Light Hadron Masses from First Principles

Stefan Krieg

<s.krieg@fz-juelich.de>

Budapest-Marseille-Wuppertal collaboration:
S. Durr, Z. Fodor, J. Frison, C. Hoelbling, S.D. Katz, T. Kurth, L. Lellouch,
Th. Lippert, K.K. Szabo, G. Vulvert

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on Particle Physics and Quantum Field Theory

Outline

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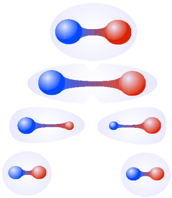
Important properties of QCD

QCD has remarkable properties:

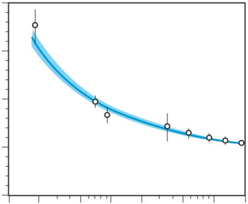


- Confinement (conformal anomaly)
- Dynamical chiral symmetry breaking of $SU_A(N_f)$ ($\langle \overline{\psi}_i \psi_i \rangle \neq 0$)
- Chiral anomaly breaking of $U_A(1)$ ($\delta \mathcal{D}\overline{\psi}_i \mathcal{D}\psi \neq 0$)

- Asymptotic freedom

$$\beta(\alpha_s) = \mu \frac{\partial \alpha_s(\mu)}{\partial \mu} = \frac{\alpha_s^2}{\pi} b_1 + \frac{\alpha_s^3}{\pi^2} b_2 + \ldots$$

$$b_1 = -\left[\frac{11}{6} C_A - \frac{2}{3} \sum_R n_R T_R \right]$$



Definition of QCD

The Lagrangian of Quantum Chromodynamics (QCD)

$$\mathcal{L}_E^{QCD} = \frac{1}{2g^2}\mathrm{Tr}\left[G_{\mu\nu}\, G_{\mu\nu}\right] - \sum_{i=1}^{N_f} \overline{\psi}_i \left(\not{D} - m_i\right) \psi_i$$
$$+ i\theta \frac{1}{16\pi^2 g^2}\mathrm{Tr}\left[G_{\mu\nu}\, G_{\rho\sigma}\epsilon_{\mu\nu\rho\sigma}\right].$$

contains all possible (renormalizable) operators that are compatible with the defining symmetries of QCD:

- Poincaré symmetry
- SU(3) (color) gauge invariance
- global $SU_V(N_f) \times U_V(1) \times SU_A(N_f)\{\times U_A(1)\}$ (massless case)
- if $\theta = 0$ C,P and T

Definition of QCD

Given the action, observables can be extracted from path-integral (PI) correlation functions

$$\begin{aligned} \langle \mathcal{O} \rangle^{F,G}_{QCD} &= \int \mathcal{D}\overline{\psi}\mathcal{D}\psi\mathcal{D}A\, \mathcal{O}(\overline{\psi},\psi,A)\ \exp\left\{ iS^{QCD}(\overline{\psi},\psi,A)\right\} \\ &= \int \mathcal{D}A \left(\prod_{i=1}^{N_f} \det[D(m_i)] \right) \langle \mathcal{O}(A)\rangle^F \ \exp\left\{ iS^{QCD}_G(A)\right\} \end{aligned}$$

- The integration of the Grassmann-variables yields the fermionic determinant.
- After performing a Wick-rotation to imaginary time, the action transforms

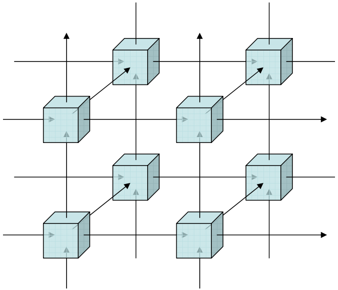
$$iS^{QCD} \rightarrow -S^{QCD}_E$$

  and becomes *real* ($\Rightarrow$ LQCD simulations)

