

# Exploratory calculations of baryon resonances and exotic charmonia from Lattice QCD using Lüscher's method

Daniel Mohler

Hirscheegg,  
January 15th, 2018



- 1 Introduction and motivation
  - Recent progress in Lattice QCD simulations
  - Coordinated Lattice Simulations (CLS)
  - Illustrative example:  $\rho$  resonance and relevance to  $(g - 2)_\mu$
- 2 Exploratory calculations for charmonium resonances and bound states
  - Previous results for the  $\chi'_{c0} / X(3915)$
  - Towards charmonium resonances from coupled-channel simulations
- 3 Exploratory calculations for baryon resonances
  - Previous results
  - Challenges
  - Towards coupled-channel results for the  $\Lambda(1405)$
- 4 Conclusions and Outlook

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# Lattice Quantum Chromodynamics: What do we calculate?

Regularization of QCD by a 4-d Euclidean space-time lattice. (Kenneth Wilson 1974)

Provides a calculational method for QCD



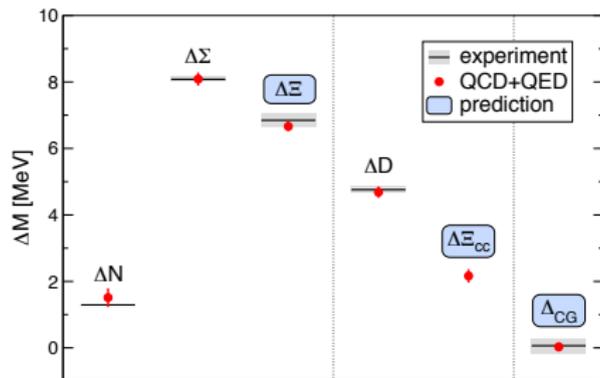
Euclidean correlator of two Hilbert-space operators  $\hat{O}_1$  and  $\hat{O}_2$ .

$$\begin{aligned}\langle \hat{O}_2(t)\hat{O}_1(0) \rangle &= \sum_n e^{-t\Delta E_n} \langle 0|\hat{O}_2|n\rangle \langle n|\hat{O}_1|0\rangle \\ &= \frac{1}{Z} \int \mathcal{D}[\psi, \bar{\psi}, U] e^{-S_E} O_2[\psi, \bar{\psi}, U] O_1[\psi, \bar{\psi}, U]\end{aligned}$$

- Path integral over the Euclidean action  $S_{E,QCD}[\psi, \bar{\psi}, U]$ ; (a sum over quantum fluctuations)
- Can be evaluated with *Markov Chain Monte Carlo* (using methods well established in statistical physics)

# Recent progress in Lattice QCD

- Dynamical simulations with 2+1(+1) flavors of sea quarks
- Simulations at physical pion (light-quark) masses
- Isospin splitting and QCD+QED simulations
- Improved heavy quark actions for charm



BMW Collaboration, Borsanyi et al. Science 347 1452 (2015)

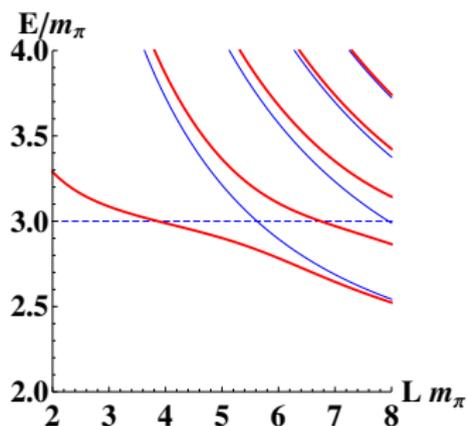
# Progress from an old idea: Lüscher's finite-volume method

M. Lüscher Commun. Math. Phys. 105 (1986) 153;  
Nucl. Phys. B 354 (1991) 531; Nucl. Phys. B 364 (1991) 237.

*Basic observation:* Finite volume, multi-particle energies are shifted with regard to the free energy levels due to the interaction

$$E = E(p_1) + E(p_2) + \Delta_E$$

- Energy shifts encode scattering amplitude(s)
- Original method: Elastic scattering in the rest-frame in multiple spatial volumes  $L^3$
- Coupled 2-hadron channels well understood
- $2 \leftrightarrow 1$  and  $2 \leftrightarrow 2$  transitions well understood (example  $\pi\pi \rightarrow \pi\gamma^*$ )
- significant progress for 3-particle scattering  
→ see talk by Akaki Rusetsky



# Fully systematic calculation vs. exploratory study

Important lattice systematics from

- Taking the *continuum limit*:  $a(g, m) \rightarrow 0$
- Taking the *infinite volume limit*:  $L \rightarrow \infty$
- Calculation at (or extrapolation to) the physical pion mass

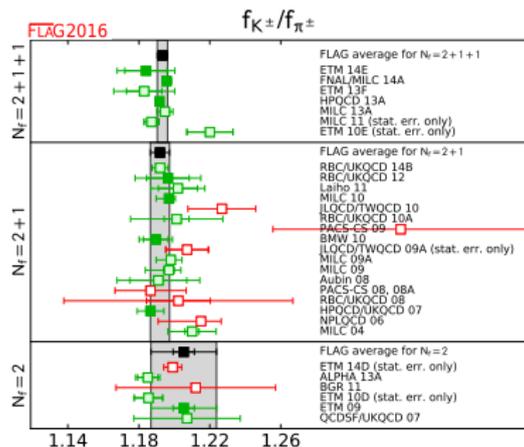
I cover many *exploratory* results

- Should be compared only qualitatively to experiment
- Provide an outlook on future Lattice QCD results

Example for fully systematic results:

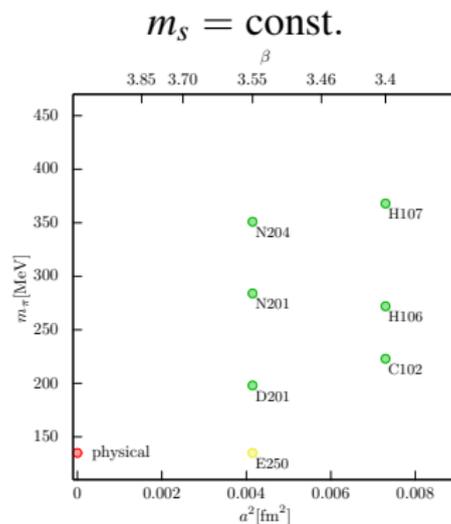
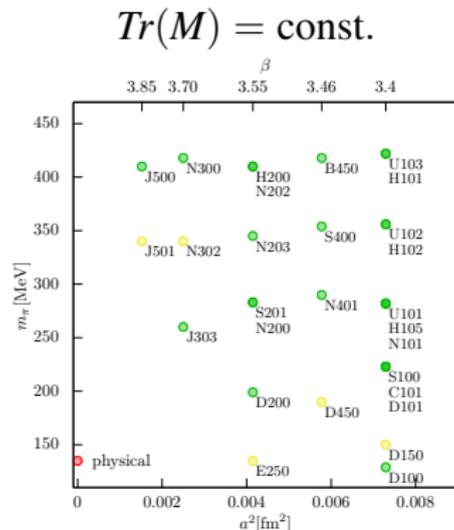
- Flavor physics results listed in the FLAG review

