Hadron Physics from Lattice Simulations

I. Concepts of lattice field theory

regularisation, simulation, numerical measurements

II. Lattice QCD results for the hadron spectrum

from quenched to dynamical quarks

results to %-level

III. Summary and outlook

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I. Lattice Field Theory

Functional integral formulation of Quantum Field Theory in Euclidean space

(Wick rotation to imaginary time $\rightarrow$ link to stat. mechanics):

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

$$e^{-S_{\mathrm{E}}[\Phi]}/Z = \text{probability of field configuration } [\Phi]$$

Lattice regularisation

discrete Euclidean space, lattice spacing a $\rightarrow$ momentum cutoff π/a

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

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

Lattice Simulations

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

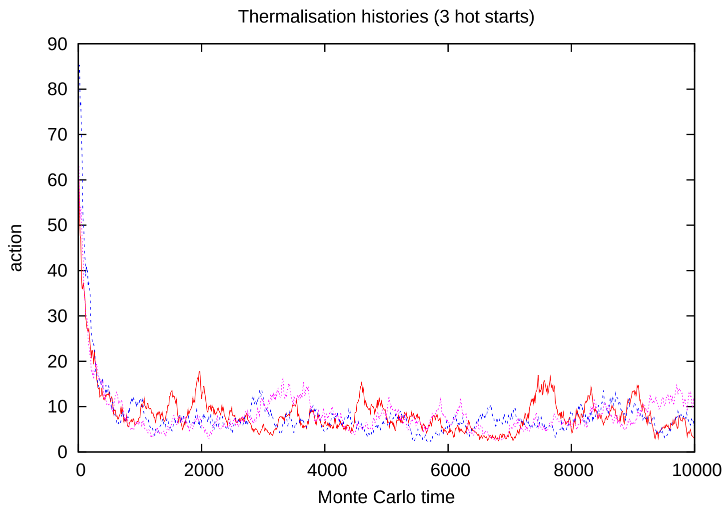
Sum over this set $\rightarrow$ measure observables up to

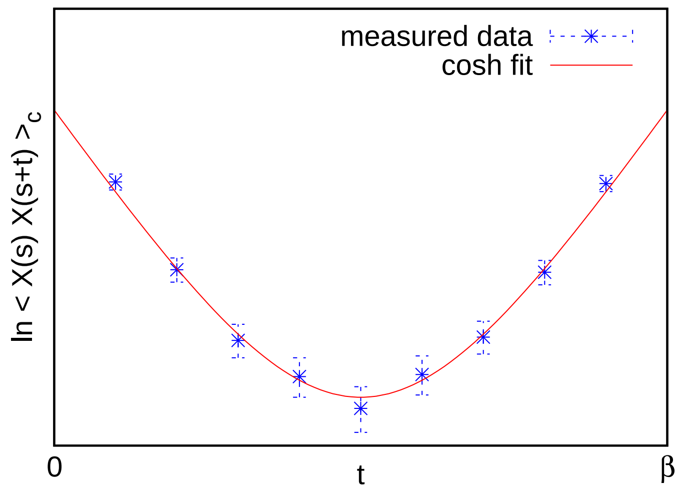
- statistical errors $\propto 1/\sqrt{\text{number of configurations}}$
- systematic errors (finite a, finite volume), vary and extrapolate

Non-perturbative ! Results at finite coupling strength.
Works at 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”).
First discard many steps, until the right regime is attained (“thermalisation”).
Then pick well separated (“de-correlated”) conf's to measure observables.





