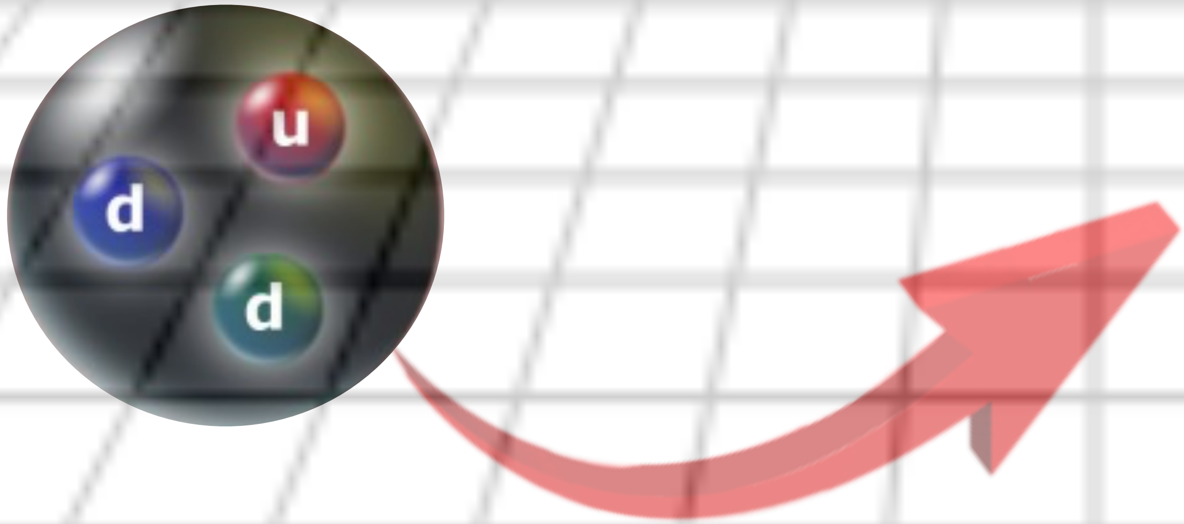


Nucleon-nucleon scattering from lattice QCD: history, progress, resolutions

Amy Nicholson
UNC, Chapel Hill

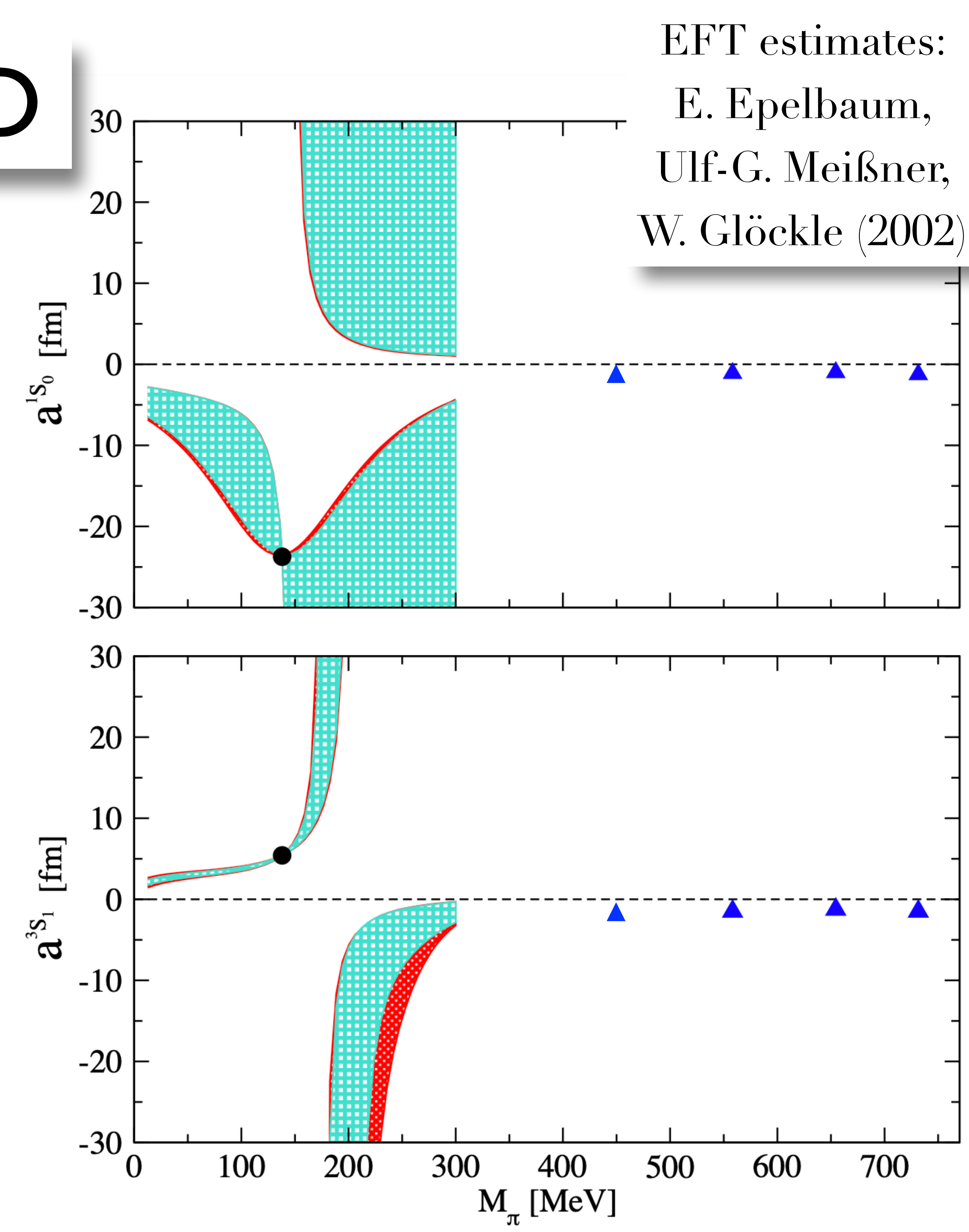
BaSc

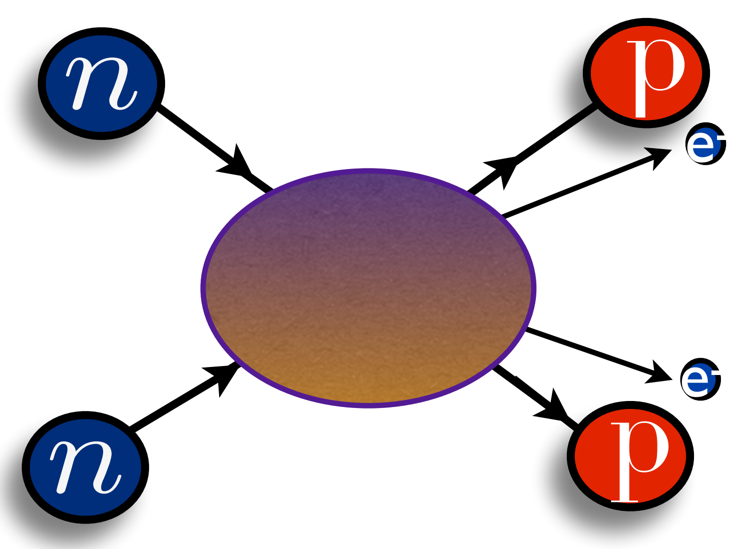
INT Program: Accessing and Understanding the QCD Spectra
March 22, 2023

CoSMoN

NN scattering from LQCD

- Build quantitative connection between QCD & nuclear physics
  - requires interplay between LQCD & many-body approaches
  - NN scattering should be a benchmark
  - Phase shifts required for infinite volume matching of NN MEs





PHYSICAL REVIEW LETTERS **120,** 202001 (2018)

Editors' Suggestion Featured in Physics

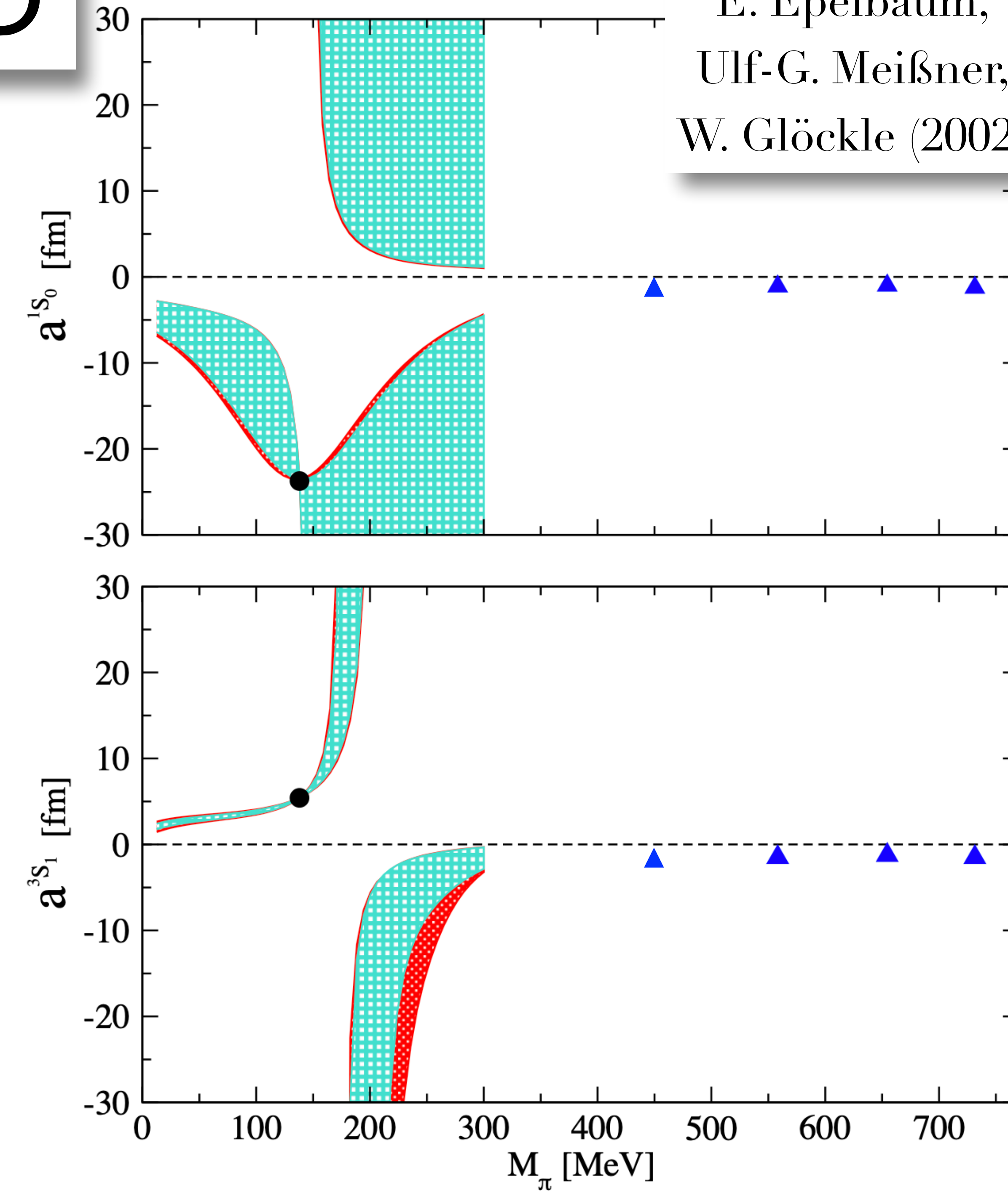
New Leading Contribution to Neutrinoless Double-β Decay

Vincenzo Cirigliano,[1] Wouter Dekens,[1] Jordy de Vries,[2] Michael L. Graesser,[1]
Emanuele Mereghetti,[1] Saori Pastore,[1] and Ubirajara van Kolck[3,4]

NN scattering from LQCD

- Build quantitative connection between QCD & nuclear physics
  - requires interplay between LQCD & many-body approaches
  - NN scattering should be a benchmark
  - Phase shifts required for infinite volume matching of NN MEs
- Must have full control over 2-body systems
  - How do we project onto desired states?
  - How do we disentangle signals from closely spaced energy levels?