<http://itpwiki.unibe.ch/flag/>



# CLS 2+1 flavor ensembles: Overview

Bruno et al. JHEP 1502 043 (2015); Bali et al. PRD 94 074501 (2016)

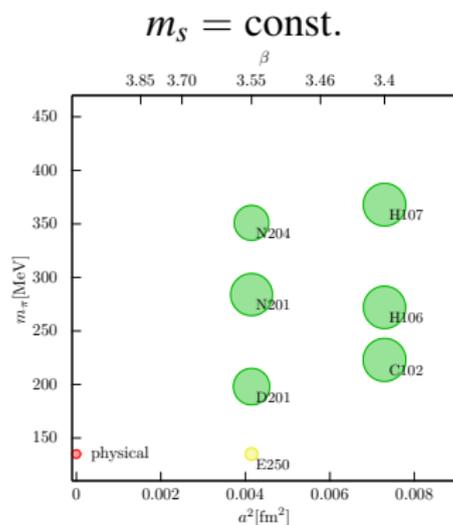
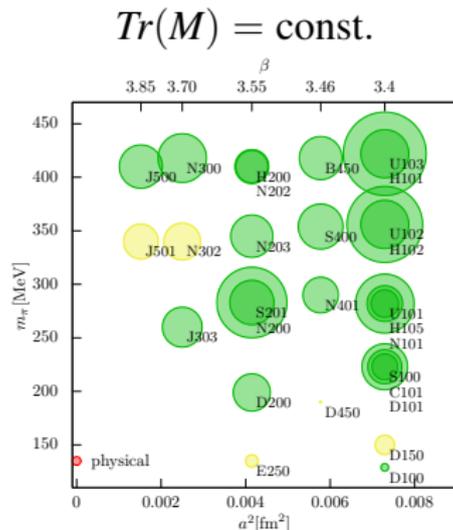


plots by Jakob Simeth, RQCD

- Letters in the name denote the aspect ratio  $T/L$ ; First digit encodes  $\beta$
- Ensembles at 5 lattice spacings and with a range of  $M_\pi \leq 420\text{MeV}$
- Ensembles to control (or exploit) finite volume effects

# CLS 2+1 flavor ensembles: Statistics – area $\propto$ MDU

Bruno et al. JHEP 1502 043 (2015); Bali et al. PRD 94 074501 (2016)



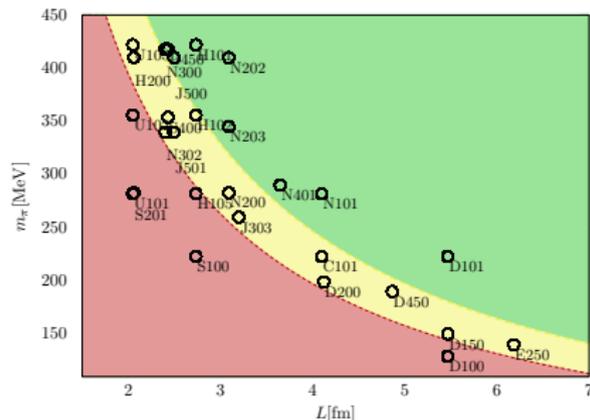
plots by Jakob Simeth, RQCD

- > 4000 MDU for many ensembles  
Typically save 1 configuration every 4 MDU
- target statistics chosen considering largest  $\tau_{int}$  (often YM action density)

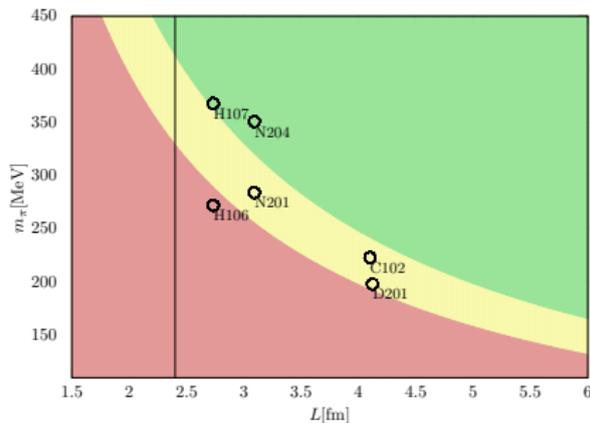
# CLS 2+1 flavor ensembles: Volumes used

Bruno *et al.* JHEP 1502 043 (2015); Bali *et al.* PRD 94 074501 (2016)

$Tr(M) = \text{const.}$



$m_s = \text{const.}$



plots by Jakob Simeth, RQCD

- red:  $m_\pi L \leq 4$ ; yellow:  $4 \leq m_\pi L \leq 5$ ; green  $5 \leq m_\pi L$
- Most ensembles with  $m_\pi L \geq 4$
- Some smaller volumes to check finite size effects

# A non-exotic example: The $\rho$ meson

$\rho(770)$  [6]

Mass  $m = 775.26 \pm 0.25$  MeV  
Full width  $\Gamma = 149.1 \pm 0.8$  MeV

$$J^{PC} = 1^{+}(1^{- -})$$

For  $2m_{\pi} \leq m_{\rho} \leq 4m_{\pi}$  the original Lüscher formalism is applicable

$\rho(770)$ DECAY MODES	Fraction ( $\Gamma_i/\Gamma$ )
$\pi\pi$	$\sim 100$

Correlation matrix built from both quark-antiquark  $\rho$  and  $\pi\pi$  interpolators:

$$C(t) = \begin{pmatrix} \langle \rho(t)\rho(0)^\dagger \rangle & \langle \rho(t)(\pi\pi)(0)^\dagger \rangle \\ \langle (\pi\pi)(t)\rho(0)^\dagger \rangle & \langle (\pi\pi)(t)(\pi\pi)(0)^\dagger \rangle \end{pmatrix}$$

Where we use  $\rho^0$  and  $\pi^+\pi^-$  type interpolators:

$$\rho^0(P, t) \propto \sum_{\mathbf{x}} e^{-i\mathbf{P}\cdot\mathbf{x}} (\bar{u}\mathbf{a} \cdot \gamma u - \bar{d}\mathbf{a} \cdot \gamma d)(\mathbf{x}, t)$$

$$(\pi\pi)(t) = \pi^+(\mathbf{p}_1, t)\pi^-(\mathbf{p}_2, t) - \pi^-(\mathbf{p}_1, t)\pi^+(\mathbf{p}_2, t)$$

