

# Lattice QCD and Baryon Spectroscopy

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# Outline

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## ◆ Lattice QCD

- ◆ Background, actions, observables, ...

## ◆ Methodology

- ◆ Group theory and operator design
- ◆ Variational method
- ◆ Ensembles, parameter and analysis

## ◆ Numerical Results

- ◆ Octet and decuplet
- ◆ Other  $\pm$ -parity, spin-1/2 and 3/2 states
- ◆ Roper from full QCD

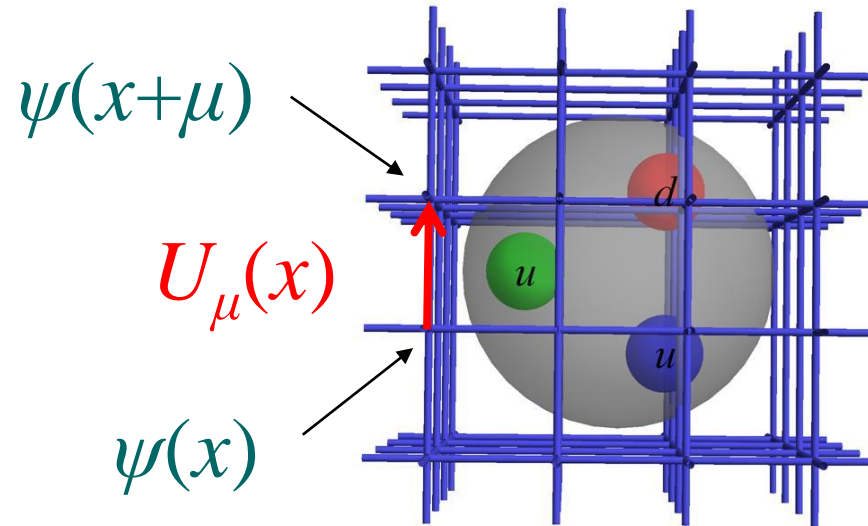
## ◆ Conclusions and Outlook

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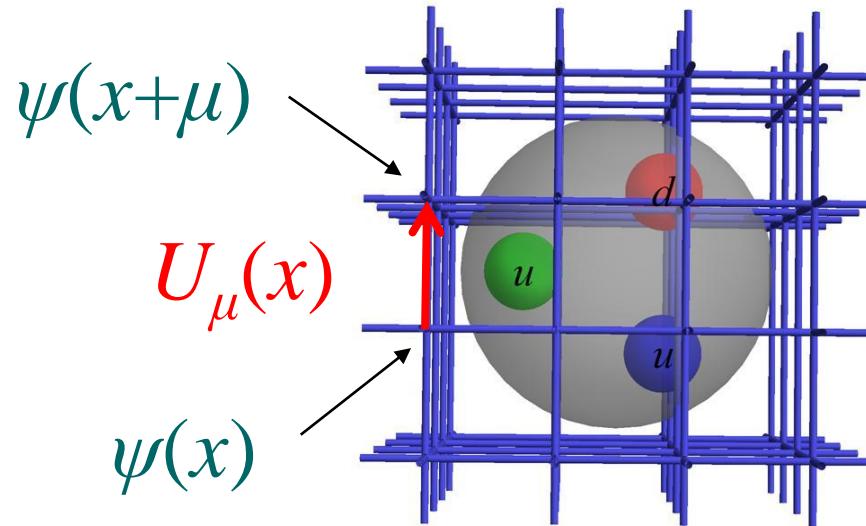
# Lattice QCD

- ◆ Lattice QCD is a discrete version of continuum QCD theory



# Lattice QCD

- ◆ Lattice QCD is a discrete version of continuum QCD theory



- ◆ Physical observables are calculated from the path integral

$$\langle 0|O(\bar{\psi}, \psi, A)|0\rangle = \frac{1}{Z} \int [dA][d\bar{\psi}][d\psi] O(\bar{\psi}, \psi, A) e^{i \int d^4x \mathcal{L}^{\text{QCD}}(\bar{\psi}, \psi, A)}$$

- ◆ Use Monte Carlo integration combined with the “importance sampling” technique to calculate the path integral.
- ◆ Take  $a \rightarrow 0$  and  $V \rightarrow \infty$  in the continuum limit

# Lattice QCD

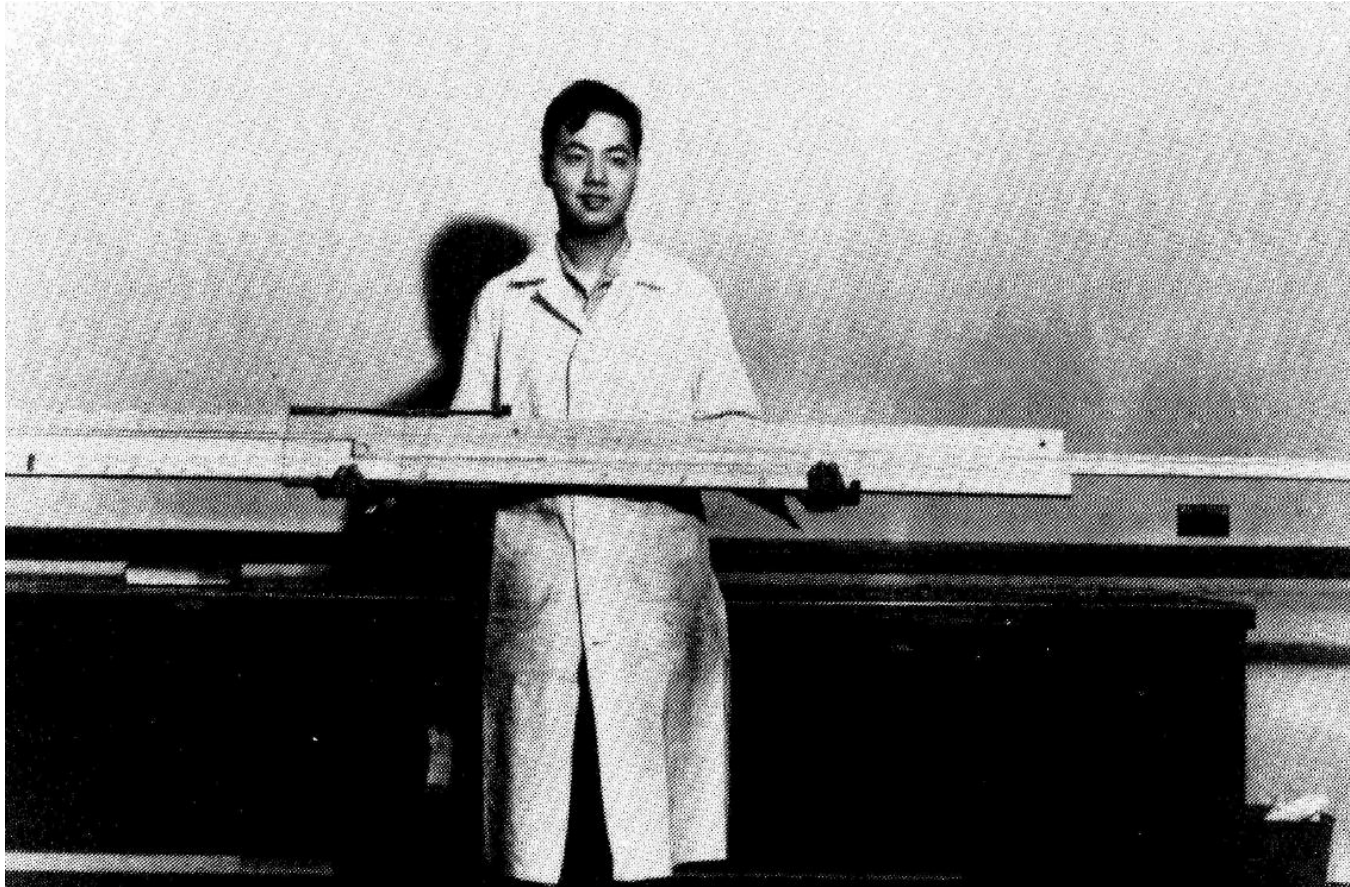
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- ◆ A wide variety of first-principles QCD calculations can be done:  
In 1970, Wilson wrote down the original lattice action
- ◆ Progress is limited by computational resources...  
but assisted by advances in algorithms.

# Lattice QCD

T.D. Lee uses an “analog computer” to calculate stellar radiative transfer equations



# Lattice QCD

2007: The 13 Tflops cluster at Jefferson Lab



Other joint lattice resources within the US: Fermilab, BNL.  
Non-lattice resources open to USQCD: ORNL, LLNL, ANL.

# Lattice QCD

- ◆ Lattice QCD is computationally intensive

$$\text{Cost} \approx \left(\frac{L}{\text{fm}}\right)^5 L_s \left(\frac{\text{MeV}}{M_\pi}\right) \left(\frac{\text{fm}}{a}\right)^6 \left(C_0 + C_1 \left(\frac{\text{fm}}{a}\right) \left(\frac{\text{MeV}}{M_K}\right)^2 + C_2 \left(\frac{a}{\text{fm}}\right)^2 \left(\frac{\text{MeV}}{M_\pi}\right)^2\right)$$

Norman Christ, LAT2007

- ◆ Current major US 2+1-flavor gauge ensemble generation:
  - ◆ MILC: staggered,  $a \sim 0.06$  fm,  $L \sim 3$  fm,  $M_\pi \sim 250$  MeV
  - ◆ RBC+UKQCD: DWF,  $a \sim 0.09$  fm,  $L \sim 3$  fm,  $M_\pi \sim 330$  MeV
- ◆ Chiral domain-wall fermions (DWF) at large volume (6 fm) at physical pion mass may be expected in 2011
- ◆ But for now...  
need a pion mass extrapolation  $M_\pi \rightarrow (M_\pi)_{\text{phys}}$   
(use chiral perturbation theory, if available)



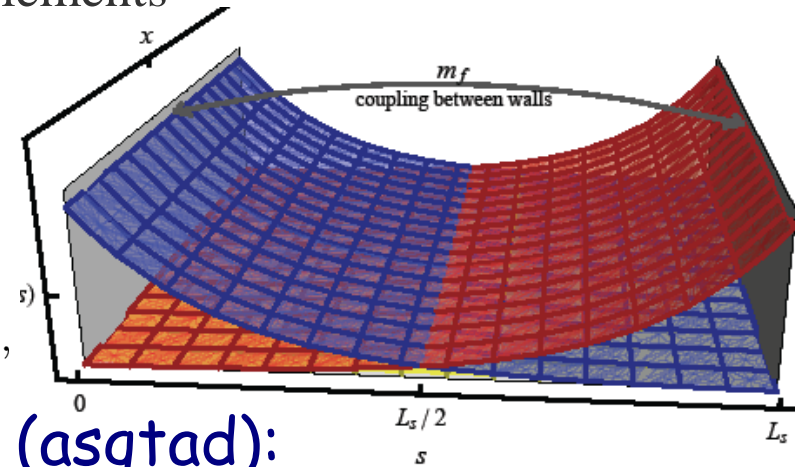
# Lattice Fermion Actions

## ◆ Chiral fermions (e.g., Domain-Wall/Overlap):

- ◆ Automatically  $O(a)$  improved, good for spin physics and weak matrix elements
- ◆ Expensive

$$D_{x,s;x',s'} = \delta_{x,x'} D_{s,s'}^\perp + \delta_{s,s'} D_{x,x'}^\parallel$$

$$D_{s,s'}^\perp = \frac{1}{2}[(1 - \gamma_5)\delta_{s+1,s'} + (1 + \gamma_5)\delta_{s-1,s'} - 2\delta_{s,s'}] \\ - \frac{m_f}{2}[(1 - \gamma_5)\delta_{s,L_s-1}\delta_{0,s'} + (1 + \gamma_5)\delta_{s,0}\delta_{L_s-1,s'}],$$



## ◆ (Improved) Staggered fermions (asqtad):

- ◆ Relatively cheap for dynamical fermions (good)
- ◆ Mixing among parities and flavors or “tastes”
- ◆ Baryonic operators a nightmare — not suitable

