum limit) and quark masses m_ℓ, m_s (chiral limit)

- baryon masses m: nucleon (N), lambda (Λ), sigma (Σ), xi (Ξ), black points=physical values
- combined chiral and continuum fit
  $\rightarrow$ visualized here: only extrapolation to physical light quark mass $m_\ell \rightarrow m_{\ell,physical}$
- note: pion mass $M_\pi^2 \sim m_\ell$: $m_\ell \rightarrow m_{\ell,physical} \longleftrightarrow M_\pi^2 \rightarrow M^2_{\pi,physical} \approx 135MeV/c^2$

Light Baryon Spectrum



Results of fits for masses of baryons: nucleon (N), lambda (Λ), sigma (Σ), xi (Ξ), omega (Ω)

- comparison of previous results from BMWc collaboration from 2008 and our recent results (RQCD 2022)
- black horizontal lines represent experimental data

Lattice QCD: Hard- and Software

Hardware

- JURECA-BOOSTER@Jülich: Intel KNL
- JUWELS@Jülich: Intel Skylake
- JUWELS-BOOSTER@Jülich: Nvidia A100
- SuperMUC-NG@Munich: Intel Skylake
- QPACE3@UR: Intel KNL
- QPACE4@UR: ARM (Fujitsu A64FX)
- FRITZ@FAU

Storage and data management: Peta Bytes of data

- 126,000 configurations (975 TB) stored at Zeuthen and redundantly at Regensburg (on tape)
- analysis files stored at Regensburg $\sim$ 1.2 PB and a lot a JSC
- tools are available for backing up data (reading and writing to tape), scripts are used for automated data handling
- configurations are available for users outside CLS upon request

Software

- C/C++, Python
- high performance solver: multigrid solvers (DD-αAMG, IDFLS)
- software packages: openQCD, Chroma, GRID + GPT (open source)

Summary

Standard Model

- excellent agreement of experimental and theoretical results
- Standard Model is believed to be incomplete
  $\rightarrow$ search for little deviation from the Standard Model
- high precision results needed in both experiments and theory

This project

- high precision results from Lattice QCD necessary
- need to control all systematic uncertainties in Lattice QCD simulations
- finite volume effects is a relevant source of systematics at the precision reached now
  $\rightarrow$ see calculated baryon masses

$\Rightarrow$ a good understanding of finite volume effects is needed

$\Rightarrow$ fritz@fau: perfect environment to perform this important, intermediate scale project