EFT estimates:
E. Epelbaum,
Ulf-G. Meißner,
W. Glöckle (2002)



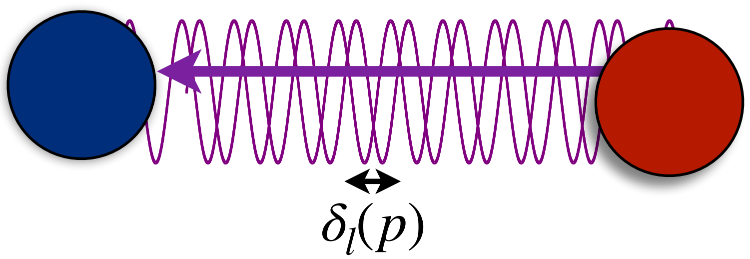
Two methods for computing phase shifts

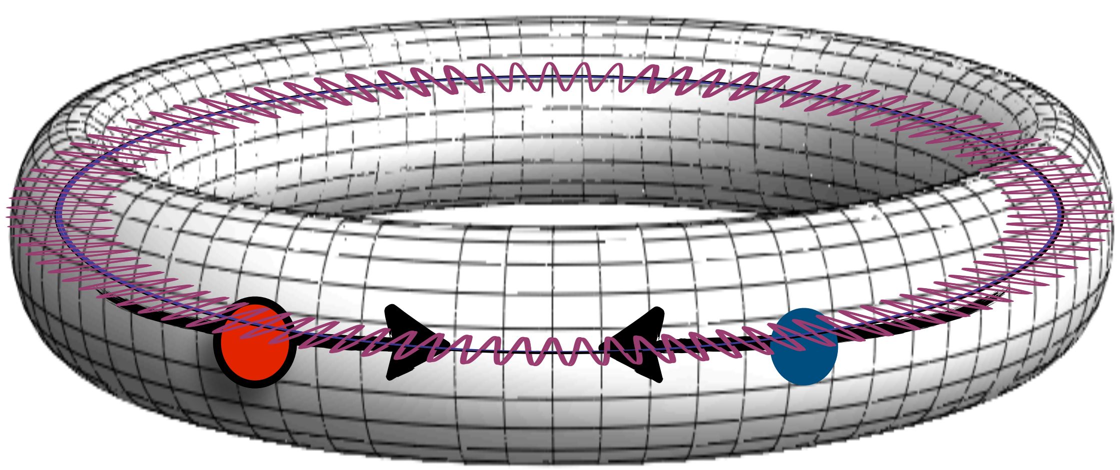
Spectroscopy + Lüscher Method

Potential Method

Two methods for computing phase shifts

Spectroscopy + Lüscher Method



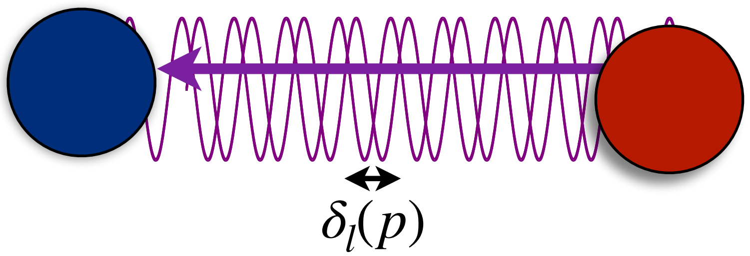


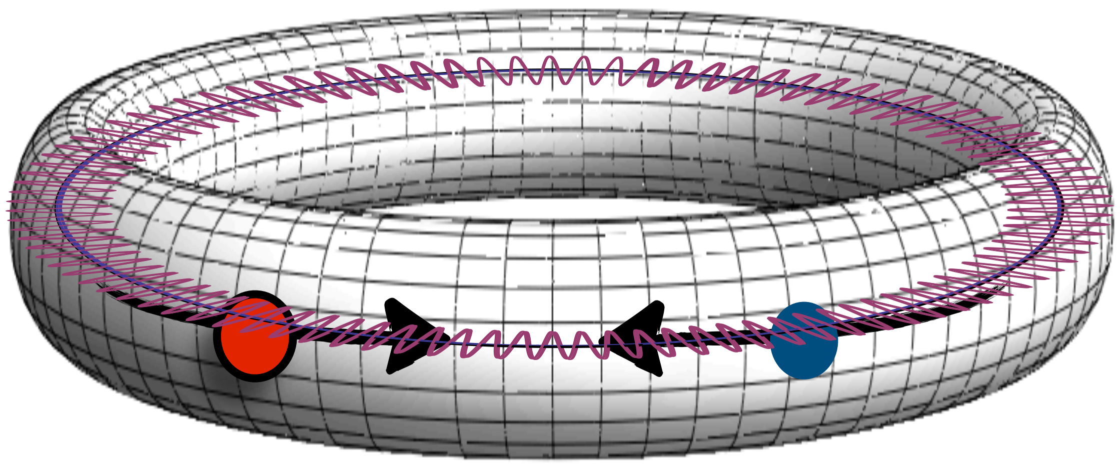
Quantization condition:

$$\det\left[F(E,\mathbf{P},L)^{-1}+\mathscr{K}(E)\right]=0$$

Two methods for computing phase shifts

Spectroscopy + Lüscher Method





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Known geometric function

Two methods for computing phase shifts

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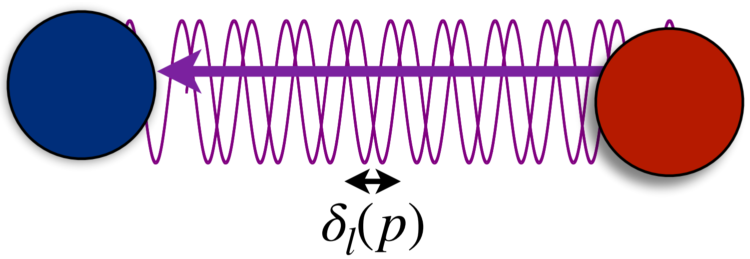

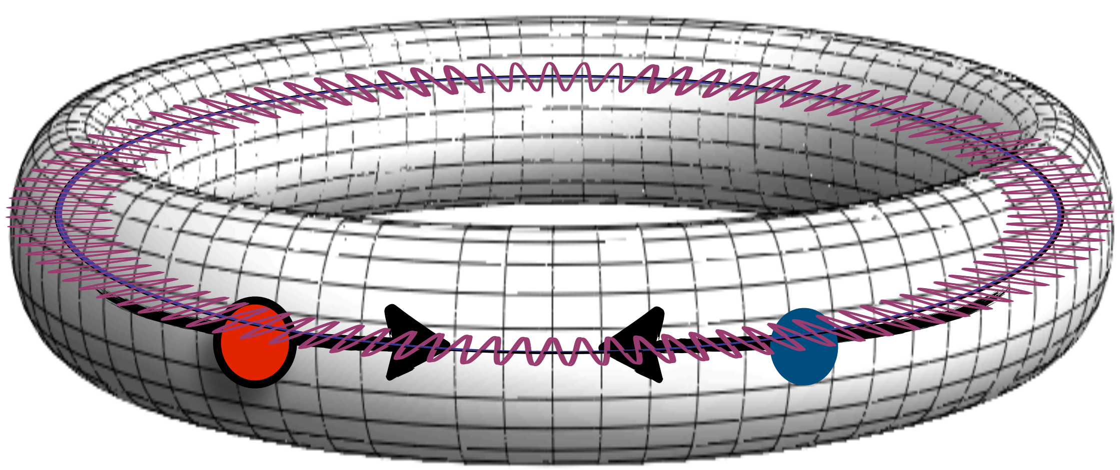

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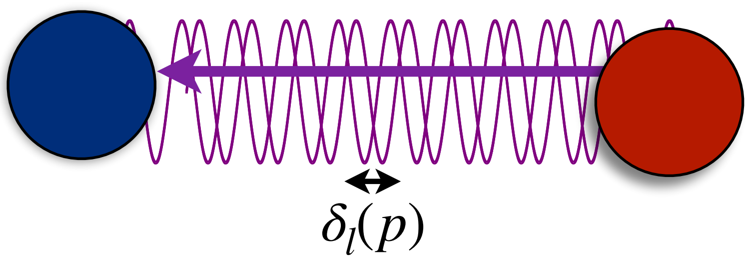
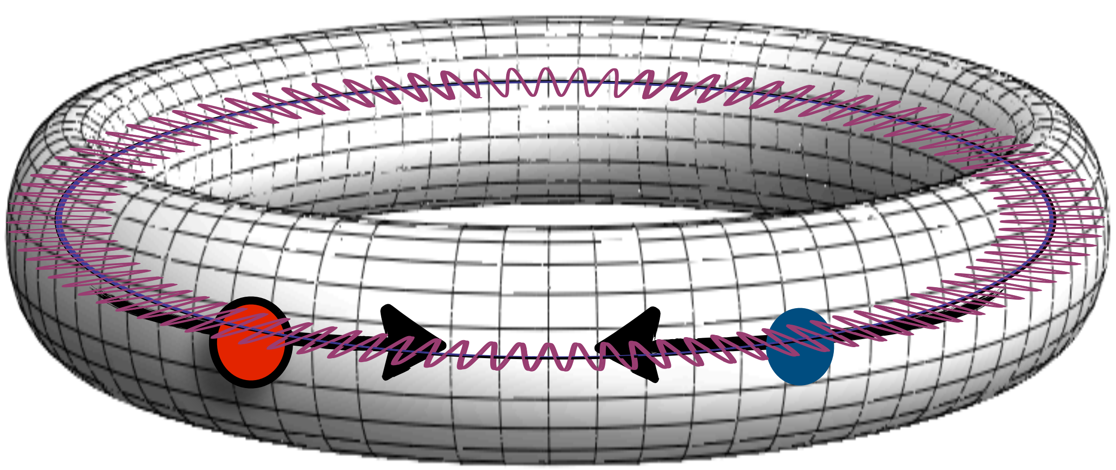
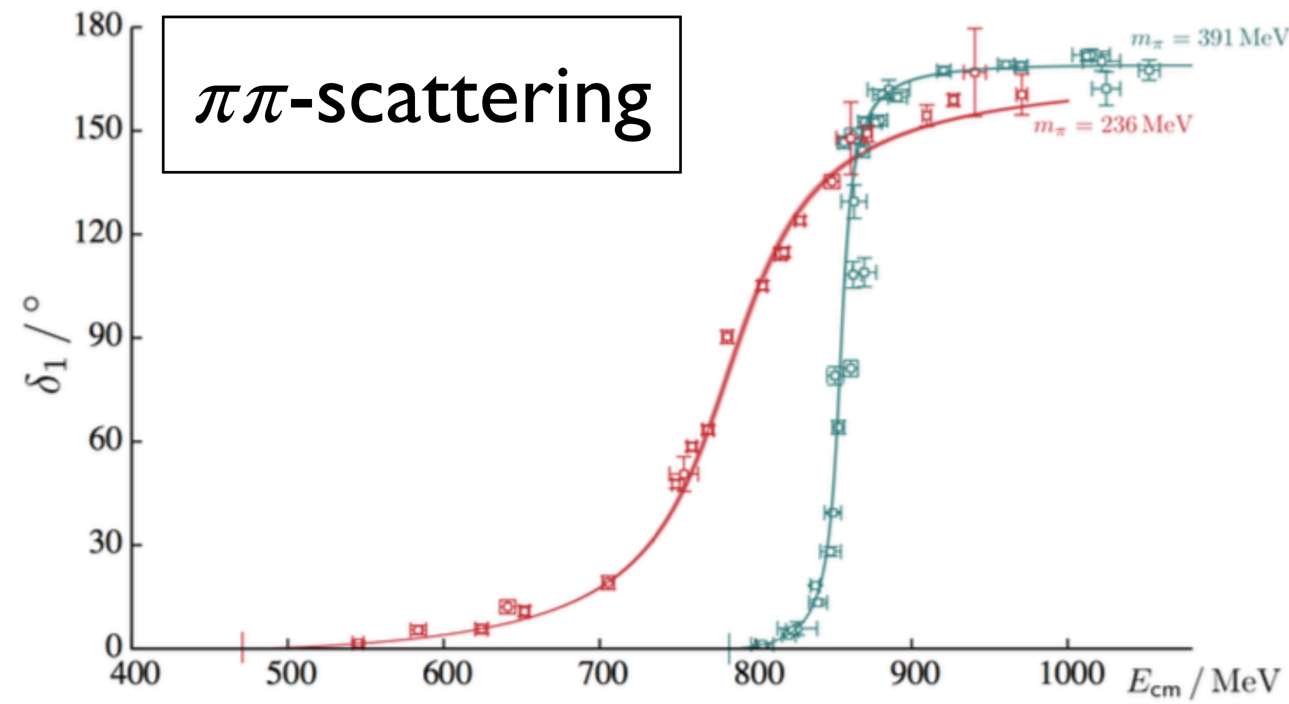