## ◆ Wilson/Clover action:

- ◆ Moderate cost; explicit chiral symmetry breaking

## ◆ Twisted Wilson action:

- ◆ Moderate cost; isospin mixing

# Mixed Action Parameters

## ◆ Mixed action:

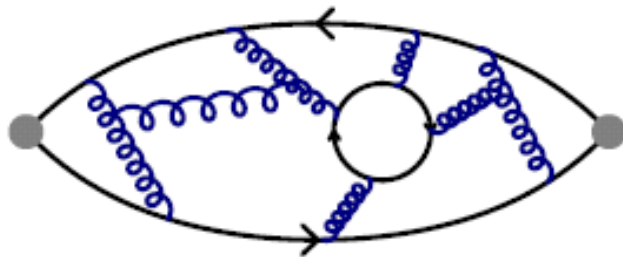
- ◆ Staggered sea (cheap) with domain-wall valence (chiral)
- ◆ Match the sea Goldstone pion mass to the DWF pion
- ◆ Only mixes with the “scalar” taste of sea pion
- ◆ Free light quark propagators (LHPC & NPLQCD)

## ◆ In this calculation:

- ◆ Pion mass ranges 300–750 MeV
- ◆ Volume fixed at 2.6 fm, box size of  $20^3 \times 32$
- ◆  $a \approx 0.125$  fm,  $L_s = 16$ ,  $M_5 = 1.7$
- ◆ HYP-smearred gauge fields

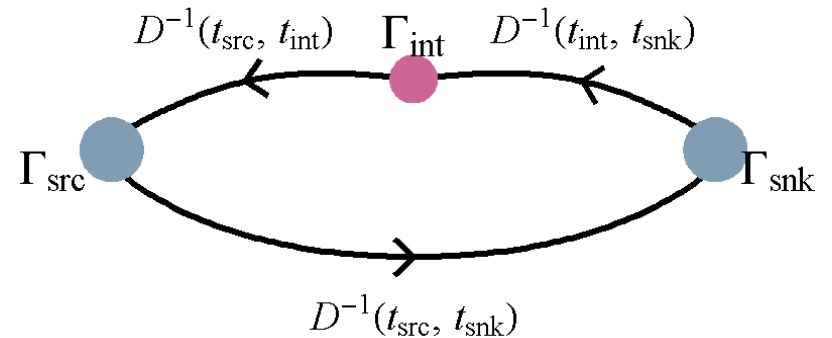
# Lattice QCD: Observables

- ◆ Two-point Green function  
e.g. spectroscopy



$$\sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{\text{snk}}) J(X_{\text{src}}) \rangle_{\alpha, \beta}$$

- ◆ Three-point Green function  
e.g. form factors, structure functions, ...

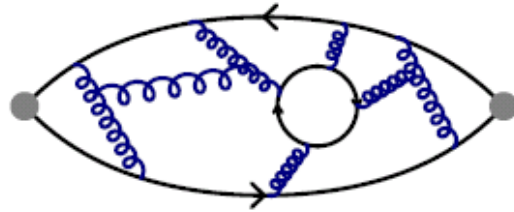


$$\sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{\text{snk}}) O(X_{\text{int}}) J(X_{\text{src}}) \rangle_{\alpha, \beta}$$

# Lattice QCD: Observables

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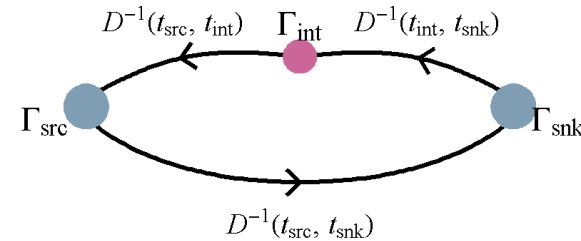
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## ◆ Three-point Green function

e.g. form factors, structure functions, ...



$$\sum_{\alpha,\beta} \Gamma^{\alpha,\beta} \langle J(X_{\text{snk}}) O(X_{\text{int}}) J(X_{\text{src}}) \rangle_{\alpha,\beta}$$

After taking spin and momentum projection

(ignore the variety of boundary condition choices)

Two-point correlator

$$\sum_n Z_{n,B} e^{-E_n(\vec{P})t}$$

Three-point correlator

$$\sum_n \sum_{n'} Z_{n',B}(p_f) Z_{n,A}(p_i) \times \text{FF's} \times e^{-(t_f-t)E'_n(\vec{p}_f)} e^{-(t-t_i)E_n(\vec{p}_i)}$$

At large enough  $t$ , the ground-state signal dominates.

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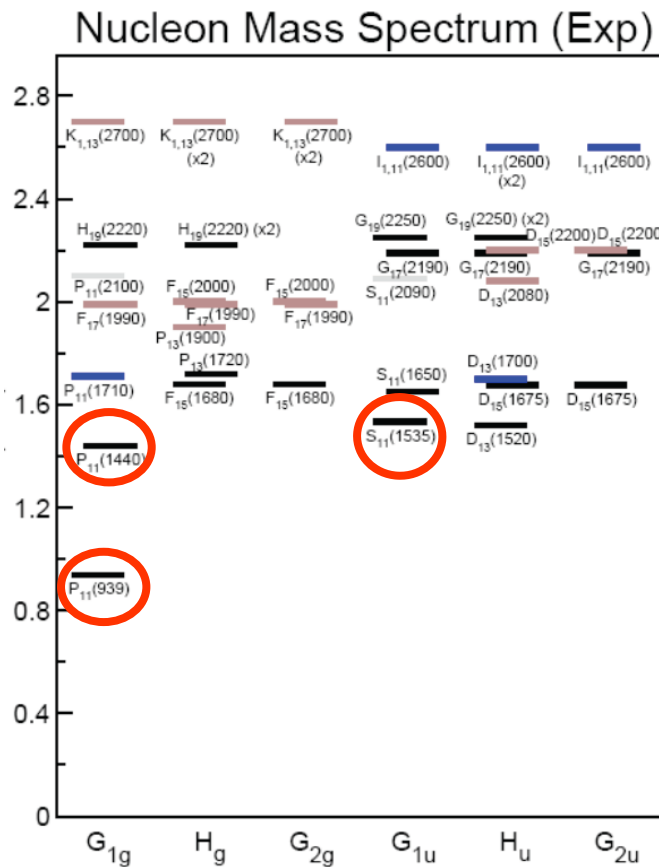
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# Motivations and Methodology

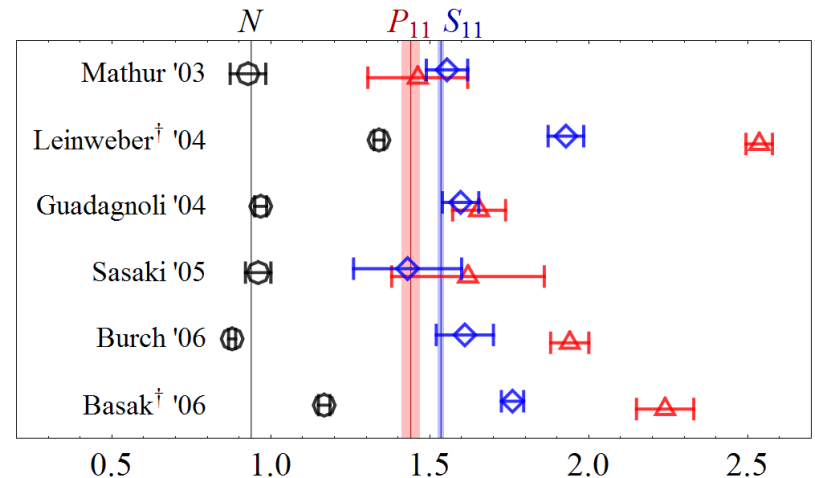
# Why Baryons?

## Lattice QCD spectrum

- ◆ Successfully calculates many ground states (*Nature*, ...)
- ◆ Nucleon spectrum, on the other hand... not quite



## Example: $N$ , $P_{11}$ , $S_{11}$ spectrum



# Strange Baryons

- ◆ Strange baryons are of particular interest; challenging even to experiment
- ◆ Example from *PDG Live*:

## $\Xi$ BARYONS ( $S = -2, I = 1/2$ )

		$\Xi^0 = u s s, \Xi^- = d s s$			
$\Xi^0$	$1/2(1/2^+)$ ****	$\Xi(1820) D_{13}$	$1/2(3/2^-)$ ***	$\Xi(2370)$	$1/2(?)^? \cdot^{**}$
$\Xi^-$	$1/2(1/2^+)$ ****	$\Xi(1950)$	$1/2(?)^?$ ***	$\Xi(2500)$	$1/2(?)^? \cdot^*$
$\Xi(1530) P_{13}$	$1/2(3/2^+)$ ****	$\Xi(2030)$	$1/2(\geq 5/2^?)$ ***	• — OMITTED FROM SUMMARY TABLE	
$\Xi(1620)$	$1/2(?)^? \cdot^*$	$\Xi(2120)$	$1/2(?)^? \cdot^*$		
$\Xi(1690)$	$1/2(?)^? \cdot^{**}$	$\Xi(2250)$	$1/2(?)^? \cdot^{**}$		

## $\Omega$ BARYONS ( $S = -3, I = 0$ )

		$\Omega^- = s s s$	
$\Omega^-$	$0(3/2^+)$ ****		
$\Omega(2250)^-$	$0(?)^?$ ***		
$\Omega(2380)^-$	$\cdot^{**}$		
$\Omega(2470)^-$	$\cdot^{**}$		

# Operator Design

- ◆ All baryon spin states wanted:  $j = 1/2, 3/2, 5/2, \dots$
- ◆ Rotation symmetry is reduced due to discretization  
rotation  $O(3) \Rightarrow$  octahedral  $O_h$  group

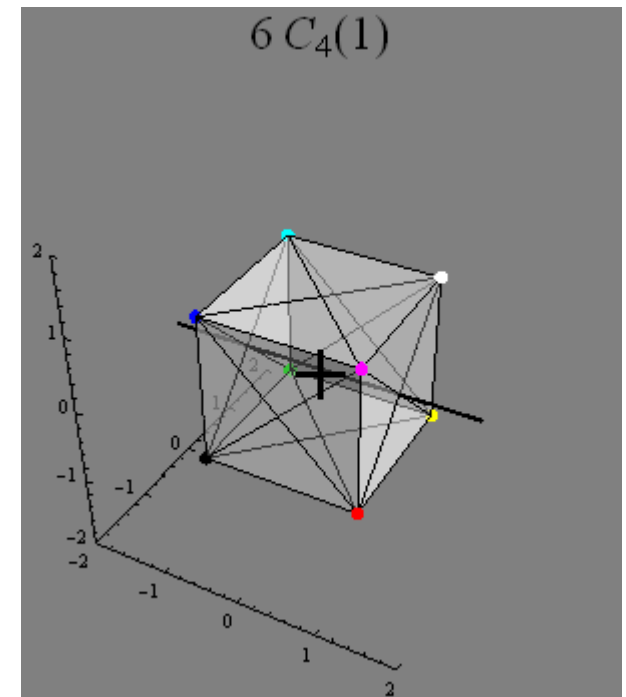
	I	J	6 $C_4$	8 $C_6$	8 $C_2$	6 $C_9$	6 $C'_9$	12 $C'_4$
$A_1$	1	1	1	1	1	1	1	1
$A_2$	1	3	-2	1	0	-1	1	0
E	2	1	1	1	-1	-1	-1	0
$G_1$	2	0	1	-1	1	-2	1	0
$G_2$	2	-4	0	1	0	0	1	-1
$T_1$	3	2	0	0	1	1	-1	-1
$T_2$	3	3	0	-1	-1	1	1	0
H	4	-3	-1	0	0	0	-1	1