With this set, measure *e.g.* a 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* $M = E_1 - E_0 = \{$Mass of particle described by $X\} = 1/\xi$

Lattice Gauge Theory

E.g. scalar field $\Phi_x \in \mathbb{C}$, action

$$S[\Phi] = \frac{1}{2} a^4 \sum_{x,y} \Phi_x^* M_{xy} \Phi_y + \frac{\lambda}{4!} a^4 \sum_x |\Phi_x|^4$$

$$M_{xy} = \sum_{\mu=1}^{d} \frac{-\delta_{x+\hat{\mu},y} - \delta_{x-\hat{\mu},y} + 2\delta_{x,y}}{a^2} + m^2 \delta_{x,y}$$

$|\hat{\mu}| = a$, vector in μ-direction. Discrete version of $-\partial^2 + m^2$

Global symmetry $\Phi_y \to \exp(\mathrm{i} g \varphi)\, \Phi_y$
is promoted to local symmetry (gauge symmetry) $\Phi_y \to \exp(\mathrm{i} g \varphi_y) \Phi_y$
if we replace the δ-links as

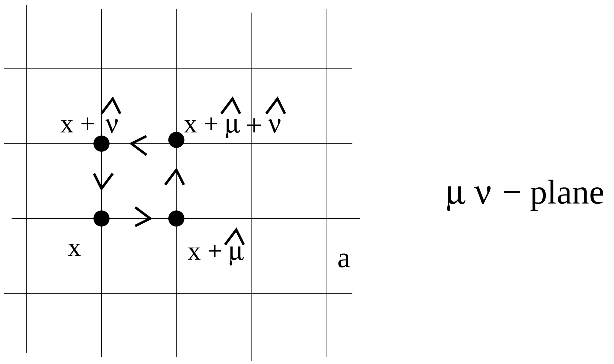
$$\Phi_x^* \Phi_{x+\hat{\mu}} \to \Phi_x^* U_{x,\mu} \Phi_{x+\hat{\mu}} \;, \qquad U_{x,\mu} \in \mathrm{U}(1)$$

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

Discrete covariant derivative; regularised system is gauge invariant !
"Compact link variables" $\in$ gauge group

Pure Gauge Action

$$\text{Plaquette variable :} \quad U_{x,\mu\nu} := U^*_{x,\nu} U^*_{x+\hat{\nu},\mu} U_{x+\hat{\mu},\nu} U_{x,\mu}$$



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

$$S_{\rm gauge}[U] = \frac{1}{4a^2} \sum_{x,\mu<\nu} (2 - U_{x,\mu\nu} - U^*_{x,\mu\nu}) \overset{\text{cont. limit}}{\rightsquigarrow} \frac{1}{4} F_{\mu\nu} F_{\mu\nu}$$

Non-Abelian Gauge Groups, *e.g.* QCD

$U_{x,\mu},\ U_{x,\mu\nu} \in \mathrm{SU}(3)$. Inverse direction: $U^\dagger_{x,\mu}$

$$S_{\rm gauge}[U] = \frac{1}{4a^2} \sum_{x,\,\mu<\nu} \Big(6 - \mathrm{Tr}[U_{x,\mu\nu} + U^\dagger_{x,\mu\nu}]\Big)$$

Regularised theory is gauge invariant, no gauge fixing needed !

{ Global symmetry: Poincaré invariance reduced to a discrete version, but recovery in continuum limit is safe. }

Fermion fields : $\bar{\Psi}_x,\ \Psi_y, \quad Z = \int \mathcal{D}\bar{\Psi}\mathcal{D}\Psi\ \exp(-\bar{\psi}_i M_{ij} \psi_j)$

i, j run over :

- space-time points $\longrightarrow$ lattice sites
- internal degrees of freedom (spinor index, ev. flavour and colour)

M contains for each spinor a (discrete, Euclidean) Dirac operator $D = \mathrm{i}\gamma_\mu D_\mu + m$

Naïve ansatz fails: $D_\mu^{\text{free, naïve}} = (\delta_{x+\hat{\mu}} - \delta_{x-\hat{\mu}})/(2a) \ \Rightarrow\ D_\mu(p) = \frac{\mathrm{i}}{a}\sin(ap_\mu)$
Doubling problem! Can be avoided by adding a discrete Laplacian ("Wilson fermion"),
but: explicit chiral symmetry breaking, additive mass renormalisation . . .