D. J. Wilson, R. A. Briceno, J. J. Dudek, R. G. Edwards and C. E. Thomas, Phys. Rev. D 92, 094502 (2015)



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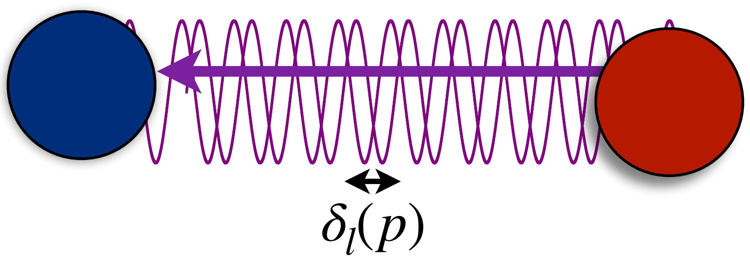
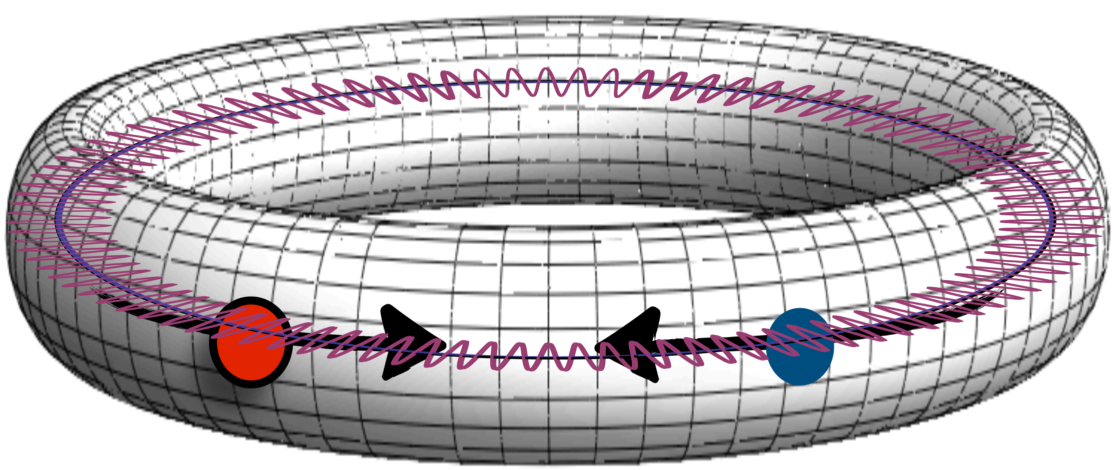
Calculate from lattice (input) — E

Output — $\mathscr{K}(E)$

Two methods for computing phase shifts

Spectroscopy + Lüscher Method





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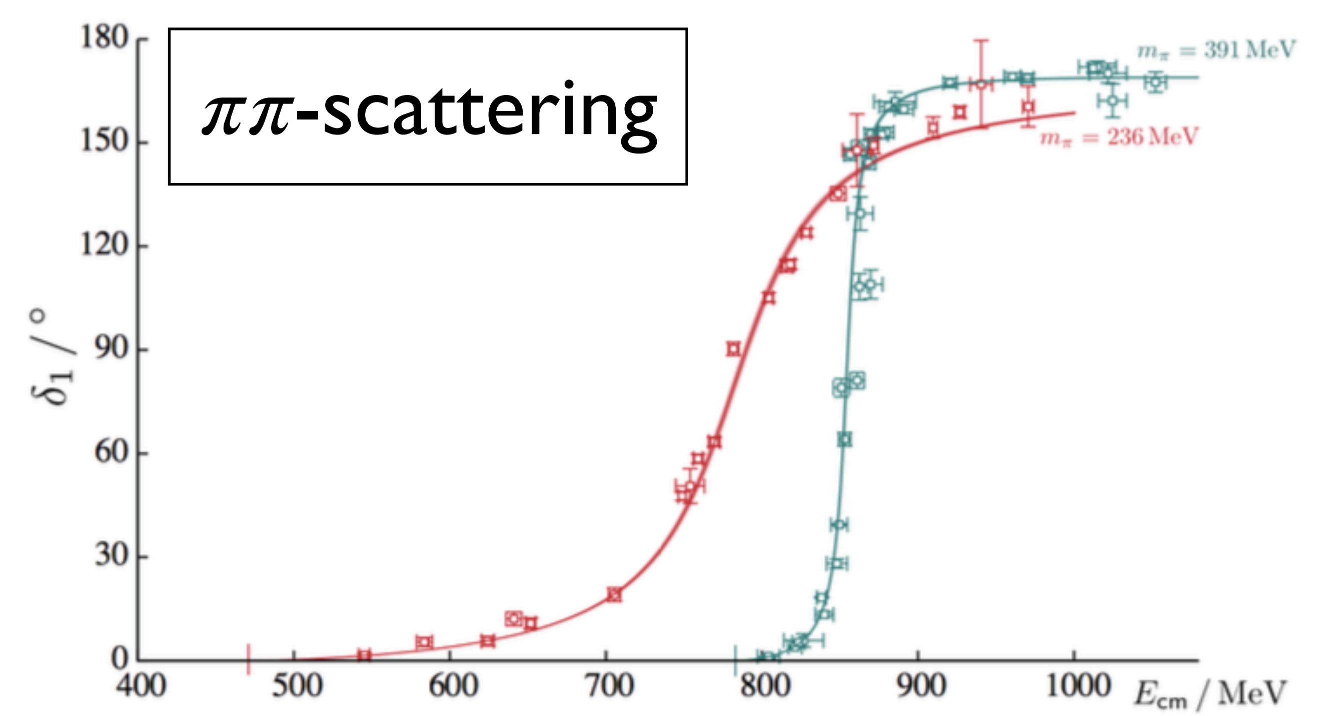

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Calculate from lattice (input)

Output

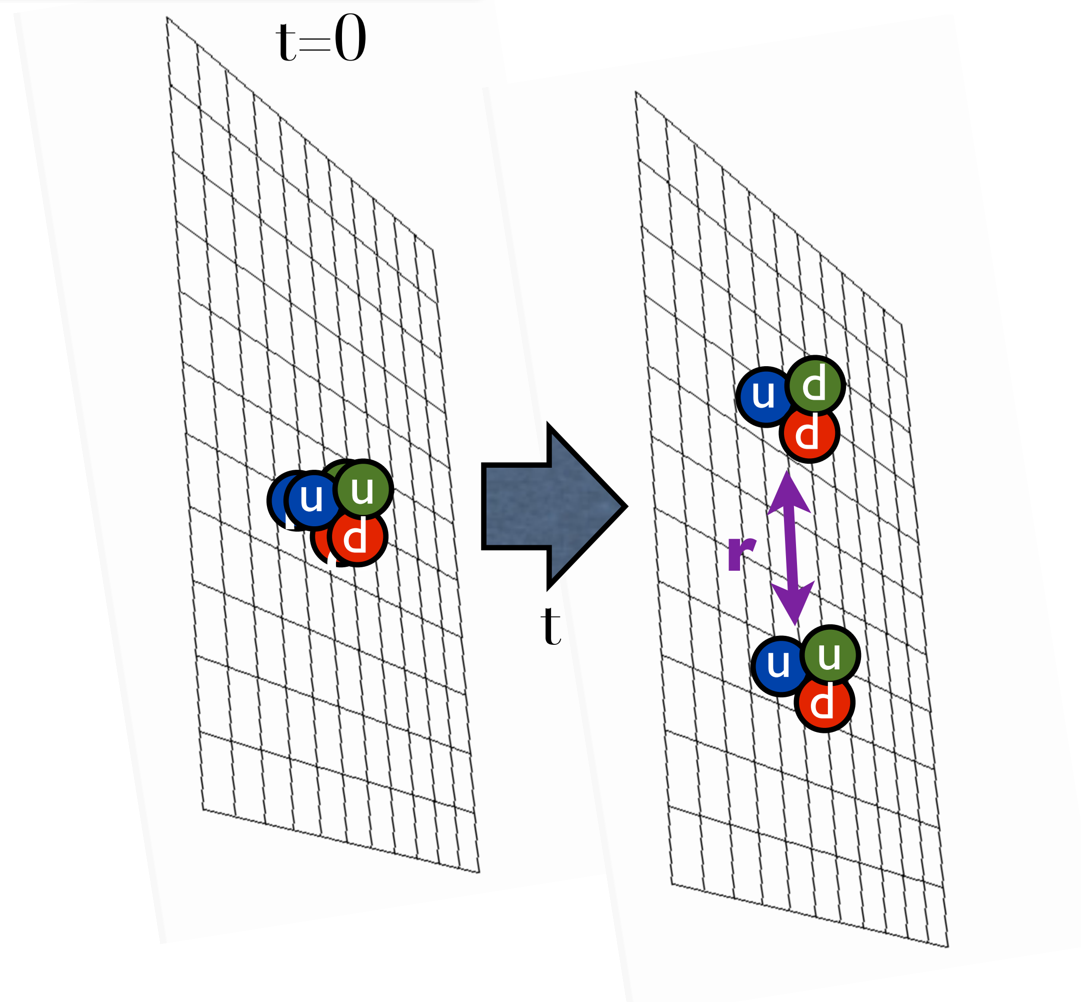
- Partial waves mix in cubic volume
- Must truncate partial wave expansion

Two methods for computing phase shifts

Potential Method

Hadrons to Atomic nuclei
HAL
from Lattice QCD

1. Create the following correlation function:



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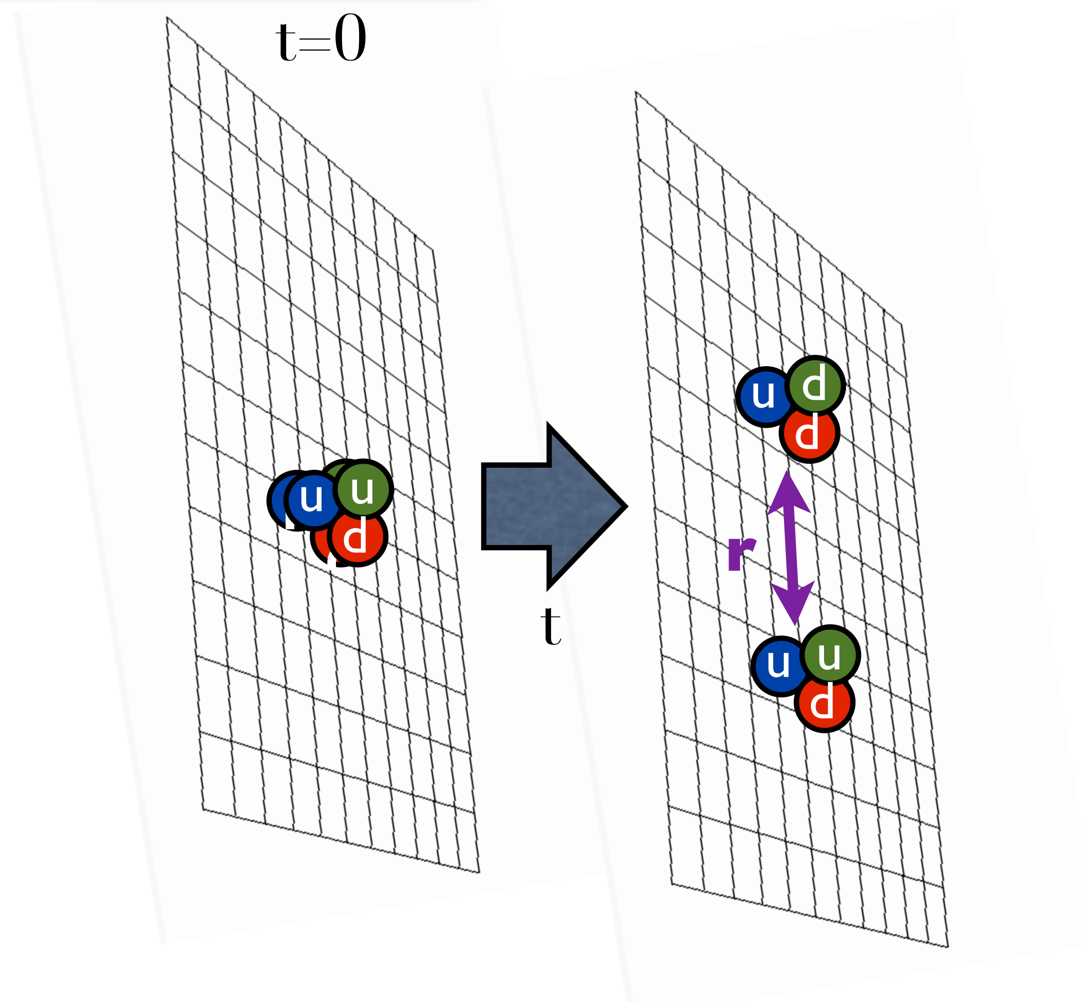

$$\lim_{t\to\infty} C_{NN}(\mathbf{r},t) \;=\; \psi_0^\dagger \times e^{-E_0 t} \times \psi_0(\mathbf{r})$$