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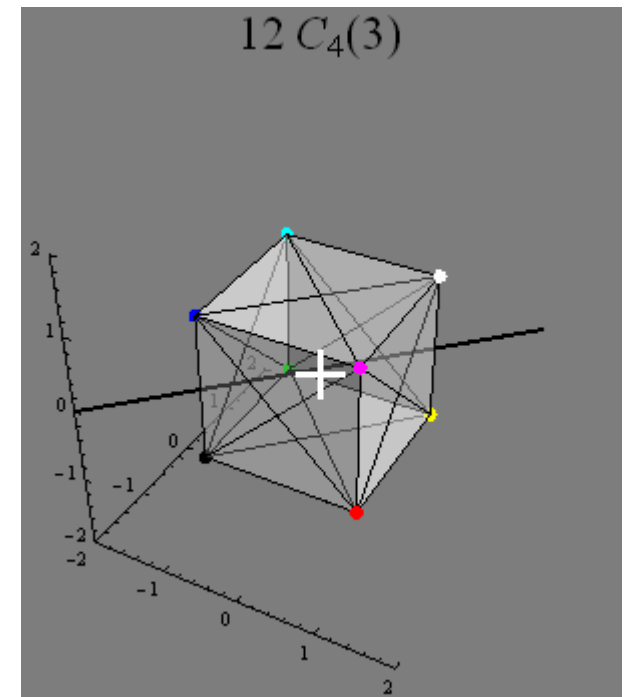
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$G_1$	2	0	1	-1	1	-2	1	0
$G_2$	2	-4	0	1	0	0	1	-1
$T_1$	3	2	0	0	1	1	-1	-1
$T_2$	3	3	0	-1	-1	1	1	0
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## Baryons

j	Irreps
$\frac{1}{2}$	$G_1$
$\frac{3}{2}$	H
$\frac{5}{2}$	$G_2 \oplus H$
$\frac{7}{2}$	$G_1 \oplus G_2 \oplus H$
$\frac{9}{2}$	$G_1 \oplus 2H$
$\frac{11}{2}$	$G_1 \oplus G_2 \oplus 2H$
$\frac{13}{2}$	$G_1 \oplus 2G_2 \oplus 2H$
$\frac{15}{2}$	$G_1 \oplus G_2 \oplus 3H$
$\frac{17}{2}$	$2G_1 \oplus G_2 \oplus 3H$
$\frac{19}{2}$	$2G_1 \oplus 2G_2 \oplus 3H$
$\frac{21}{2}$	$G_1 \oplus 2G_2 \oplus 4H$
$\frac{23}{2}$	$2G_1 \oplus 2G_2 \oplus 4H$

# Operator Design

## ◆ The basic building blocks

$$\bar{B}_{\alpha\beta\gamma}^{ABC}(x) = \bar{\psi}_{\alpha}^{A,i} \bar{\psi}_{\beta}^{B,j} \bar{\psi}_{\gamma}^{C,k} \epsilon^{ijk}$$

- ◆  $A, B, C$ : quark flavor
- ◆  $i, j, k$ : color
- ◆  $\alpha, \beta, \gamma$ : Dirac indices

## ◆ Project onto irreducible representations (irreps)

$$\bar{B}_{\lambda}^{\Lambda,n}(x) = \Gamma_{\lambda}^{\Lambda,n}(\alpha, \beta, \gamma) \bar{B}_{\alpha,\beta,\gamma}(x)$$

- ◆  $\Lambda$ : irrep
- ◆  $\lambda \in [1, \dim(\Lambda)]$
- ◆  $n$ : element of interoperating op

Flavor	$G_{1g/u}(2)$	$H_{g/u}(4)$
$N$	3	1
$\Delta$	1	2
$\Lambda$	4	1
$\Sigma$	4	3
$\Xi$	4	3
$\Omega$	1	2

## ◆ Correlator matrix

$$C_{\Lambda}^{m,n}(t) = \sum_{\vec{x}} \sum_{\lambda} \langle 0 | B_{\lambda}^{\Lambda,m}(\vec{x}, t) \bar{B}_{\lambda}^{\Lambda,n}(0) | 0 \rangle$$

## ◆ For more details and extended-link operators:

*S. Basak et al., Phys. Rev. D72, 094506 (2005)*

# Variational Method

C. Michael, Nucl. Phys. B 259, 58 (1985)

M. Lüscher and U. Wolff, Nucl. Phys. B 339, 222 (1990)

- ◆ Construct the matrix

$$C_{ij}(t) = \langle 0 | \mathcal{O}_i(t)^\dagger \mathcal{O}_j(0) | 0 \rangle$$

- ◆ The  $\mathcal{O}_i$  could be different choices of operator or smearing parameters

- ◆ Solve for the generalized eigensystem of

$$C(t_0)^{-1/2} C(t) C(t_0)^{-1/2} v = \lambda(t, t_0) v$$

with eigenvalues

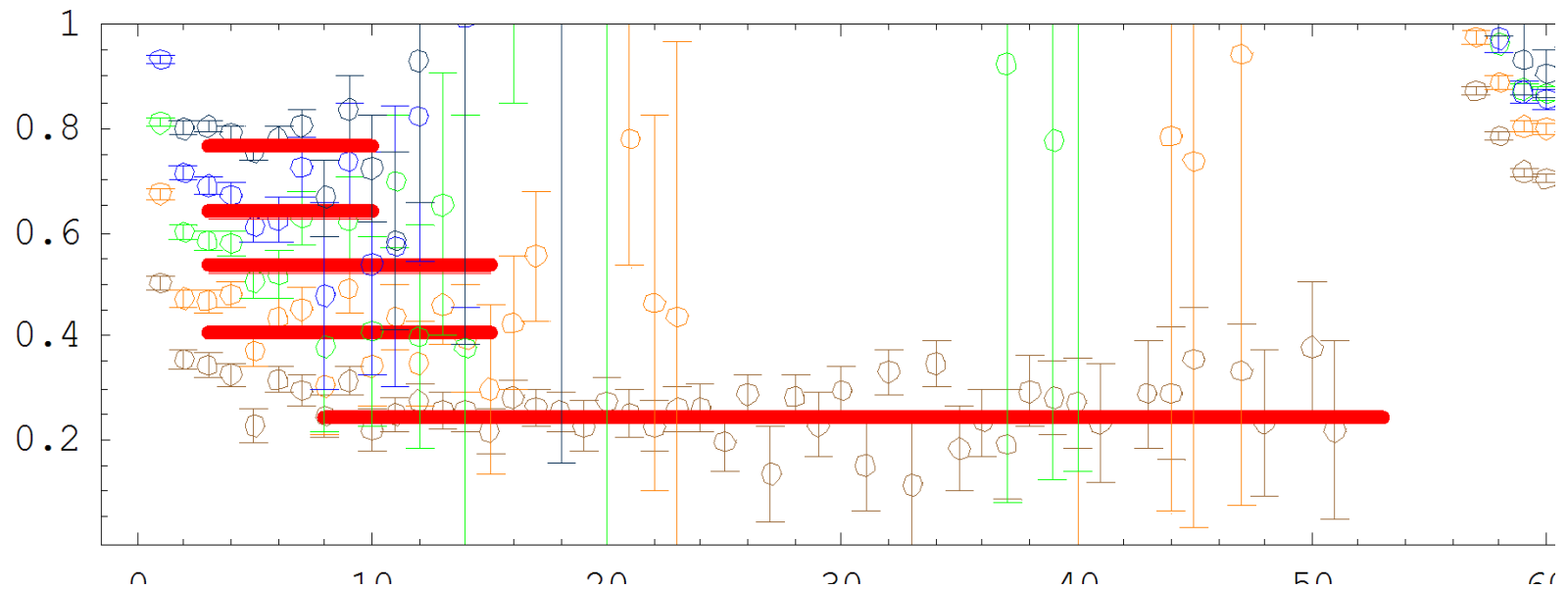
$$\lambda_n(t, t_0) = e^{-(t-t_0)E_n} (1 + \mathcal{O}(e^{-|\delta E|(t-t_0)}))$$

- ◆ At large  $t$ , the signal of the desired state dominates.

# Variational Method

## Quenched Anisotropic ( $a_t^{-1} \sim 6$ GeV)

- ◆ Clover action, 680 MeV pion
- ◆ Example:  $5 \times 5$  smeared-smeared correlator matrices
- ◆ Fit them individually with exponential form (red bars)
- ◆ Plotted along with effective masses

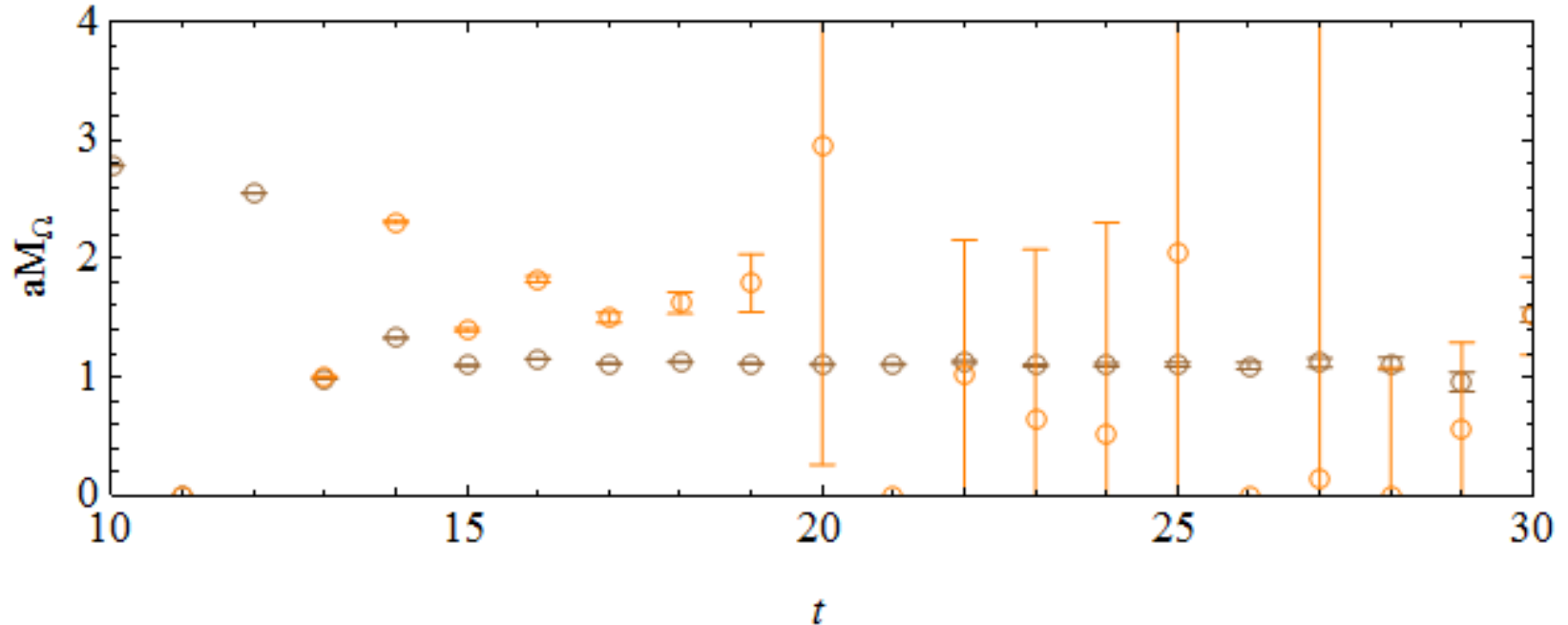


# Variational Method

## Mixed Action ( $a_t^{-1} \sim 1.6 \text{ GeV}$ )

◆ Example: ( $\sim 350 \text{ MeV}$  pion)