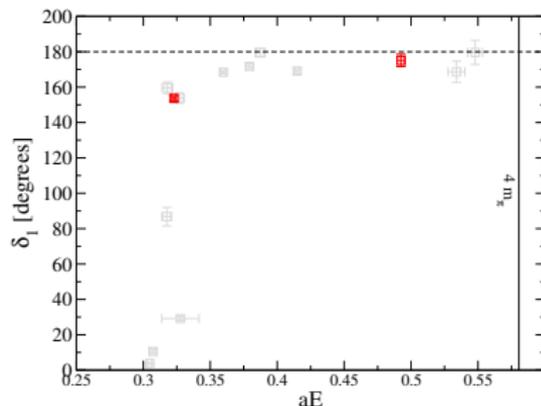
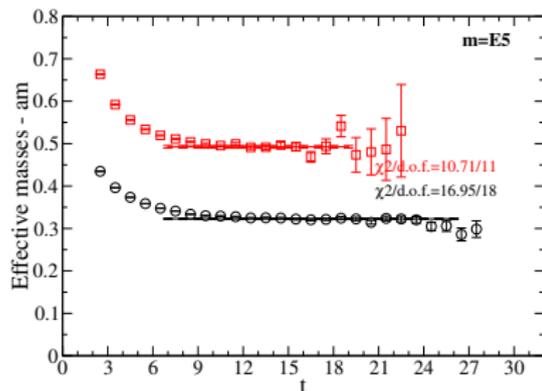
$$\pi^+(p, t) \propto \sum_{\mathbf{x}} e^{-i\mathbf{p}\cdot\mathbf{x}} \bar{d}\gamma_5 u(\mathbf{x}, t)$$

# A non-exotic example: The $\rho$ meson

- Lüscher quantization condition

$$\delta_1(k) + \phi\left(\frac{L}{2\pi}k\right) = n\pi \quad \text{with} \quad E_{cm}(k) = 2\sqrt{k^2 + m_\pi^2}$$

- In this simple case of elastic scattering:  
one phase-shift point for each energy level

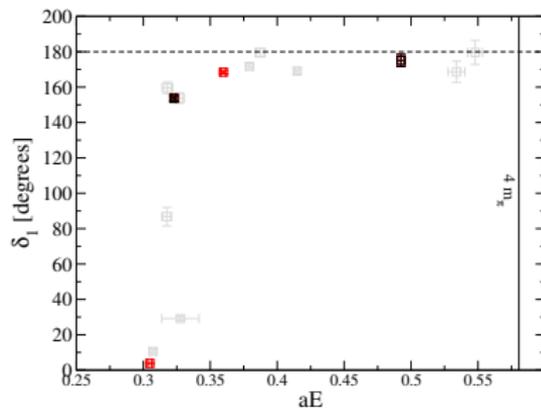
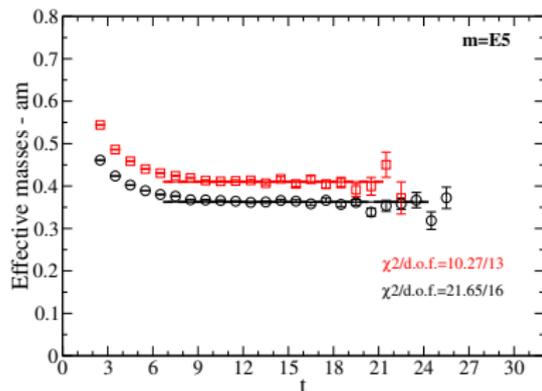


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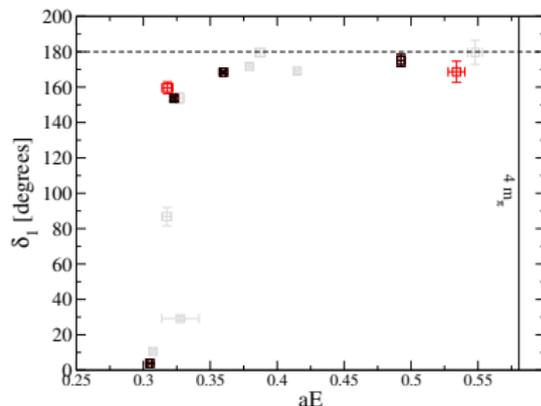
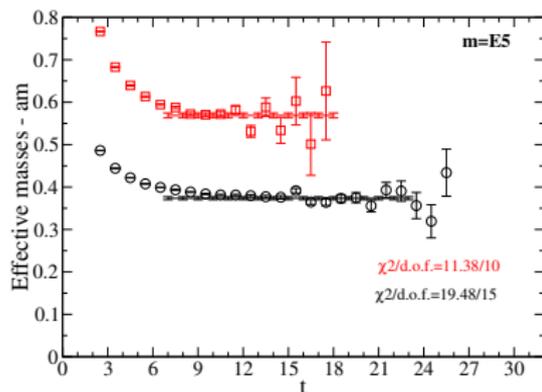


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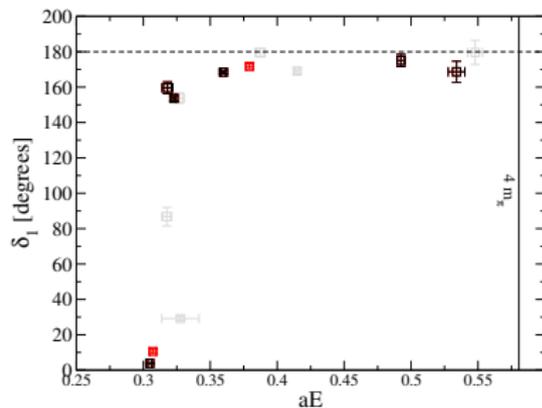
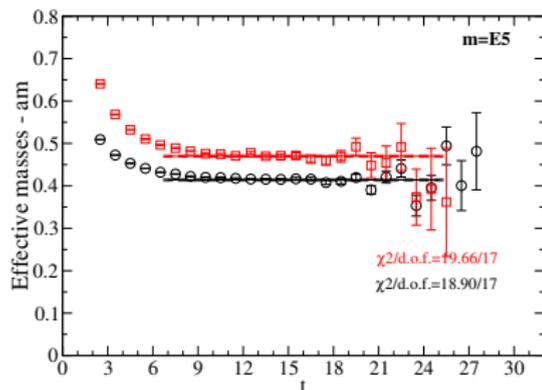


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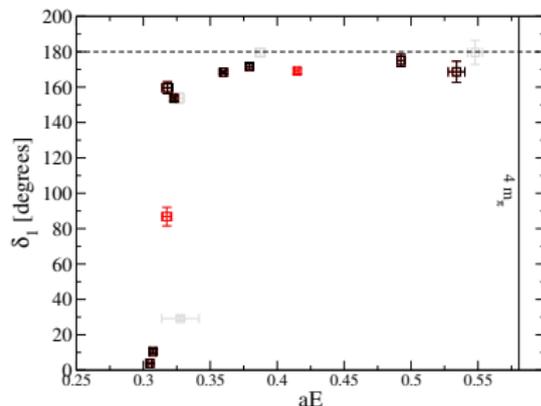
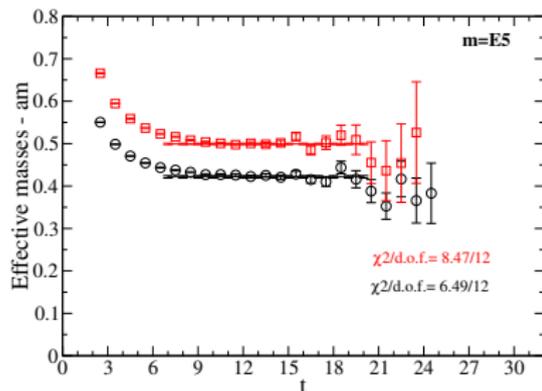


