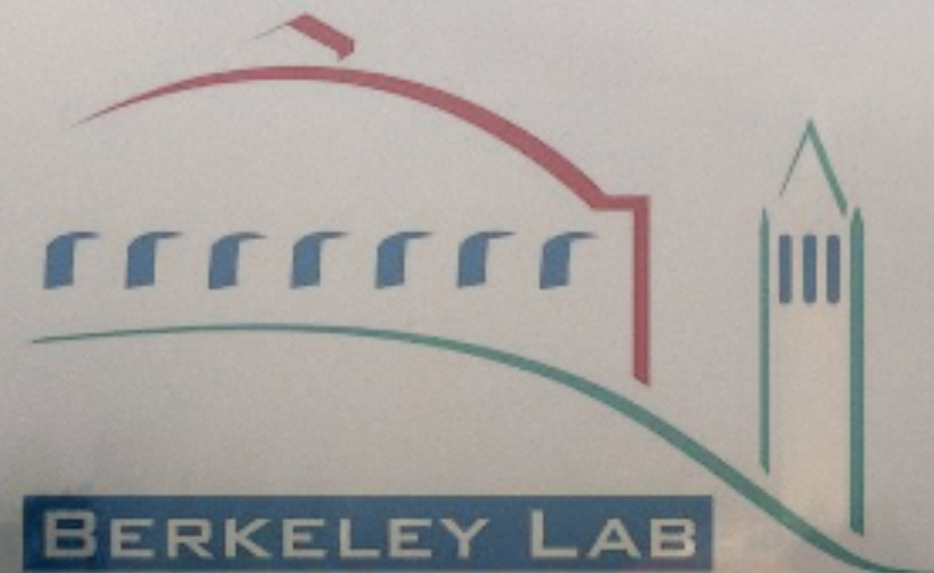


# To bind or not to bind: A question of various two-nucleon interpolators

Lattice 2023: FNAL

3<sup>rd</sup> August, 2023

André Walk-Loud





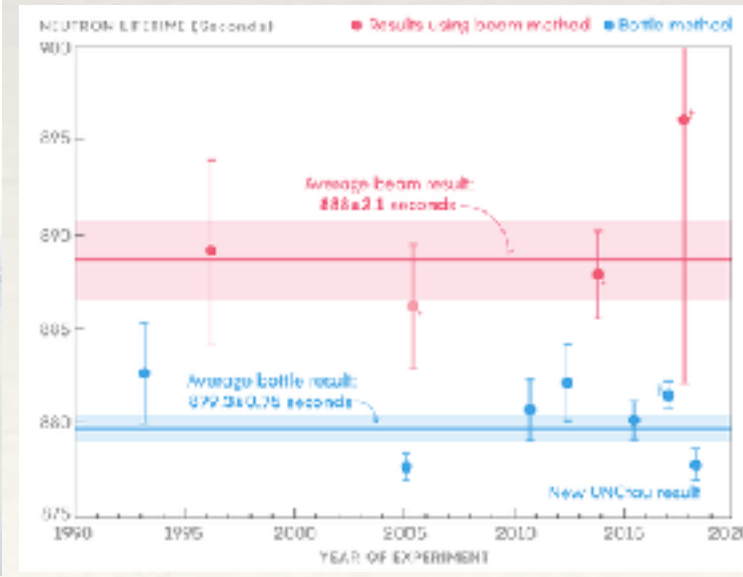
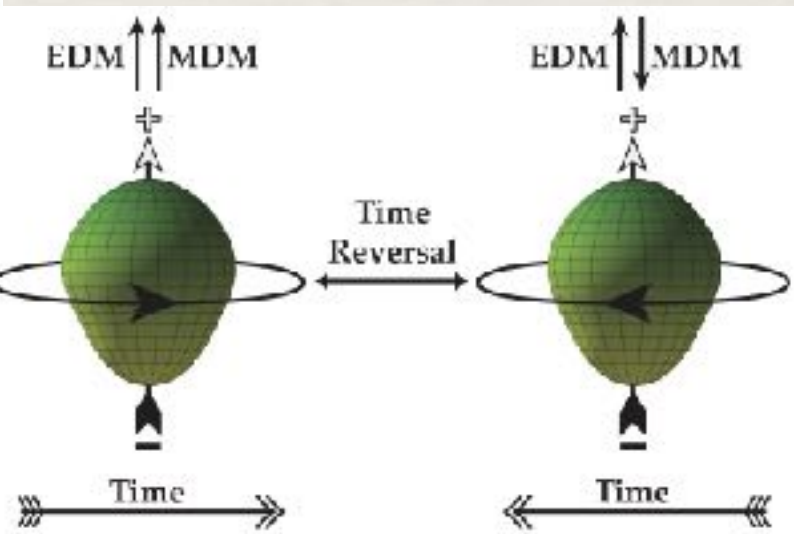
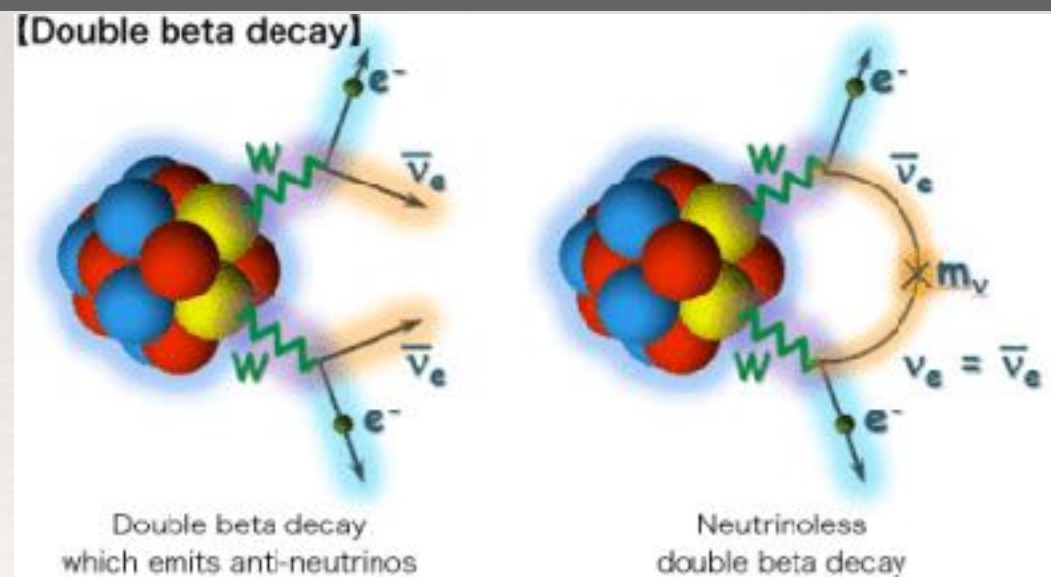
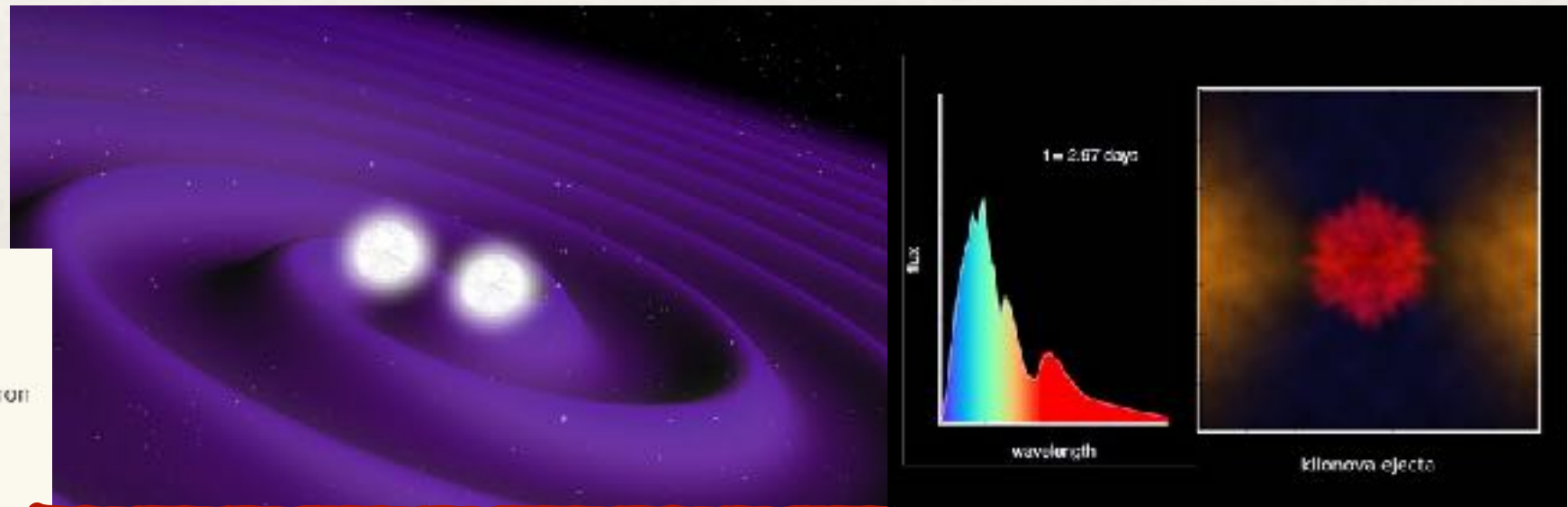
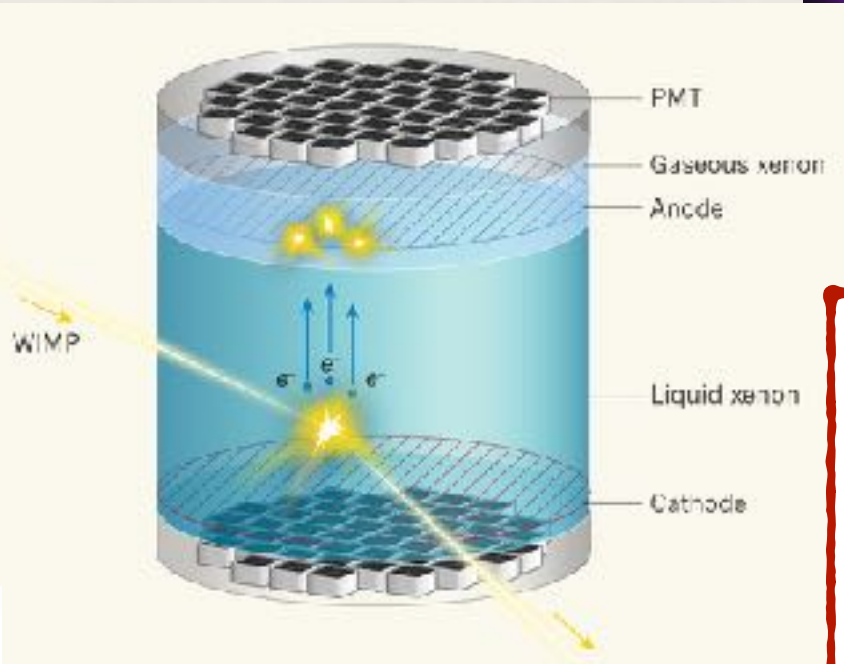
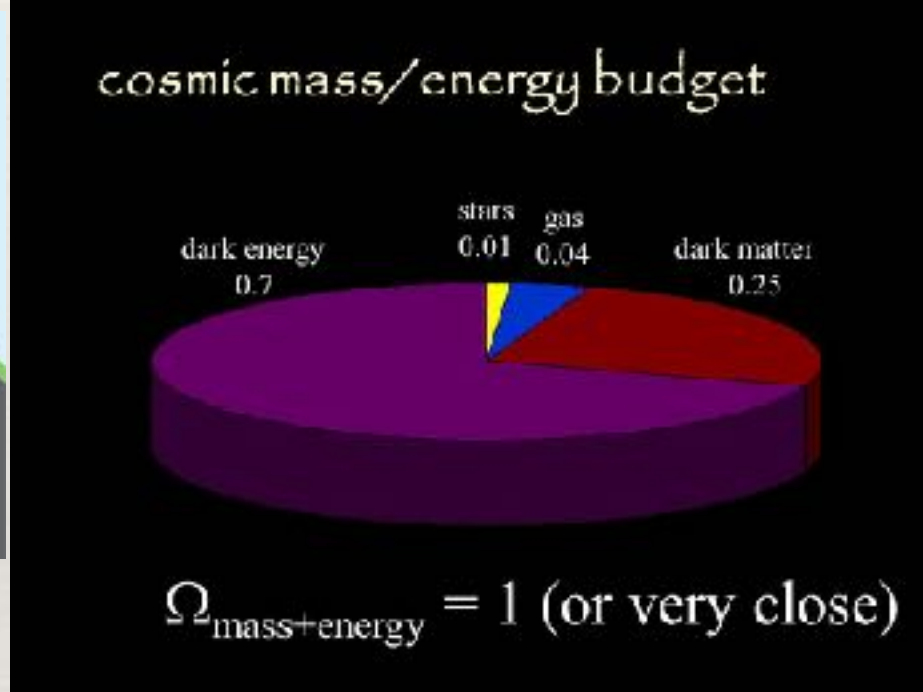
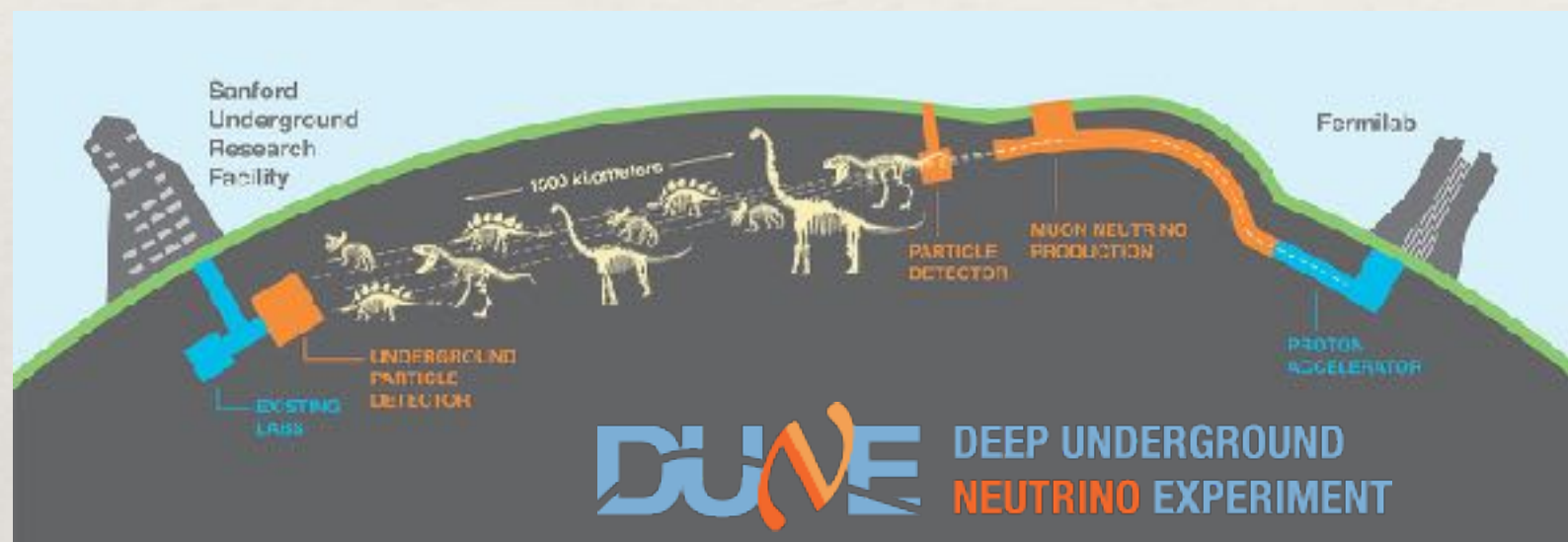
Understanding the emergence of nuclear physics has the potential to be relevant to a broad set of nuclear and particle physics experimental programs

Why is the universe composed of matter? (and not anti-matter)

Does dark matter interact with matter? (beyond gravitationally)