Omega  $2 \times 2$  smeared-smeared operator correlator matrices

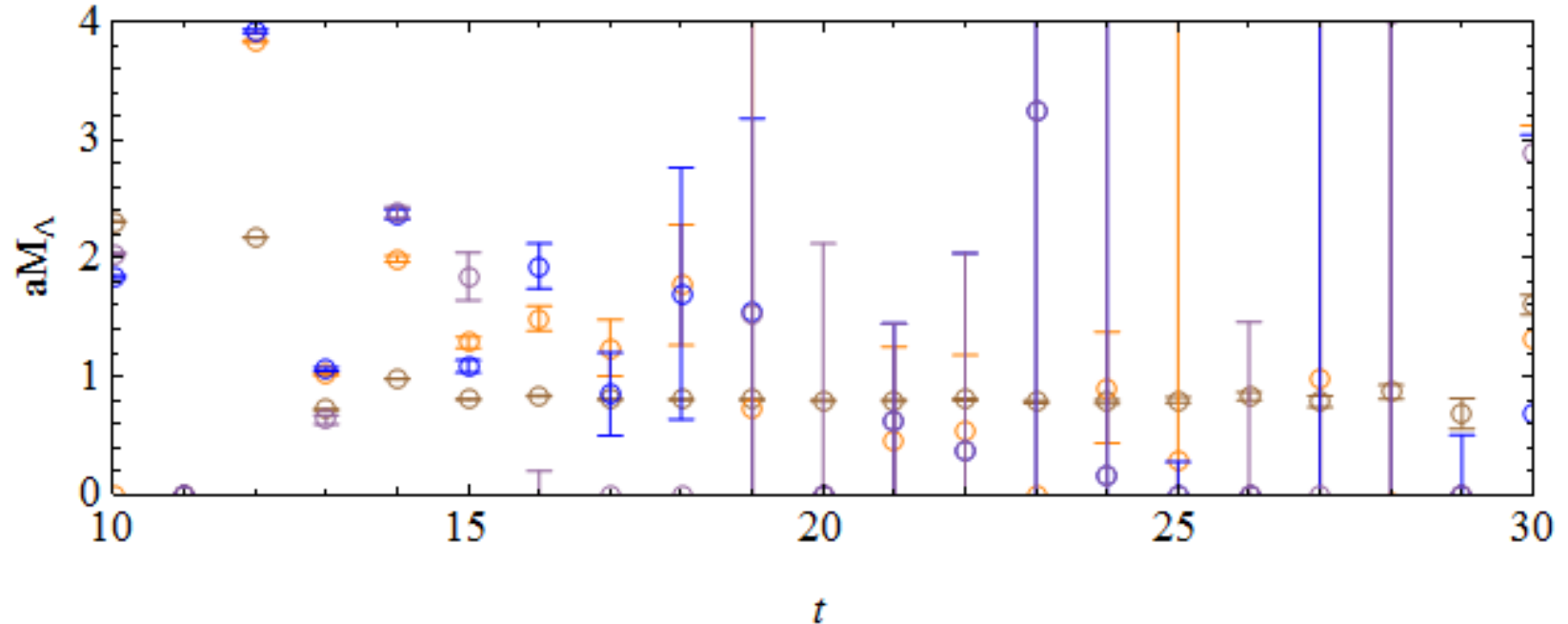


# Variational Method

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- ◆ Example: ( $\sim 350 \text{ MeV}$  pion)

Lambda  $4 \times 4$  smeared-smeared operator correlator matrices



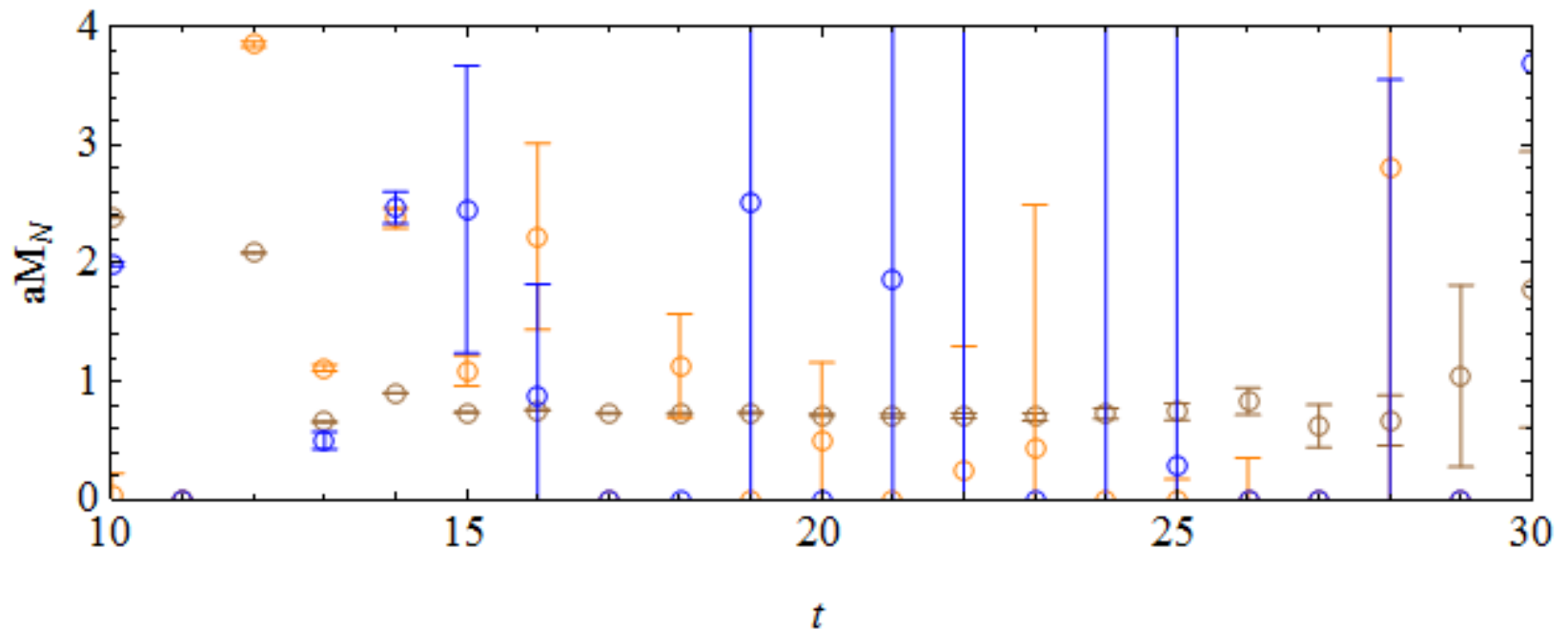


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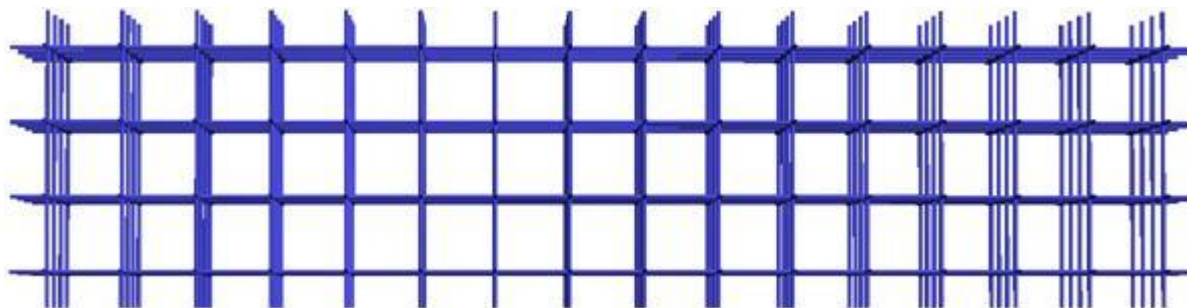
Nucleon  $3 \times 3$  smeared-smeared operator correlator matrices



- ◆ Unfortunately, we cannot see a clear radial excited state

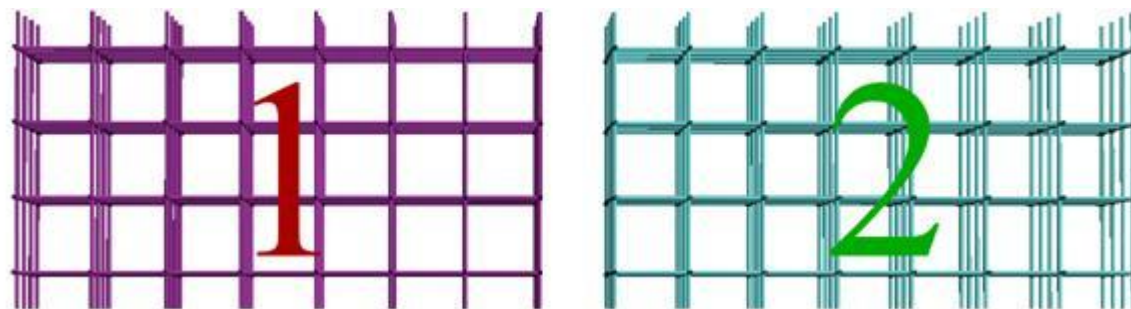
# Ensembles and Parameters

- ◆ Mixed action: DWF on staggered sea
- ◆ Pion mass ranges 300–750 MeV
- ◆  $a \approx 0.125$  fm,  $L_s = 16$ ,  $M_5 = 1.7$
- ◆ Volume fixed at 2.6 fm, box size of  $20^3 \times 32$  chopped



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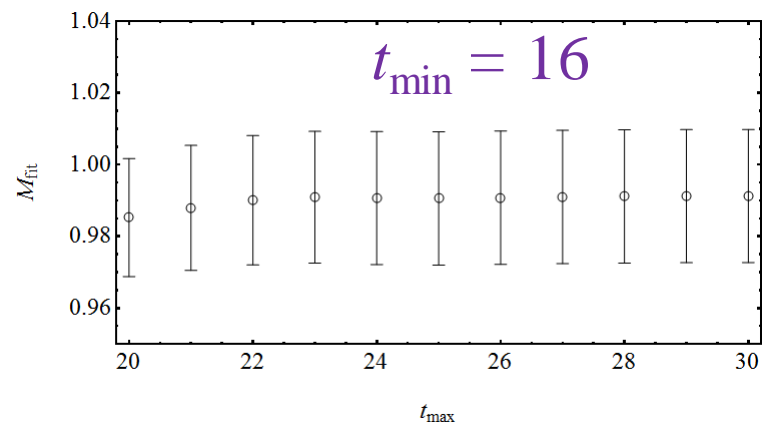
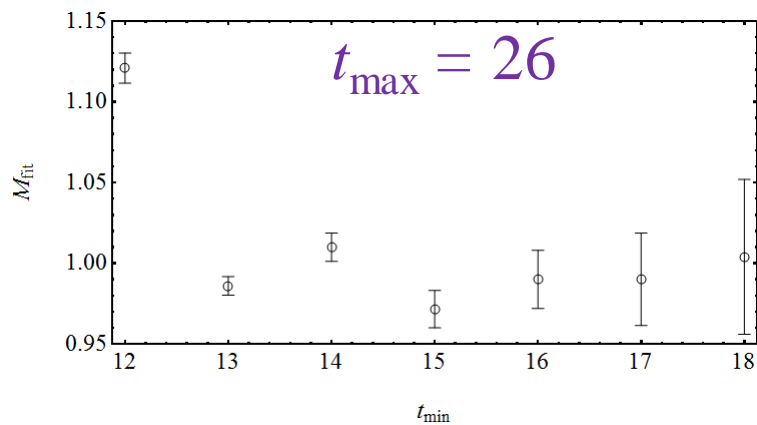


ensem	m007	m010	m020	m030	m040	m050
Conf.	3489	3693	1455	700	324	425

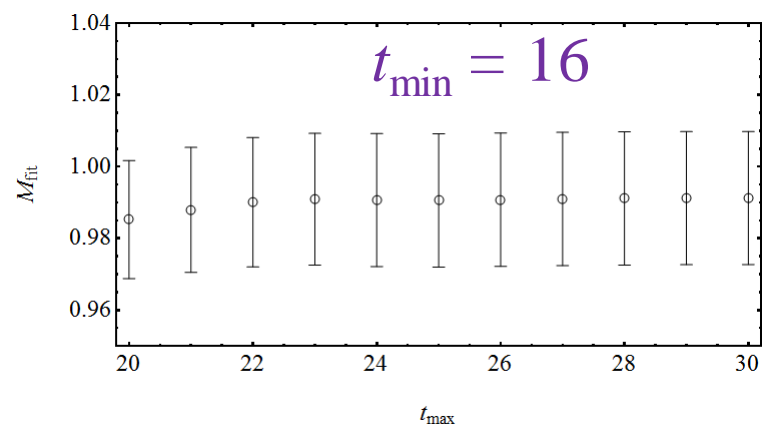
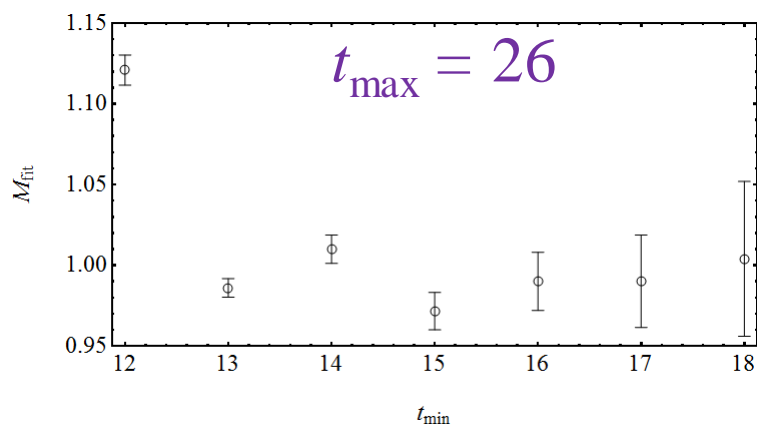
- ◆ HYP-smearred gauge fields, Gaussian operator smearing