Remedy (for vector theories, like QCD): preserve lattice modified chiral symmetry,
solutions are known, but tedious to simulate.

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

With gauge interaction: covariant derivative D_μ

Components $\bar{\psi}_i,\ \psi_j$ anti-commute, represented by Grassmann variables

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

$\Rightarrow$ Computer does not deal with Grassmann variables, we "only" need $\det M$, 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 $M[U]^{-1}$

Pure gauge: action shift for local update $[U] \rightarrow [U']$ can be computed locally $\rightarrow$ fast

With fermions tedious, in QCD: quarks cost $O(100)$ times more compute time.

Lattice QCD

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

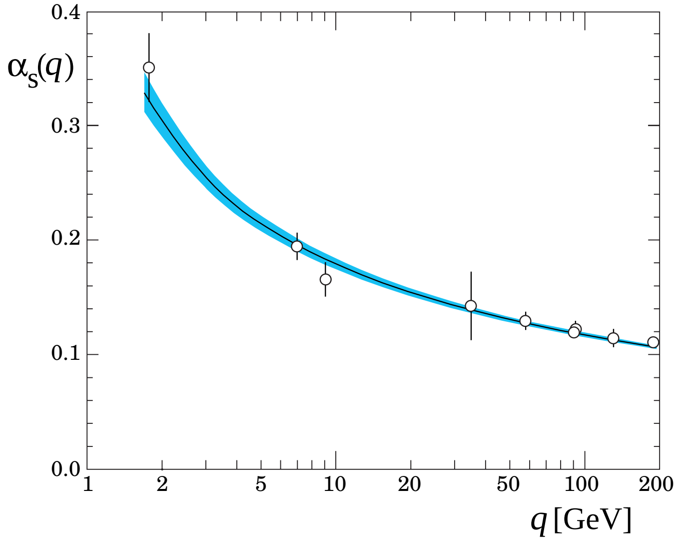
$$Z = \int \mathcal{D}U \underbrace{\det M[U] \exp(-S_{\mathrm{gauge}}[U])}_{\text{statistical weight of conf. } [U] \,\to\, \textit{Monte Carlo}}$$

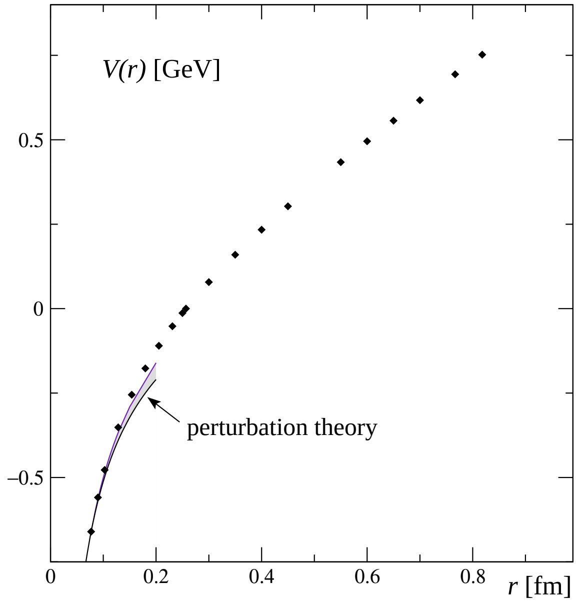
Measure correlation functions, *e.g.* of pseudoscalar density $P = \bar{\Psi}\gamma_5\Psi$

$\langle P_x \, P_y \rangle_{\mathrm{c}} \propto \exp(-M_\pi |x-y|) \;\Rightarrow\;$ pion mass M_π

$\Rightarrow$ Explicit results for hadron masses, matrix elements, decay constants, cross-over: confinement $\leftrightarrow$ de-confinement, topological susceptibility ... REALLY based on QCD.