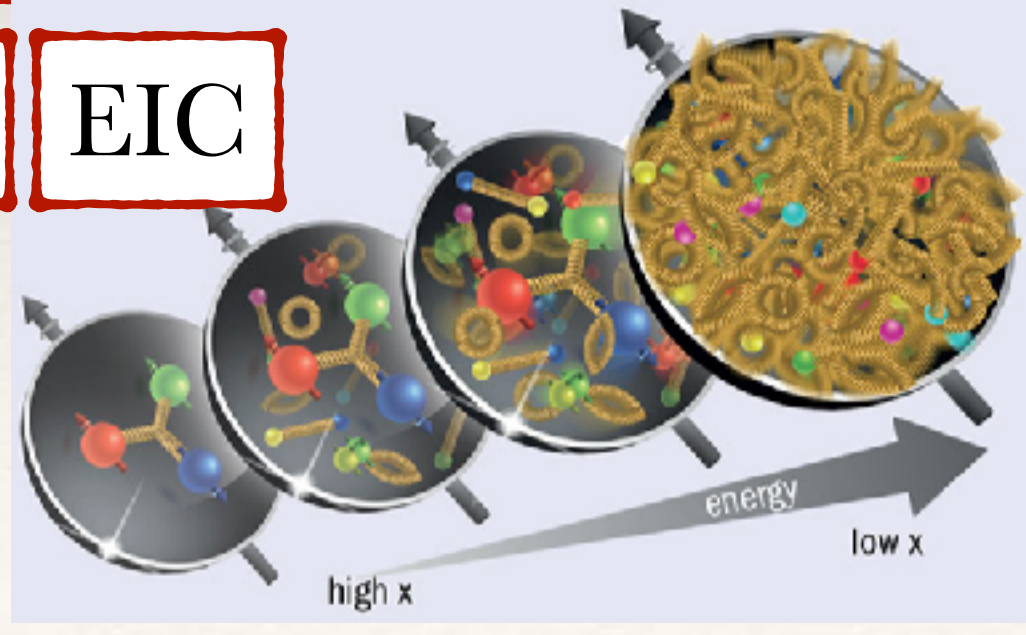
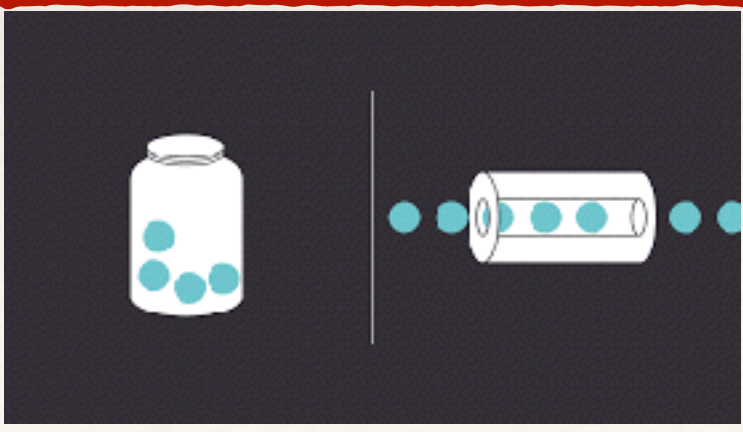
What are the properties of dense nuclear matter?

What are the properties of the proton?



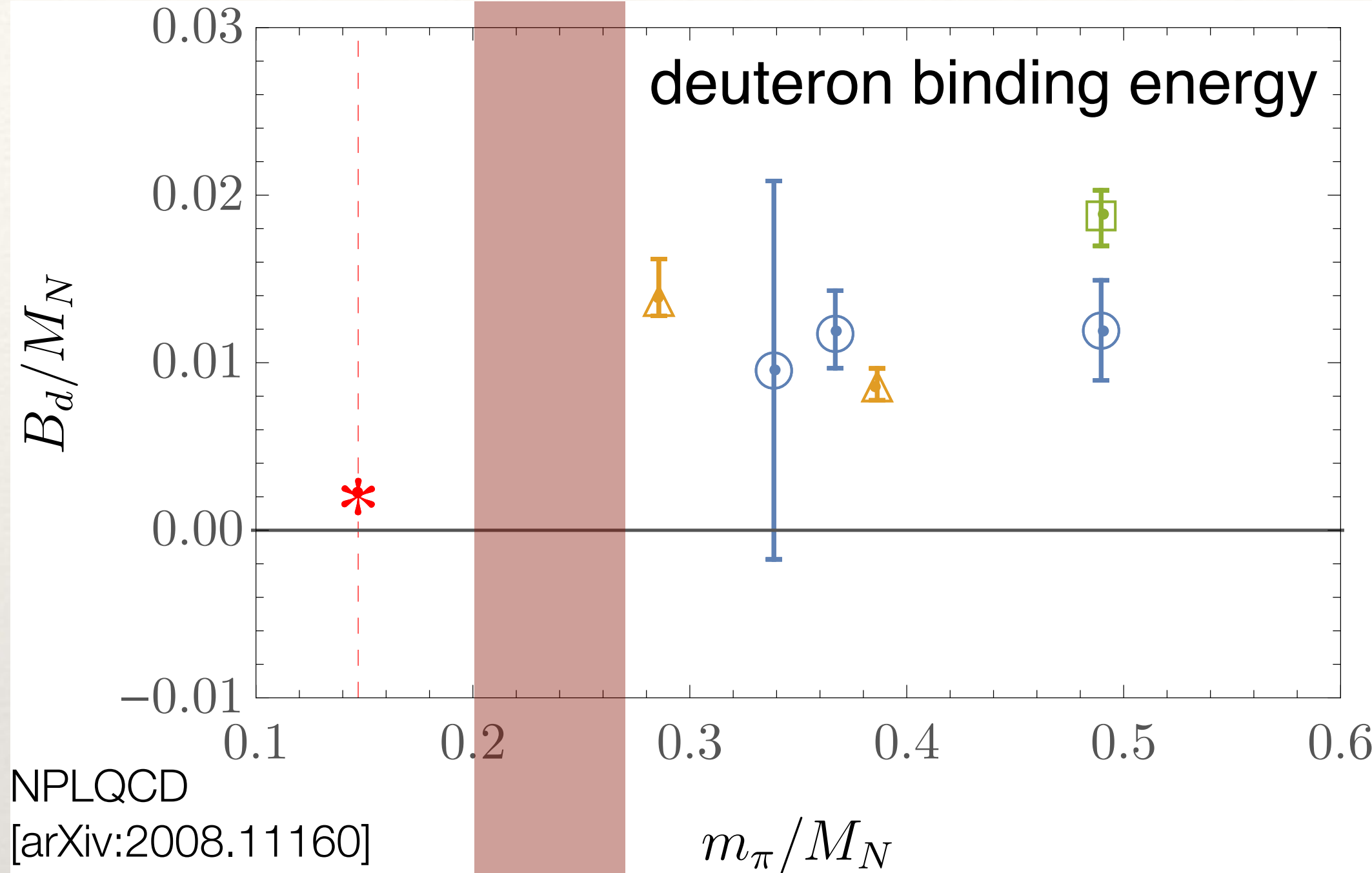
neutron lifetime

EIC





This seemingly simple problem has proved remarkably challenging to undertake



Estimated upper range of validity of NN EFT

**LQCD Results with (deeply) bound di-nucleons**

- 2006 NPLQCD - first dynamical LQCD calculations of NN
- 2011 NPLQCD  $M_\pi \approx 390$  MeV
- 2012 Yamazaki et al.  $M_\pi \approx 510$  MeV
- 2012 NPLQCD  $M_\pi \approx 800$  MeV
- 2015 Yamazaki et al.  $M_\pi \approx 310$  MeV
- 2015 CalLat  $M_\pi \approx 800$  MeV + P,D,F waves
- 2015 NPLQCD  $M_\pi \approx 450$  MeV
- 2020 NPLQCD  $M_\pi \approx 450$  MeV

**LQCD Results without bound di-nucleons (or inconclusive)**

- 2012 HAL QCD  $M_\pi \approx 710$  MeV
- 2012 HAL QCD  $M_\pi \approx 469 - 1171$  MeV
- 2019 "Mainz"  $M_\pi \approx 960$  MeV
- 2020 CoSMoN  $M_\pi \approx 714$  MeV
- 2021 NPLQCD  $M_\pi \approx 800$  MeV

(blue = work I was involved in)



# Challenges for NN calculations that are particularly difficult

- Exponential decay of signal with respect to the variance

- $\frac{S}{N}(t) \approx \frac{1}{\sqrt{N}} e^{-A(M_N - \frac{3}{2}m_\pi)t}$

- Physics of interest (interaction energies) are at the per-mille level of the total energy  
Deuteron:  $B_D \approx 2.2$  MeV,  $E_{NN} \approx 2$  GeV

- The excited state energy gap is set by kinetic energy of nucleons, much smaller than the typical inelastic excited state energy

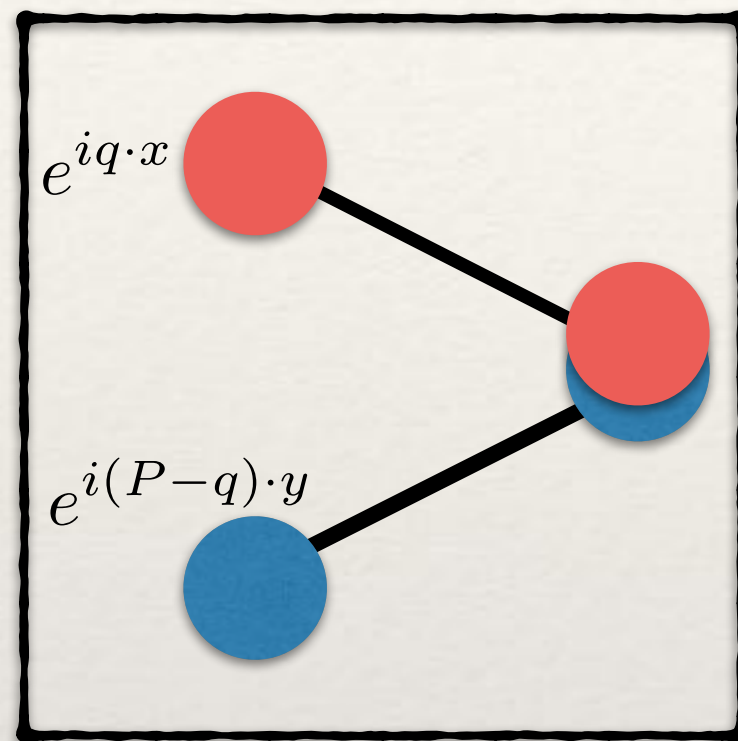
- pion production threshold becomes very close to  $2M_N$  at  $m_\pi^{\text{phys}}$

- short-time is polluted by excited states (as can be intermediate times) while late times are too noisy to resolve signals - and we must precisely determine a per-mille contribution to the total energy



To simplify the problems - work at  $m_u = m_d = m_s \approx m_s^{\text{phys}}$

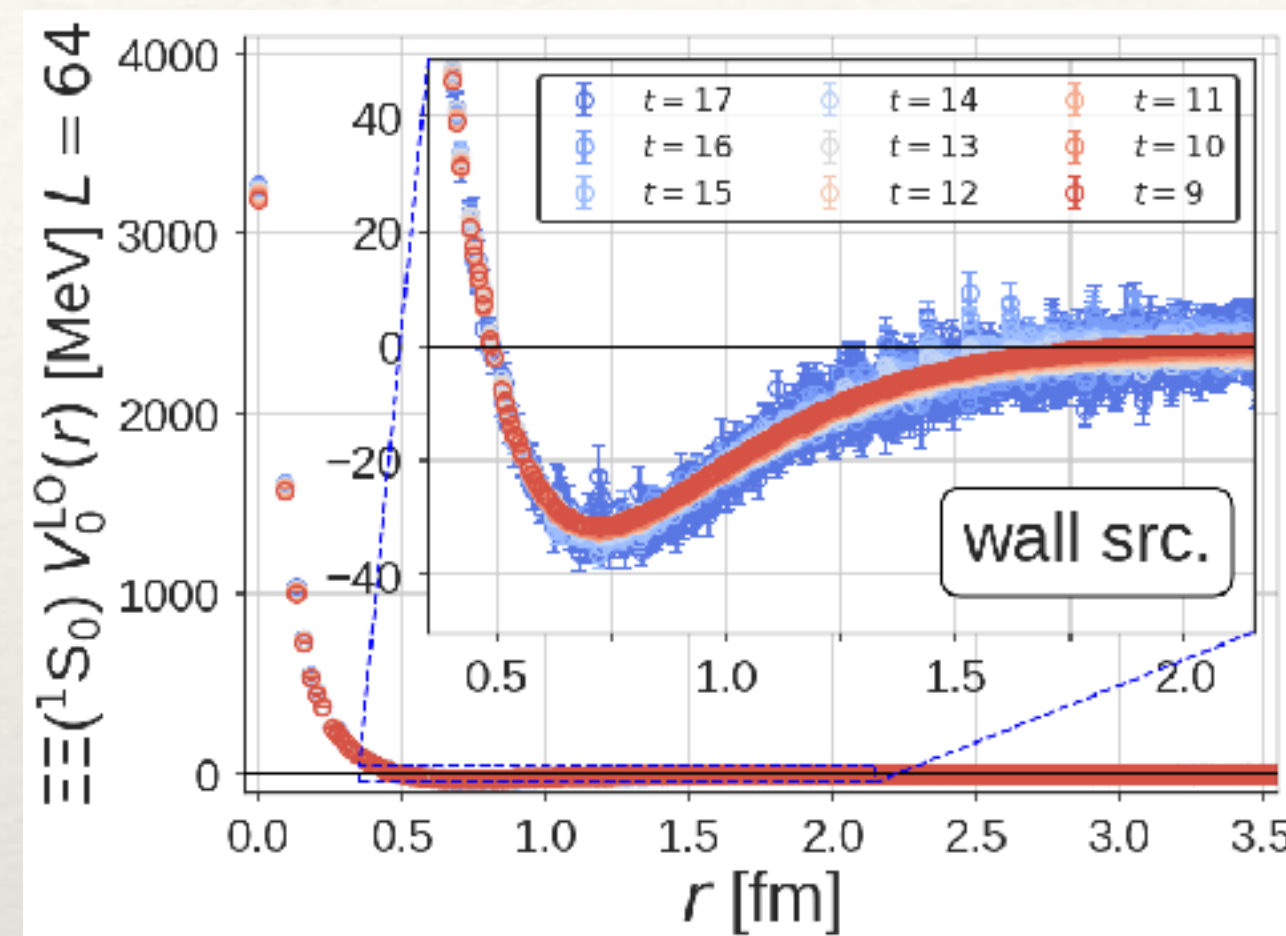
NPLQCD,  
Yamazaki et al.,  
CalLat (2015)



Compact, hexa-quark  
creation operator

Deep bound di-nucleons

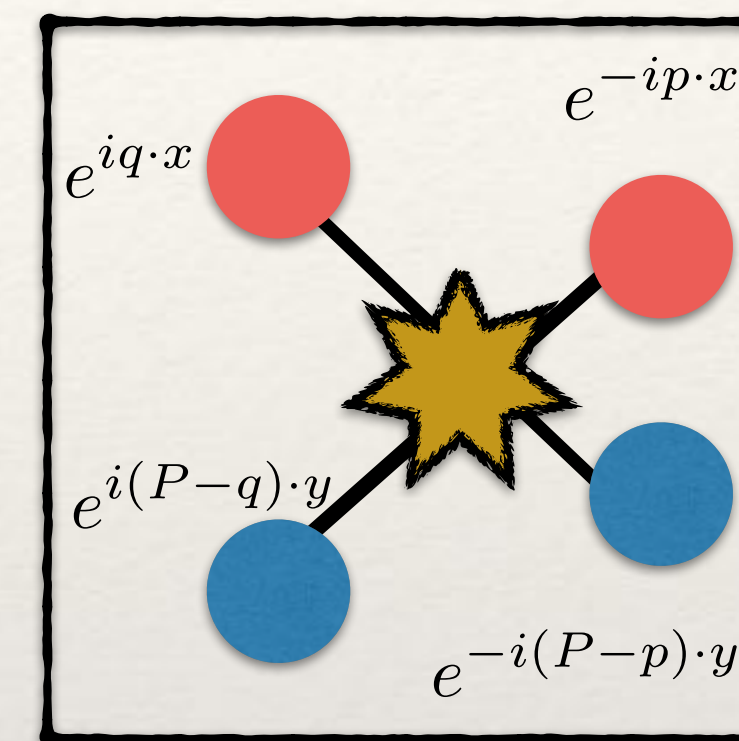
HAL QCD Potential



diffuse - wall source

no bound state

“Mainz” (Distillation)  
CoSMoN (stochastic LapH)  
NPLQCD (sparsened momentum)



momentum-space  
creation & annihilation  
positive-definite correlation matrix

no bound state



# To simplify the problems - work at $m_u = m_d = m_s \approx m_s^{\text{phys}}$

- ❑ So far, no study of all methods on the same ensemble (different actions, masses, lattice spacings...)
- ❑ difficult to draw conclusions
- ❑ especially given the recent “Mainz” results [Green, Hanlon, Junnarkar, Wittig, PRL 127 - 2103.01054]

- ❑ I will report on our (CoSMoN/BaSc) efforts to study most methods on a single ensemble