# Consistent Analyses

- Systematic error due to fit range
- Example: Nucleon @ 350 MeV



- Example: Delta @ 350 MeV



# Consistent Analyses

- ◆ Oscillating effective mass is related to transfer matrix with 5<sup>th</sup>-dimensional mass term  
→ treat as a lattice artifact

- ◆ Solution: oscillating term + one excited state

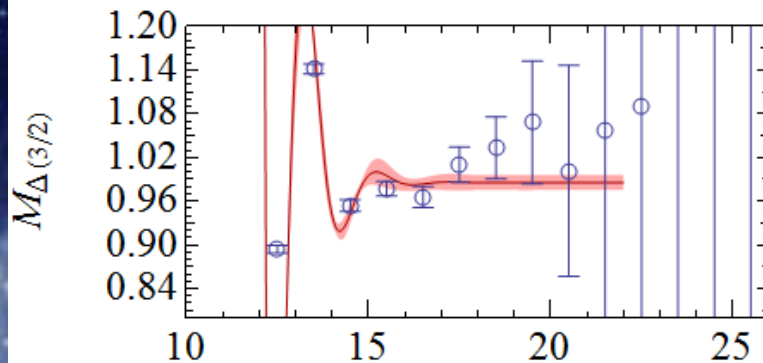
$$C(t) = \sum_{n=0}^1 A_n \exp[-M_n \times (t - t_{\text{src}})] + A_{\text{osc}} (-1)^t \exp[-M_{\text{osc}} \times (t - t_{\text{src}})].$$

J. Negele et al. LAT2007, 078

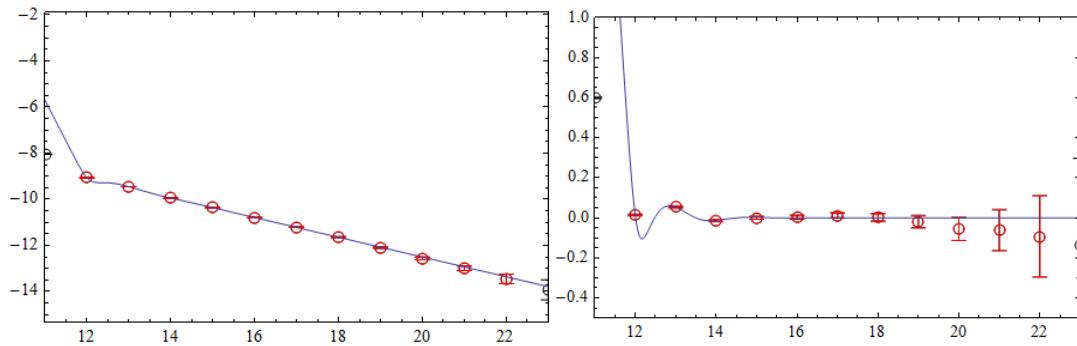
- ◆ Example: Delta @ 350 MeV pion ensemble

$$\chi^2/\text{dof} = 0.69$$

“effective” mass

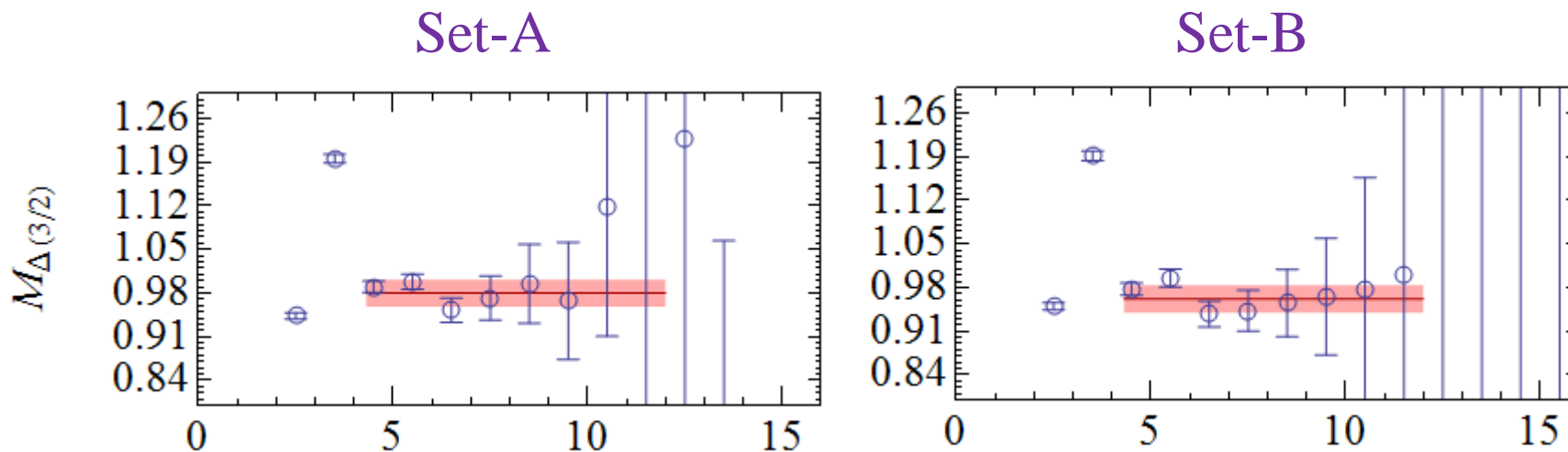


log corr. (ground-state removed)



# Consistent Analyses

- ◆ Chopped lattice? Example: Delta @350 MeV
  - ◆ Set A:  $20^3 \times 64$ , 4 sources, 224 confs.
  - ◆ Set B: chopped  $20^3 \times 32$ , 620 confs.



- ◆ Consistent results in both cases

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# Ground-State Results

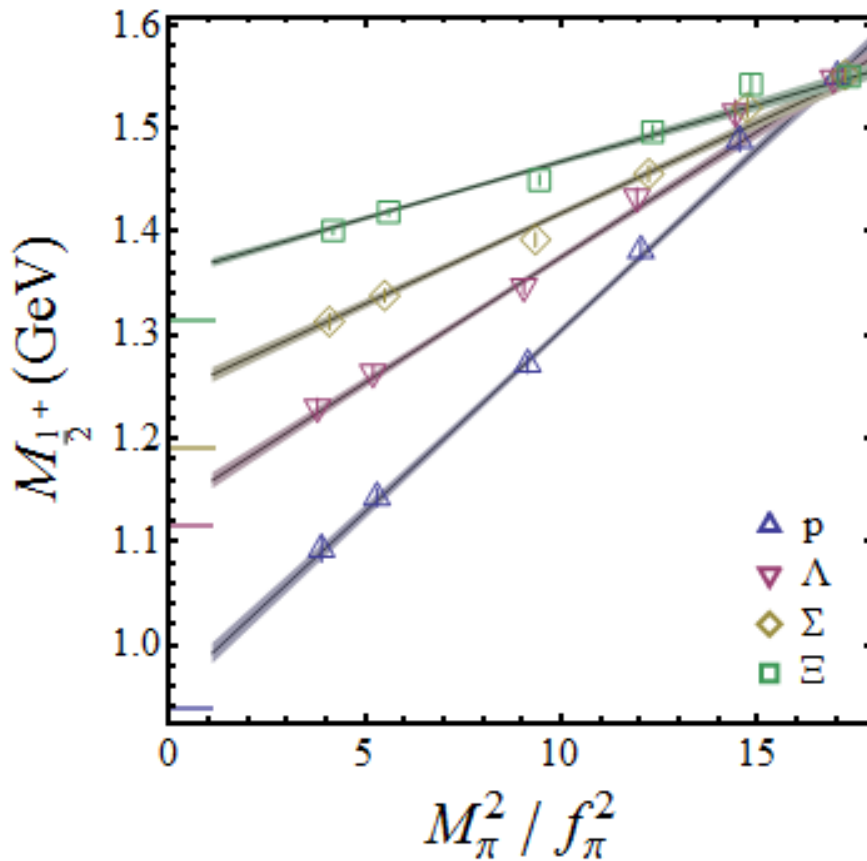
work with

Lattice Hadron Physics Collaboration (LHPC)

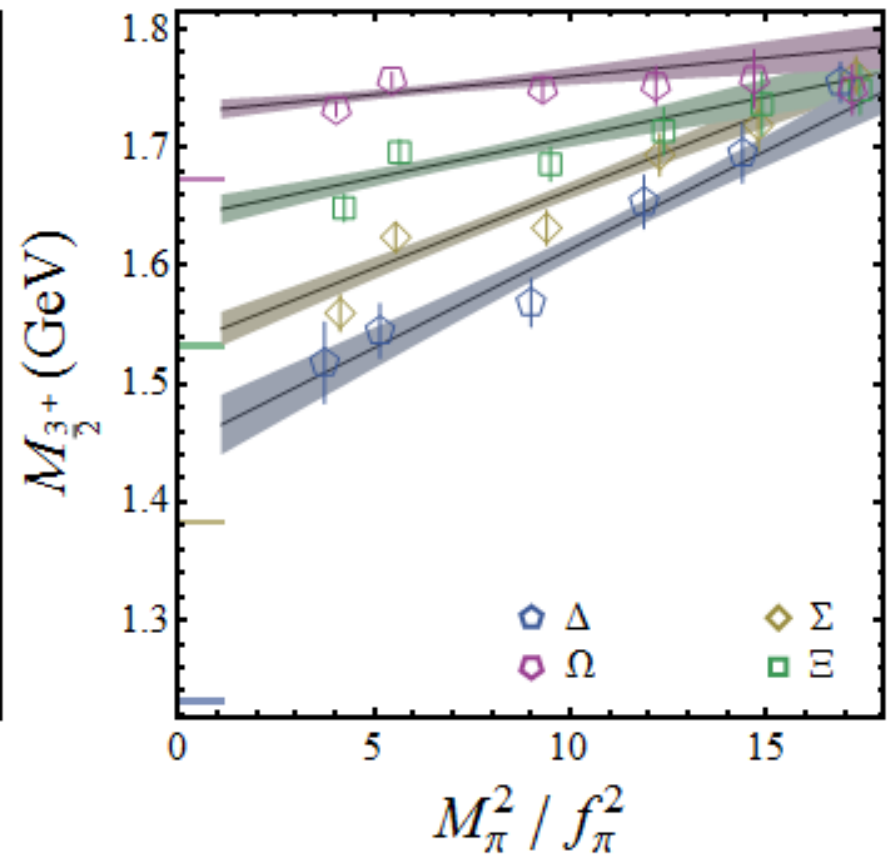


# Octets and Decuplets

◆ Spin-1/2



◆ Spin-3/2



# Multiplet Mass Relations

## ◆ SU(3) flavor symmetry breaking

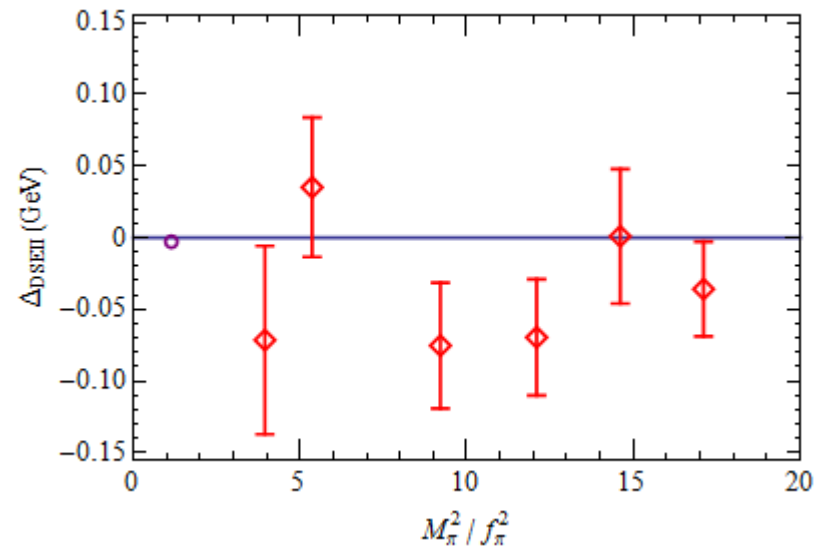
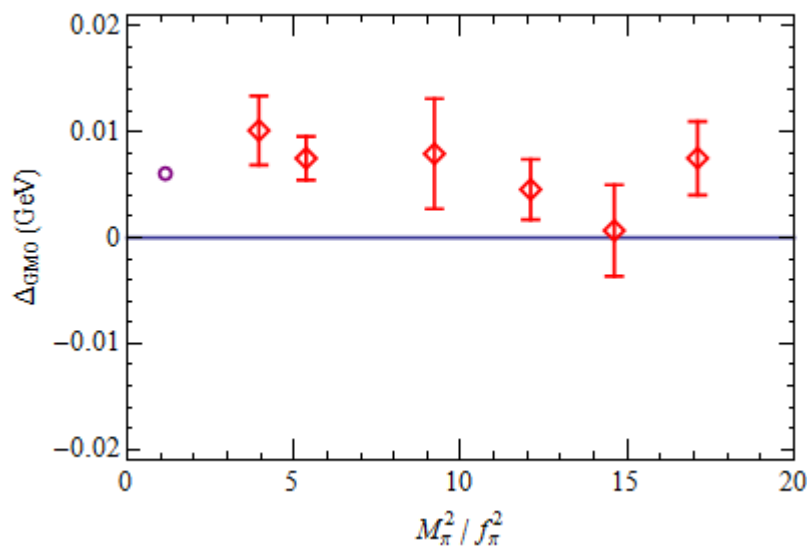
### ◆ Gell-Mann-Okubo relation

$$\Delta_{GMO} = \frac{3}{4}M_{\Lambda} + \frac{1}{4}M_{\Sigma} - \frac{1}{2}M_N - \frac{1}{2}M_{\Xi}$$