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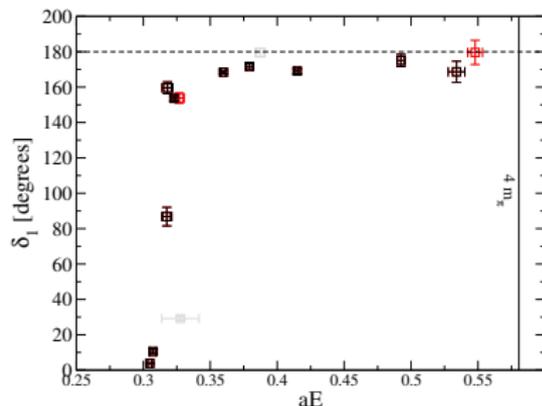
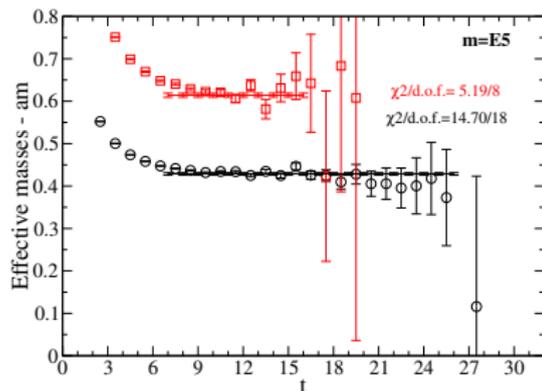


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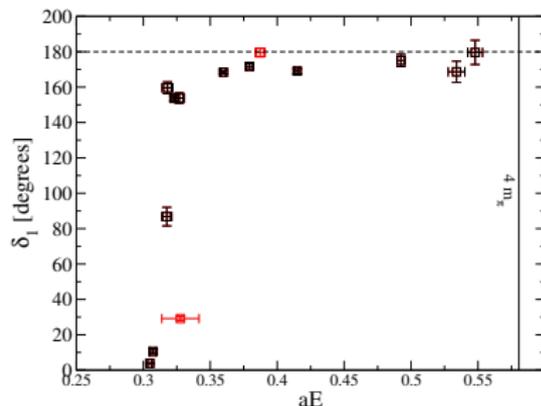
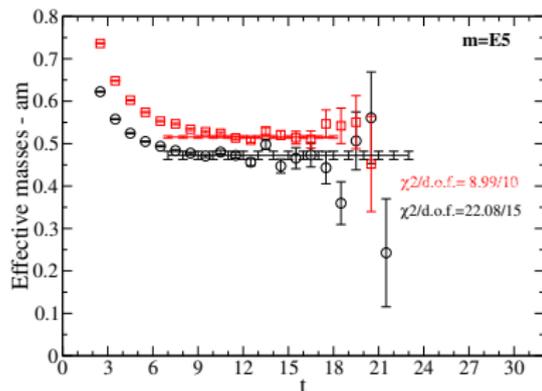


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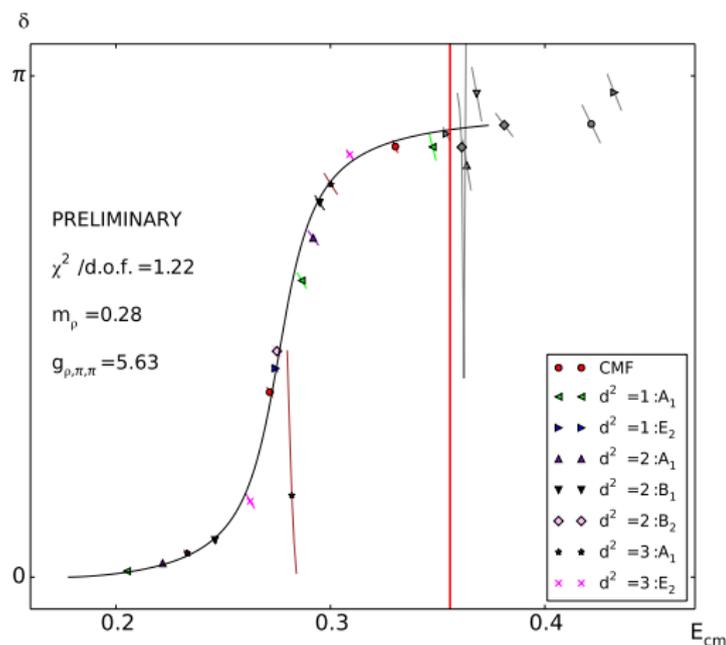
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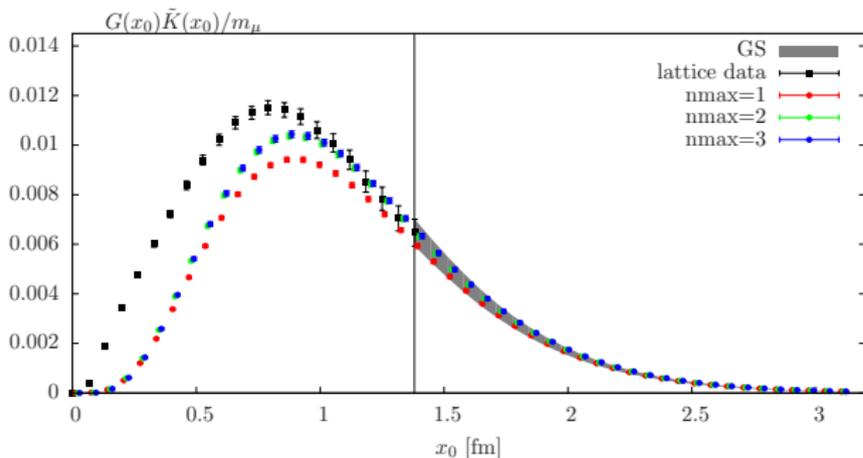
# Similar results with $m_\pi \approx 265$ MeV



Data from Felix Erben, Mainz

- Treats all correlations correctly, see [arXiv:1710.03529](https://arxiv.org/abs/1710.03529)
- Different fits for final publications: Breit-Wigner, Gounaris-Sakurai, ...

# $(g - 2)_\mu$ and the large $x_0$ behavior of the vector correlator

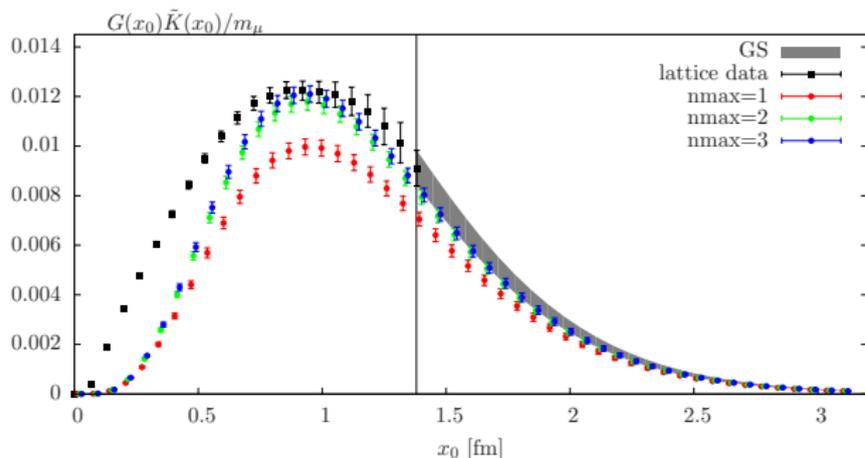


Previous determination from arXiv:1705.01775  
New analysis from Felix Erben.