- ❑ sLapH

- ❑ hexa-quark

- ❑ displaced local source (CalLat)

- ❑ HAL QCD

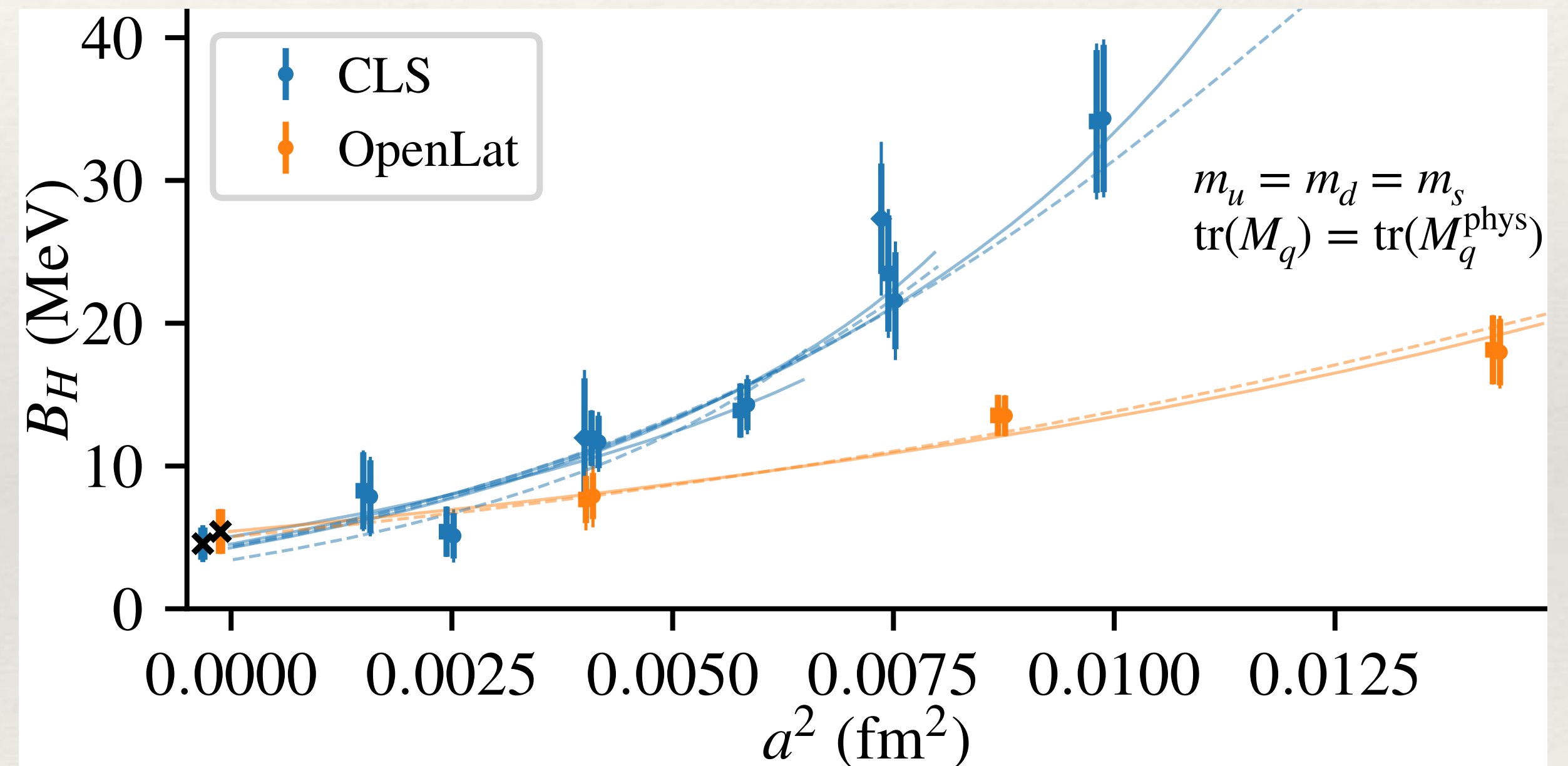


figure courtesy of J. Green



# Our Lattice Action

- We generated an ensemble with the CLS action  
Lüscher-Weisz gauge action, non-perturbative  $O(a)$  improved clover-Wilson fermions
- $m_u = m_d = m_s \approx m_s^{\text{phys}} \longrightarrow m_\pi \approx 714 \text{ MeV}$   
 $a \approx 0.086 \text{ fm}, V = 48^3 \times 96$
- The intent was to make a physical volume similar to that used by NPLQCD  
single stout-smear, tadpole improved, iso-clover fermion action  
@ SU(3) symmetric  $m_\pi \approx 806 \text{ MeV}$   
 $a \approx 0.145 \text{ fm}, V = 32^3 \times 48$



# stochastic Laplacian Heaviside (sLapH) Method

- “Distillation” — Peardon et al. PRD 80 (2009) [0905.2160]

quark propagator

$$\sum_i^N |\lambda_i\rangle\langle\lambda_i| \rho(t_0, x_0)$$

$|\lambda\rangle$  — eigenvectors of 3D gauge-covariant Laplacian  
 $\rho(t_0, x_0)$  — smeared quark-source

holding smearing fixed in physical units  $\rightarrow, N \propto L^3$

- “sLapH” — Morningstar et al. PRD 83 (2011) [1104.3870]

quark propagator

$$\sum_j^{N_\eta} |\eta_j\rangle\langle\eta_j| \sum_i^N |\lambda_i\rangle\langle\lambda_i| \rho(t_0, x_0)$$

introduce stochastic noise-basis between LapH space and quark lines

number of stochastic noises,  $N_\eta$ , is independent of volume

introduces more noise to correlation functions

adds some complexity/cost to constructing hadrons and contracting them



# stochastic Laplacian Heaviside (sLapH) Method

with either method — construct hadron interpolating fields in momentum space at the source as well as sink

- Expected levels for  $I = 0$ ,  $S = 0$ ,  $B = 2$ ,  $P = 0$ , and  $T_{1g}$  irrep
- Momentum squared in parentheses (units  $(2\pi/L)^2$ ) in particle content

$E/m_N$	Multiplicity	Particle Content
2.00000000	(1)	$N(0) N(0)$
2.03441931	(2)	$N(1) N(1)$
2.06826590	(3)	$N(2) N(2)$
2.10156746	(2)	$N(3) N(3)$
2.13434948	(2)	$N(4) N(4)$
2.16663555	(5)	$N(5) N(5)$
2.19844753	(5)	$N(6) N(6)$
2.26072895	(3)	$N(8) N(8)$
2.29123489	(5)	$N(9B) N(9B)$
2.29123489	(2)	$N(9A) N(9A)$
2.31017370	(2)	$\Delta(0) \Delta(0)$
2.32133997	(5)	$N(10) N(10)$
2.34003514	(5)	$\Delta(1) \Delta(1)$

- Expected levels for  $I = 1$ ,  $S = 0$ ,  $B = 2$ ,  $P = 0$ , and  $A_{1g}$  irrep
- Momentum squared in parentheses (units  $(2\pi/L)^2$ ) in particle content

$E/m_N$	Multiplicity	Particle Content
2.00000000	(1)	$N(0) N(0)$
2.03441931	(1)	$N(1) N(1)$
2.06826590	(1)	$N(2) N(2)$
2.10156746	(1)	$N(3) N(3)$
2.13434948	(1)	$N(4) N(4)$
2.16663555	(1)	$N(5) N(5)$
2.18722722	(1)	$N(1) \Delta(1)$
2.19844753	(1)	$N(6) N(6)$
2.21889309	(2)	$N(2) \Delta(2)$
2.25010523	(1)	$N(3) \Delta(3)$
2.26072895	(1)	$N(8) N(8)$
2.28088292	(1)	$N(4) \Delta(4)$
2.29123489	(1)	$N(9B) N(9B)$
2.29123489	(1)	$N(9A) N(9A)$
2.31017370	(1)	$\Delta(0) \Delta(0)$

tables courtesy of C. Morningstar

at this pion mass ( $m_\pi \approx 714$  MeV), pion-production is heavier still!



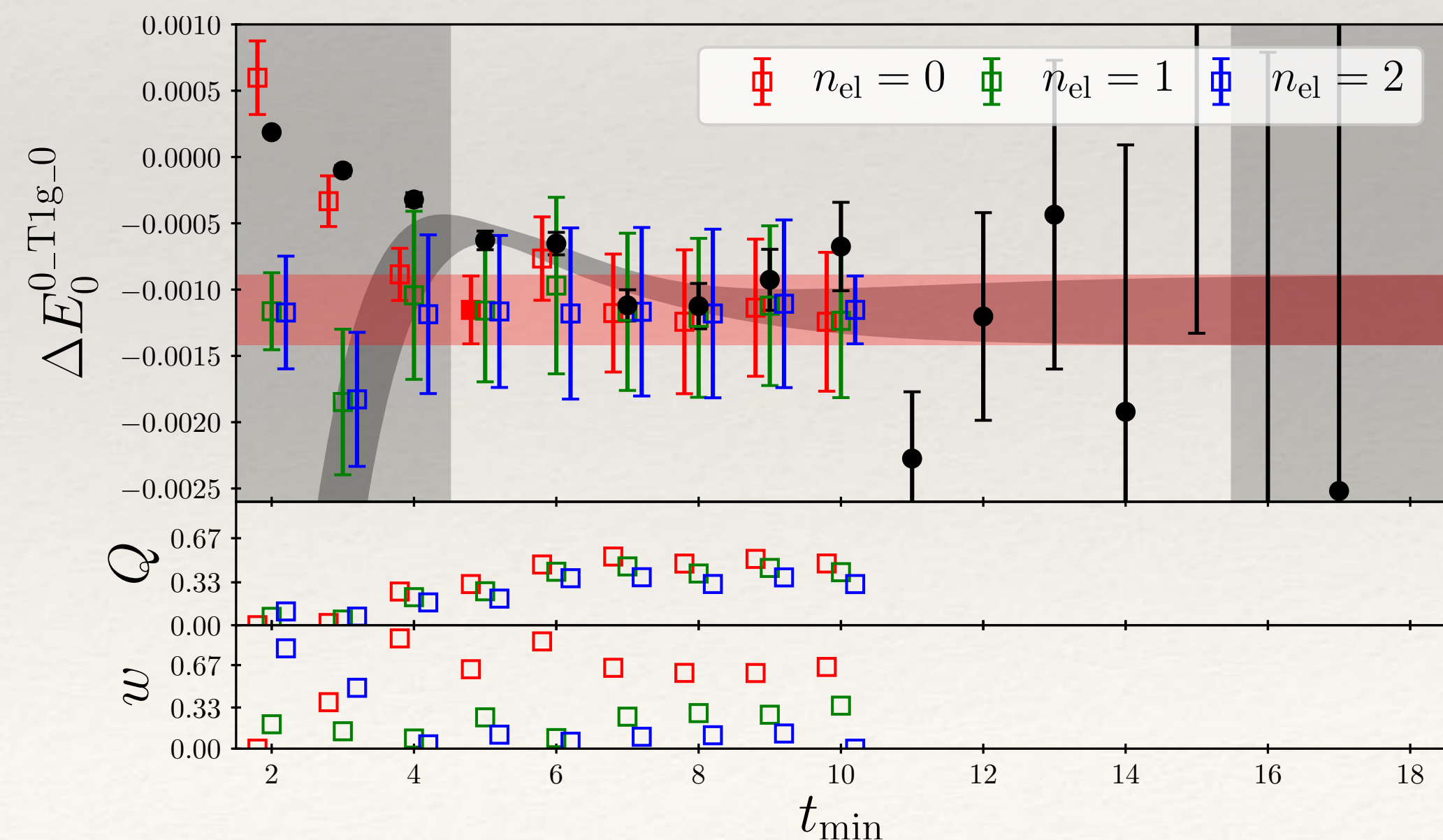
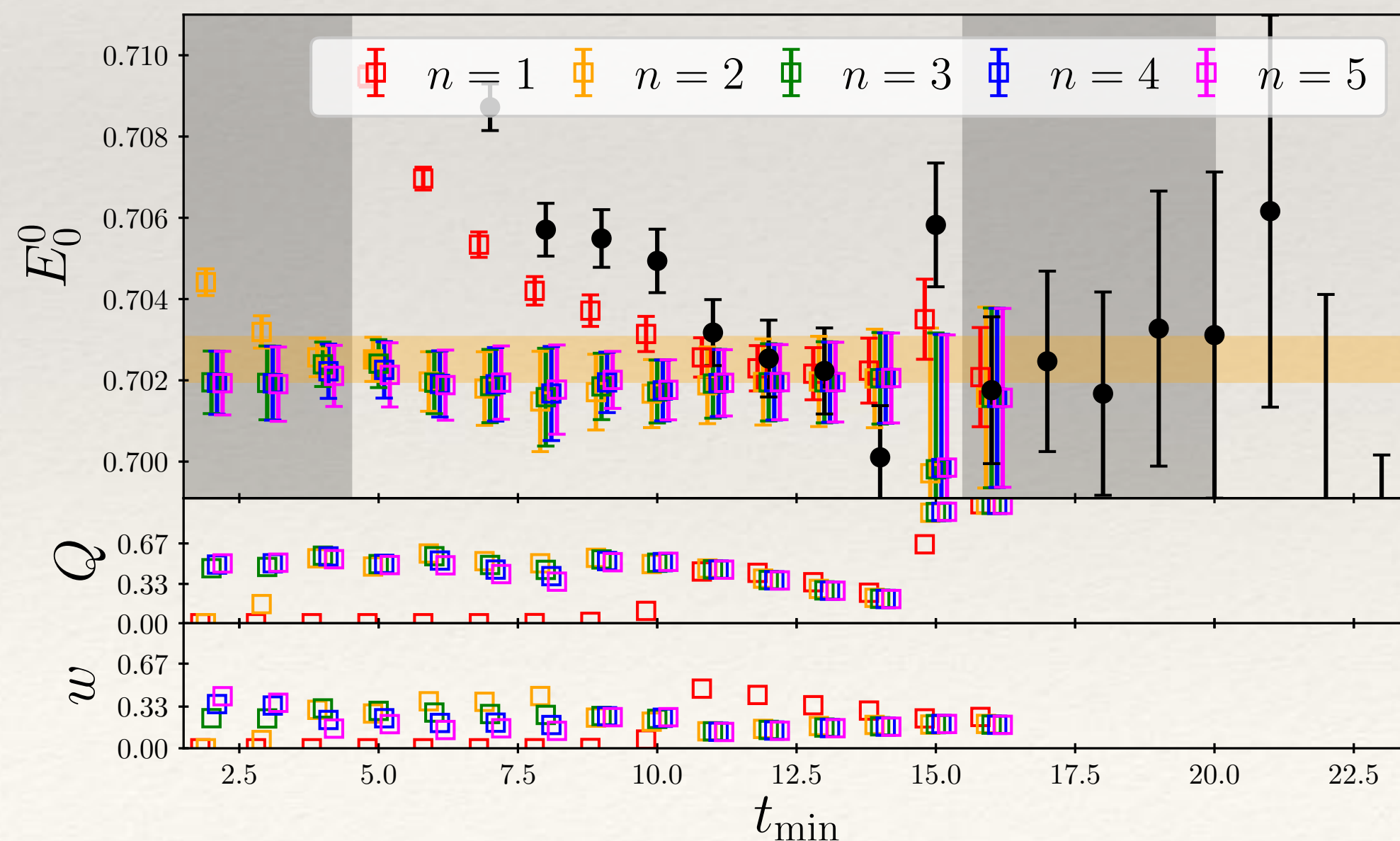
# our results circa 2020 [2009.11825]

- 2 streams of 401 configurations each  
4 time-sources per configuration  
forward propagating correlators only
- Our results are not precise enough to  
fit NN and N separately  
— we have to rely upon fitting the ratio  
correlator

$$C_N(t, p) = A_0(p)e^{-E_0(p)t} \left[ 1 + \sum_{n=1}^N r_n e^{-\Delta E_n(p)t} \right]$$

$$R_{NN}(t) = B_0 e^{-\Delta E_0^{NN} t} \frac{1 + \sum_{n=1}^N r_n^{NN} e^{-\Delta E_n^{NN} t}}{(1 + \sum_p r_p e^{-\Delta E_p t})(1 + \sum_q r_q e^{-\Delta E_q t})}$$