### ◆ Decuplet Equal Spacing relation

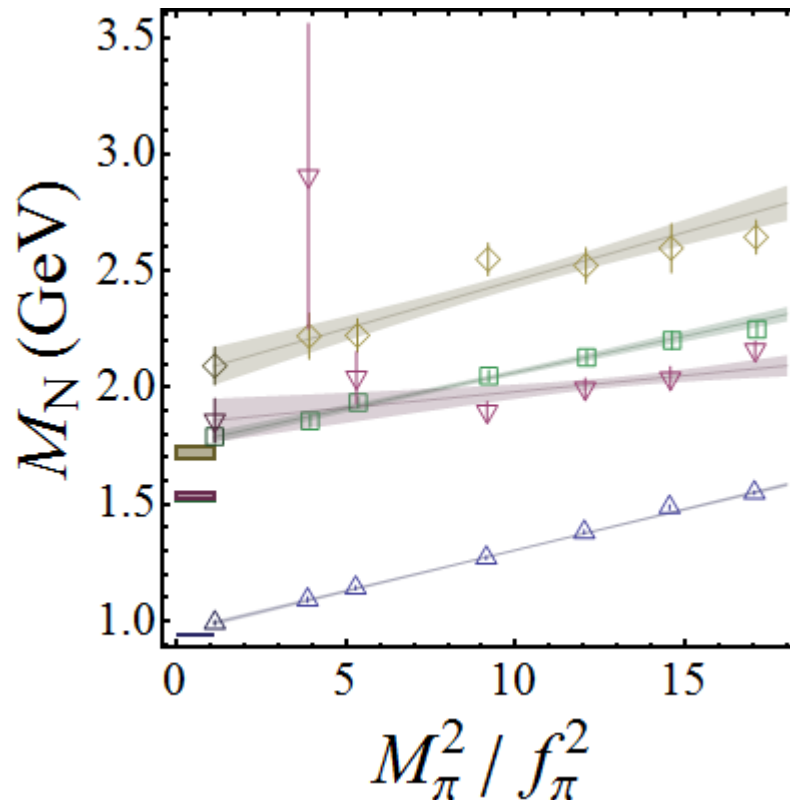
$$\Delta_{DESI} = \frac{1}{2}(M_{\Sigma^*} - M_{\Delta}) + \frac{1}{2}(M_{\Omega} - M_{\Xi^*}) - M_{\Xi^*} + M_{\Sigma^*}$$

## ◆ Mass differences are close to experimental numbers



# General Spectroscopy

- ◆ The non-strange baryons ( $N$ )
- ◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$
- ◆  $N$   $N(1535)$   $N(1720)$   $N(1520)$

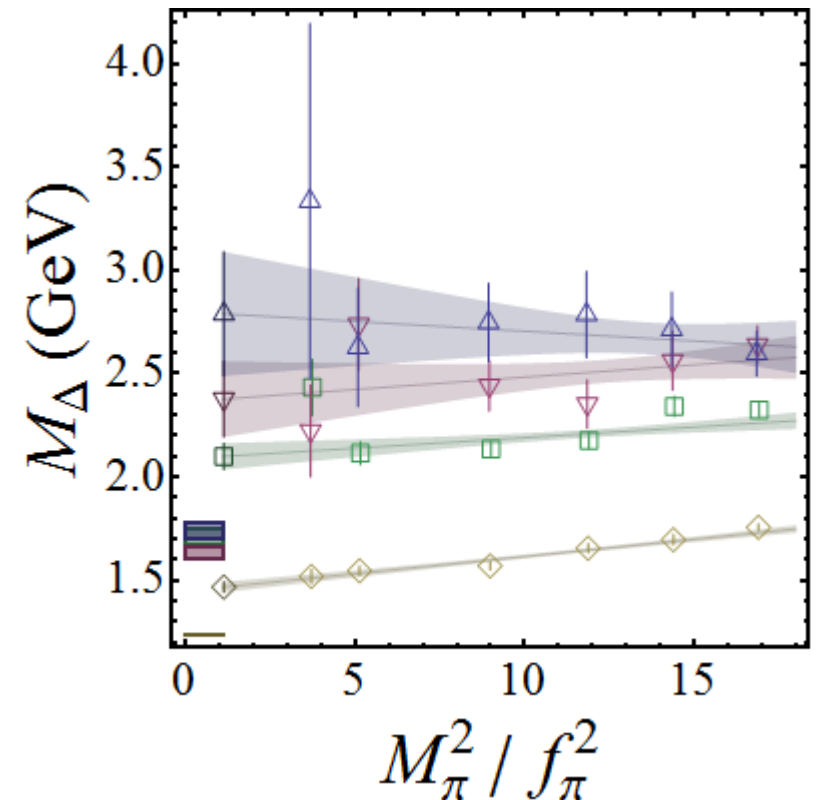
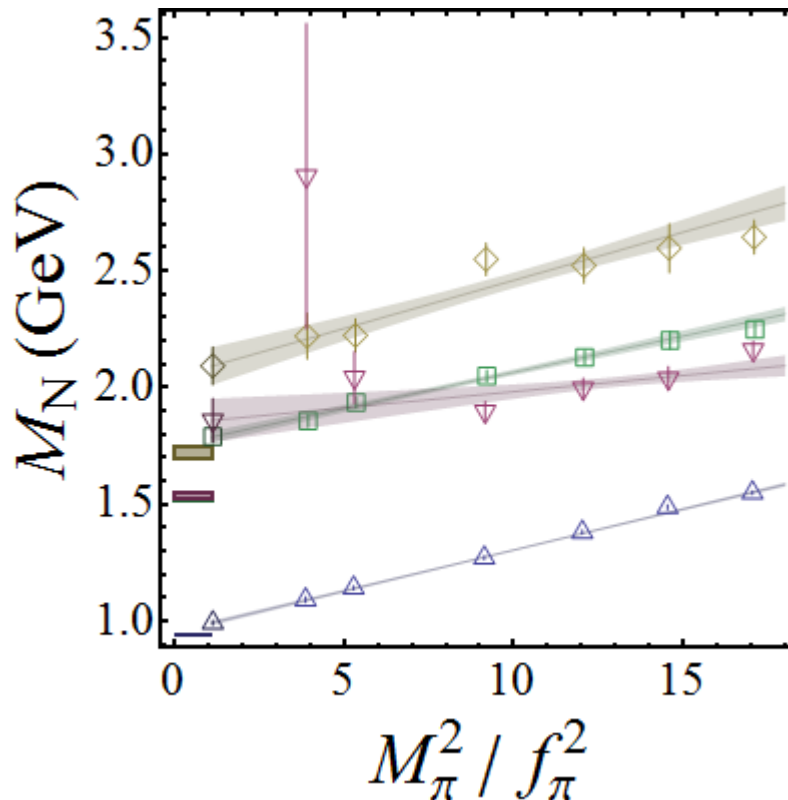


# General Spectroscopy

◆ The non-strange baryons ( $N$  and  $\Delta$ )

◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$

◆	$N$	$N(1535)$	$N(1720)$	$N(1520)$
◆		$\Delta(1620)$	$\Delta$	$\Delta(1700)$

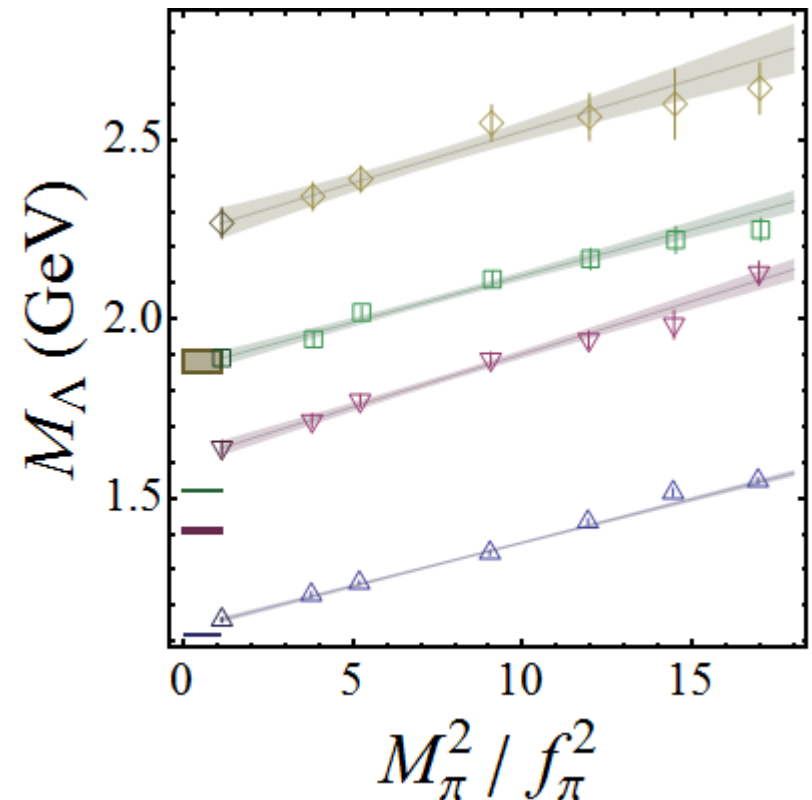
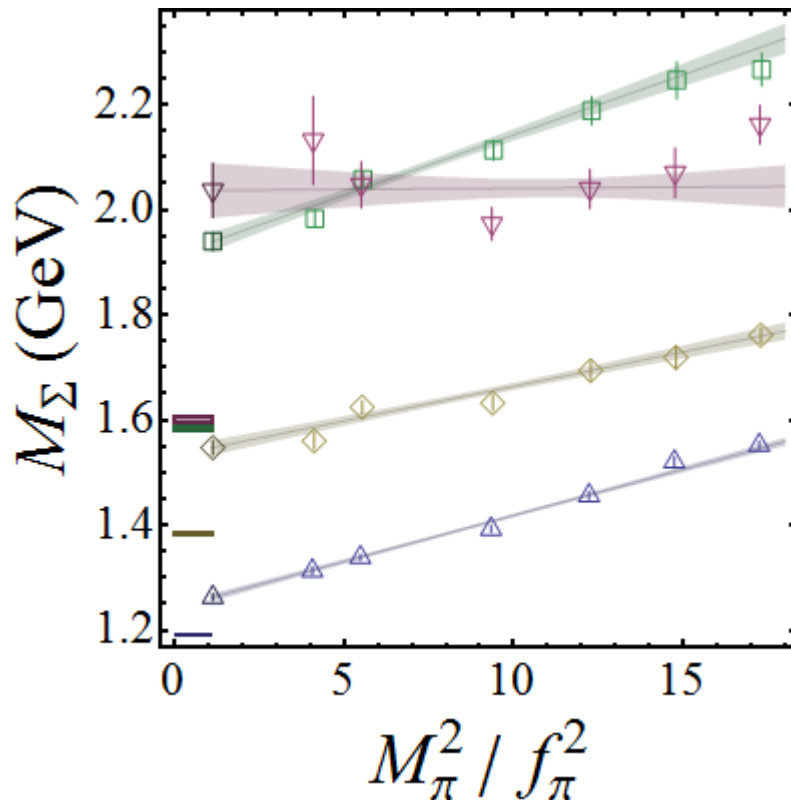