The Lattice and the classical Wilson gauge action

$$S_{WG} = g_0^{-2} \sum_{x,\mu\nu} \left[N_c - \Re \,\mathrm{Tr} \left[U_\mu(x) U_\nu(x + a\,\hat{\mu}) U_\mu^\dagger(x + a\,\hat{\nu}) U_\nu^\dagger(x) \right] \right]$$

$$\begin{aligned} U_\mu(x) &= \exp\{ia\tau^a A_\mu^a(x)\} \\ U_{\mu\nu}(x) &= \mathbf{1} + i(a^2 G_{\mu\nu} + \mathcal{O}(a^3)) \\ &\quad -\frac{1}{2} a^4 G_{\mu\nu}^2 + \mathcal{O}(a^5) \\ S_{WG} &= \frac{1}{2g_0^2} \sum_x \mathrm{Tr}\left[G_{\mu\nu} G_{\mu\nu}\right] + \mathcal{O}(a^2) \end{aligned}$$



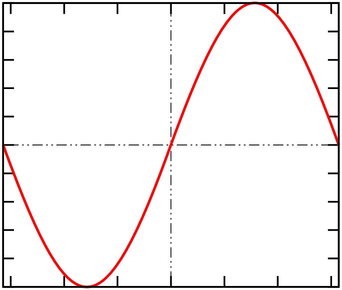
- Quarks live on the lattice points
- Gluons not only live on the links, they *are* the links

Symmetries

Discretization should preserve as many symmetries as possible.

It cannot preserve

- SO(4) (→ Poincaré) invariance, but the lattice variant: the cubic group W(4)
- **Nielsen Ninomiya theorem:** Fermion action cannot preserve translational invariance and chiral symmetry while being real, local and bilinear



Latter problem is usually solved by **explicitly breaking** chiral symmetry in some fashion.

The Wilson fermion action

- Wilson solved doubling problem by adding a *continuum irrelevant* operator (the terms proportional to r)

$$
\begin{aligned}
S_{WF} &= a^4 \sum_{xy} \bar{\psi}(x) M_{Wxy} \psi(y) \\
M_{Wxy} &= \delta_{x,y} - \kappa \sum_{\mu} \left[(r - \gamma_\mu) U_\mu(x) \delta_{x,y+a\hat{\mu}} + (r + \gamma_\mu) U_\mu^\dagger(x) \delta_{x,y-a\hat{\mu}} \right] \\
M_W &\propto am_0 - a\not{D} + \mathcal{O}(a^3) + r a^2 D^2 + \mathcal{O}(a^3)
\end{aligned}
$$

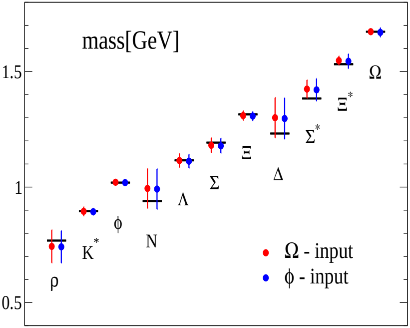
- In other words by **explicitly breaking** chiral symmetry :

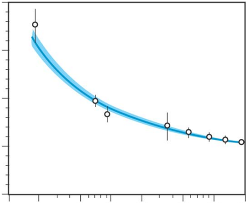
$$
\begin{aligned}
(\gamma_5 M_W + M_W \gamma_5)_{xy} &= \delta_{x,y} - r\kappa \sum_{\mu} \left[U_\mu(x) \delta_{x,y+a\hat{\mu}} + U_\mu^\dagger(x) \delta_{x,y-a\hat{\mu}} \right] \\
S_W(p) &= \left[m_0 a + 4r - \sum_{\mu} (r \cos ap_\mu - i\gamma_\mu \sin ap_\mu) \right]
\end{aligned}
$$

- **Problem:** Additive quark mass renormalization, *critical slowing down*
- Improved actions & algorithms required (25 year effort by the field)

Status

- Asymptotic freedom: good agreement between theory and experiment (perturbative methods)