- Data from Lüscher analysis  $\rightarrow$  more accurate determination of the large  $x_0$  behavior
- Reduces uncertainty of lattice determination of the HVP contribution
- Lellouch-Lüscher yields timelike pion form factor

H.B. Meyer, PRL **107**, 072002 (2011)

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# $\chi'_{c0}$ and $X/Y(3915)$

$X(3915)$   
was  $\chi_{c0}(3915)$

$$I^G(J^{PC}) = 0^+(0 \text{ or } 2^{++})$$

Mass  $m = 3918.4 \pm 1.9$  MeV

Full width  $\Gamma = 20 \pm 5$  MeV ( $S = 1.1$ )

PDG interpreted  $X(3915)$  as a **regular charmonium** ( $\chi'_{c0}$ )

- Some of the reasons to doubt this assignment:

Guo, Meissner Phys. Rev. **D86**, 091501 (2012)

Olsen, PRD 91 057501 (2015)

- No evidence for fall-apart mode  $X(3915) \rightarrow \bar{D}D$
- Spin splitting  $m_{\chi_{c2}(2P)} - m_{\chi_{c0}(2P)}$  too small
- Large OZI suppressed  $X(3915) \rightarrow \omega J/\psi$
- Width should be significantly larger than  $\Gamma_{\chi_{c2}(2P)}$
- Zhou *et al.* (PRL 115 2, 022001 (2015)) argue that what is dubbed  $X(3915)$  is the spin 2 state already known and suggests that a broader state is hiding in the experiment data.
- Observation of an alternative  $\chi_{c0}(2P)$  by Belle:

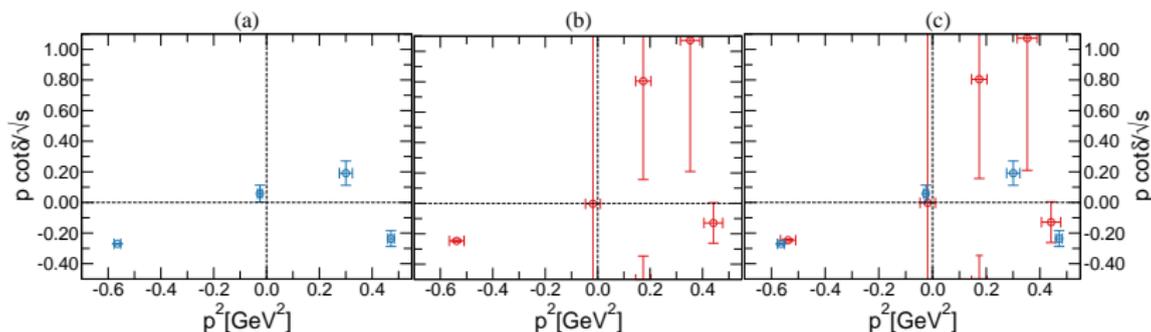
Chilikin *et al.* PRD 95 112003 (2017)

$$M = 3862^{+26+40}_{-32-13} \text{ MeV}$$

$$\Gamma = 201^{+154+88}_{-067-82} \text{ MeV}$$

# $\chi'_{c0}$ : Exploratory lattice calculation

Lang, Leskovec, DM, Prelovsek, JHEP 1509 089 (2015)



- Assumes only  $\bar{D}D$  is relevant
- Lattice data suggests a fairly narrow resonance with  $3.9\text{GeV} < M < 4.0\text{GeV}$  and  $\Gamma < 100\text{MeV}$
- Future experiment and lattice QCD results needed to clarify the situation

# $\chi'_{c0}$ : Improvements and challenges

with G. Bali, S. Collins, M. Padmanath, S. Piemonte, S. Prelovsek

## Improvements:

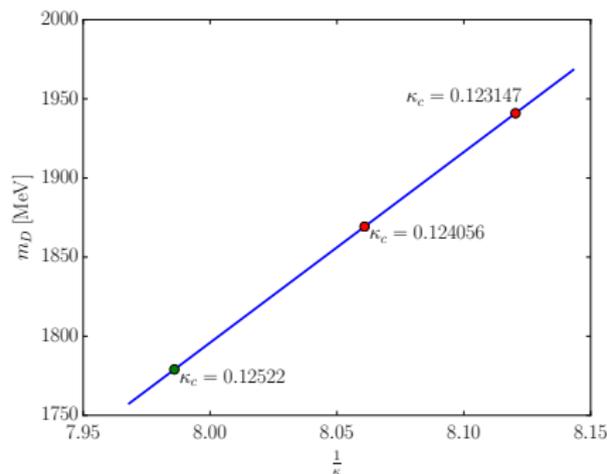
- High-precision determinations of the energy splittings needed  
→ significantly improve statistics by using CLS ensembles
- Bigger density of energy level needed  
→ Calculation in multiple volumes: CLS ensembles U101, H105, N101  
→ Add information from moving frames
- Treatment as a single-channel problem only sensible if  $X(3915)$  is indeed a spin-2 state  
→ consider coupled channel  $D\bar{D}$ ,  $J/\psi\omega$  and  $D_s\bar{D}_s$

## Challenges:

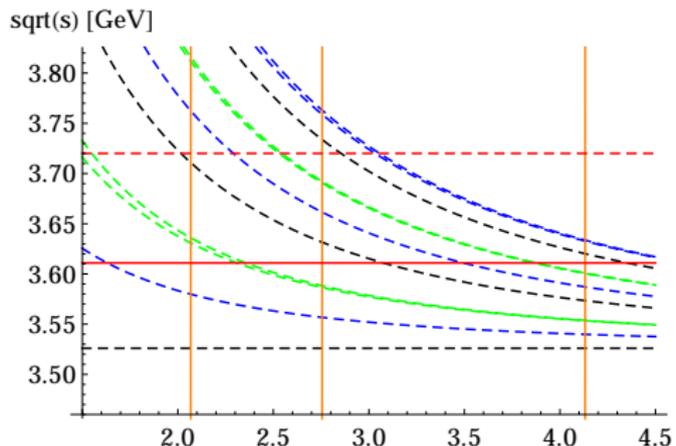
- Need strategy for dealing with (largish) discretization effects
- $Tr(M) = \text{const.}$  trajectory means  $D_s\bar{D}_s$  threshold lower