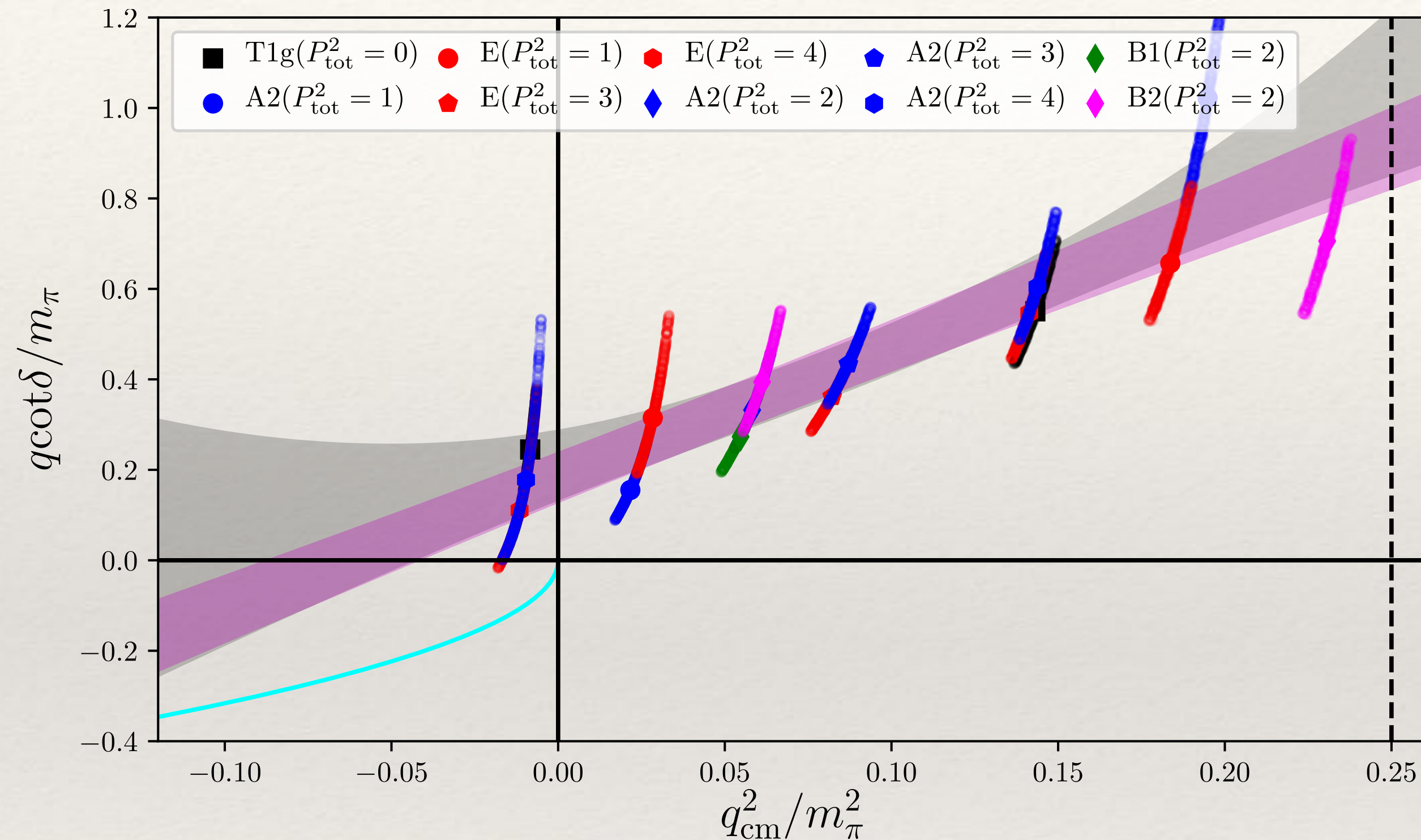
$$N_n = 1, \quad N_{nn}^{\text{inel}} = 1$$





# our results circa 2020 [2009.11825]

- 16 energy levels with (expected) negligible overlap with non S-wave



- We find a virtual bound state (like dineutron) - a purely imaginary solution with negative sign

$$\frac{q_-^{\text{deut}}}{m_\pi} = -i0.132(32)$$

- We can infer the size of the potential from causality and unitarity: Wigner PRD 98 (1955), Phillips and Cohen PLB 390 (1997)

$$r_0 \leq 2 \left[ R - \frac{R^2}{a} + \frac{R^3}{3a^2} \right], \quad m_\pi R \gtrsim 2.0, \quad R \gtrsim 0.55 \text{ fm}$$



# Updates since 2009.11825

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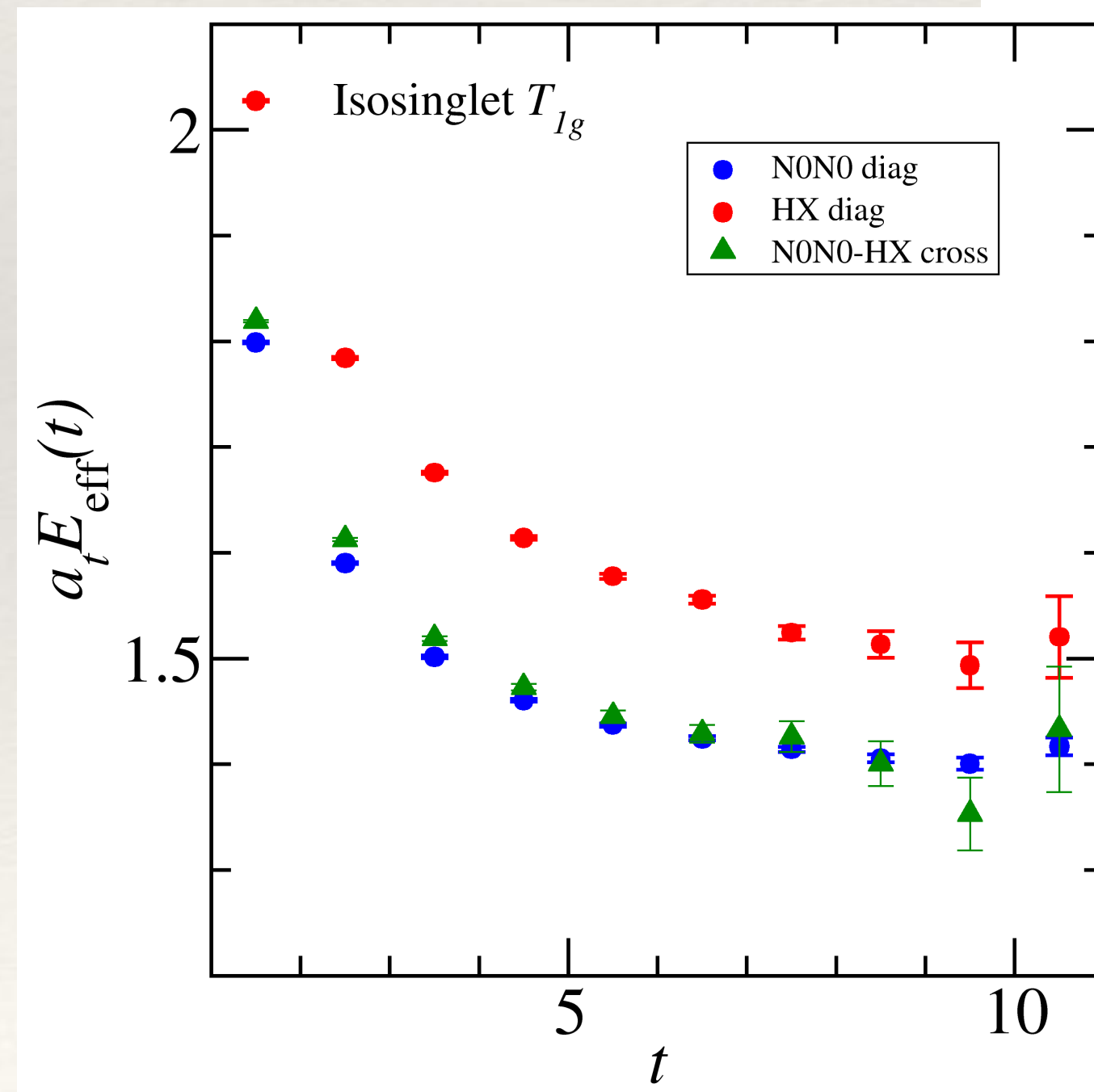
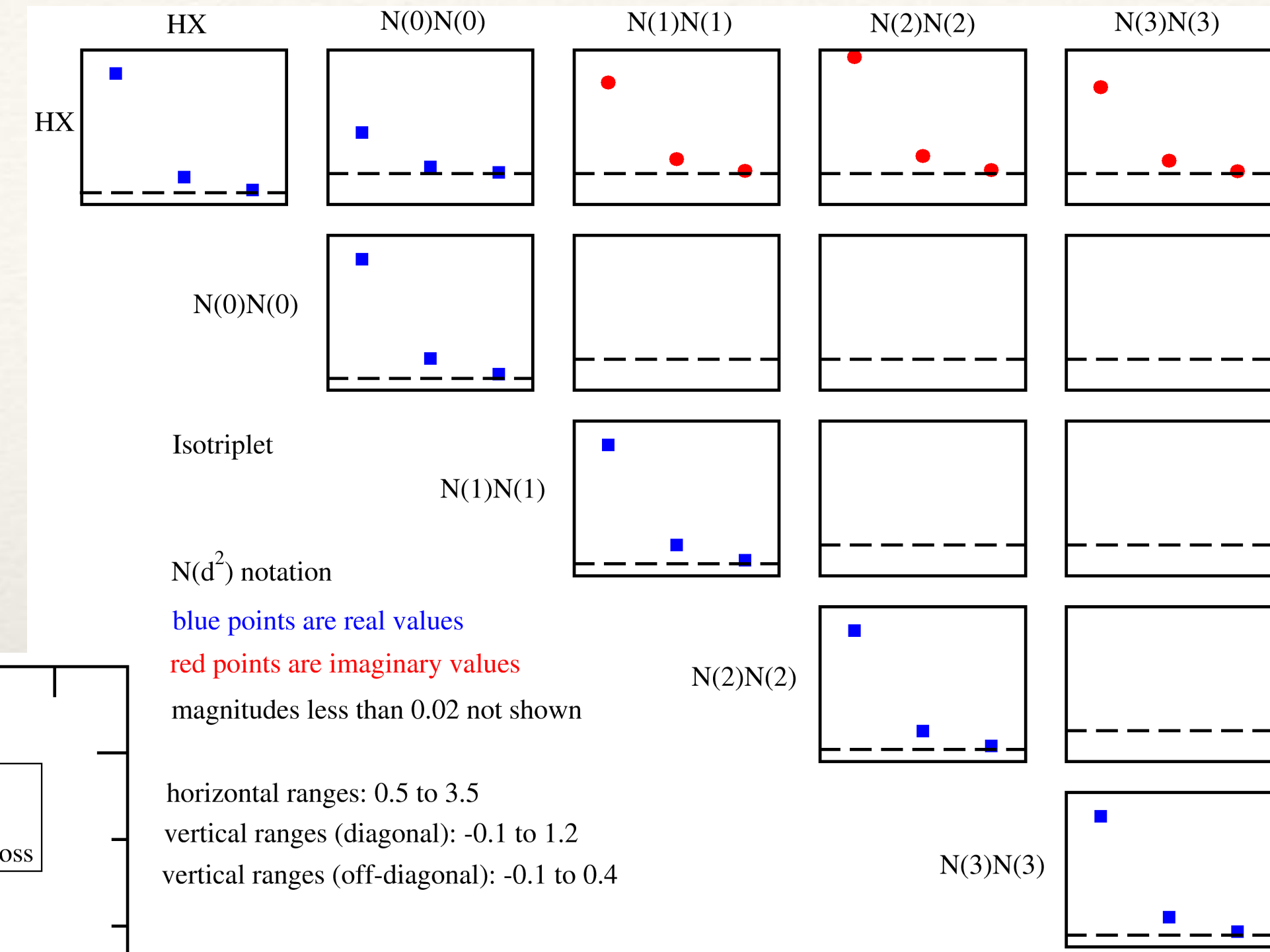
- ❑ Our goal is to compare and contrast (nearly) all methods in the literature on a single ensemble
  - ❑ add hexaquark interpolator to the basis
  - ❑ compare with p-sink / hexaquark source off-diagonal only (NPLQCD, Yamazaki et al, CalLat)
  - ❑ compare with p-sink / displaced NN source off-diagonal (CalLat)
  - ❑ increase statistics of sLapH method
  - ❑ compare with HAL QCD potential



# Updates since 2009.11825 — add hexaquark to basis

(thanks to C. Morningstar and S. Skinner)

- hexaquark (HX) operator has more excited state contamination and is noisier than the  $N(0)N(0)$  correlator
- The off-diagonal  $N(0)N(0)$  — HX correlator has similar behavior to diagonal  $N(0)N(0)$  correlator
- This is in contrast to what NPLQCD/CalLat find
  - lattice action
  - quark smearing





# Updates since 2009.11825 — add hexaquark to basis

(thanks to C. Morningstar and S. Skinner)

- hexaquark (HX) operator strongly overlaps with highest state in the spectrum (top left)
- $N(p)N(p)$  operators mostly overlap onto a single state, with some mixing (except with highest state)



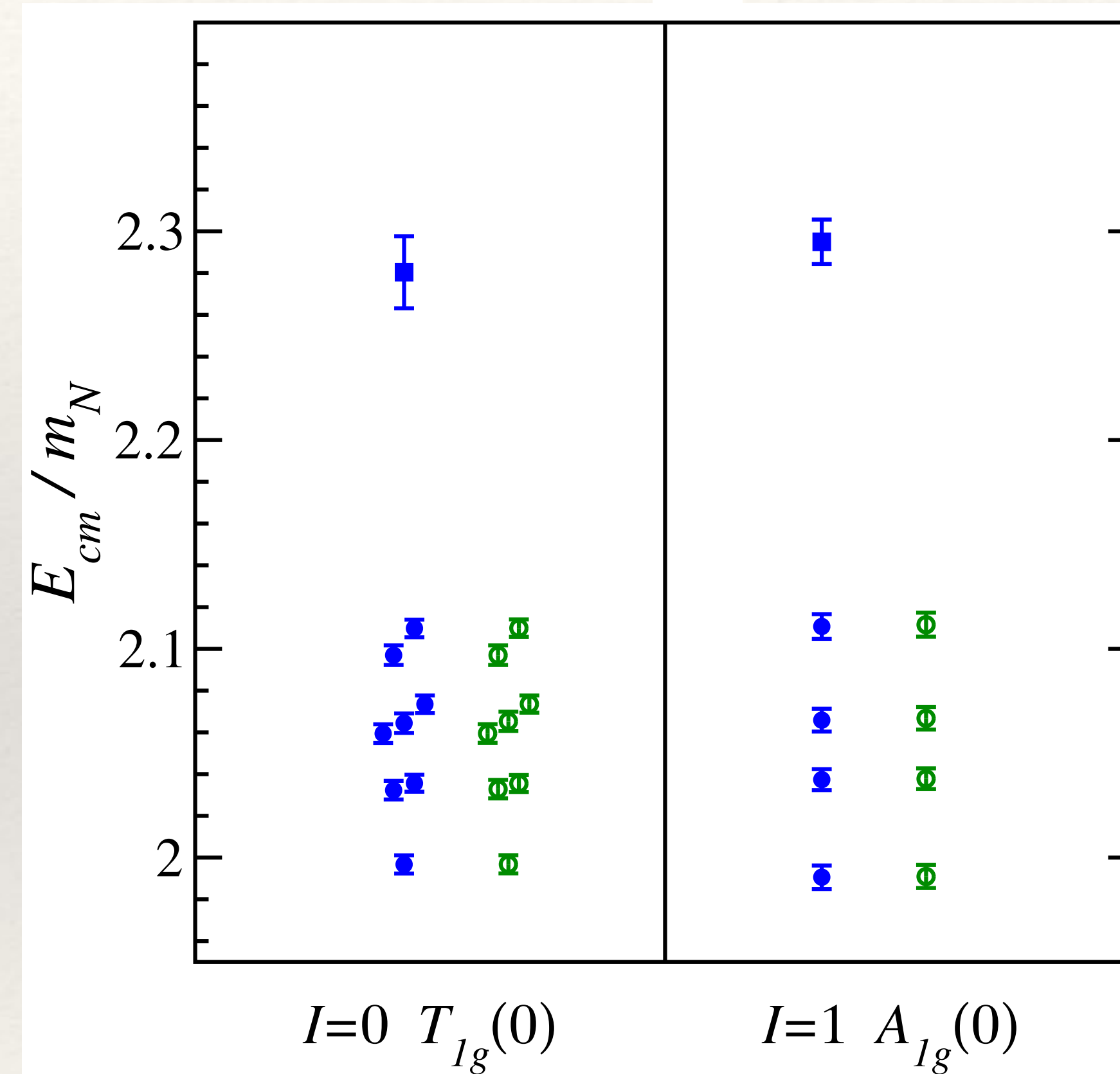
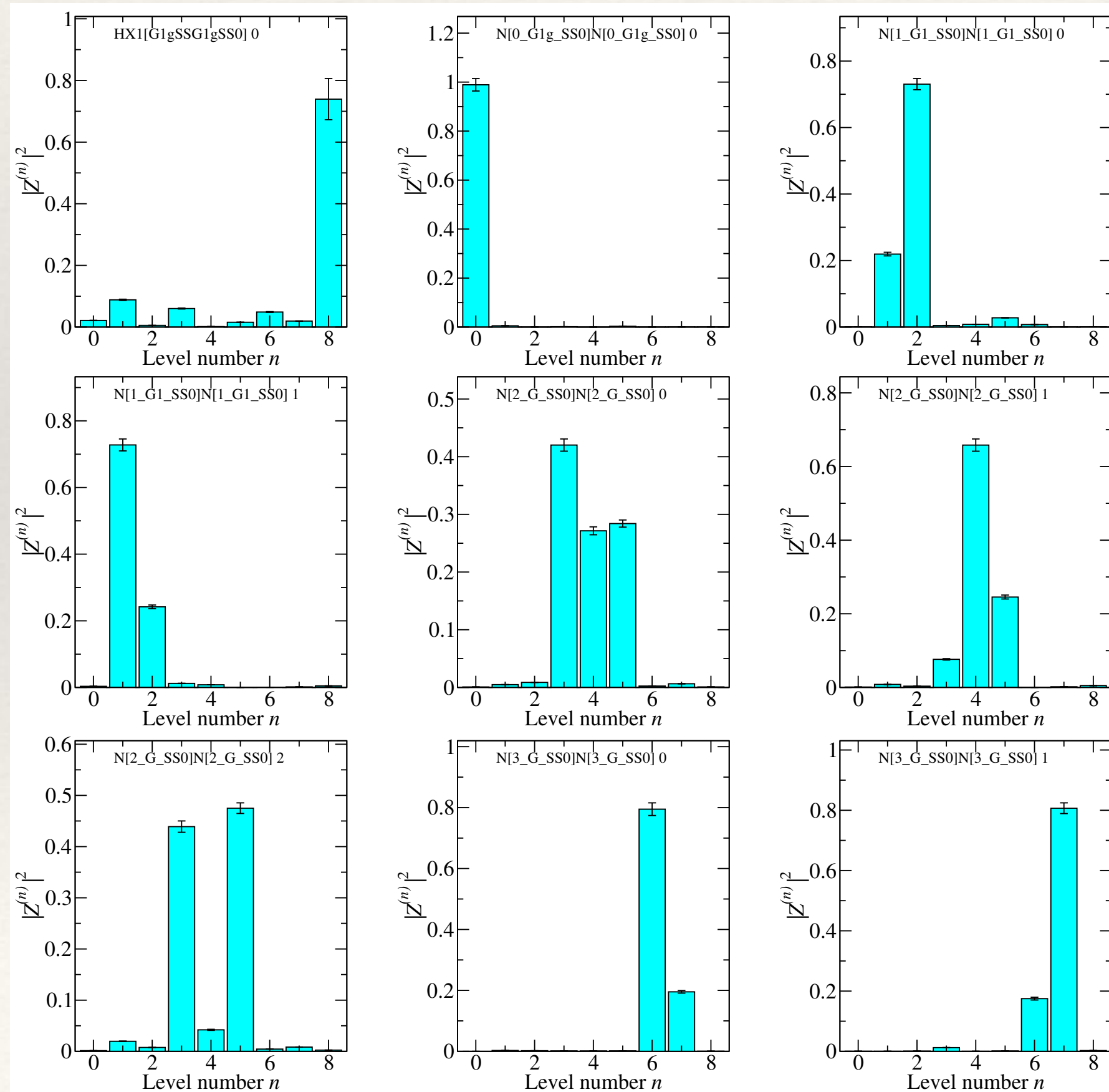
E w/out HX