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



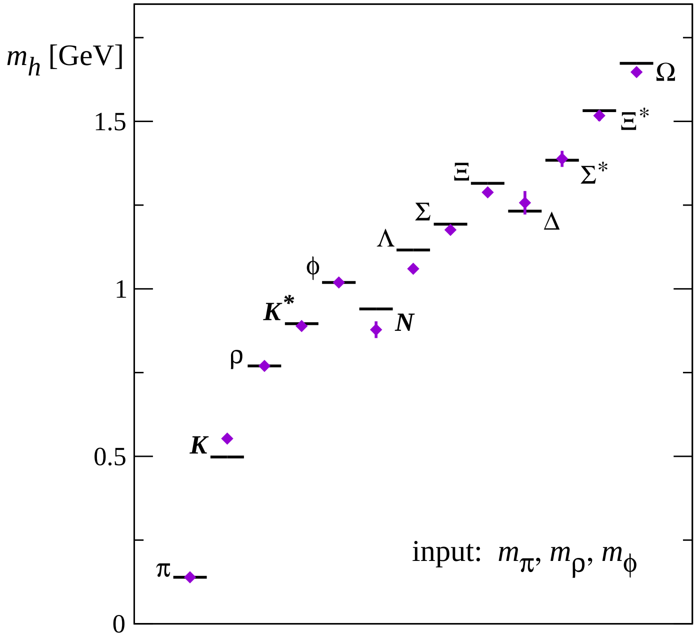


- Left: strong coupling $\alpha_s(q) = g_s^2(q)/4\pi$ at transfer momentum q

  Fit: $\alpha_s(q) \propto 1/\ln(q/\Lambda_{QCD})$ $\quad (\Lambda_{QCD} \approx 250\ \mathrm{MeV})$

- Right: the potential between static quarks; numerical results demonstrate confinement

  No *analytic* proof so far, millennium problem



Hadron Masses :

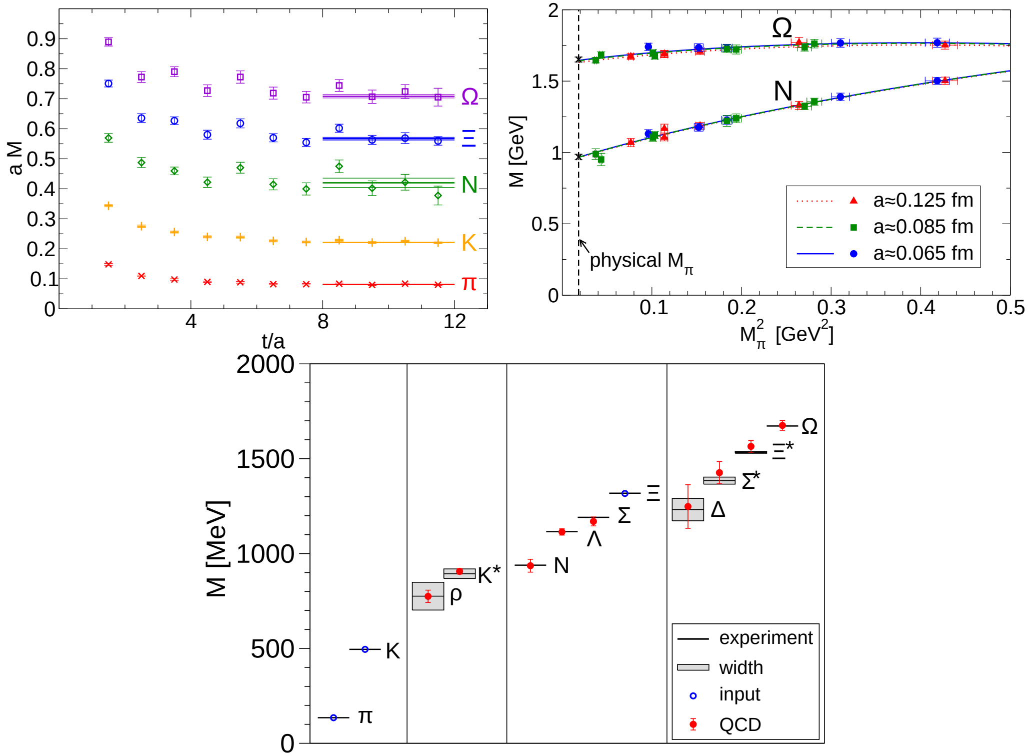
Status: year 2002 (CP-PACS Collaboration), "quenched" simulations
(generate conf's with $\det M = 1$)