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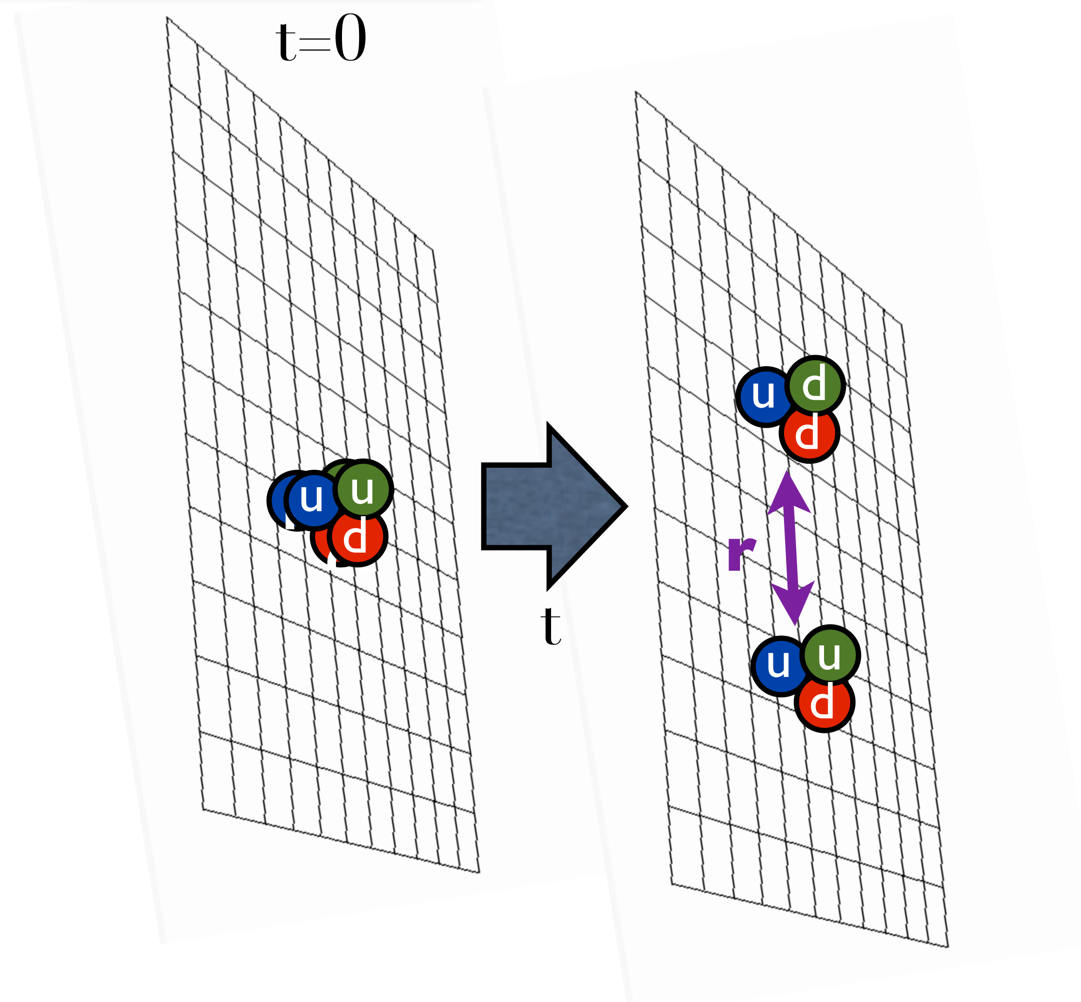

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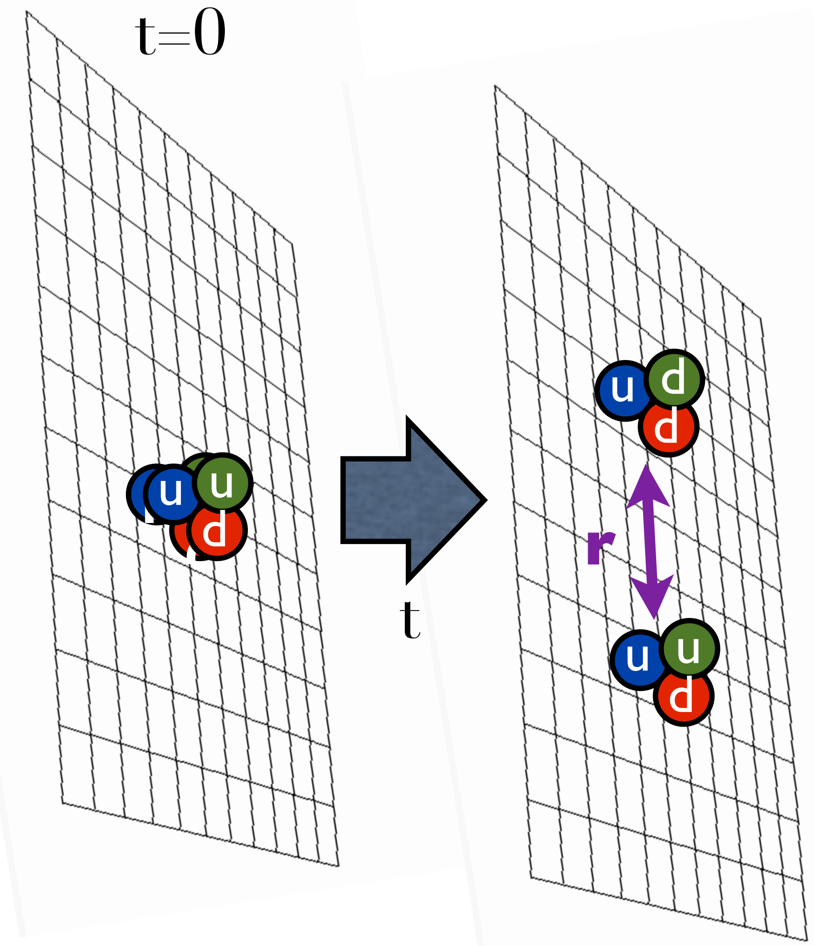

2. Plug NBS wave-function into Schrödinger Eq. to determine the potential:

$$\left[\frac{\mathbf{p}^2}{2\mu} - H_0\right] \psi_{\mathbf{p}}(\mathbf{r}) = \int d^3r' \, U(\mathbf{r},\mathbf{r}') \, \psi_{\mathbf{p}}(\mathbf{r}') \longleftarrow \psi_0(\mathbf{r})$$

Two methods for computing phase shifts

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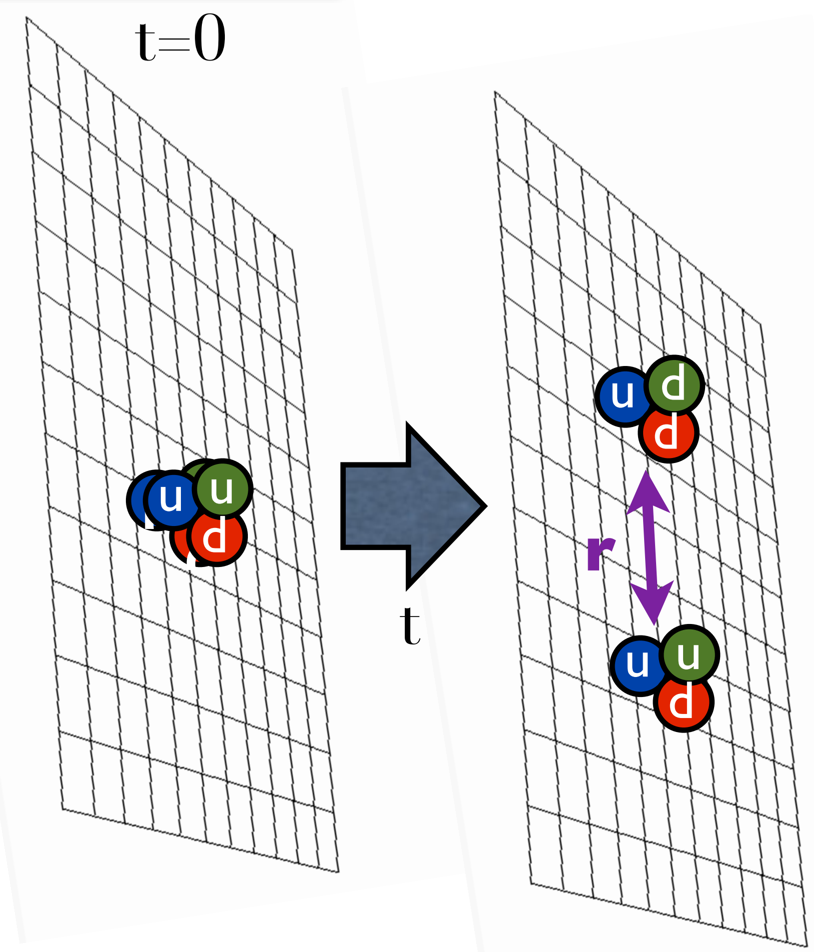

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3. Determine scattering phase shifts

Two methods for computing phase shifts

Potential Method

In practice:

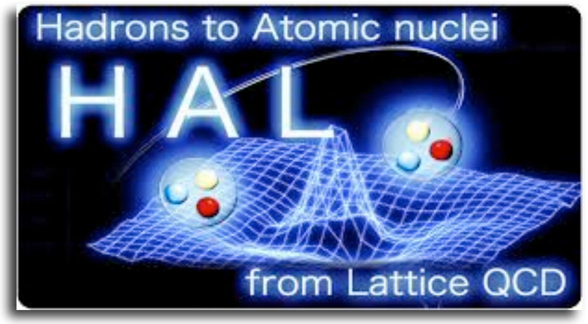
$$R(\mathbf{r}, t) = \frac{C_{NN}(\mathbf{r}, t)}{\left(C_N(\mathbf{r}, t)\right)^2}$$

(same type of input as Luscher)

Schrodinger Eq: $\left\{-H_0 - \frac{\partial}{\partial t}\right\} R(\mathbf{r}, t) = \int d^3r' \, U(\mathbf{r}, \mathbf{r}') R(\mathbf{r}', t)$

Two methods for computing phase shifts

Potential Method



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$$U(\mathbf{r}, \mathbf{r}') = V_C(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}') + \mathcal{O}(\nabla_{\mathbf{r}}^2/\Lambda^2)$$

Uncontrolled approximation

Two methods for computing phase shifts

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Uncontrolled approximation

Nearly continuous phase shifts, only need to eliminate inelastic excited states

Lüscher Method

Potential Method

History: are there bound states at $m_\pi \sim 800$ MeV?

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Lüscher Method

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Potential Method

Uncontrolled systematics

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Potential Method

Uncontrolled systematics

Relatively few assumptions….but input energies must be correct!

History: are there bound states at $m_\pi \sim 800$ MeV?