E with HX



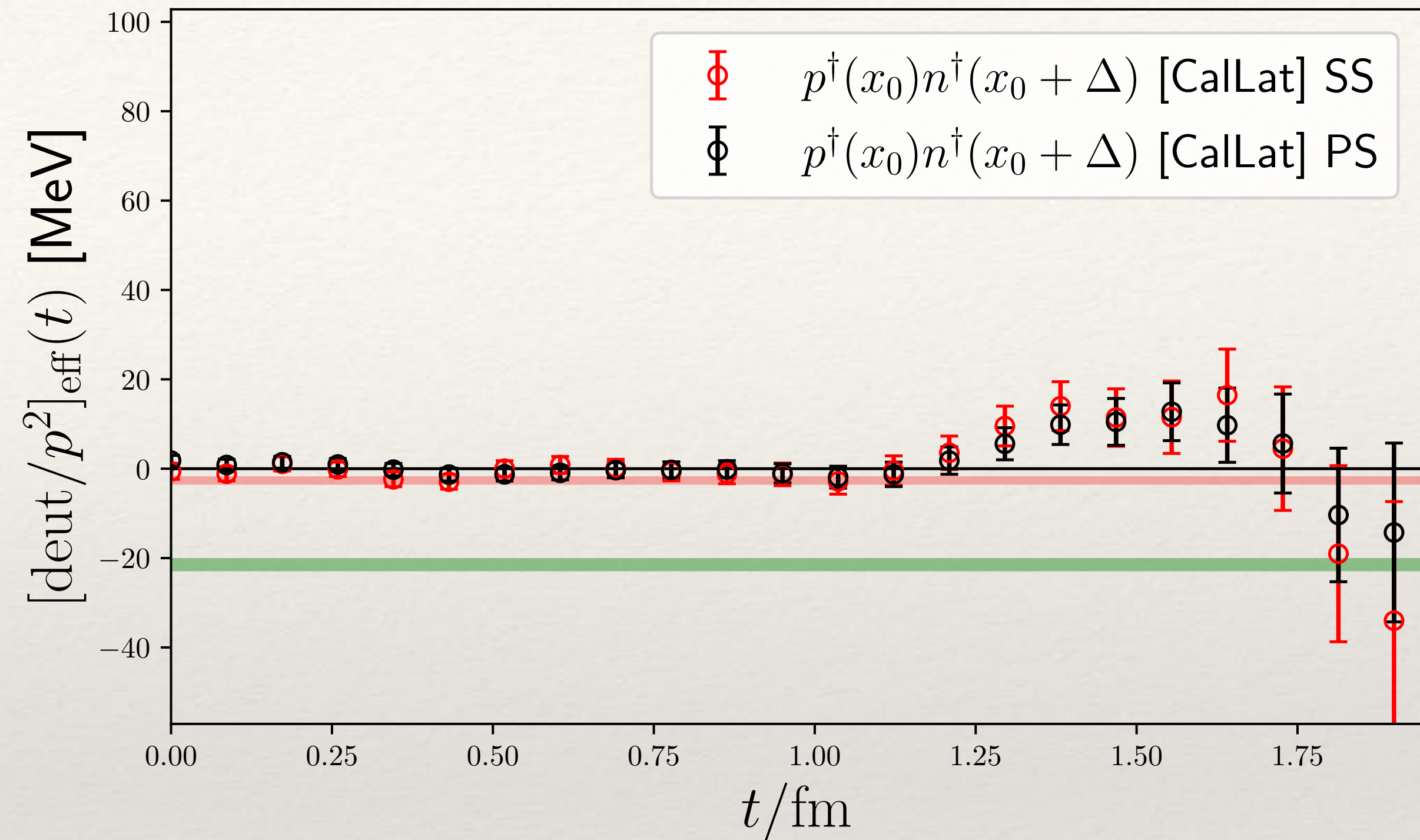
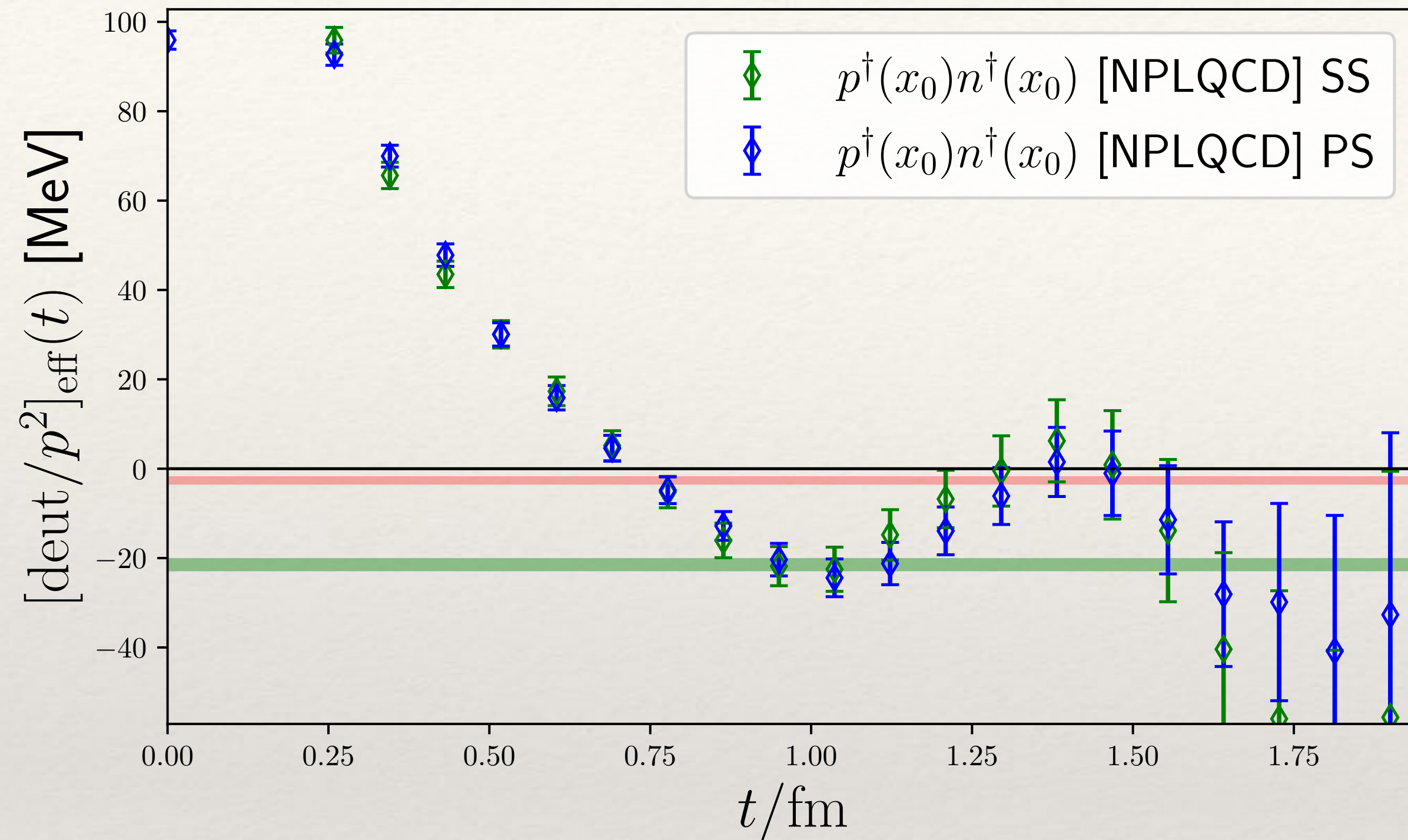
HX dominated state

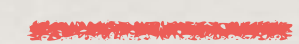



- we find the HX operator is NOT needed to determine the low-lying NN spectrum



# Updates since 2009.11825 — compare with local/displaced NN source



 sLapH g.s. energy in  $T_{1g}$  from 2009.11825

 NPLQCD (2012, 2017) / CalLat (2015) g.s. energy from local NN creation operator

- pulling  $p^\dagger(x_0)n^\dagger(x_0 + \Delta)$  apart at creation leads to significantly different excited state contamination
- extracting stable  $\Delta E$  is challenging
- local  $p^\dagger(x_0)n^\dagger(x_0)$  strongly couples to NN-inelastic states that are unique to NN (not N on its own) e.g.  $\Delta\Delta$



# Updates since 2009.11825 — increased statistics with sLapH

---

- ❑ 2 streams of 401 configurations each  
4 time-sources per configuration
- ❑ 4 streams, 1490 total configs  
8 time-sources per configuration
- ❑ Additionally, introduce more sophisticated “conspiracy” fit model
- ❑ It is observed that the excited states strongly cancel in the ratio correlator, suggesting a “conspiracy” of cancellation between most excited states in the numerator and denominator
- ❑ Build a fit function that mimics this observation



# Updates since 2009.11825 — “conspiracy” model

- Assume a good approximation for NN correlator is from the product of the individual nucleon correlators

$$C_{NN}(t) \approx C_{N_1}(t)C_{N_2}(t)$$

$$C_{NN}(t) \approx A_0^1 e^{-E_0^1 t} \left[ 1 + \sum_{n=1}^{N_1-1} r_n^1 e^{-\Delta E_n^1 t} \right] A_0^2 e^{-E_0^2 t} \left[ 1 + \sum_{n=1}^{N_2-1} r_n^2 e^{-\Delta E_n^2 t} \right]$$

- For simplicity - consider using a single excited state for the individual nucleons then, we can construct a fit function for NN with 2 excited states:

$$C_{NN}(t) = B_{00} e^{-(2E_0 + \Delta E_{00})t} + B_{01} e^{-(E_0 + E_1 + \delta E_{10})t} + B_{11} e^{-(2E_1 + \delta E_{11})t}$$

and similar for more excited states



# Updates since 2009.11825 — “conspiracy” model

- Assume a good approximation for NN correlator is from the product of the individual nucleon correlators

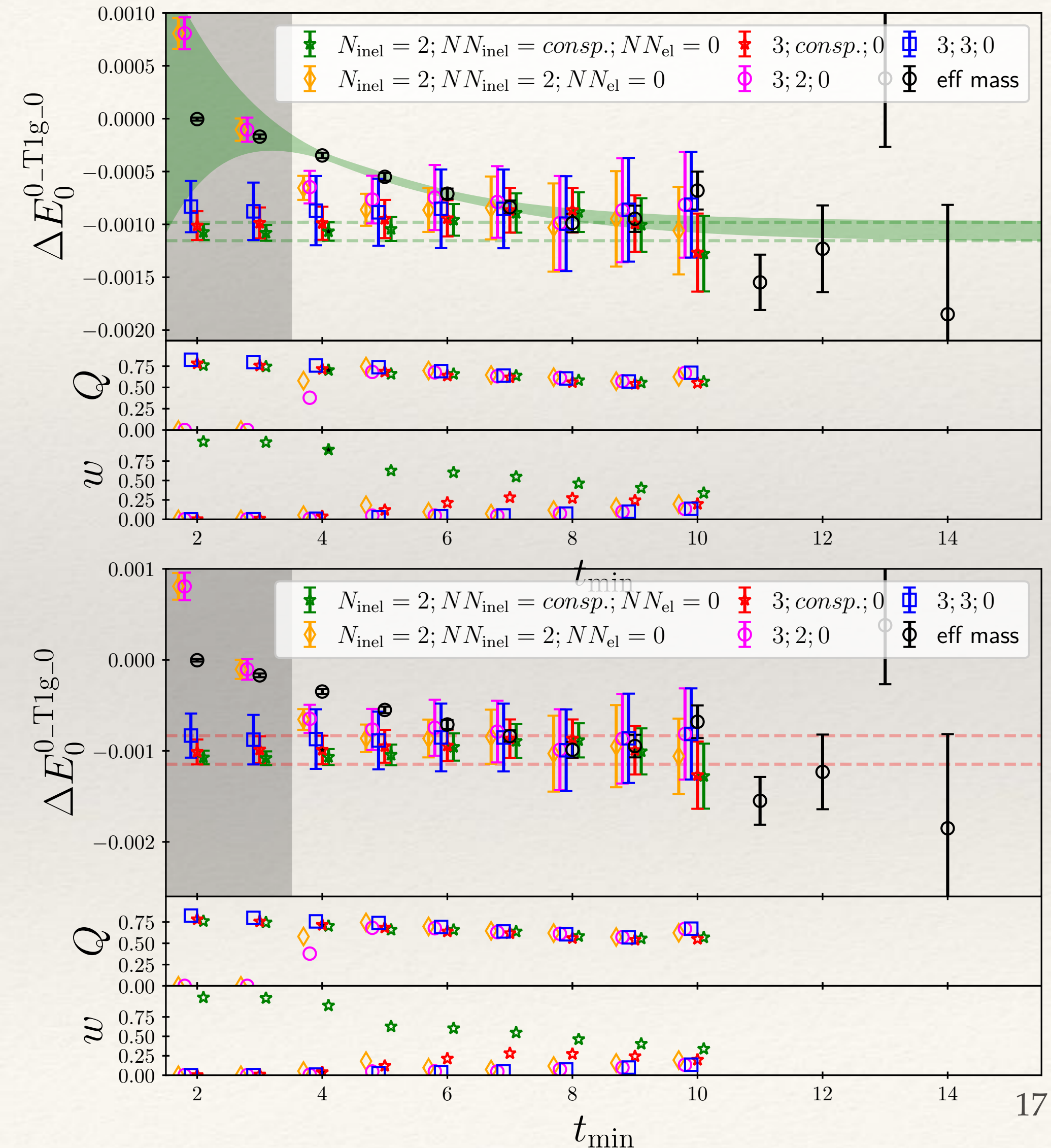
$$C_{NN}(t) \approx C_{N_1}(t)C_{N_2}(t)$$

$$C_{NN}(t) \approx A_0^1 e^{-E_0^1 t} \left[ 1 + \sum_{n=1}^{N_1-1} r_n^1 e^{-\Delta E_n^1 t} \right] A_0^2 e^{-E_0^2 t} \left[ 1 + \sum_{n=1}^{N_2-1} r_n^2 e^{-\Delta E_n^2 t} \right]$$