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

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

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

Dynamical quarks (det M included), *e.g.* Budapest-Marseilles-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 $\mathrm{M_{Nucleon}} = \mathbf{936(25)(22)\ MeV}$ vs. 939 MeV in Nature (statistical) (systematic) error.

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

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:

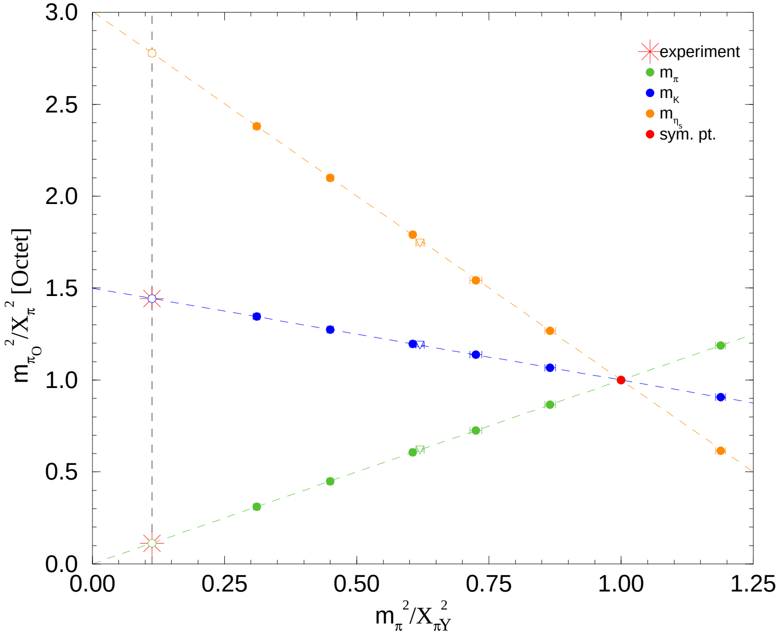
1. Start from a $SU(3)_{\mathrm{flavour}}$ symmetric point: $m_u^R = m_d^R = m_s^R$, $M_\pi = M_K$
2. Approach physical point with $m_l^R - m_s^R$ splitting while keeping

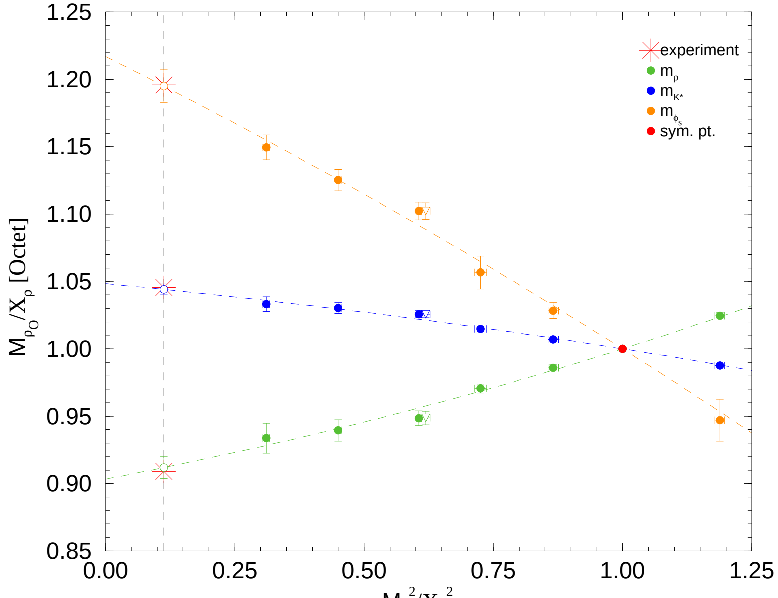
   $X_\pi^2 := \frac{1}{3}(M_\pi^2 + 2M_K^2) \approx \mathrm{const.} \approx (411\ \mathrm{MeV})^2$ (centre of mass^2 in meson octet)