Lüscher Method

Potential Method

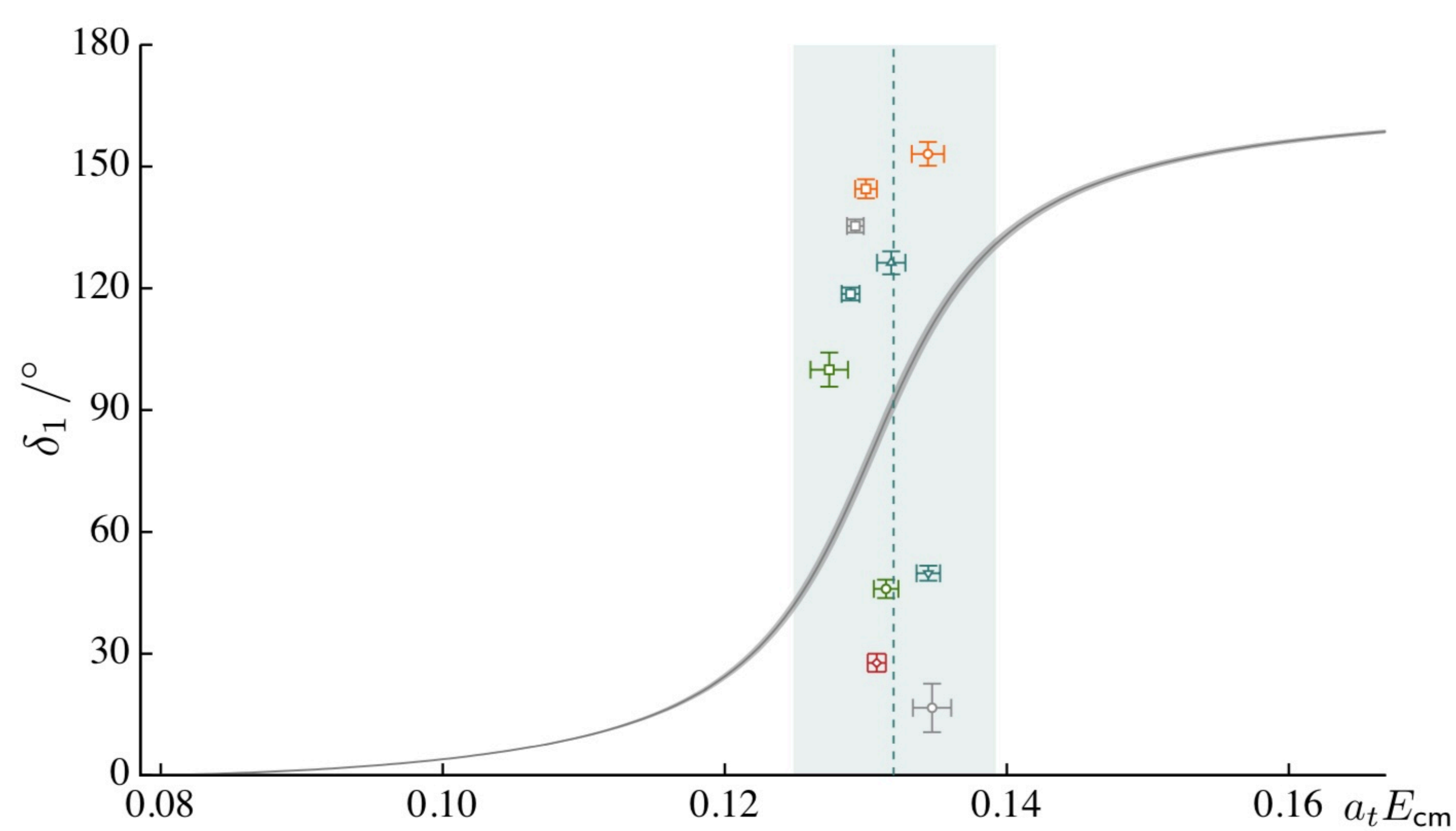
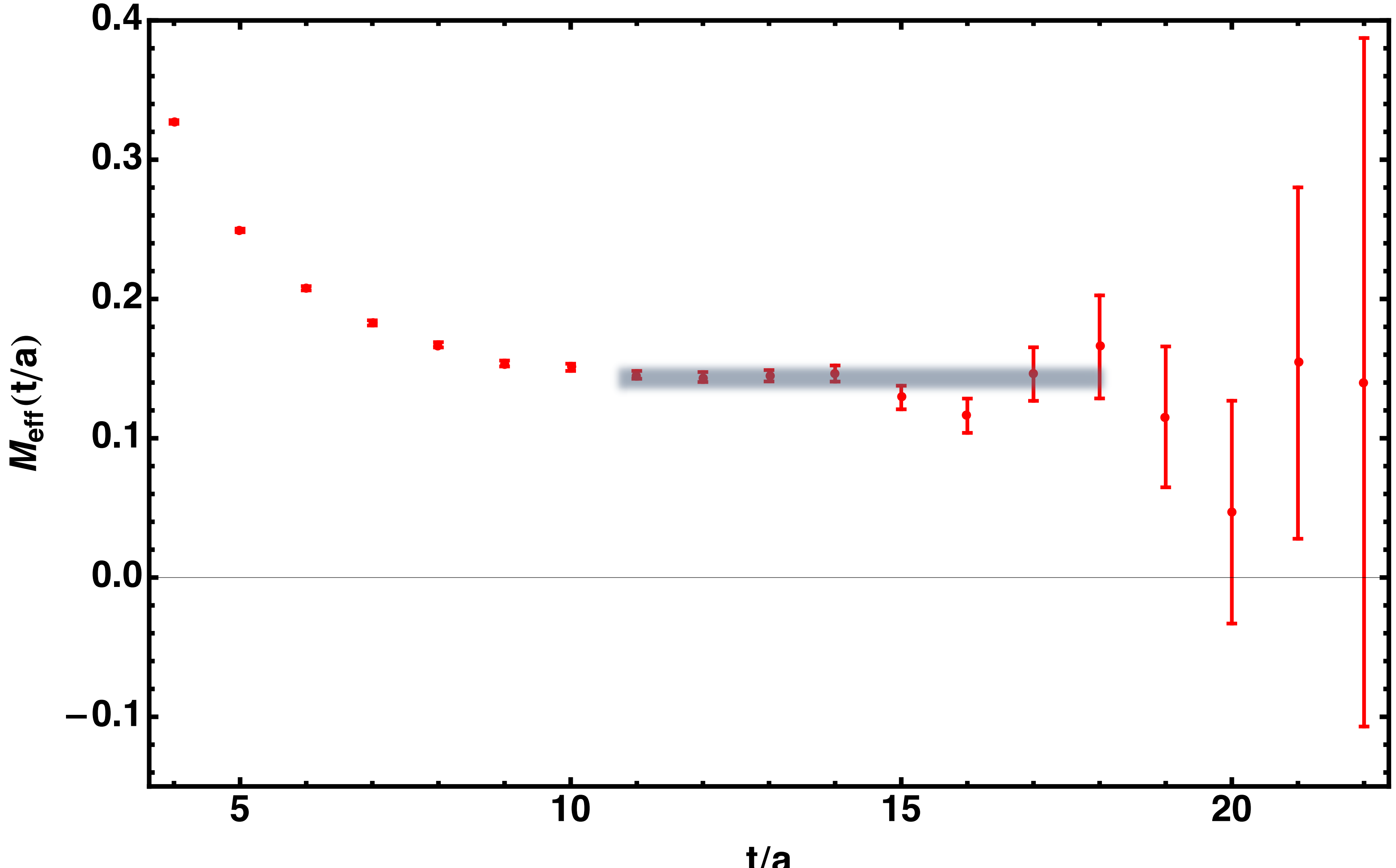


Figure from: Wilson, et al, Phys. Rev. D 92, 094502 (2015)

Calculating Spectra



Effective mass plot:

$$M_{\text{eff}} \equiv \ln \frac{C(t)}{C(t+1)} \xrightarrow[t\to\infty]{} E_0$$

Long time limit = zero temperature

$$C(t) = A_0 e^{-E_0 t} + A_1 e^{-E_1 t} + A_2 e^{-E_2 t} + A_3 e^{-E_3 t} + \cdots$$

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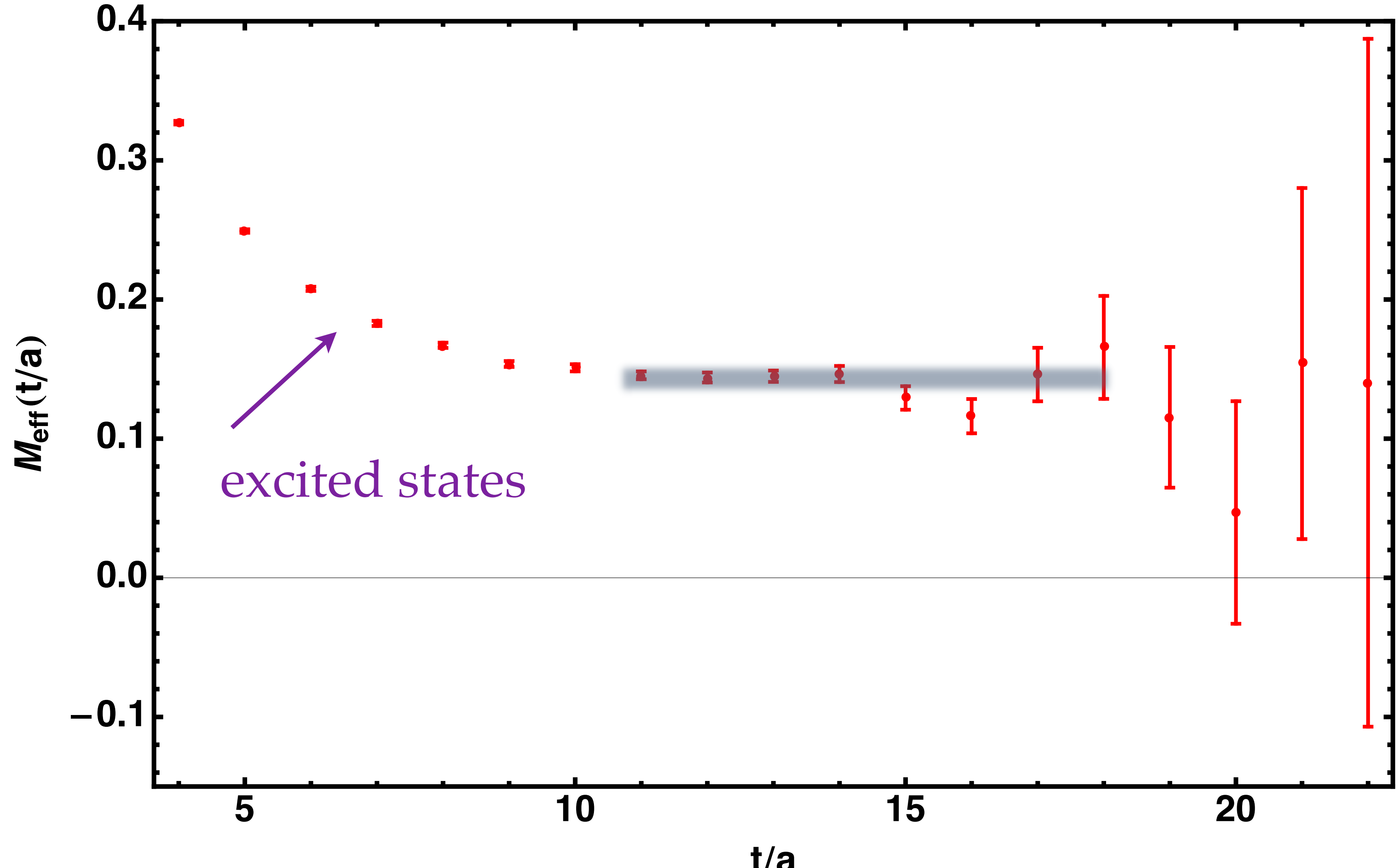

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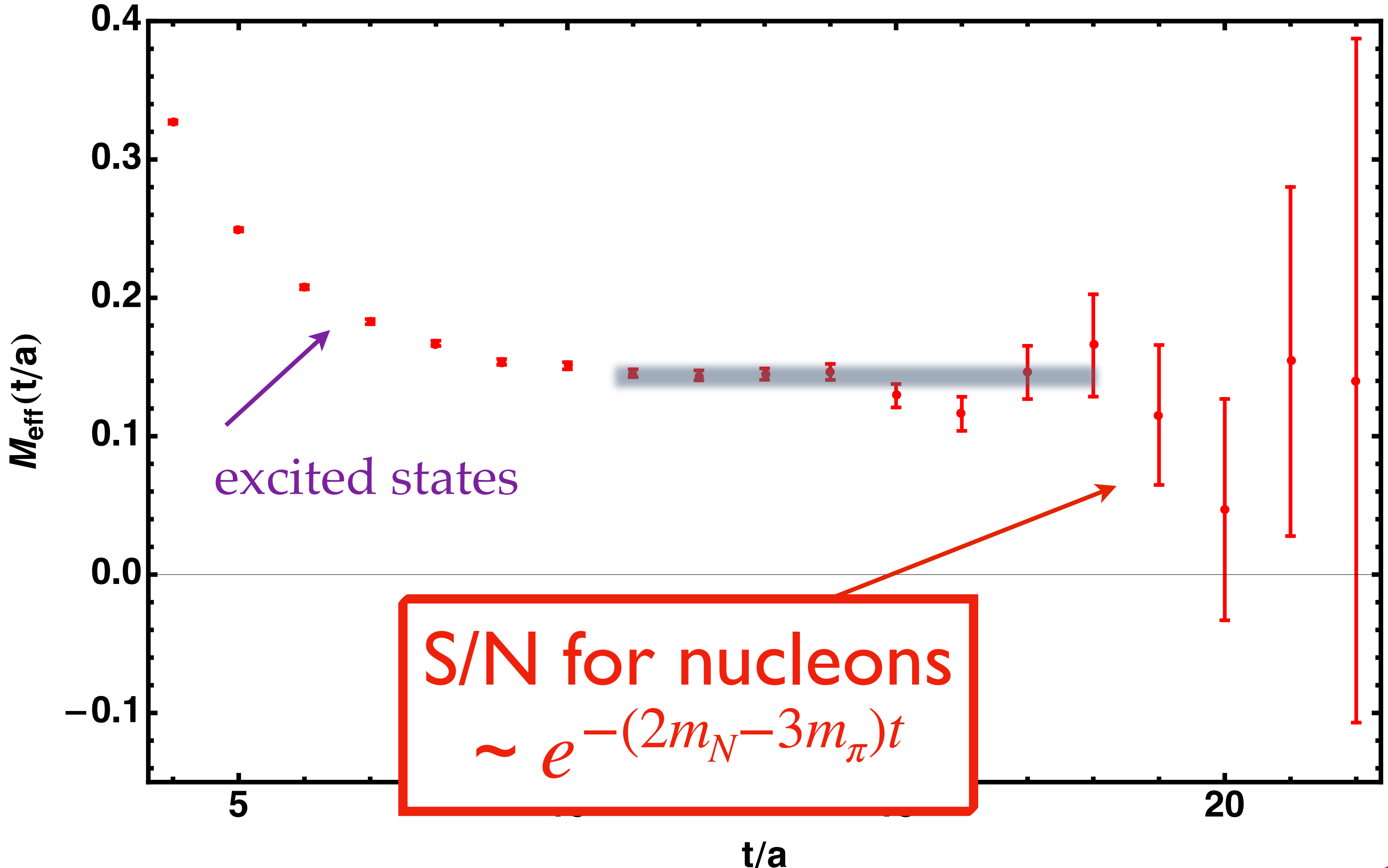