# General Spectroscopy

◆ The singly strange baryons: ( $\Sigma$  and  $\Lambda$ )

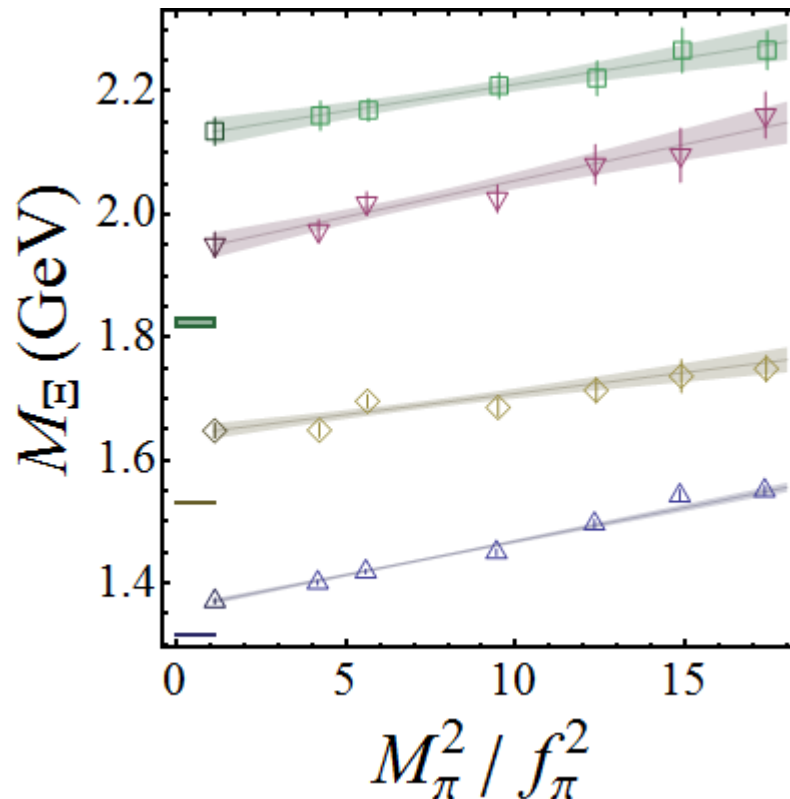
◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$

◆	$\Sigma$	$\Sigma(1620)$	$\Sigma^*$	$\Sigma(1580)$
◆	$\Lambda$	$\Lambda(1405)$	$\Lambda(1890)$	$\Lambda(1520)$



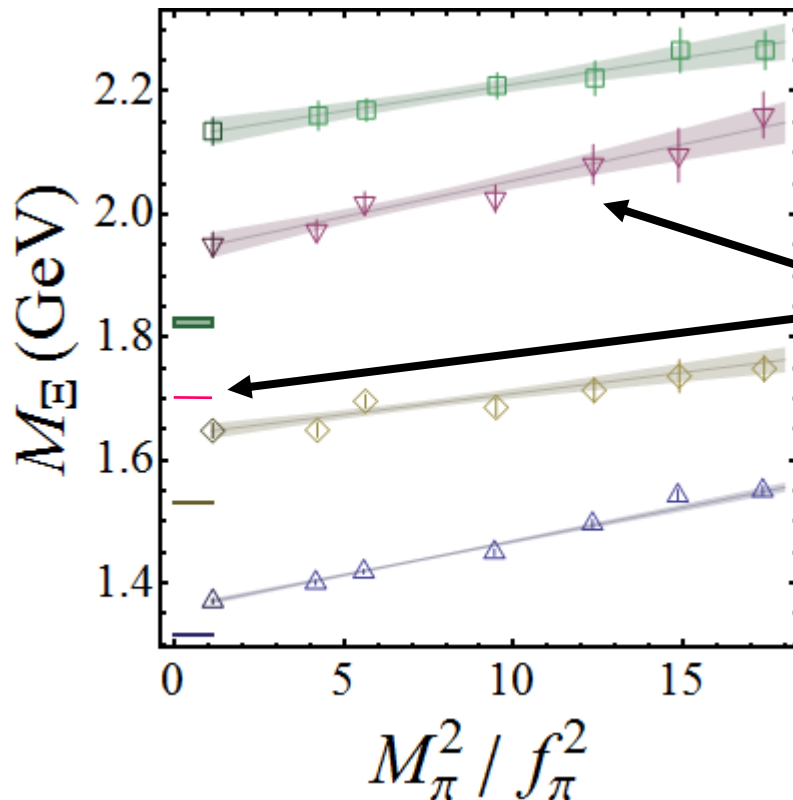
# General Spectroscopy

- ◆ The less known baryons ( $\Xi$  )
- ◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$
- ◆  $\Xi$   $\Xi(1690)?$   $\Xi(1530)$   $\Xi(1820)$



# General Spectroscopy

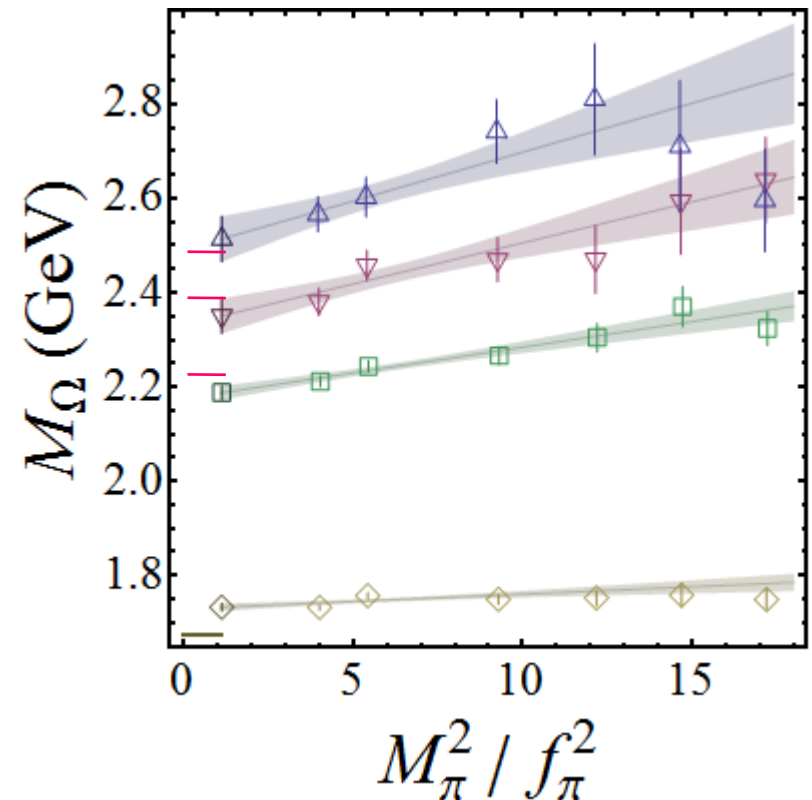
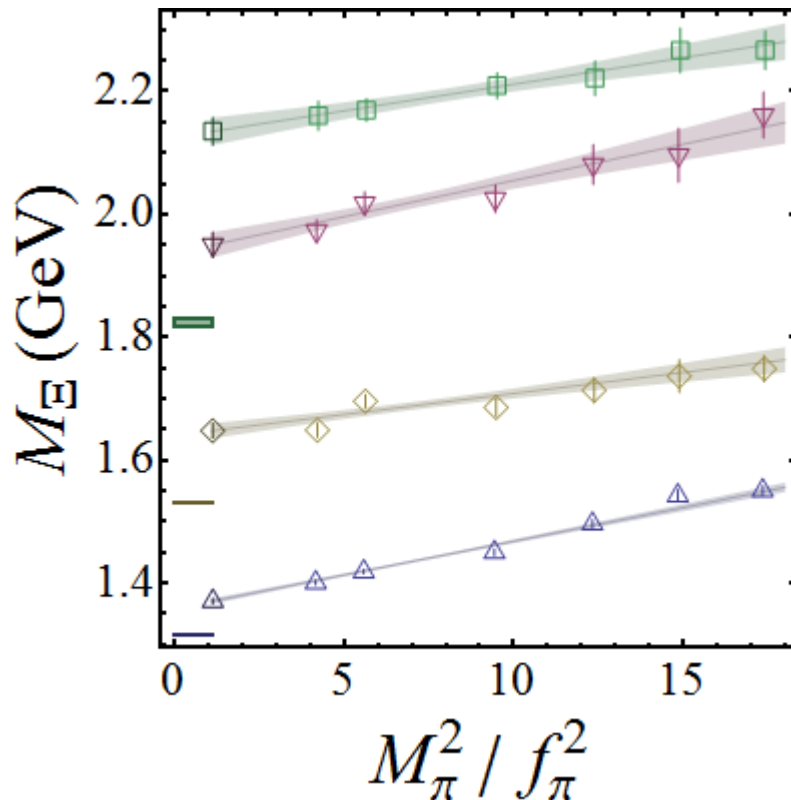
- ◆ The less known baryons ( $\Xi$  )
- ◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$
- ◆  $\Xi$   $\Xi(1690)?$   $\Xi(1530)$   $\Xi(1820)$



- ◆ Babar at MENU 2007:  
 $\Xi(1690)^0$  negative parity  
 $-1/2$

# General Spectroscopy

- ◆ The less known baryons ( $\Xi$  and  $\Omega$ )
- ◆ Symbols:  $J^P = 1/2^+$   $\triangle$ ,  $1/2^-$   $\nabla$ ,  $3/2^+$   $\diamond$ ,  $3/2^-$   $\square$ 
  - ◆  $\Xi$   $\Xi(1690)?$   $\Xi(1530)$   $\Xi(1820)$
  - ◆ Could they be  $\Omega(2250)$ ,  $\Omega(2380)$ ,  $\Omega(2470)?$





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# Excited-State Results

## Roper Puzzles

# What is the Roper?

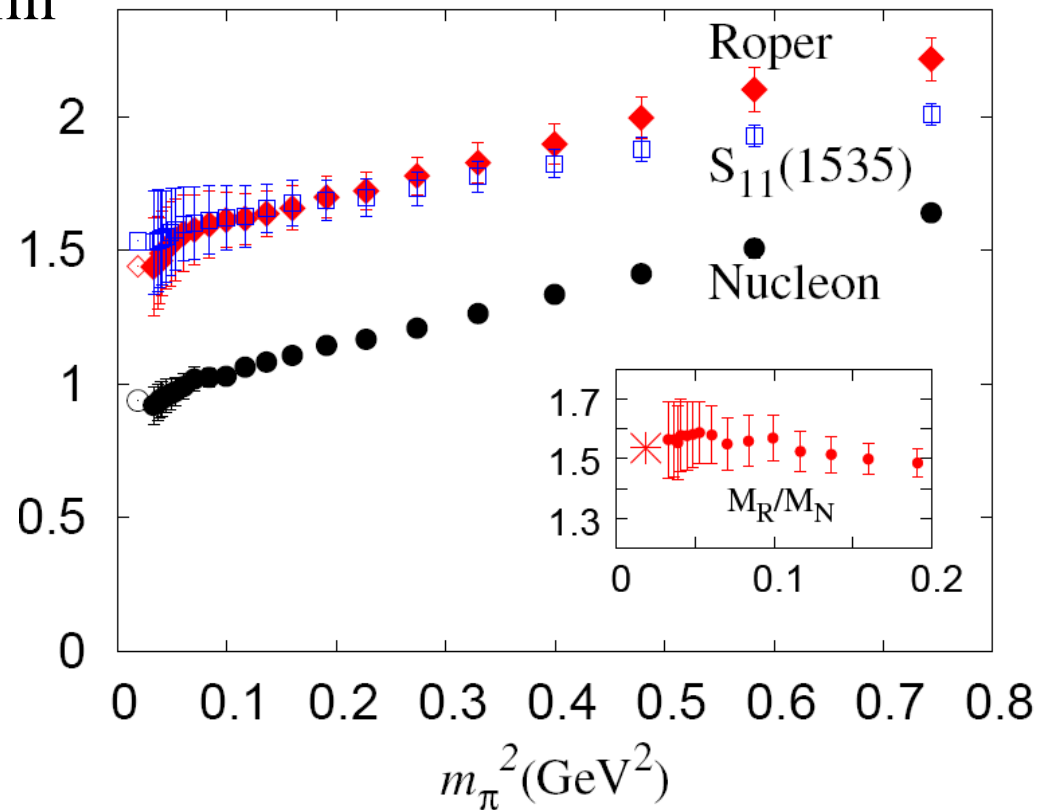
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- ◆ First positive-parity excited state of the nucleon
- ◆ Unusual feature: 1<sup>st</sup> excited state is lower than its negative-parity partner!
- ◆ Long-standing puzzle
  - ◆ Quark-gluonic (hybrid) state [*C. Carlson et al. (1991)*]
  - ◆ Five-quark (meson-baryon) state [*O. Krehl et al. (1999)*]
  - ◆ Constituent quark models (many different specific approaches)
  - ◆ and many other models...
- ◆ Lattice gauge theory
  - ◆ Many early quenched calculations failed to extract the correct Roper mass
  - ◆ Kentucky group (with lightest pion mass = 180 MeV) got  $M_{\text{Roper}} = 1462(157) \text{ MeV}$