# Charm-quark mass tuning and expected energy levels

D-meson mass as a function of the charm-quark hopping parameter  $\kappa_c$



Expected energy levels: CLS-ensembles  
U101, H105, N101

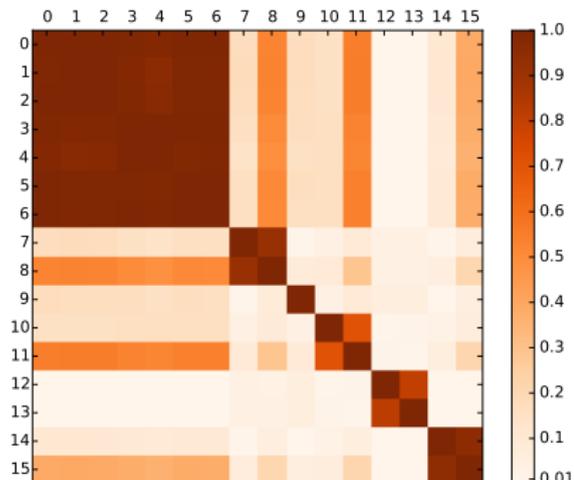


- Currently: Low statistics results on U101
- For these results: Charm quark tuning by RQCD
- Will add further charm-quark masses if needed

# Interpolator basis

$$A_1^{++} (J^{PC} = 0^{++}, 4^{++}, \dots)$$

Label n	Operator
0	$\bar{q} q$
1	$\bar{q} \gamma_i \overleftrightarrow{\nabla}_i q$
2	$\bar{q} \gamma_i \gamma_t \overleftrightarrow{\nabla}_i q$
3	$\bar{q} \overleftrightarrow{\nabla}_i \overleftrightarrow{\nabla}_i q$
4	$\bar{q} \overleftrightarrow{\Delta} \overleftrightarrow{\Delta} q$
5	$\bar{q} \overleftrightarrow{\Delta} \gamma_t \overleftrightarrow{\nabla}_i q$
6	$\bar{q} \overleftrightarrow{\Delta} \gamma_i \gamma_t \overleftrightarrow{\nabla}_i q$
7	$O^{\bar{D}(0)D(0)} \sim \bar{c} \gamma_5 l \bar{l} \gamma_5 c$
8	$O^{\bar{D}(0)D(0)} \sim \bar{c} \gamma_5 \gamma_t l \bar{l} \gamma_5 \gamma_t c$
9	$O^{\bar{D}(p)D(-p)} \sim \bar{c} \gamma_5 l \bar{l} \gamma_5 c$
10	$O^{\bar{D}^*(0)D^*(0)} \sim \bar{c} \gamma_t l \bar{l} \gamma_t c$
11	$O^{\bar{D}^*(0)D^*(0)} \sim \bar{c} \gamma_i \gamma_t l \bar{l} \gamma_i \gamma_t c$
12	$O^{J/\psi(0)\omega(0)} \sim \bar{c} \gamma_t c \bar{l} \gamma_t l$
13	$O^{J/\psi(0)\omega(0)} \sim \bar{c} \gamma_i \gamma_t c \bar{l} \gamma_i \gamma_t l$
14	$O^{\bar{D}_s(0)D_s(0)} \sim \bar{c} \gamma_5 s \bar{s} \gamma_5 c$
15	$O^{\bar{D}_s(0)D_s(0)} \sim \bar{c} \gamma_5 \gamma_t s \bar{s} \gamma_5 \gamma_t c$



# A first look at mass splittings

*Preliminary results:* Energy splittings from 120 configurations of U101

	$\kappa_c = 0.12522$	$\kappa_c = 0.12315$	Experiment
$m_{J/\Psi} - m_{\eta_c}$	106.9(0.6)(1.1)	98.0(0.5)(1.1)	113.2(0.7)
$m_{D_s^*} - m_{D_s}$	131.3(1.9)(1.4)	118.4(2.0)(1.3)	143.8(0.4)
$m_{D^*} - m_D$	127.8(3.9)(1.4)	115.1(4.1)(1.2)	140.66(10)
$2m_{\overline{D}} - m_{\overline{c\overline{c}}}$	912.0(7.6)(9.8)	939.7(8.1)(10.1)	882.4(0.3)
$2M_{\overline{D}_s} - m_{\overline{c\overline{c}}}$	1011.7(4.2)(10.9)	1036.0(4.5)(11.1)	1084.8(0.6)
$m_{D_s} - m_D$	47.2(2.1)(0.5)	45.7(2.2)(0.5)	98.87(29)

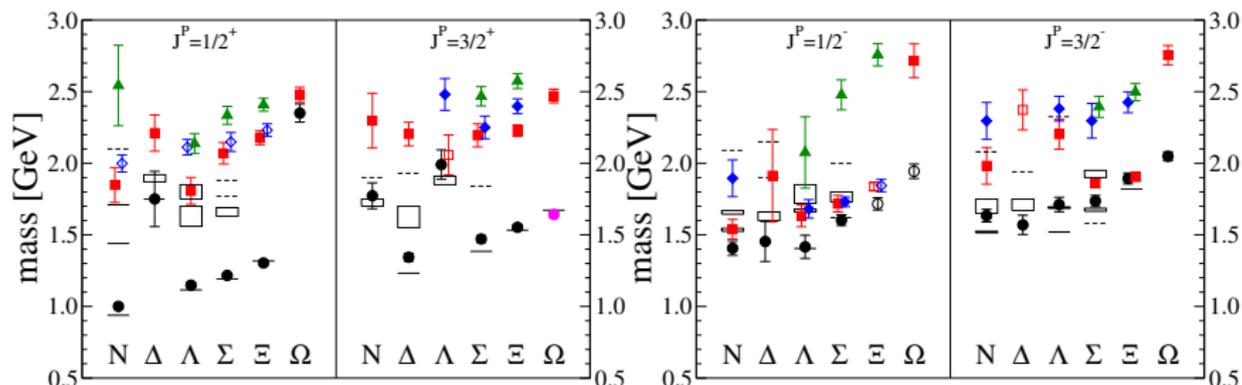
- Unphysical  $m_{D_s} - m_D$  creates a special challenge!

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# Results from 3-quark interpolating fields

- Many older results from 3-quark interpolators

Example: Engel, Lang, DM, Schäfer, PRD 87 074504 (2013)  
 $\Lambda'$ 's in Engel *et al.* PRD 87 034502 (2013)



- OK at heavy quark masses where states are stable
- Typically no indications of close-by scattering thresholds
- Experience from meson sector: Spectrum not only incomplete but wrong!