- Good evidence in the non-perturbative domain (e.g. CP-PACS '07, $N_f=2+1$, $210\mathrm{MeV} \leq M_\pi \leq 730\mathrm{MeV}$, $a \simeq 0.087\,\mathrm{fm}$, $L \lesssim 2.8\,\mathrm{fm}$, $M_\pi L \simeq 2.9$)
- However, systematic errors not under control

Outline

Importance Sampling

- After Wick-rotation, the exponent of the Boltzmann-factor in the path-integral is positive

$$\exp\left\{iS^{QCD}\right\} \to \exp\left\{-S_E^{QCD}\right\}$$

- The path-integral is now equivalent to a partition sum of statistical mechanics
- The Boltzmann-weight can now be interpreted as probability
- The expectation value of an operator can thus be written

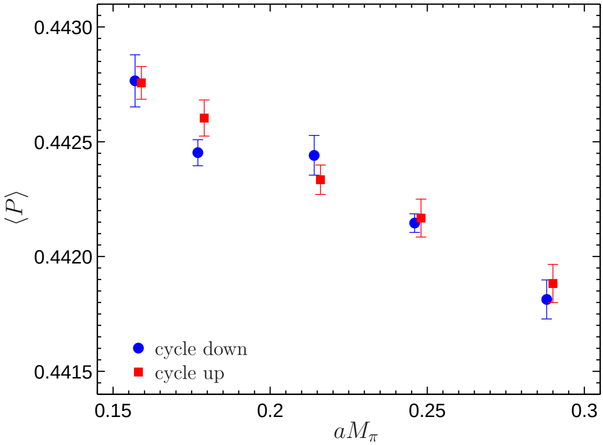
$$\langle \mathcal{O} \rangle_{F,G} = \sum_{i=0}^{\infty} \langle \mathcal{O}(A_i) \rangle_F \,,$$

if A_i has the probability $p \propto \exp\{-S_E^{QCD}(A_i)\}$ to appear in the ensemble of A's

Simulation algorithm: Details

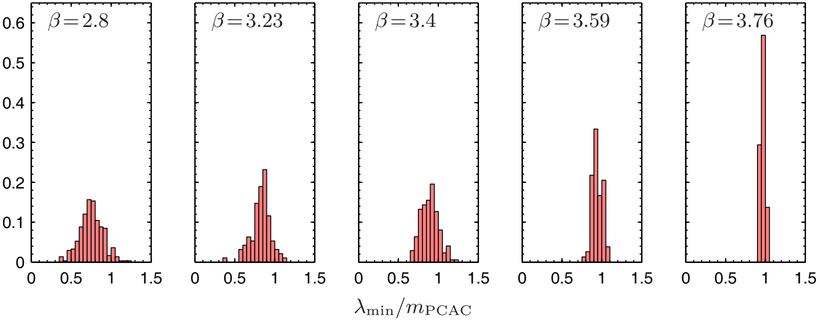
- Action
  - Clover tree level improved Wilson fermions
  - Symanzik improved gauge action
  - Stout links
- Algorithm
  - Rational HMC for strange quark
  - Mass preconditioning (“Hasenbusch trick”)
  - Multi scale integration scheme (“Sexton-Weingarten”)
  - Omelyan integrator (“non equidistant leap frog”), increasing integration precision
  - Mixed precision inverters

Algorithm stability: absence of phase transitions



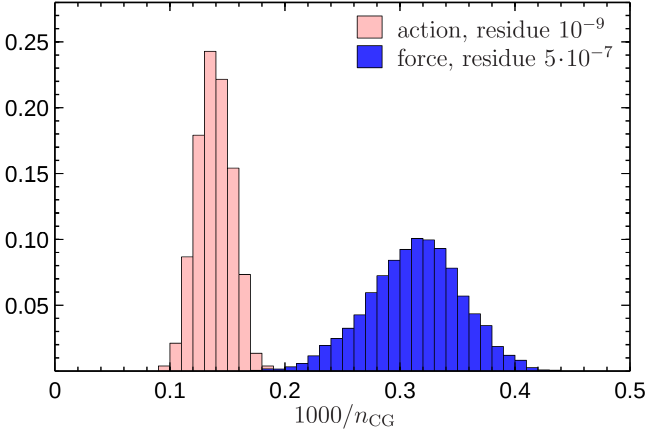
Lattices: $M_\pi \approx 240 - 440$ MeV, $a \approx 0.136$ fm