- For simplicity - consider using a single excited state for the individual nucleons then, we can construct a fit function for NN with 2 excited states:

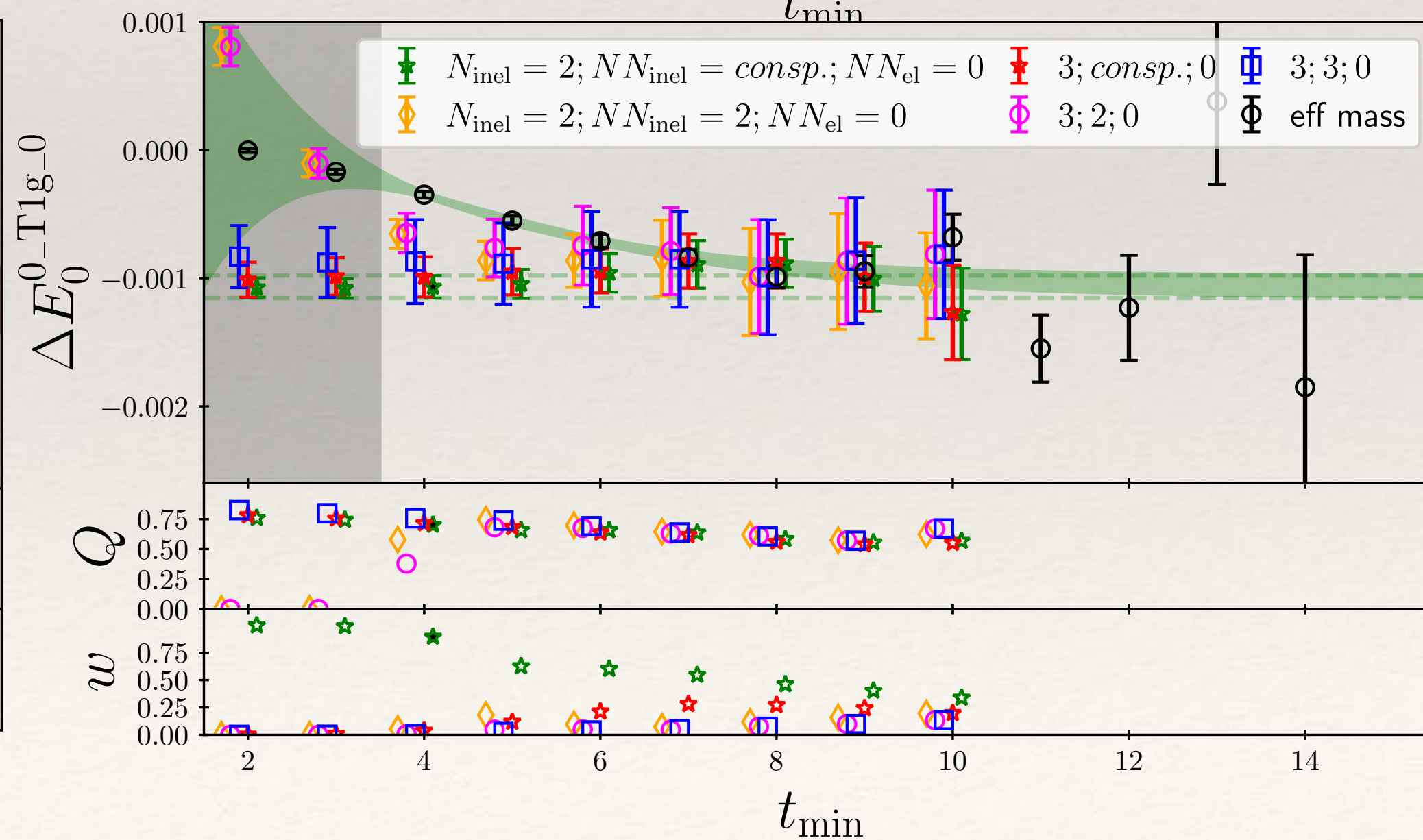
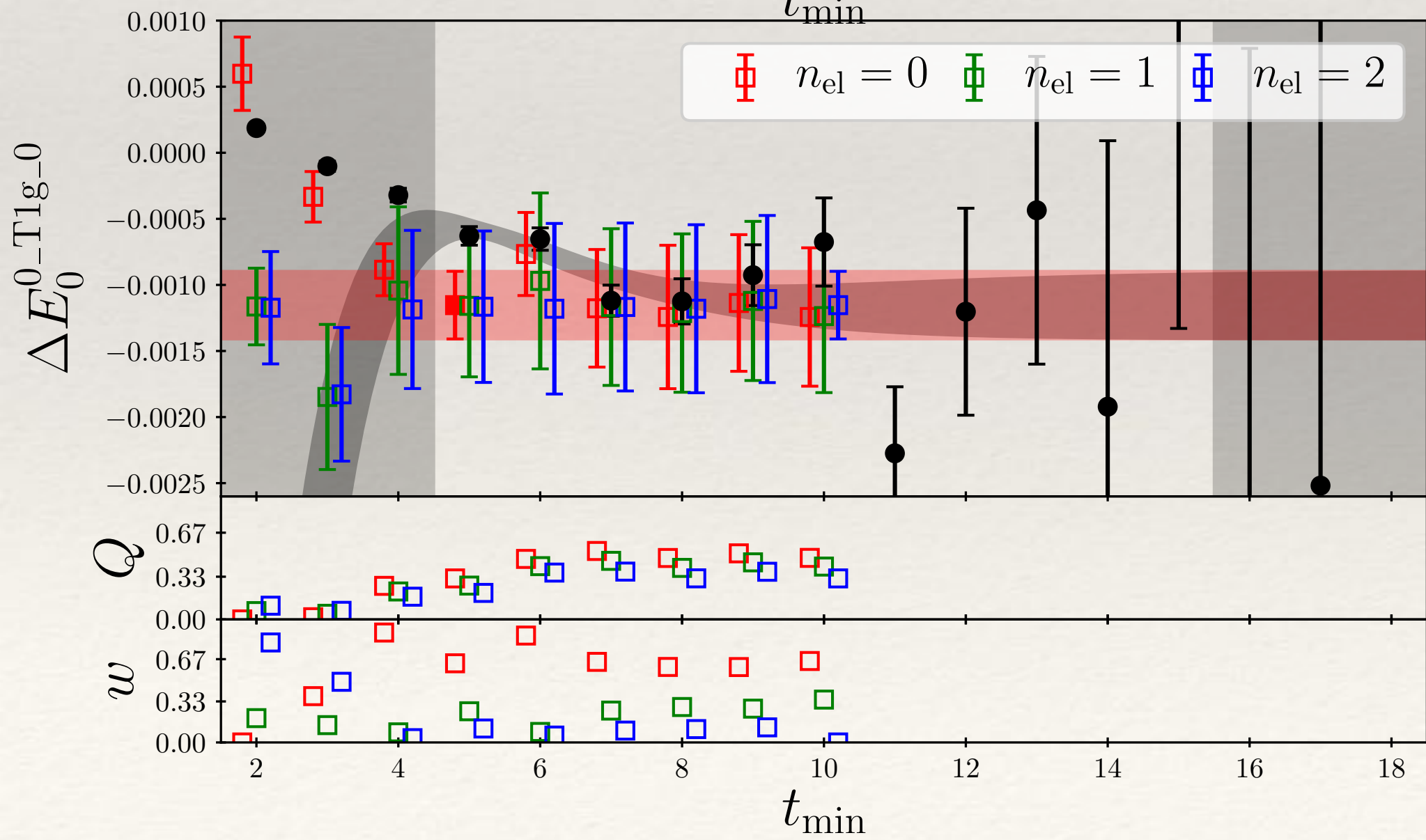
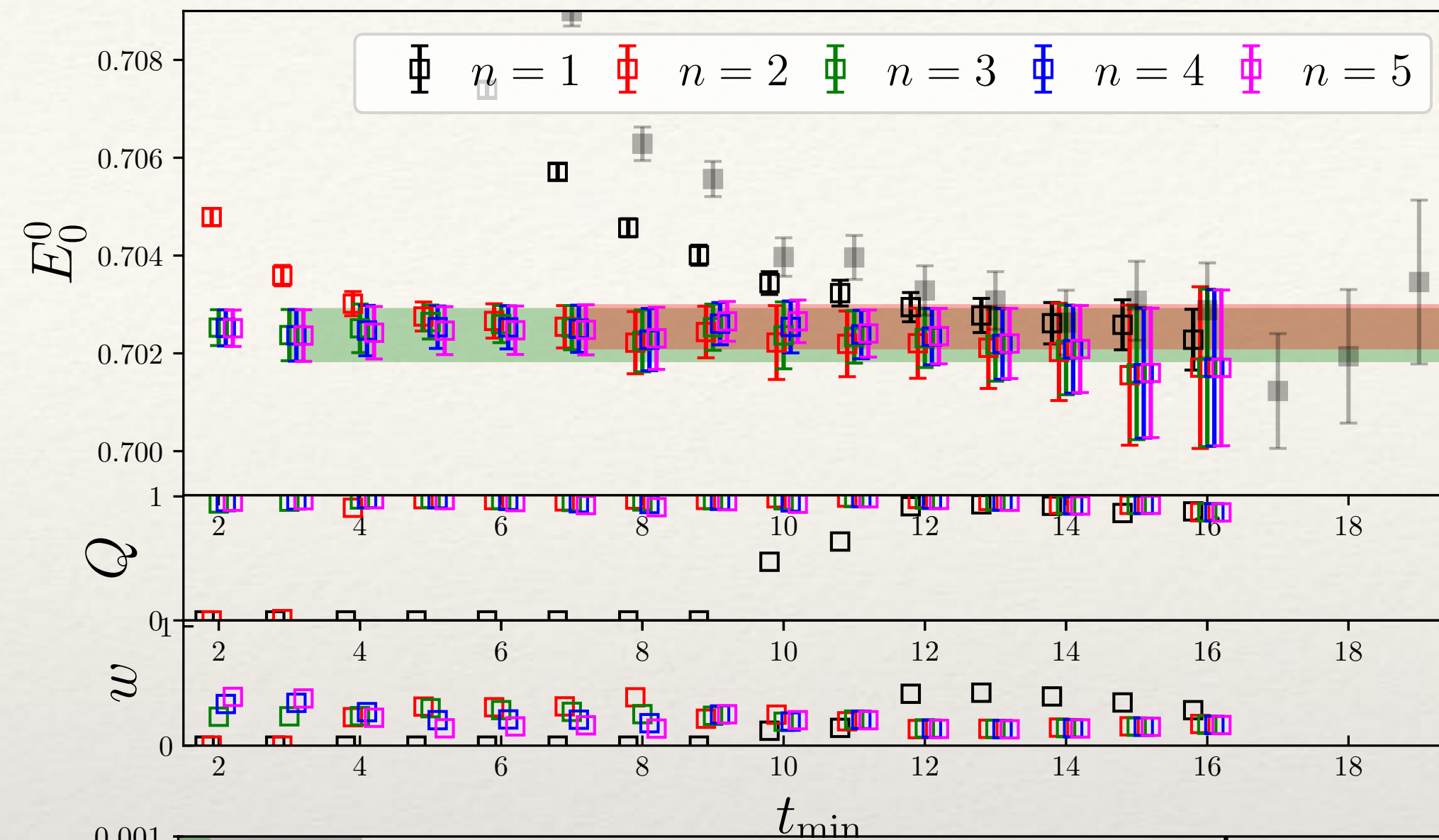
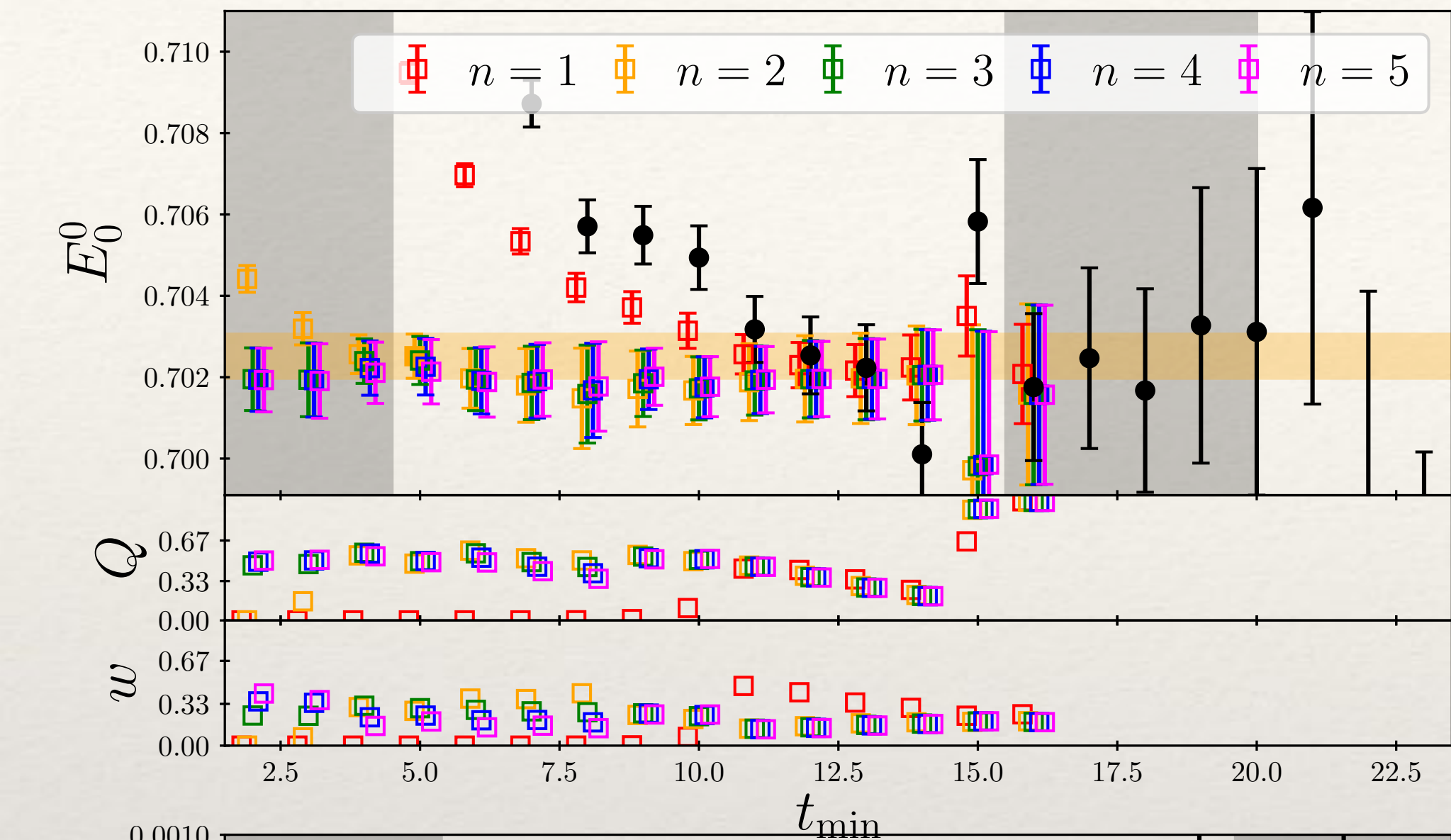
$$C_{NN}(t) = B_{00} e^{-(2E_0 + \Delta E_{00})t} + B_{01} e^{-(E_0 + E_1 + \delta E_{10})t} + B_{11} e^{-(2E_1 + \delta E_{11})t}$$