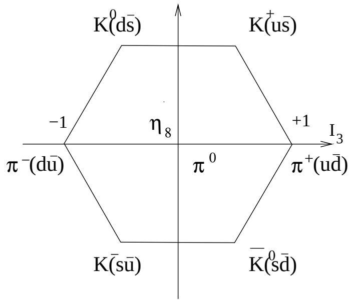
   m_l^R resp. M_π down, m_s^R resp. M_K up;

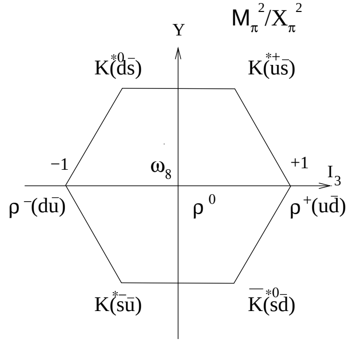
   extrapolation constrained and stable, guided by χPT

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



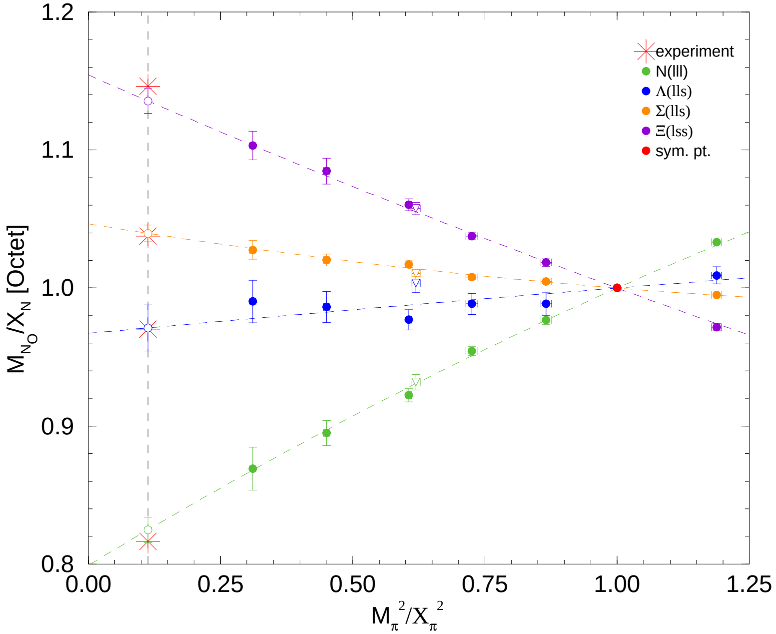


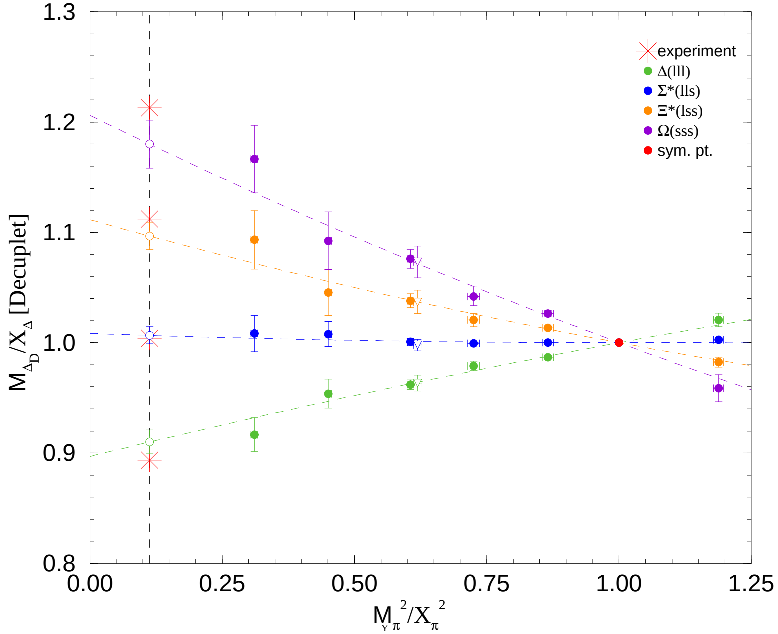


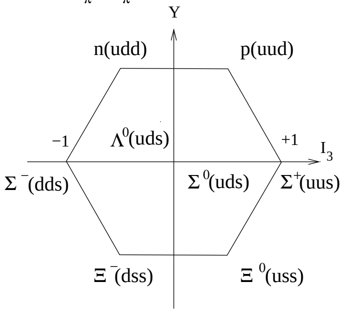


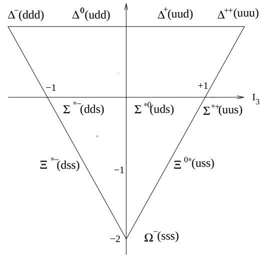
pseudo-scalars π, K, η_s ($\bar{s}s$, hypothetical) vector mesons ρ, K^*, ϕ