λ_{min}^{-1} distribution



$\mapsto$ Simulations

Algorithm stability: distribution of $1/n_{CG}$



Lattice: $m_\pi = 190$ MeV, $a = 0.088$ fm, 64×48^3 ($m_\pi L \geq 4$)

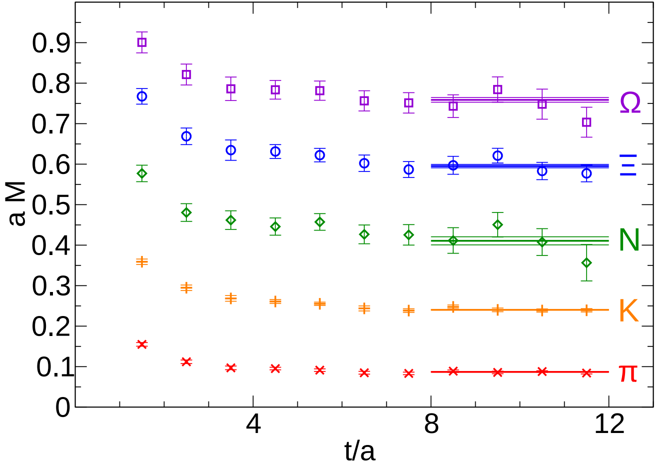
Extracting particle masses

- Masses are extracted from the formula:

$$
\begin{aligned}
\langle P(t)|P(0)\rangle &= \langle P(0)|\,\exp\{-\mathcal{H}t\}\,|P(0)\rangle \\
&= \sum_i \frac{\langle P(0)|i\rangle\,\langle i|P(0)\rangle}{2E_i}\exp\{-E_i t\} \\
&\rightarrow \frac{\langle P(0)|0\rangle\,\langle 0|P(0)\rangle}{2E_0}\exp\{-E_0 t\} + \mathcal{O}\left(\exp\{-E_1 t\}\right) \\
&\stackrel{\mathrm{BC}}{\rightarrow} const. \times \begin{matrix}\cosh\\ \sinh\end{matrix}\left\{E_0 t\right\}
\end{aligned}
$$

- Here P will be the zero momentum projected operator

Particle correlators



Lattice: $m_\pi = 190$ MeV, $a = 0.088$ fm, 64×48^3 ($m_\pi L \geq 4$)

Outline

Controlling **all** systematic errors

- Make sure it's QCD: Include u, d and s quarks int the simulation with an action, whose universality class is QCD.
- Go to physical quark masses: Use controlled interpolations and extrapolations of the results to physical m_{ud} and m_s
- Go to infinite volume: Use large volumes ($M_\pi L \gtrsim 4$) to guarantee small finite-size effects and at least one simulation at a significantly larger volume to confirm the smallness of these effects.
  - **And** treat the resonant states correctly.
- Go to the continuum: Use controlled extrapolations to the continuum limit, requiring that the calculations be performed at no less than three values of the lattice spacing.

Outline

Quark mass dependence

Goal:

- Extra-/Interpolate M_X (baryon/vector meson mass) to physical point (M_π, M_K)

Method:

- Use M_Ξ or M_Ω to set the scale
- Variables to parametrize M_π^2 and M_K^2 dependence of M_X:
  - Use bare masses aM_y, $y \in \{X, \pi, K\}$ and a (bootstrapped)
  - Use dimensionless ratios $r_y := \frac{M_y}{M_{\Xi/\Omega}}$ (cancellations)

We use both procedures $\rightarrow$systematic error

Quark mass dependence (ctd.)