and similar for more excited states





# Updates since 2009.11825 — “conspiracy” model



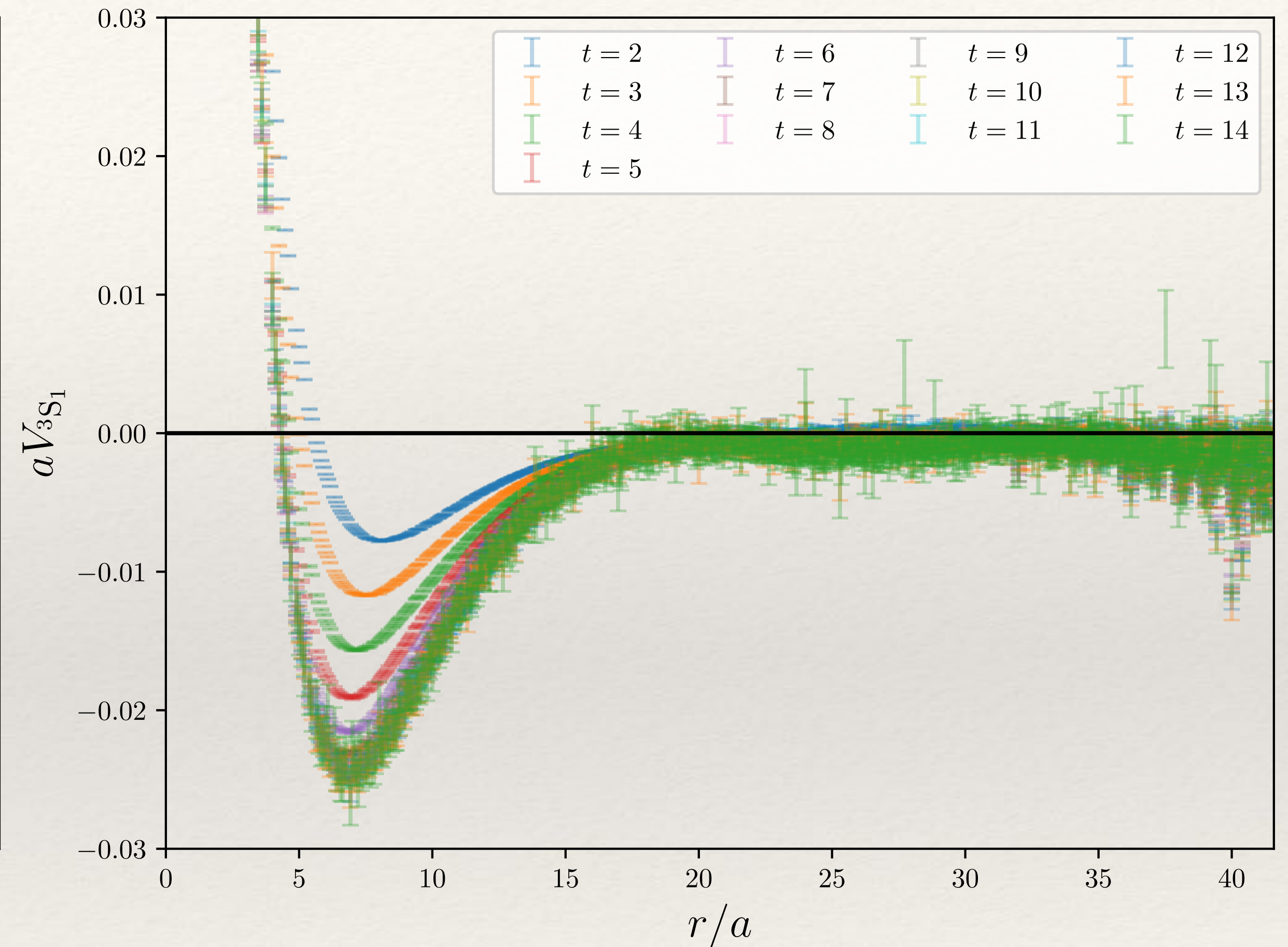
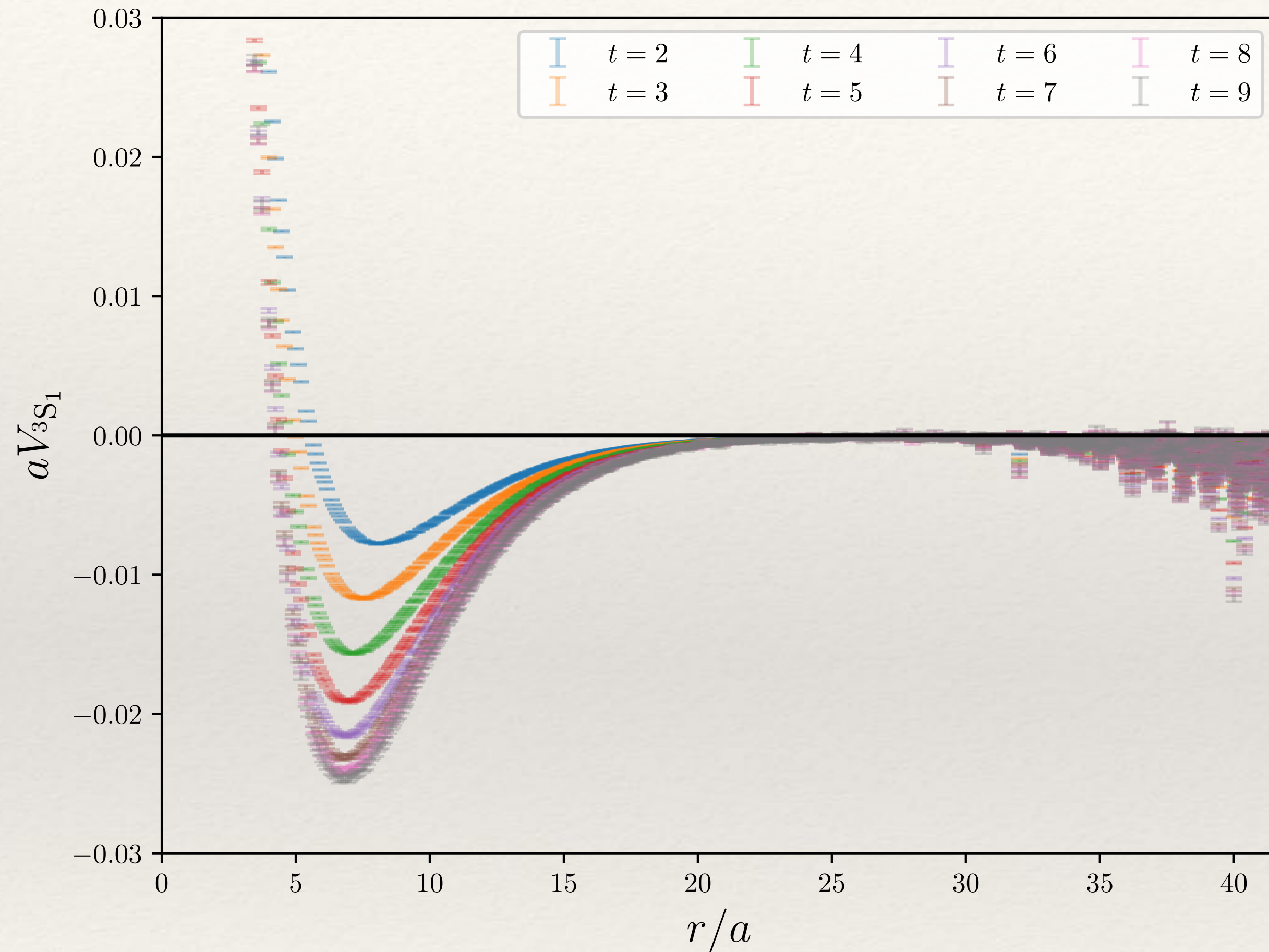
one (or more) bugs in my phase shift analysis prevent me from showing you the updated phase shift plot





# Updates since 2009.11825 — HAL QCD potential

(thanks to C. Körber, A. Meyer, A. Nicholson)

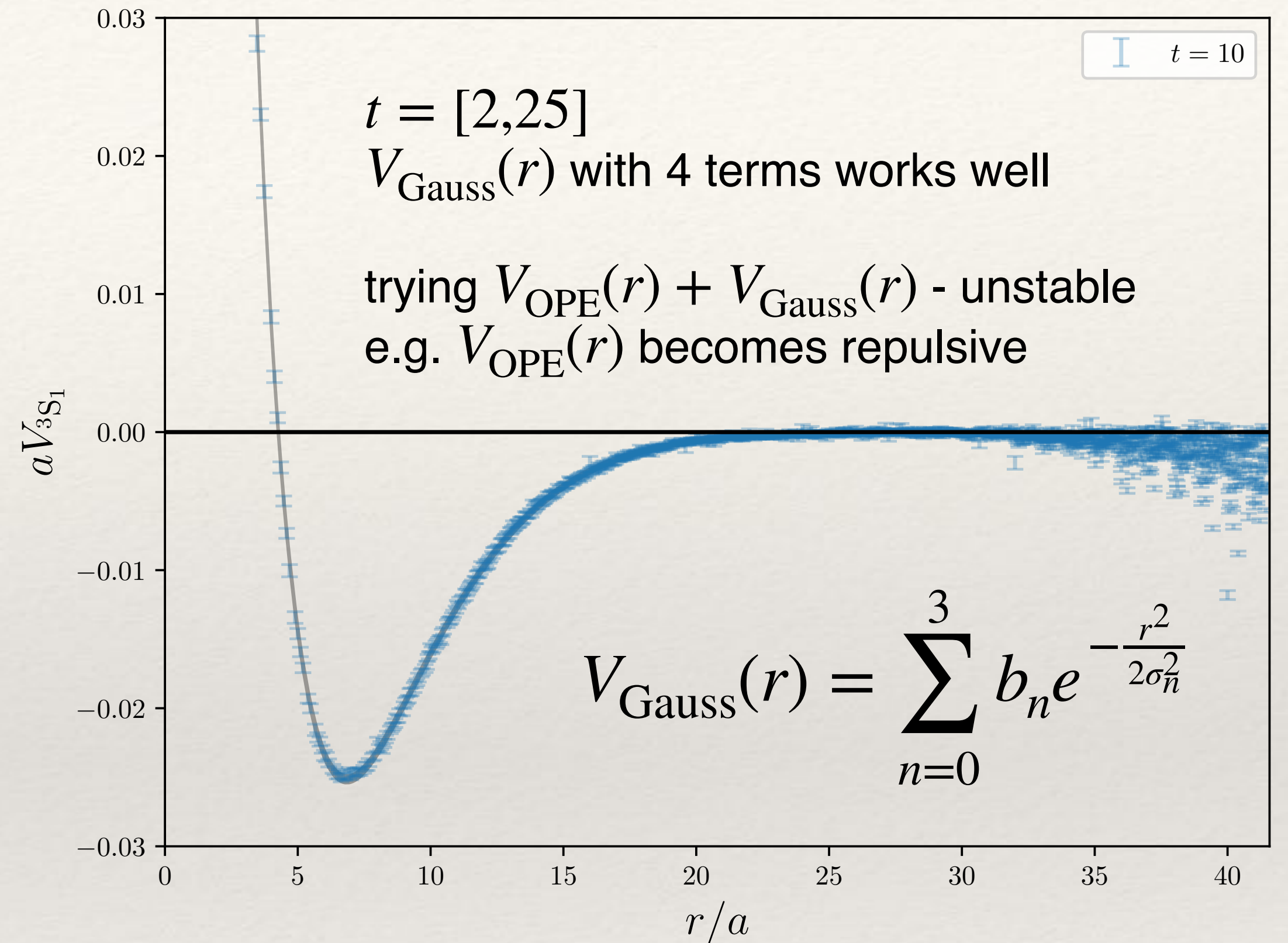
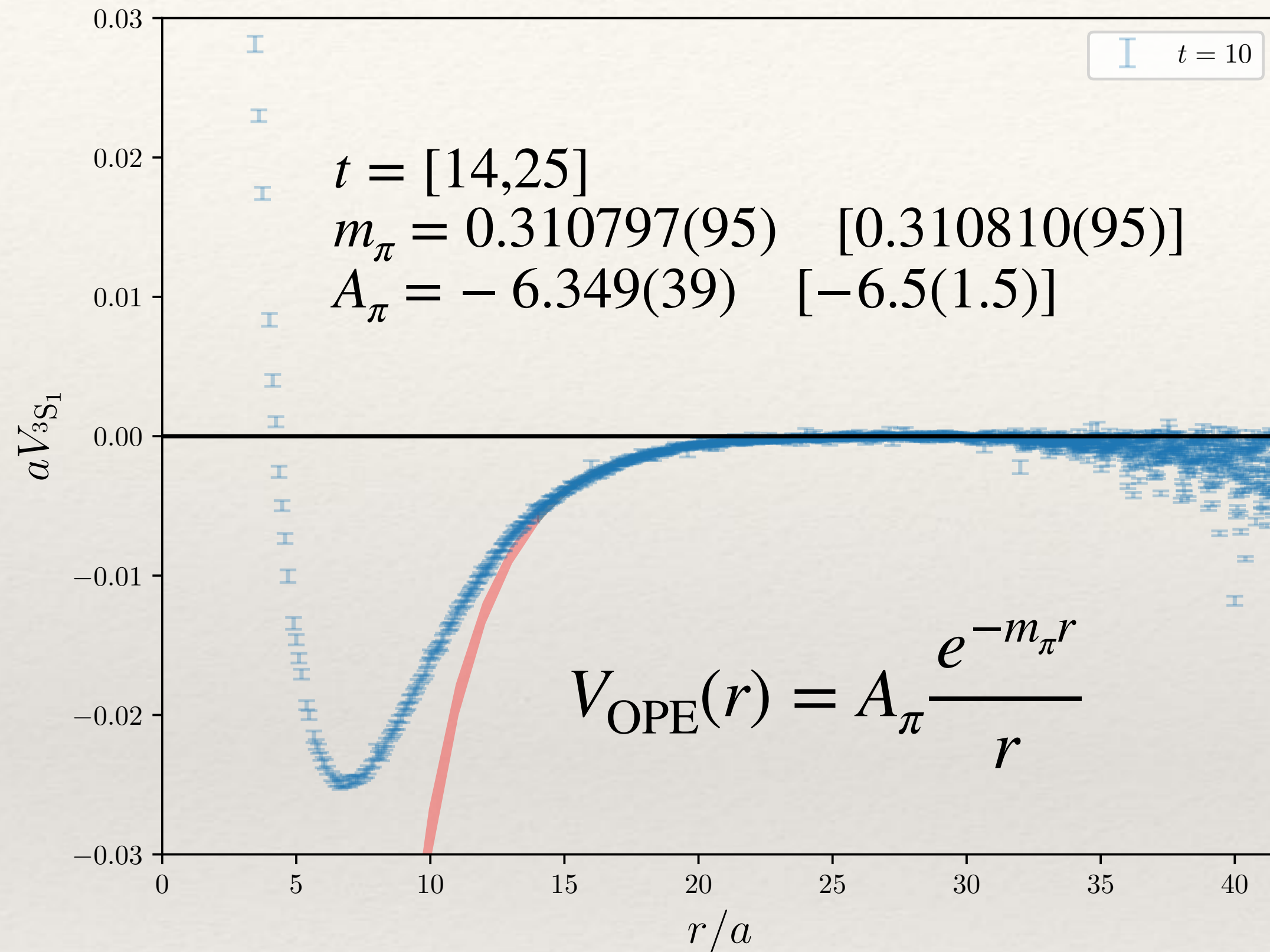


□  $m_u = m_d = m_s \approx m_s^{\text{phys}} \longrightarrow m_\pi \approx 714 \text{ MeV}$   
 $a \approx 0.086 \text{ fm}, V = 48^3 \times 96$



# Updates since 2009.11825 — HAL QCD potential

(thanks to C. Körber, A. Meyer, A. Nicholson)



□ Motivation for finding stable analytic form of the potential

□ We want to study the temporal dependence of the parameters of the potential, to see if there is some monotonic behavior that can be modeled, and used to fit  $V(t, r)$  for all  $t$  and extrapolate to  $t \rightarrow \infty$