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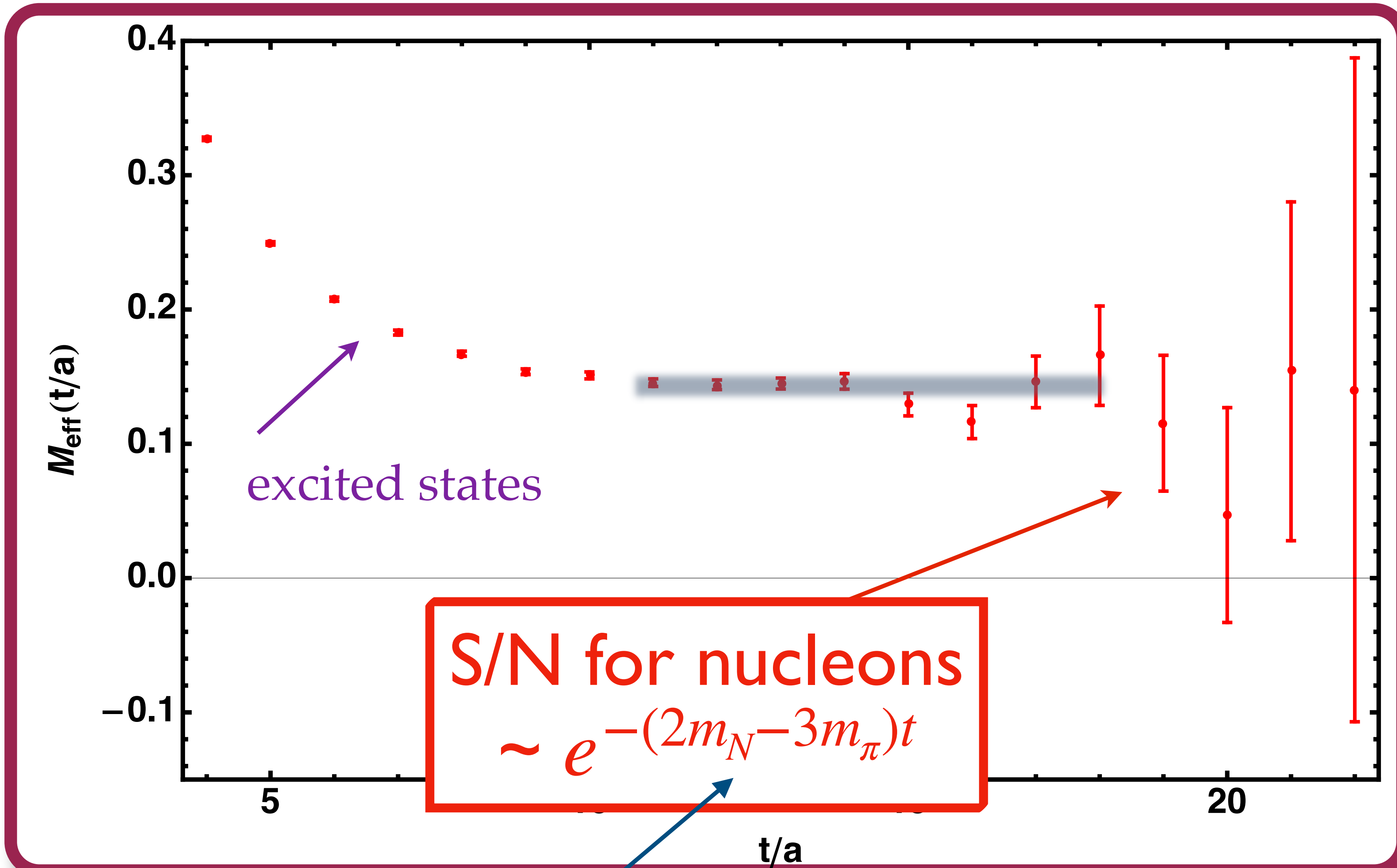

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This is why we benchmark at $m_\pi \sim$ 800MeV

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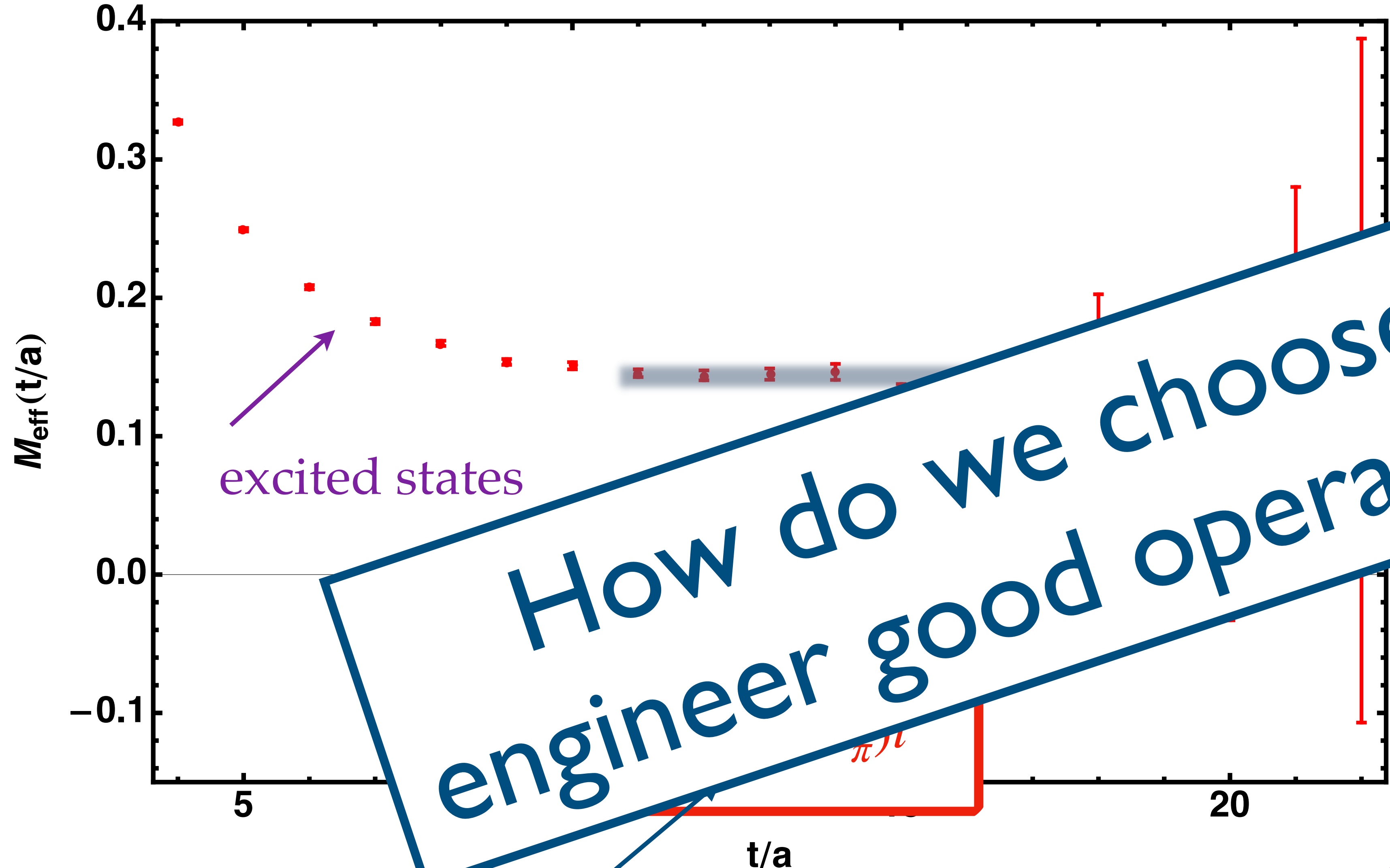

How do we choose/ engineer good operators?

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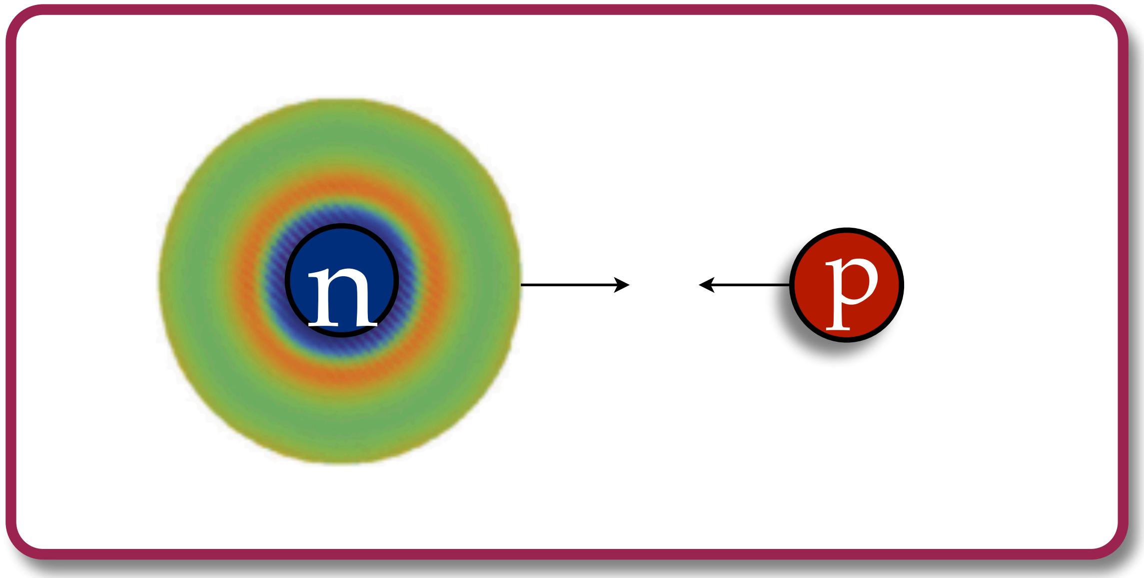
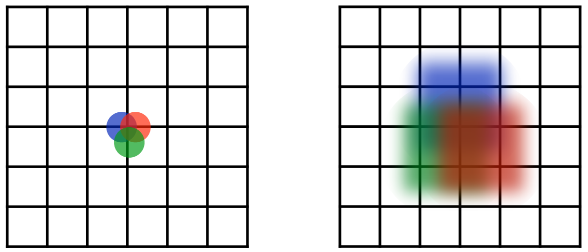
Excited state contamination



Inelastic single body
$\Delta E \sim m_\pi$

Ops: different smearings (or linear combos thereof)