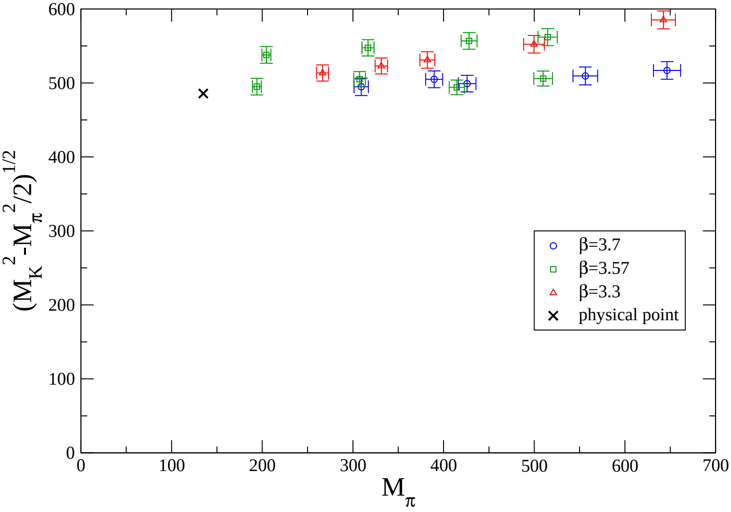
Method (ctd.):

- Parametrization: $M_X = M_X^{(0)} + \alpha M_\pi^2 + \beta M_K^2 +$ higher orders
  - Leading order sufficient for M_K^2 dependence
  - We include higher order term in M_π^2
    - Next order χPT (around $M_\pi^2 = 0$): $\propto M_\pi^3$
    - Taylor expansion (around $M_\pi^2 \neq 0$): $\propto M_\pi^4$

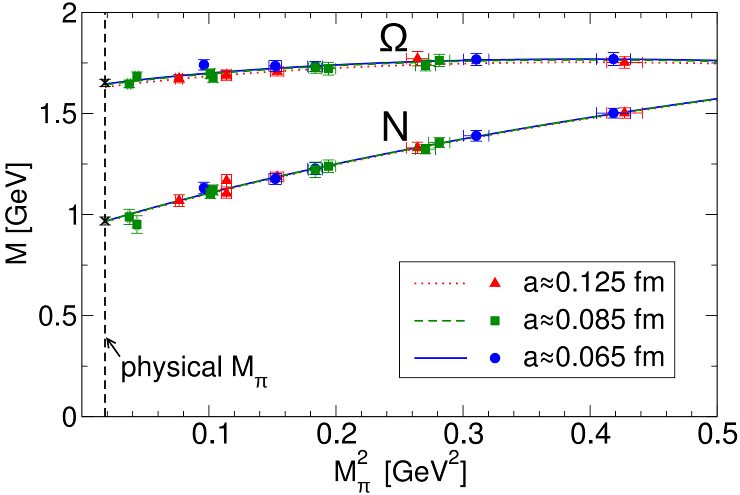
  Both procedures fine →systematic error
  No sensitivity to any order beyond these
- Vector mesons: higher orders not significant
- Baryons: higher orders significant
  - Restrict fit range to further estimate systematics:
    - Use full range, $M_\pi < 550, 450\text{MeV}$

  We use all 3 ranges →systematic error

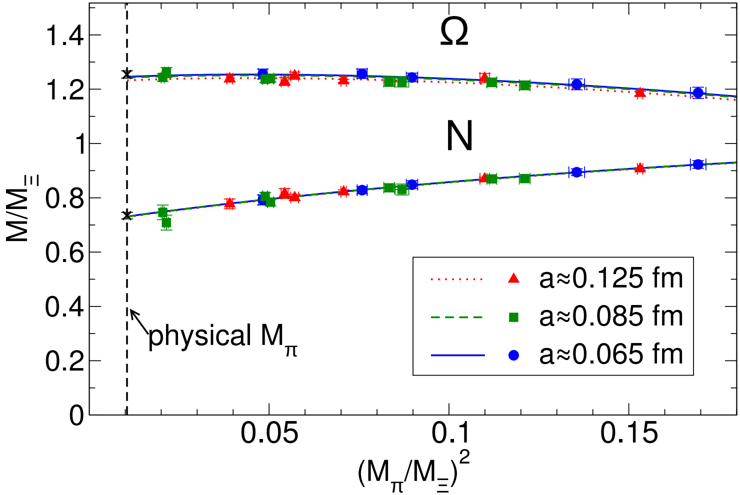
Data set


600
500
400
300
200
100
0
0
100
200
300
400
500
600
700
$(M_K^2 - M_\pi^2/2)^{1/2}$
M_π
β=3.7
β=3.57
β=3.3
physical point