# Meson-baryon scattering – challenges

- Nucleon noise to signal
  - For the nucleon we have (argument by Parisi, Lepage)

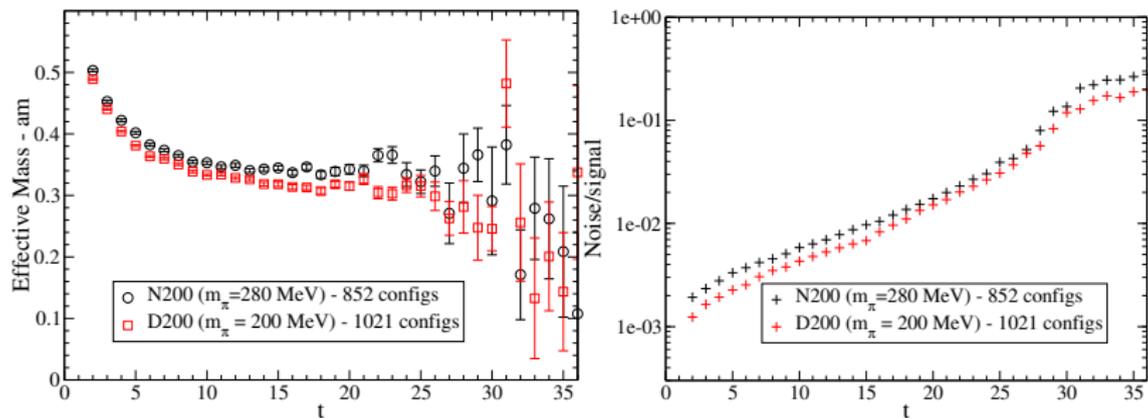
$$N\sigma_{N,\mathbf{p}=0}^2 = \langle C_N(\mathbf{p} = 0, t; m)^2 \rangle - \langle C_N(\mathbf{p} = 0, t; m) \rangle^2 \\ \propto Z_{3\pi} e^{-3m_\pi t} + Z_N^2 e^{-2m_N t}$$

- The noise to signal ratio therefore degrades exponentially

$$\frac{\sigma_N(t)}{\langle C_N(t) \rangle} \simeq \frac{1}{\sqrt{N}} e^{(m_N - \frac{3}{2}m_\pi)t}$$

- Contractions are more complicated
- Less cases where 3-particle scattering can be ignored (in a first step)

# Nucleon noise/signal



Data from Tim Harris, Konstantin Ottnad, Mainz

- Slope in (most of) plateau region does not reach asymptotic value (given by  $m_N - \frac{3}{2}m_\pi$ )
- Suggests that in practice noise/signal scaling is not as severe
- Exponential growth qualitatively observed

# Meson-baryon scattering – previous results

- S-wave pion-nucleon scattering with  $J^P = \frac{1}{2}^-$

Lang, Verduci, PRD 87 054502 (2013)

- CMF spectrum qualitatively in agreement with negative parity spectrum

- Pion-nucleon scattering in the Roper channel

Lang *et al.* PRD 95 014510 (2017)

- CMF spectrum from 3-quark,  $N(p)\pi(-p)$ , and  $N\sigma$  interpolators
- No finite volume state seen for the  $N^*(1440)$
- Results compatible with models with a dynamically generated Roper resonance from coupled channel  $N\pi, N\sigma, \Delta\pi$

- $I = \frac{3}{2}$  p-wave nucleon pion scattering and the  $\Delta(1232)$

Andersen, Bulava, Hörz, Morningstar arXiv:1710.01557

- At  $m_\pi = 280$  MeV, observe a near threshold resonance
- Coupling  $g_{\Delta N\pi}$  similar to experiment
- Should be quite feasible at lighter pion masses

# Exploratory study: $\Lambda(1405)$ , $J^P = \frac{1}{2}^-$

- PDG (4 star resonance)

$$M_\Lambda = 1405_{-1.0}^{+1.3} \text{MeV} \qquad \Gamma_\Lambda = 50.5 \pm 2.0$$

- However

- Unitarized  $\chi$ PT + Model input yields 2 poles with  $\Re \approx 1400 \text{MeV}$
- CLAS observes different line shapes for  $\Sigma^- \pi^+$ ,  $\Sigma^+ \pi^-$  and  $\Sigma^0 \pi^0$   
Interference between  $I = 0$  and  $I = 1$  amplitudes is the likely reason
- Even the  $\Sigma^0 \pi^0$  is badly described by a single Breit-Wigner
- CLAS data consistent with popular 2-pole picture
- No satisfactory lattice results (although claims exist)
- Relevant channels:  $\Sigma \pi$ ,  $N \bar{K}$  (and maybe  $\Lambda \eta$ ); simulation in isospin limit
- Goal: Explore coupled channel problem and extract scattering amplitudes from the low-lying energy spectrum

together with J. Bulava, M. Hansen, B. Hörz, C. Morningstar

# Ensemble and group theory

Current data on CLS Ensemble N200

$a$ [fm]	$T \times L^3$	$m_\pi$ [MeV]	$m_K$ [MeV]	$m_\pi L$	$N_{cnfg}$
0.0644	$128 \times 48^3$	280	460	4.3	427

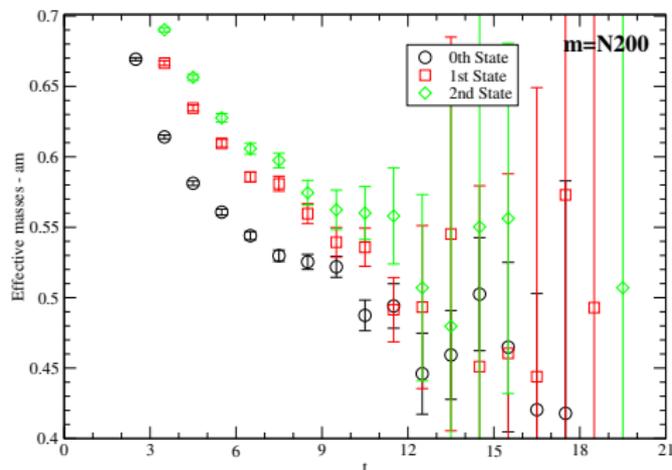
Lattice irreducible representations for a given  $J^P$

see Morningstar *et al.* arXiv:1303.6816

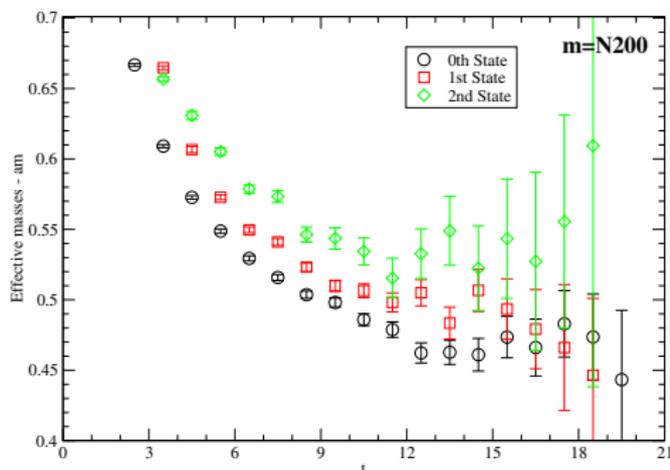
$J^P$	[000]	[00n]	[0nn]	[nnn]	
$\frac{1}{2}^+$	$G_{1g}$	$G_1$	$G$	$G$	$\Lambda, \Lambda(1600)$
$\frac{1}{2}^-$	$G_{1u}$	$G_1$	$G$	$G$	$\Lambda(1405), \Lambda(1670)$
$\frac{3}{2}^+$	$H_g$	$G_1, G_2$	$2G$	$F_1, F_2, G$	$\Lambda(1690)$
$\frac{3}{2}^-$	$H_u$	$G_1, G_2$	$2G$	$F_1, F_2, G$	$\Lambda(1520), \Lambda(1690)$