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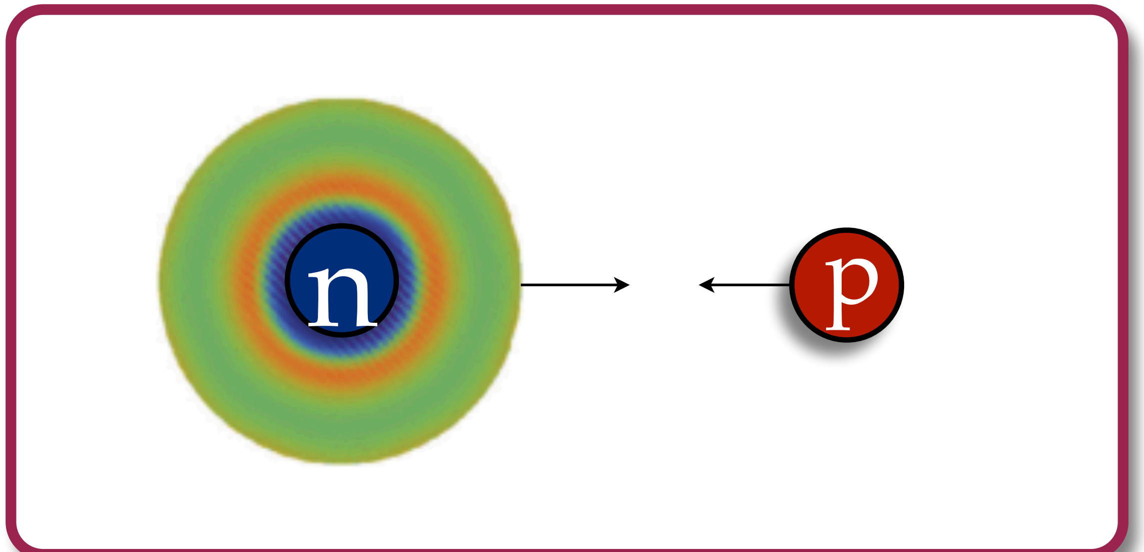

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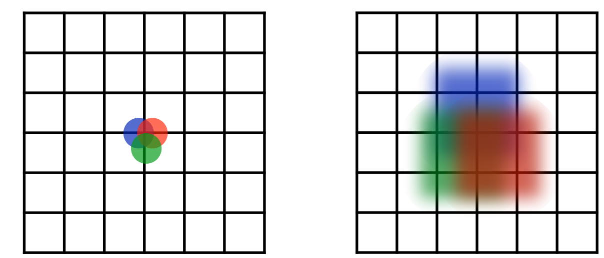
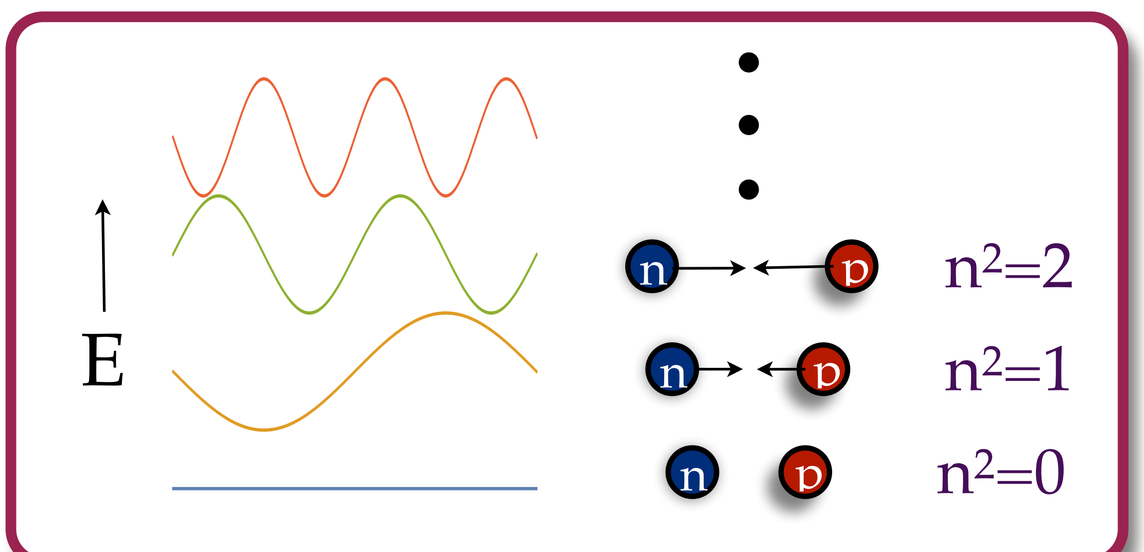
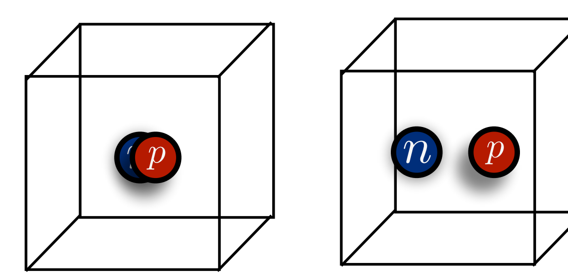




Elastic scattering (2-body)

$\Delta E \sim 50$ MeV

Ops: different spatial locations (or relative momenta)



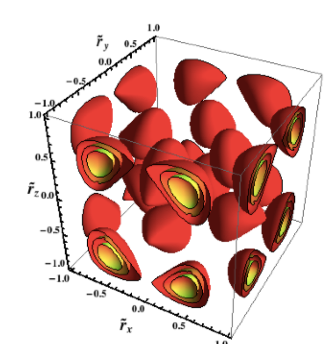
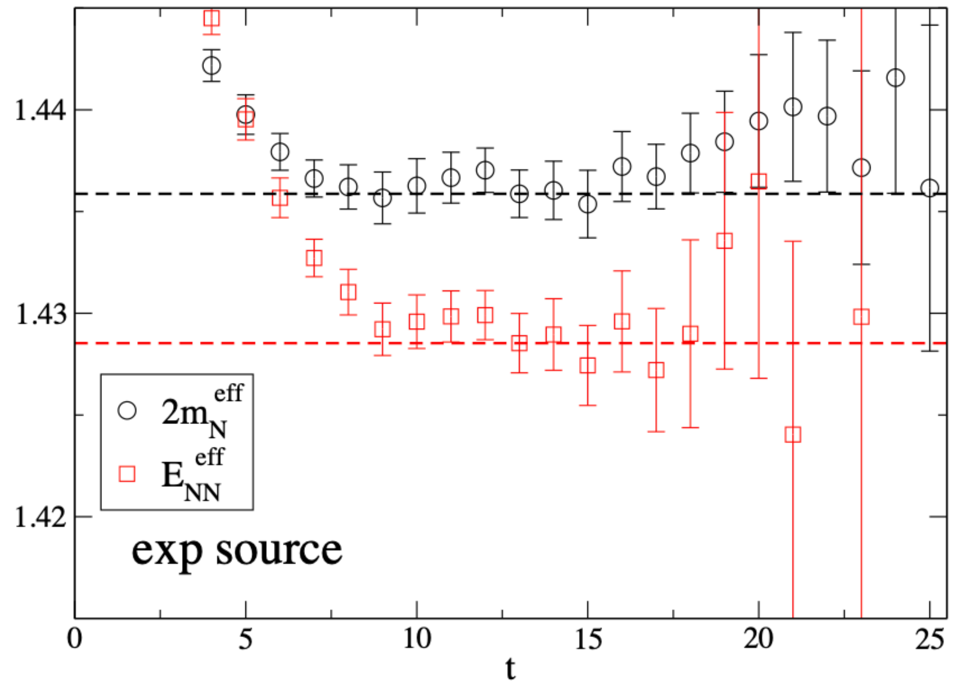
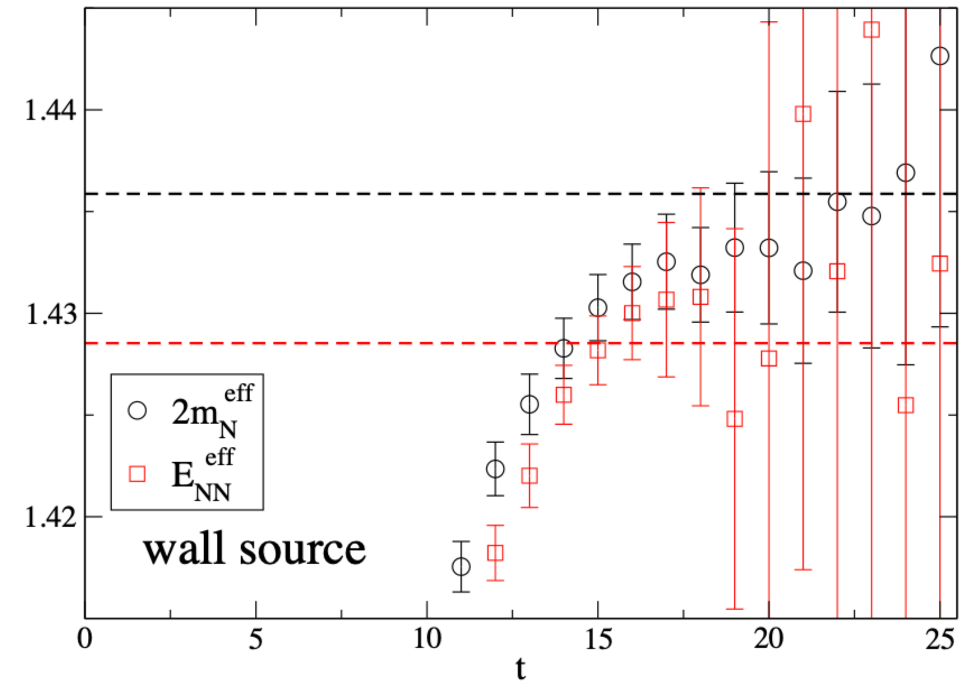


Fig: Luu & Savage (2011)

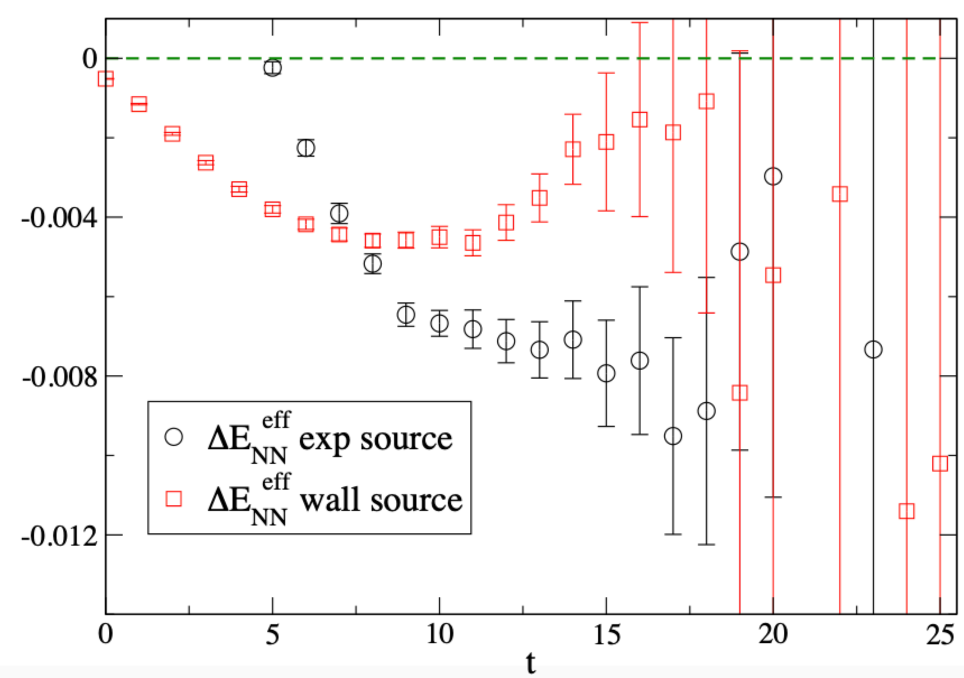
Wall vs Smeared (inelastic contributions)

PACS: NN system





Correlated difference



Yamazaki et al (2017)