Chiral fit


2
1.5
1
0.5
0
0.1
0.2
0.3
0.4
0.5
M [GeV]
M_π^2 [GeV^2]
Ω
N
physical M_π
a≈0.125 fm
a≈0.085 fm
a≈0.065 fm

Chiral fit using ratios



Outline

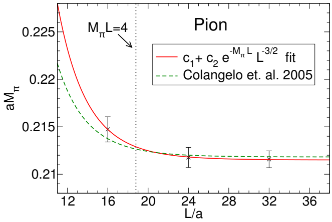
Finite volume effects from virtual pions

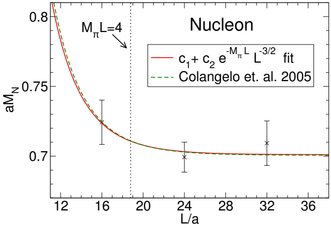
Goal:

- Eliminate virtual pion finite V effects

Method:

- Best practice: use large V
  - We use $M_\pi L \gtrsim 4$ (and one point to study finite V)
  - Effects are tiny and well described by $\frac{M_X(L)-M_X}{M_X} = cM_\pi^{1/2} L^{-3/2} e^{M_\pi L}$ Colangelo et. al., 2005





Finite volume effects in resonances

Goal:

- Eliminate spectrum distortions from resonances mixing with scattering states

Method:

- Stay in region where resonance is ground state
  - Otherwise no sensitivity to resonance mass in ground state
- Systematic treatment Lüscher, 1985-1991
  - Conceptually satisfactory basis to study resonances
  - Coupling as parameter (related to width)
- Fit for coupling (assumed constant, related to width)
  - No sensitivity on width (compatible within large error)
  - Small but dominant FV correction for light resonances

Outline

Continuum extrapolation

Goal:

- Eliminate discretization effects

Method:

- Formally in our action: $O(\alpha_s a)$ and $O(a^2)$
- But: discretization effects are tiny
  - Not possible to distinguish between $O(a)$ and $O(a^2)$

$\rightarrow$include both in systematic error

Outline

Systematic uncertainties

Goal:

- Accurately estimate total systematic error

Method:

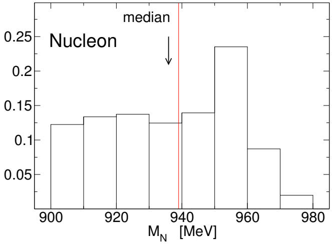
- We account for all the above mentioned effects
- When there are a number of sensible ways to proceed, we take them: Complete analysis for each of
  - 18 fit range combinations
  - ratio/nonratio fits (r_X resp. M_X)
  - $O(a)$ and $O(a^2)$ discretization terms
  - NLO χPT M_π^3 and Taylor M_π^4 chiral fit
  - 3 χ fit ranges for baryons: $M_\pi < 650/550/450$ MeV

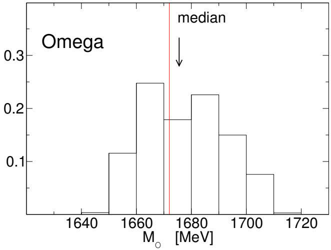
  resulting in 432 predictions for each hadron mass with each 2000 bootstrap samples for each Ξ and Ω scale setting

Systematic uncertainties (ctd.)

Method (ctd.):

- Weigh each of the 432 central values by fit quality Q
  - Median of this distribution →final result
  - Central 68% →systematic error
- Statistical error from bootstrap of the medians





Outline

Particle spectrum

BMW-collaboration, Science **322** (2008), 1224