□ Work in progress

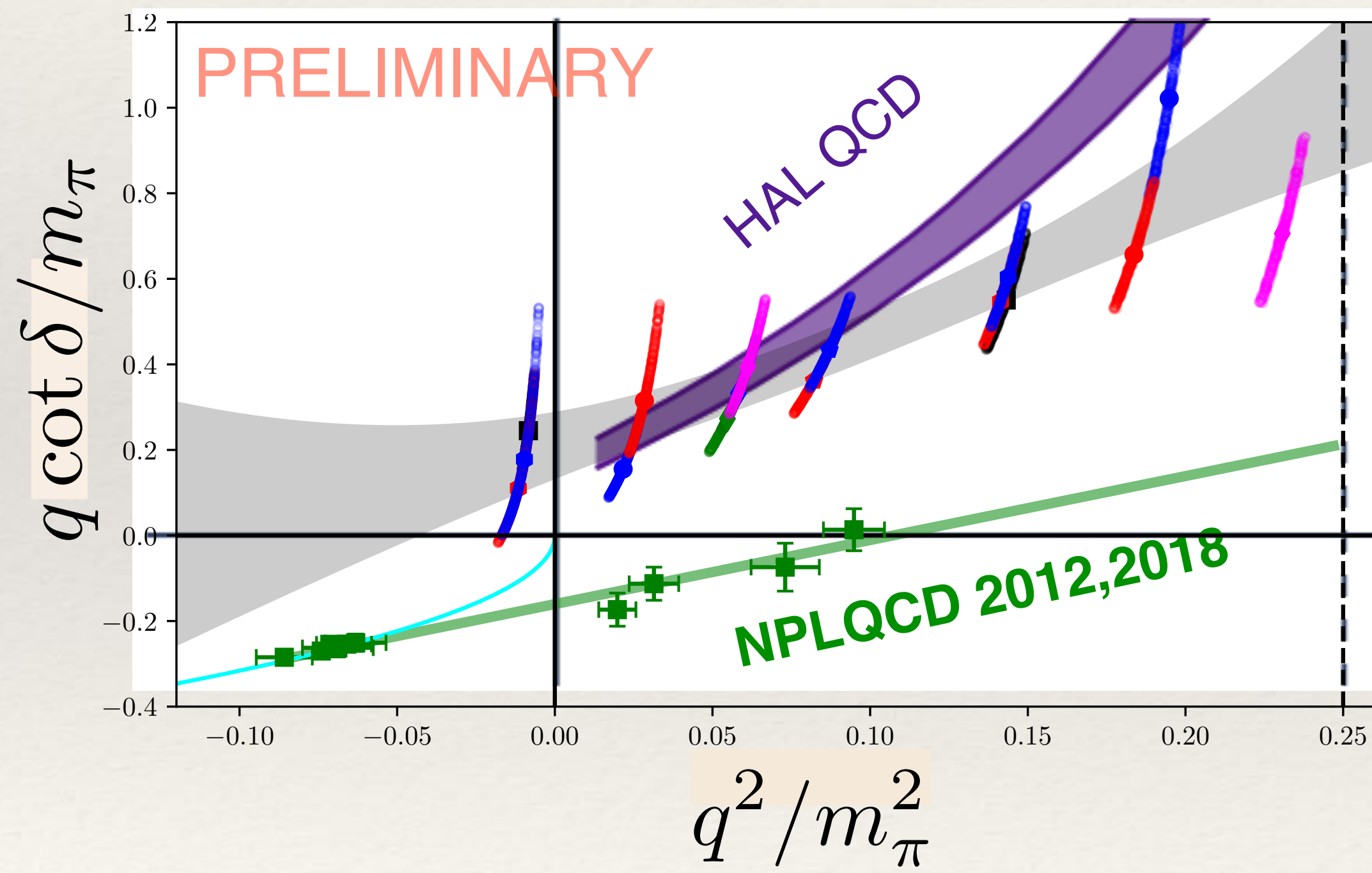


# Updates since 2009.11825 — HAL QCD potential

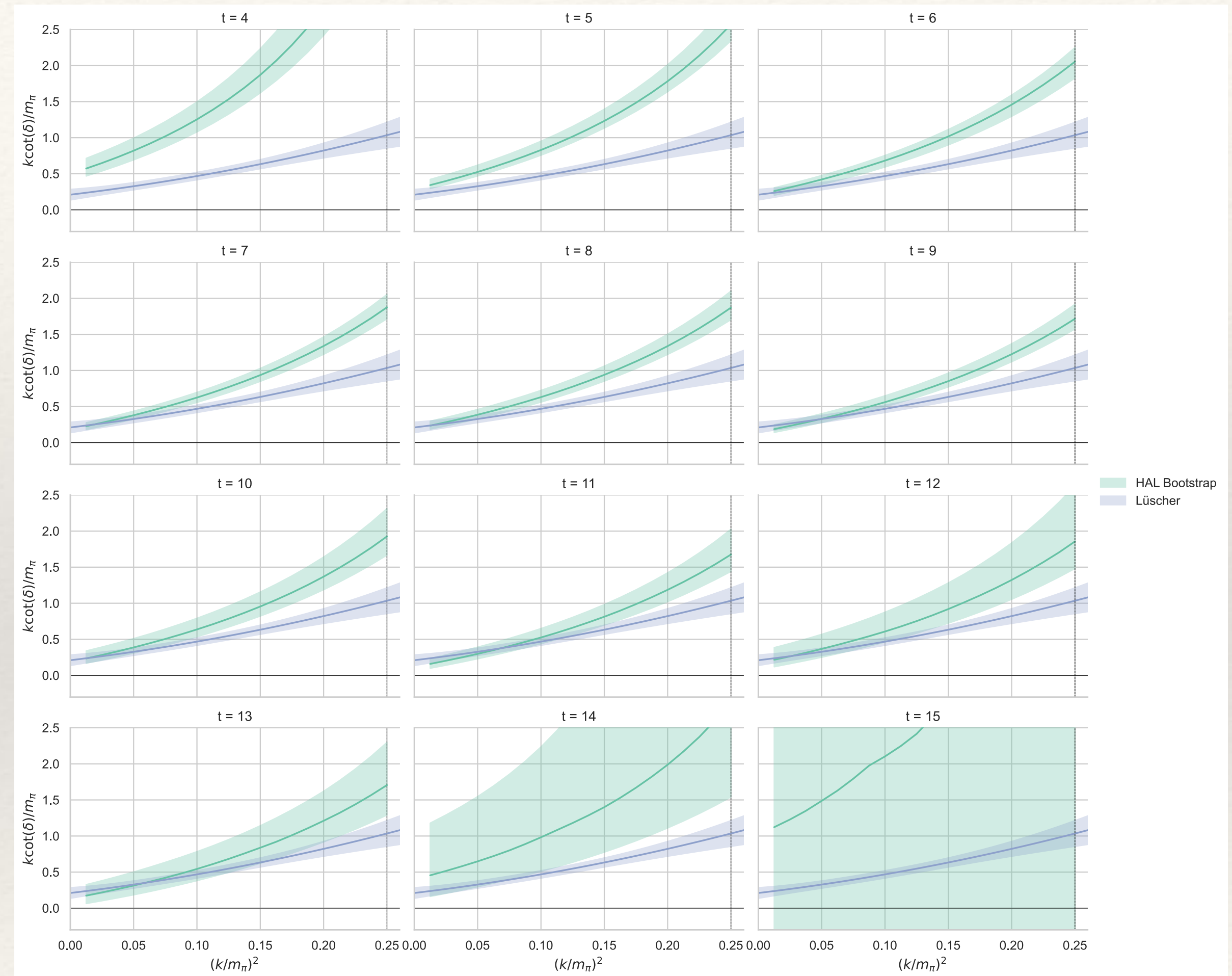
(thanks to C. Körber, A. Meyer, A. Nicholson)

- ❑ Uncorrelated fit to  $V(t, r)$
- ❑ Solve Schrödinger Equation
- ❑ Solve for asymptotic wave-function and phase shift

Lüscher

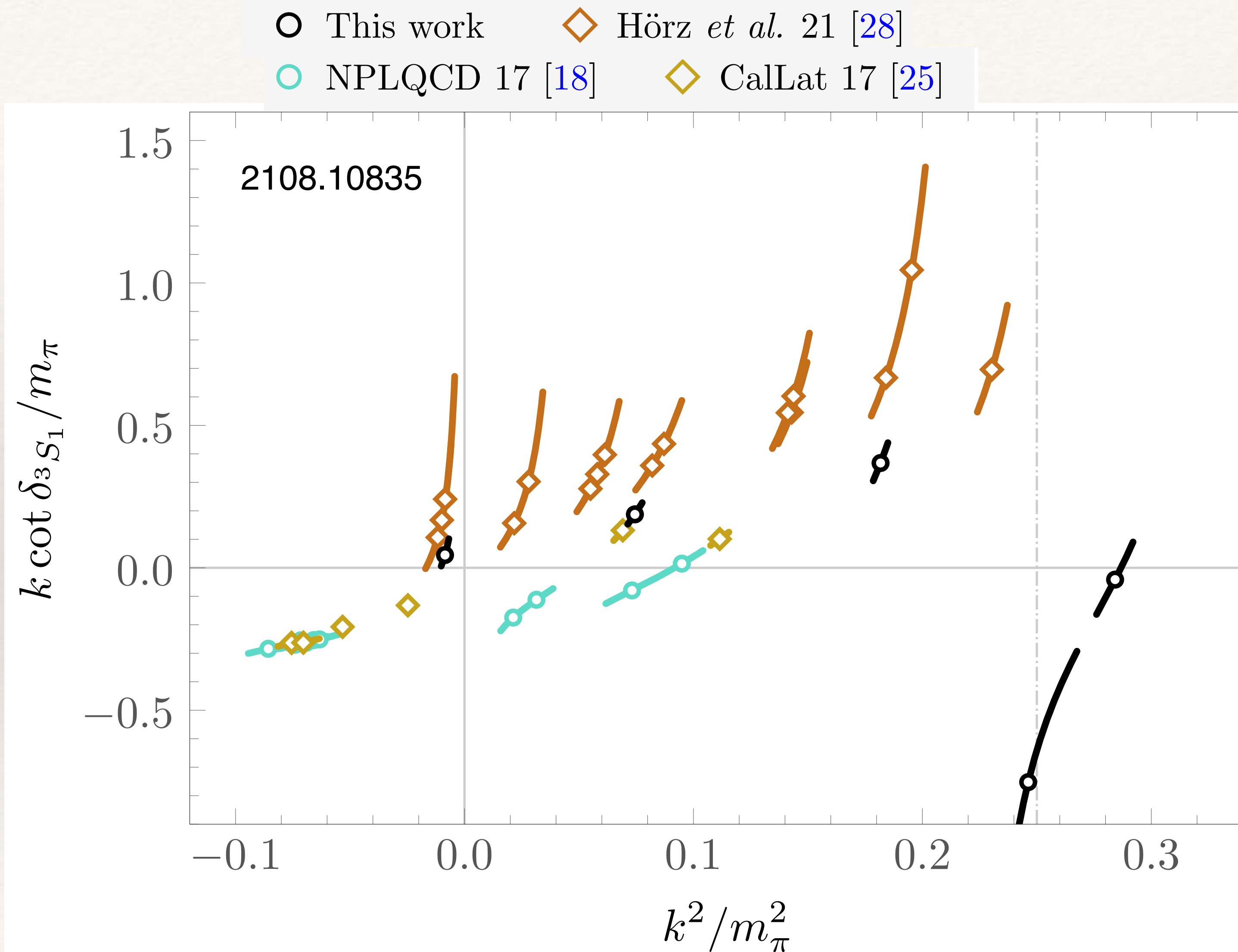
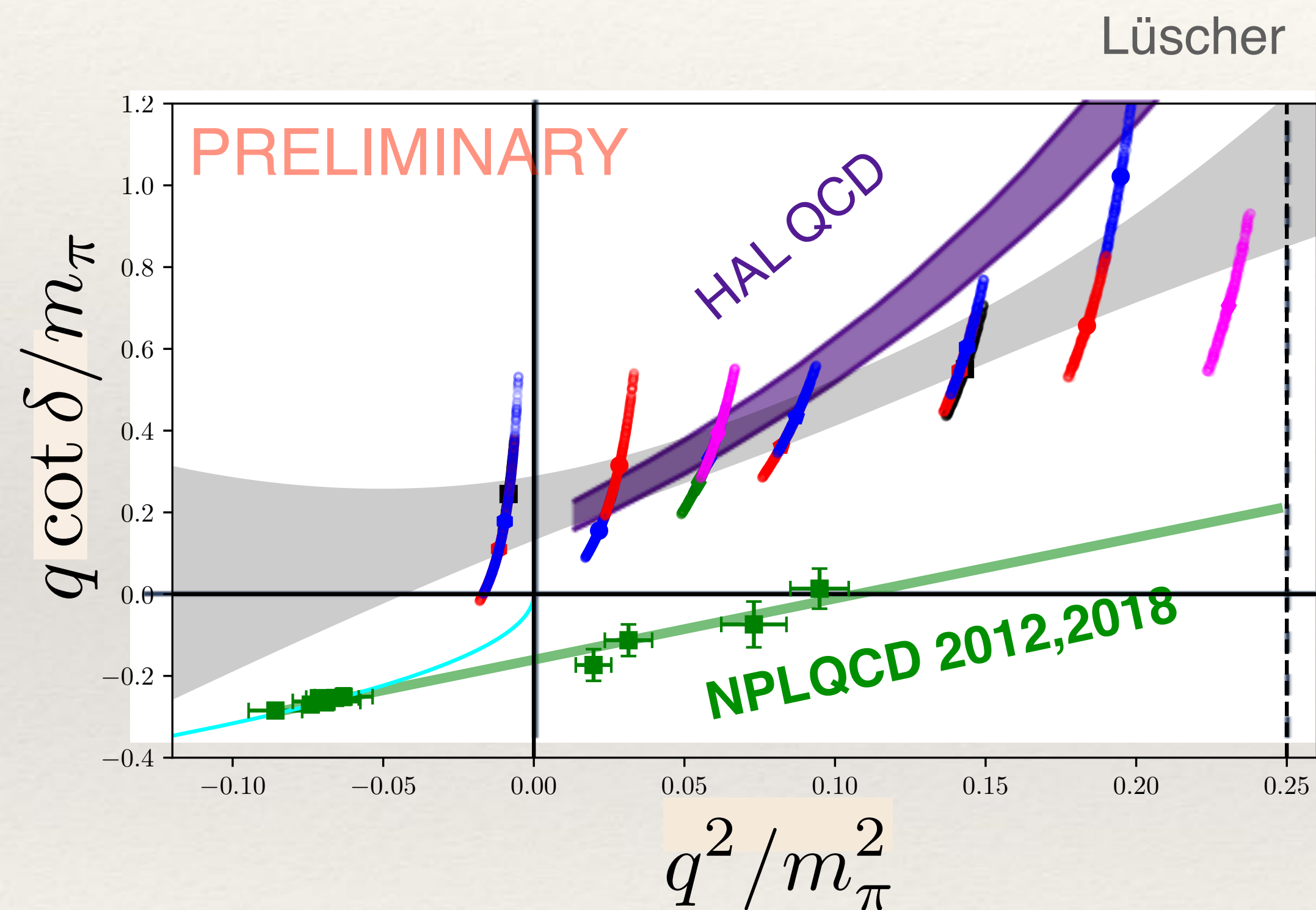


$V(t, r), t = 10$





# Updates since 2009.11825 — NPLQCD Sparsened Momentum





# To bind or not to bind?

- ❑ This is a question that is unfortunately not one we can absolutely answer - we can only find numerical evidence
- ❑ We (the community) often rely upon Lüscher quantization condition analysis of spectrum to detect inconsistent energy levels — in the case of old NPLQCD & CalLat results (at least at  $m_\pi \approx 800$  MeV), the observed spectrum did not show signs of sickness
- ❑ However, we are observing a **preponderance of evidence** that the older methods with present statistics, are yielding qualitatively incorrect spectrum —
  - I believe the old results are wrong (including those I was involved with)
  - I believe the di-nucleon system unbinds at pion masses heavier than physical
- ❑ The newer (at least newly applied to two-nucleon) methods are more expensive but, they are more robust and they yield a much richer spectrum (many more energy levels obtained in the same calculation)
- ❑ The path forward seems clear — we need to apply these methods @ lighter pion masses where they have a chance of having an impact on our understanding of NN interactions
  - ❑ To have an impact, we must have  $m_\pi \lesssim 200$  MeV



*Thank You*



# Collaborators

## CoSMoN

(Connecting the Standard Model to Nuclei)

(postdoc, grad student, undergrad)

Grant Bradley	Brown University
John Bulava	DESY
Kate Clark	NVIDIA
Zack Hall	University of North Carolina Chapel Hill
Andrew Hanlon	Brookhaven National Laboratory
Jinchen He	University of Maryland College Park
Ben Hörz	INTEL
Dean Howarth	Lawrence Berkeley National Laboratory
Bálint Joó	Oak Ridge National Laboratory
Aaron Meyer	Lawrence Livermore National Laboratory/NTN
Henry Monge-Camacho	Oak Ridge National Laboratory
Colin Morningstar	Carnegie Mellon University
Joseph Moscoso	University of North Carolina Chapel Hill
Amy Nicholson	University of North Carolina Chapel Hill
Fernando Romero-López	MIT
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