# A first look at some data: Truncating the basis

3-quark interpolators alone  
Effective masses

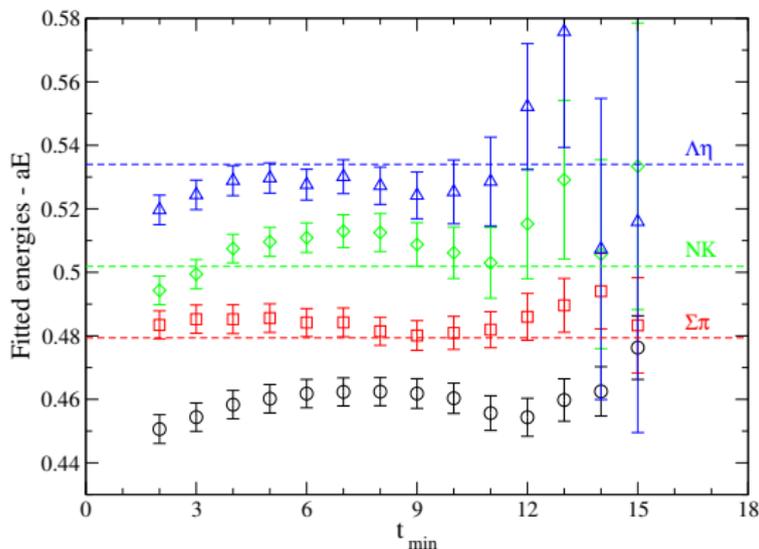


basis including  $N\bar{K}$  and  $\Sigma\pi$   
Effective masses



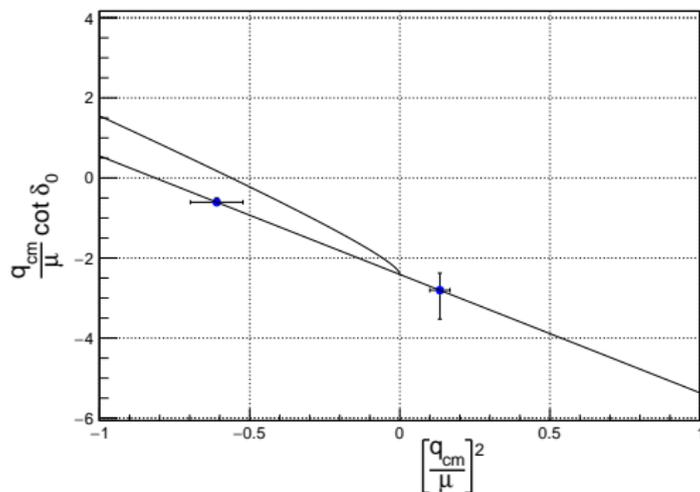
- Plot from an older dataset on 427 configurations
- Basis including meson-meson states starts to yield usable plateaus
- Even a diverse 3-quark basis does not yield the correct spectrum!

# Rest frame calculation: Fit stability



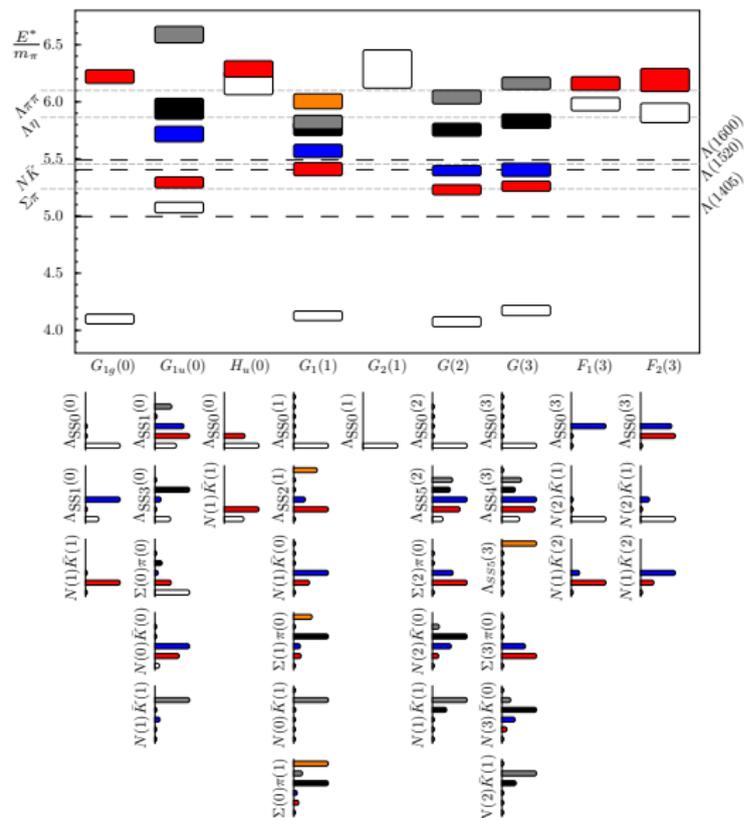
- Results for fits from  $t_{min}$  to 20
- Non-interacting levels indicated by their central value
- Correlated differences start to become significant

# Rest frame calculation: effective range approximation



- Cannot rule out the simplest scenario of one bound state below  $\Sigma\pi$
- Makes no statement about more complicated scenarios or physical  $m_\pi$

# Adding moving frames: Pattern of energy levels



- With  $Tr(M) = \text{const.}$ , expect mild chiral extrapolation of  $uds$  states
- Our  $G_1(1)$  data does not have a large enough basis (caution)
- The  $\Lambda$  ground state is seen where expected
- No indication of levels close to  $\Lambda(1600)$  in  $G_{1g}$  irrep
- No indication of levels close to  $\Lambda(1520)$  in any irrep
- Apparent absence of FV states should constrain models

## Next steps: What to expect

- Currently doubling N200 statistics ( $\approx 400$  configs  $\rightarrow \approx 800$  configs)
- Still enlarging the basis somewhat (include more 3-quark interpolators; include some  $\Lambda\eta$ )
- We plan to run more ensembles (will likely add a lighter pion mass next)
- We may add data at different lattice spacings
- Once we have bigger dataset:  
Check for consistency with model-inspired K-matrix parameterizations

- 1 Introduction and motivation
  - Recent progress in Lattice QCD simulations
  - Coordinated Lattice Simulations (CLS)
  - Illustrative example:  $\rho$  resonance and relevance to  $(g - 2)_\mu$
- 2 Exploratory calculations for charmonium resonances and bound states
  - Previous results for the  $\chi'_{c0} / X(3915)$
  - Towards charmonium resonances from coupled-channel simulations
- 3 Exploratory calculations for baryon resonances
  - Previous results
  - Challenges
  - Towards coupled-channel results for the  $\Lambda(1405)$
- 4 Conclusions and Outlook

# Conclusions

- Lüscher studies of meson-baryon scattering and for exotic charmonium-like states are very challenging
  - they require large statistics
  - coupled-channel formalism needed for even the simplest systems
- Making contact with experiment requires a variety of gauge ensembles
- Expect to see many new results over the next years
- Large potential to solve some of the puzzles surrounding hadrons with exotic properties (Roper,  $\Lambda(1405)$ , low mass charmonium-like states, ...)

Thank you!