# More on the Roper

- ◆ Kentucky's calculation
  - ◆ Quenched Iwasaki, overlap (ghost contributions are included in analysis)
  - ◆ Volume: 2.4 and 3.6 fm
  - ◆ Large range of  $m_\pi$
- ◆ Conclusive?
  - ◆ Many groups fail to see similar behaviour
  - ◆ War still going on...

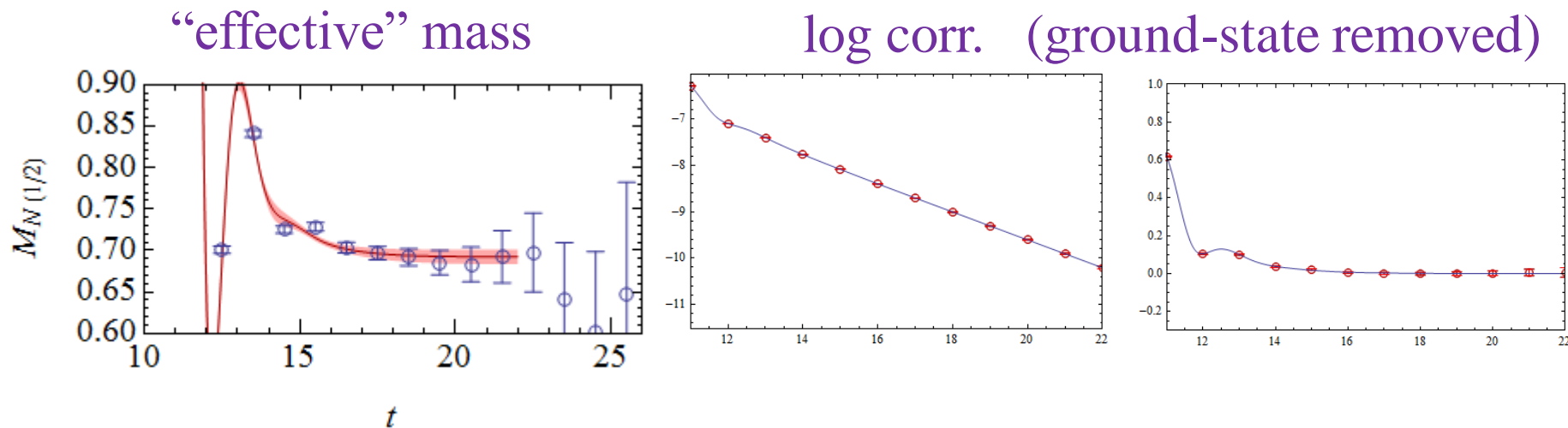


# Roper in Full QCD

- ◆ Attempt to extract Roper mass from our current data
- ◆ Analysis: oscillating term is necessary for small  $t$

$$C(t) = \sum_{n=0}^1 A_n \exp[-M_n \times (t - t_{\text{src}})] + A_{\text{osc}} (-1)^t \exp[-M_{\text{osc}} \times (t - t_{\text{src}})].$$

- ◆ Example plot (300 MeV ensemble)



- ◆ Reasonable  $\chi^2/\text{dof} < 0.6$
- ◆ Systematic error due to lack of 2<sup>nd</sup>-excited state in the fit?

# Roper in Full QCD

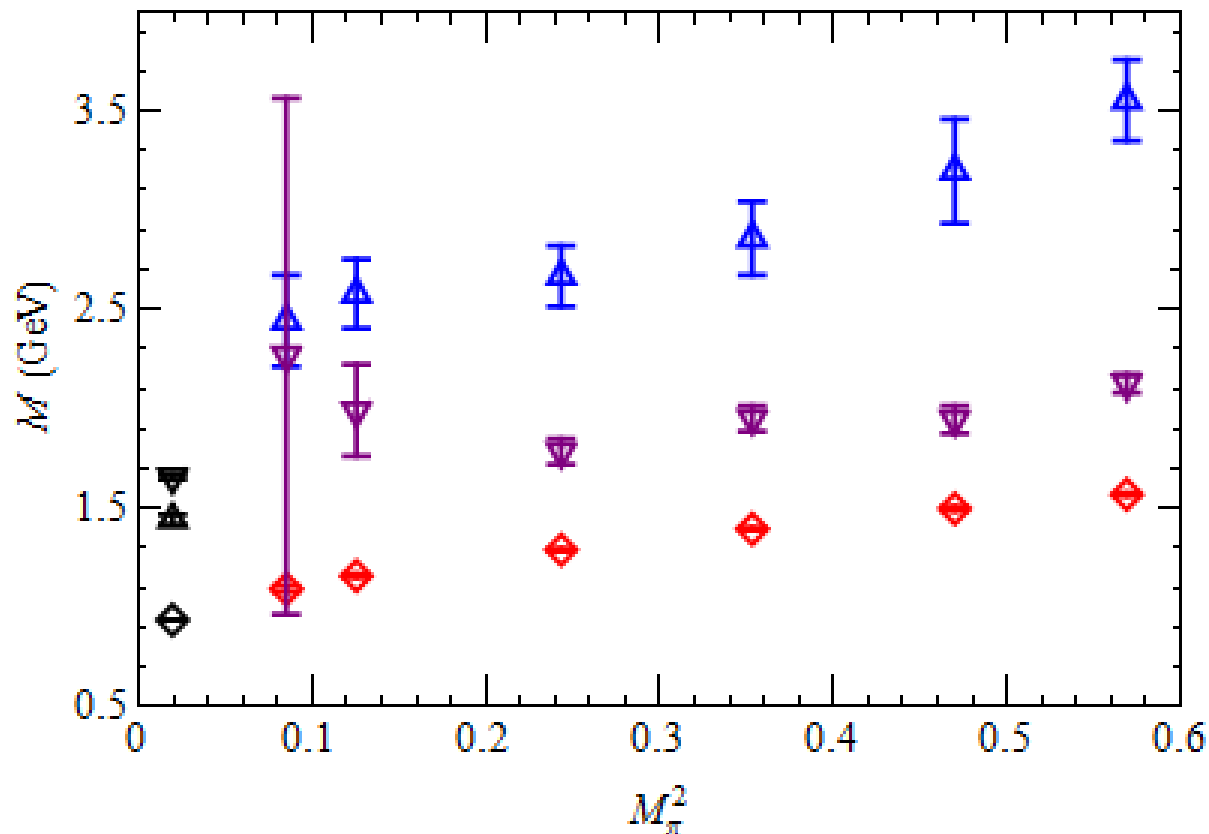
◆ Results from mixed action

◆ Symbols:  $J^P$

$1/2^+$  

$1/2^-$  

$1/2^+$  



◆ No sign of crossover occurs here

◆ Finite-volume effects starting at 350 MeV pion?

# Summary/Outlook — I

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## ◆ What we have done:

- ◆ 2+1-flavor calculations with volume around 2.6 fm
- ◆ Preliminary study with lightest pion mass 300 MeV
- ◆ Ground states of  $G_{1g/u}$  and  $H_{g/u}$  for each flavor
- ◆ Roper state calculated;  
correct mass-ordering pattern is not yet seen

## ◆ Currently in progress:

- ◆ Mixed action chiral extrapolation for octet and decuplet
- ◆ Open-minded for extrapolation to physical pion mass for other states

## ◆ In the future:

- ◆ Lower pion masses to confirm chiral logarithm drops

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# The Future

# Physical-Pion Era

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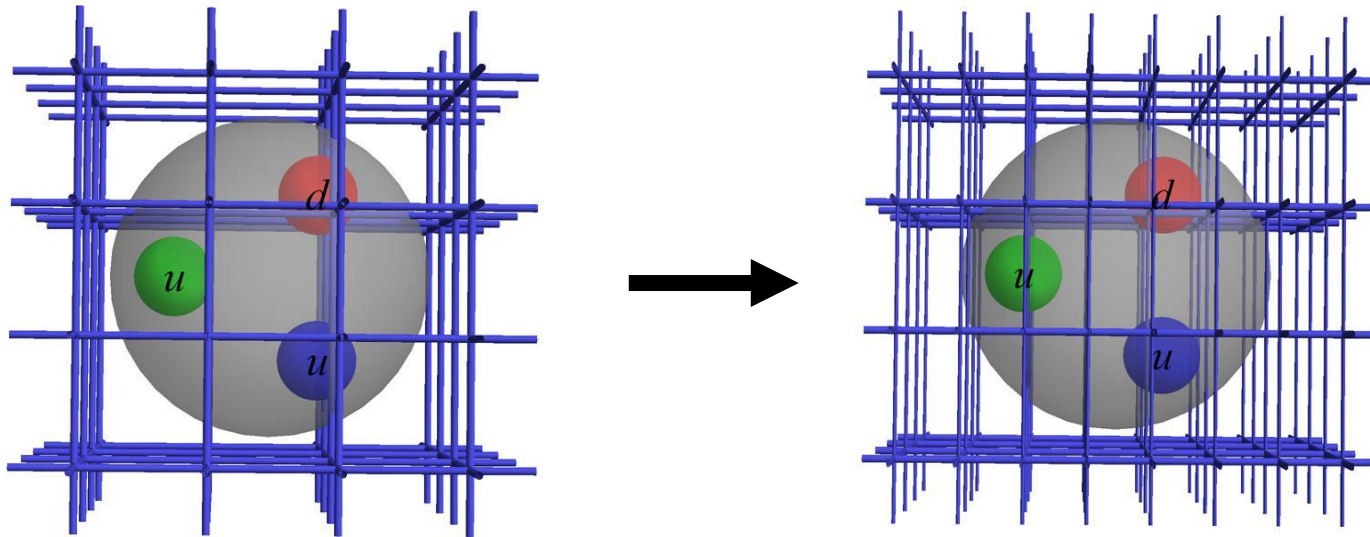
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- ◆ Physical pion mass ensembles are near
- ◆ Chiral perturbation theory will no longer be a guide, but can be judged against predictions of QCD
- ◆ Three major gauge-generation projects within US community
  - ◆ Chiral fermions:
    - DWF on Iwasaki gauge, 0.093 fm (RBC+LHPC+UKQCD)
    - Designing next generation with IBM (RBC+UKQCD)
  - ◆ Staggered fermions: MILC
    - Considering HISQ instead of the asqtad
  - ◆ Anisotropic clover lattices: LHPC
    - 2+1-flavor dynamical runs



# Anisotropic Clover Fermions

- ◆ Solution: increase resolution



- ◆ Excited-state resonances and form factors
- ◆ Glueballs, hybrids, etc.
- ◆ Nucleon scattering, four-point Green functions
- ◆ Roadmap:
  - ◆ 2012: physical pion at  $a \sim 0.10$  fm ( $72^3$ )
  - ◆ 2014: physical pion at  $a \sim 0.08$  fm ( $96^3$ )