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

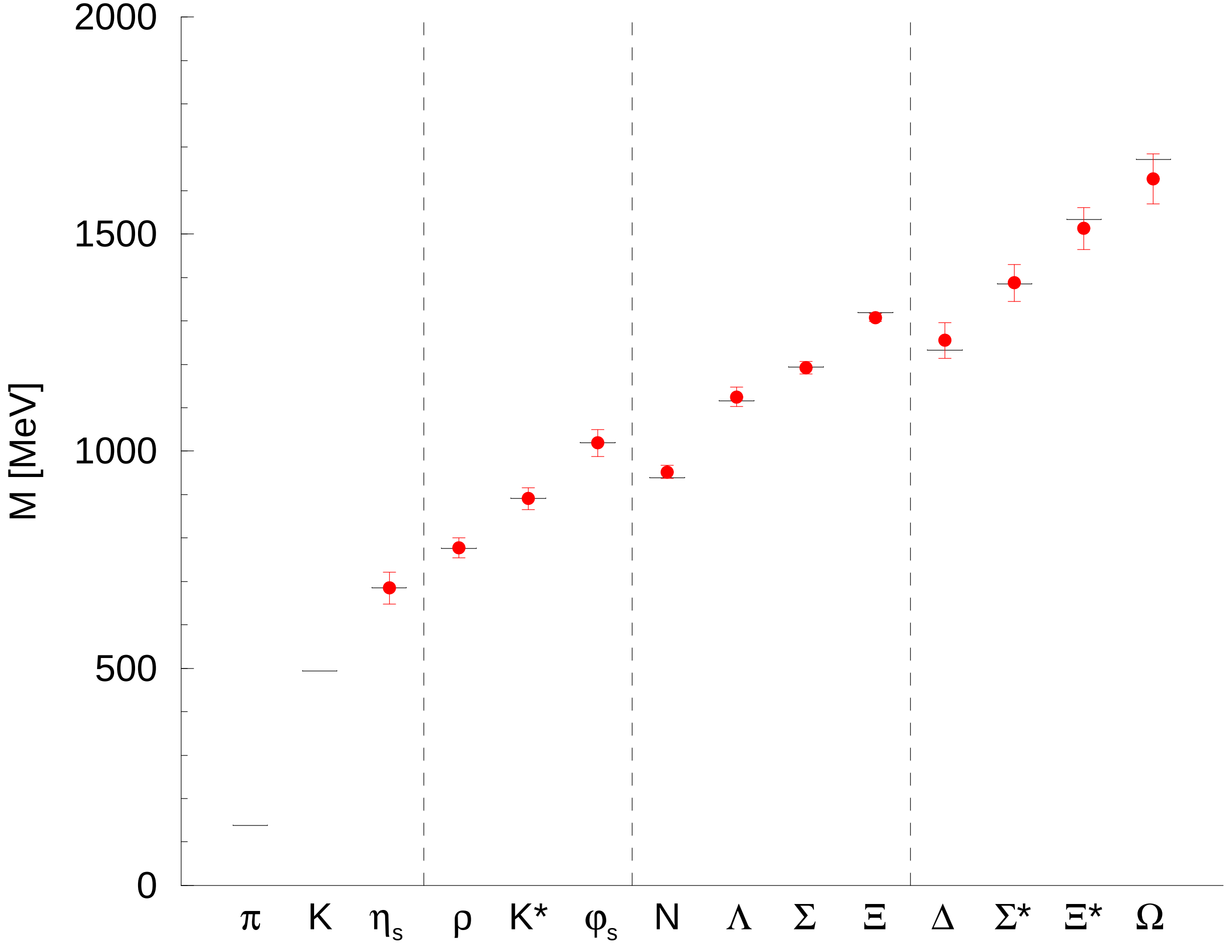








Nucleon (lll), Λ (lls), Σ (lls), Ξ (lss) Δ (lll), Σ^* (lls), Ξ^* (lss), Ω (sss)



Percent-level agreement with phen. values (black bars); M_π and M_K are input.

Summary and outlook

Lattice simulations: THE method for Quantum Field Theory beyond perturbation theory.

Developed in the 1980s, finally breakthrough in QCD (despite Wilson's pessimism).

• For the light hadron spectrum, low energy QCD is now tested from $1^{\rm st}$ principles and confirmed to percent accuracy.

Next: sub-% level, include QED effects, m_u, m_d splitting $\longrightarrow$ $M_n > M_p$

Step from post-dictions to pre-dictions:

⋆ M_{Bc} *predicted* by HPQCD (2005): $6.82(8)$ GeV; CDF (2006): $6.78(7)$ GeV.

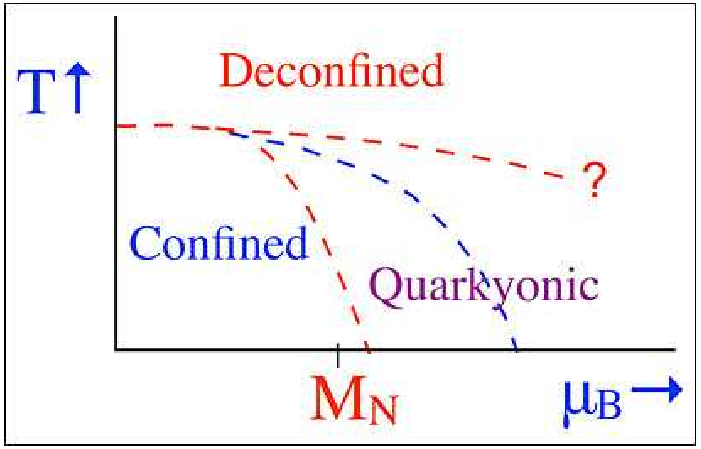
• Outstanding challenges: precision data for excited states (*e.g.* Roper resonance)

So far $a \in [0.05 \ldots 0.1]$ fm, but: $a \lesssim 0.05$ fm:
HMC algorithm gets stuck in one topological sector, not ergodic anymore

QCD phase diagram

Cross-over at $T \simeq 155 \ldots 165\,\mathrm{MeV}$ confinement $\leftrightarrow$ quark-gluon plasma, but how about high baryon density?

Unexplored, because chem. potential μ_B leads to **"sign problem"**:
$S_\mathrm{E} \in \mathbb{C} \;\Rightarrow\; \frac{1}{Z}\exp(-S_\mathrm{E}) \neq$ probability



To be solved by quantum computers ?