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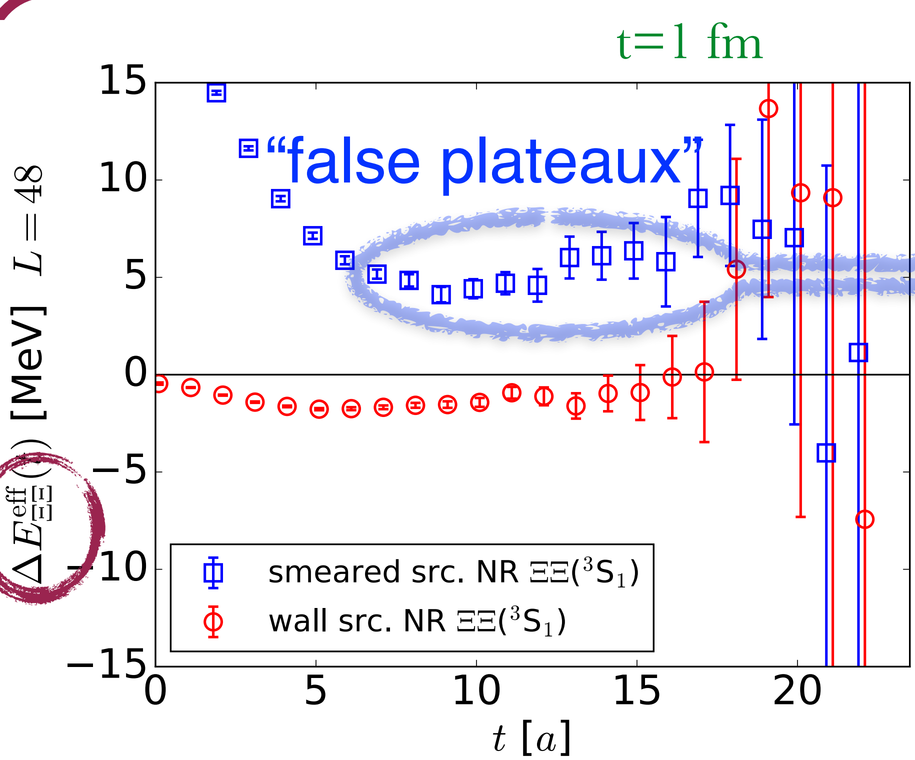
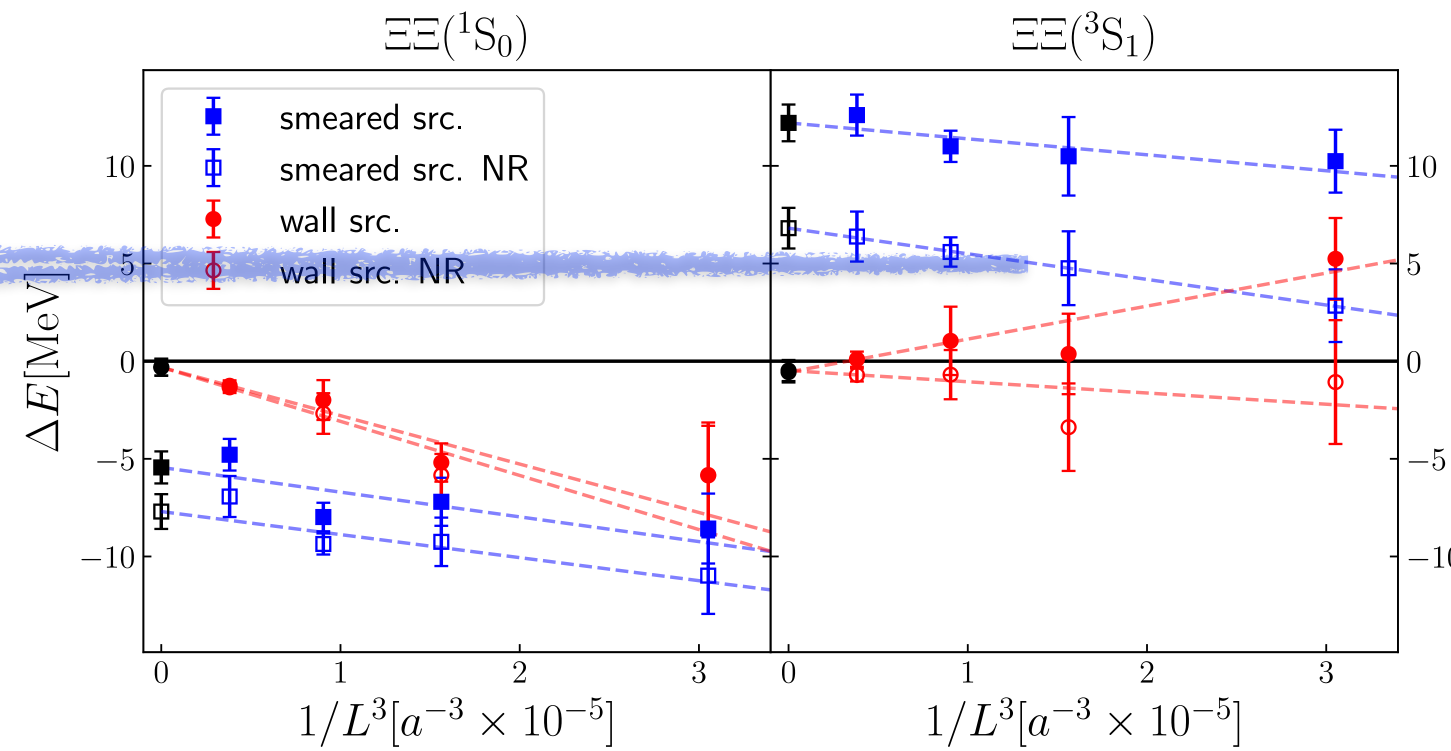
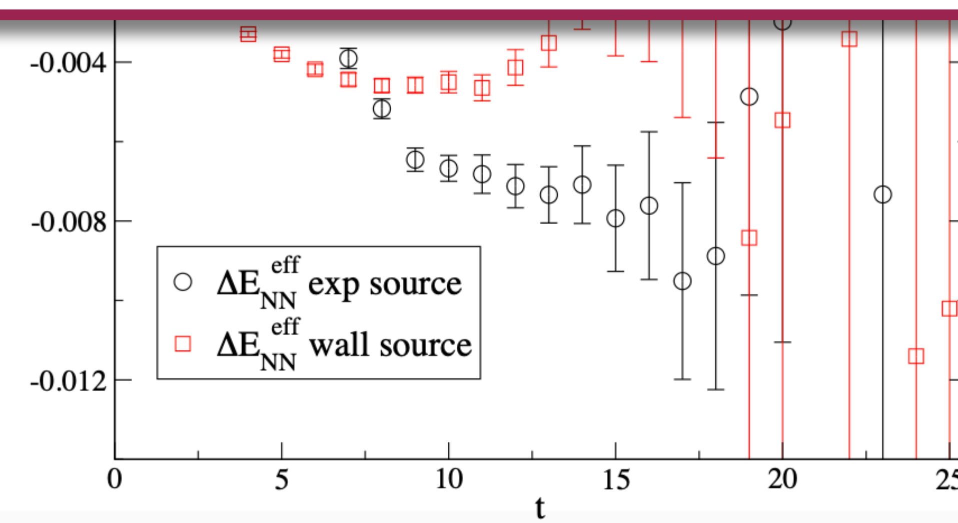


HAL QCD Consistency Checks [1703.07210]



Operator dependence of spectrum [1607.06371]

Correlated difference



Yamazaki et al (2017)

Off-diagonal vs GEVP;
Position space vs Momentum space
(elastic contributions)

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- Correlator matrix for a set of operators, $\{\mathcal{O}_i\}$: $C_{ij}(t) = \langle \mathcal{O}_i(t)\mathcal{O}_j^\dagger(0)\rangle$

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- Computationally simplest: off-diagonal "point-to-all" (hexaquark to momentum)
    - Matrix Prony (NPLQCD 2009) allows for multiple operators (generally ~2-3) to form linear combinations with better projections onto ground state
    - non-monotonic time dependence

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  - Matrix Prony (NPLQCD 2009) allows for multiple operators (generally ~2-3) to form linear combinations with better projections onto ground state
  - non-monotonic time dependence
- GEVP:
  - use full correlator matrix and find eigenvectors of $C(t_d)v_n(t_d, t_0) = \lambda_n C(t_0)v_n(t_d, t_0)$, then rotate correlator matrix using eigenvectors
  - excited state contamination on nth eigenvalue $\sim e^{-(E_{N+1}-E_n)t}$
  - large operator basis possible
  - energies approached from above with time
  - highly successful for meson systems

Expectations from EFT (in a box)

$$\mathcal{L}_{\text{eff}} = \psi^\dagger \left(i\partial_\tau + \frac{\nabla^2}{2M} \right) \psi + g_0 \left(\psi^\dagger \psi \right)^2$$

p²

Expectations from EFT (in a box)

- Two point-like nucleons interact via contact interactions

$$\mathcal{L}_{\text{eff}} = \psi^\dagger \left(i\partial_\tau + \frac{\nabla^2}{2M} \right) \psi + g_0 \left(\psi^\dagger \psi\right)^2$$

  - Valid for energies $<\sim$ m_π (same requirements as Luscher)

p^2

Expectations from EFT (in a box)

- Two point-like nucleons interact via contact interactions
  - Valid for energies <~ m_π (same requirements as Luscher)
- Calculate two-particle transfer matrix, $\mathscr{T} = e^H$, with periodic spatial BCs; diagonalize to extract the exact spectrum

$$\mathcal{L}_{\rm eff} = \psi^\dagger \left(i\partial_\tau + \frac{\nabla^2}{2M} \right) \psi + g_0 \left(\psi^\dagger \psi \right)^2$$

$$\langle pq|\mathcal{T}|p'q'\rangle = \frac{\delta_{pp'}\delta_{qq'} + \frac{g_0}{V}\delta_{p+q,p'+q'}}{\sqrt{\xi(p)\xi(q)\xi(q')\xi(p')}}$$

$$\xi(p) \equiv 1 + \frac{\Delta(q)}{M}$$

Endres, Kaplan, Lee, Nicholson (2011)

p^2

Expectations from EFT (in a box)

- Two point-like nucleons interact via contact interactions
    - Valid for energies <~ m_π (same requirements as Luscher)
- Calculate two-particle transfer matrix, $\mathscr{T} = e^{H}$, with periodic spatial BCs; diagonalize to extract the exact spectrum
    - Vary the interaction between the nucleons to investigate systems with and without a bound state

$$\mathcal{L}_{\text{eff}} = \psi^\dagger \left(i\partial_\tau + \frac{\nabla^2}{2M} \right) \psi + g_0 \left(\psi^\dagger \psi \right)^2$$

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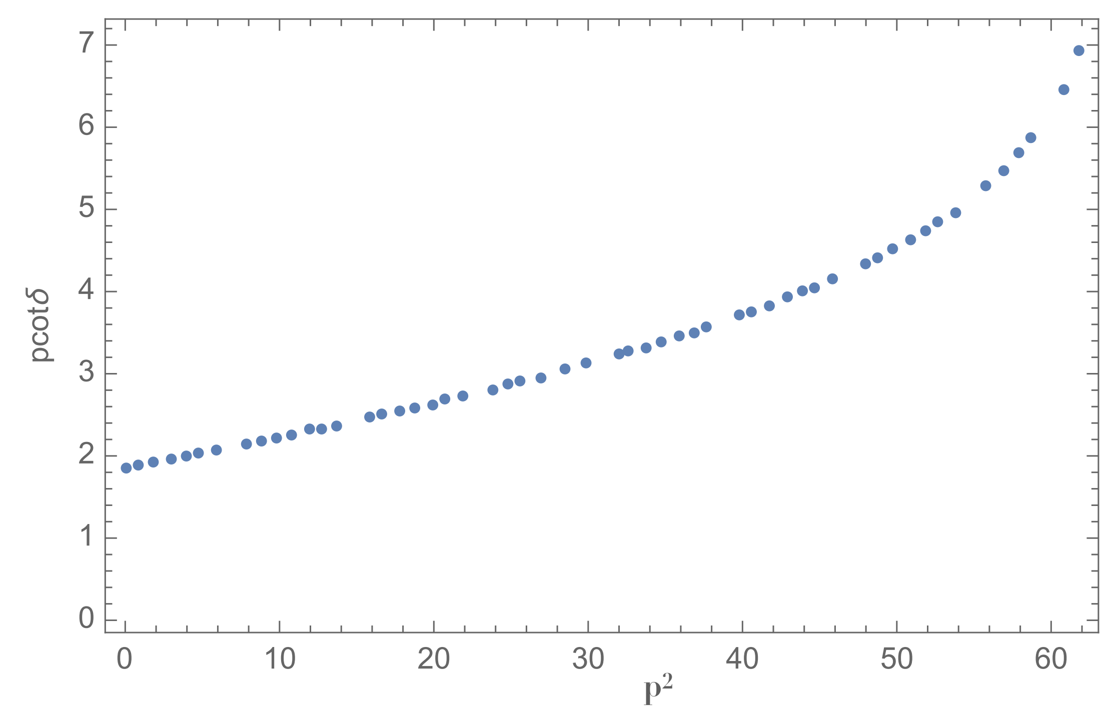
Endres, Kaplan, Lee, Nicholson (2011)



Expectations from EFT (in a box)

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  - Vary the interaction between the nucleons to investigate systems with and without a bound state
- Form correlation functions via $C(t) = (e^H)^t$
  - Investigate correlation functions for various different (elastic) ops for different physical scenarios

$$\mathcal{L}_{\text{eff}} = \psi^\dagger \left(i\partial_\tau + \frac{\nabla^2}{2M} \right) \psi + g_0 \left(\psi^\dagger \psi \right)^2$$

$$\langle pq|\mathcal{T}|p'q'\rangle = \frac{\delta_{pp'}\delta_{qq'} + \frac{g_0}{V}\delta_{p+q,p'+q'}}{\sqrt{\xi(p)\xi(q)\xi(q')\xi(p')}}$$

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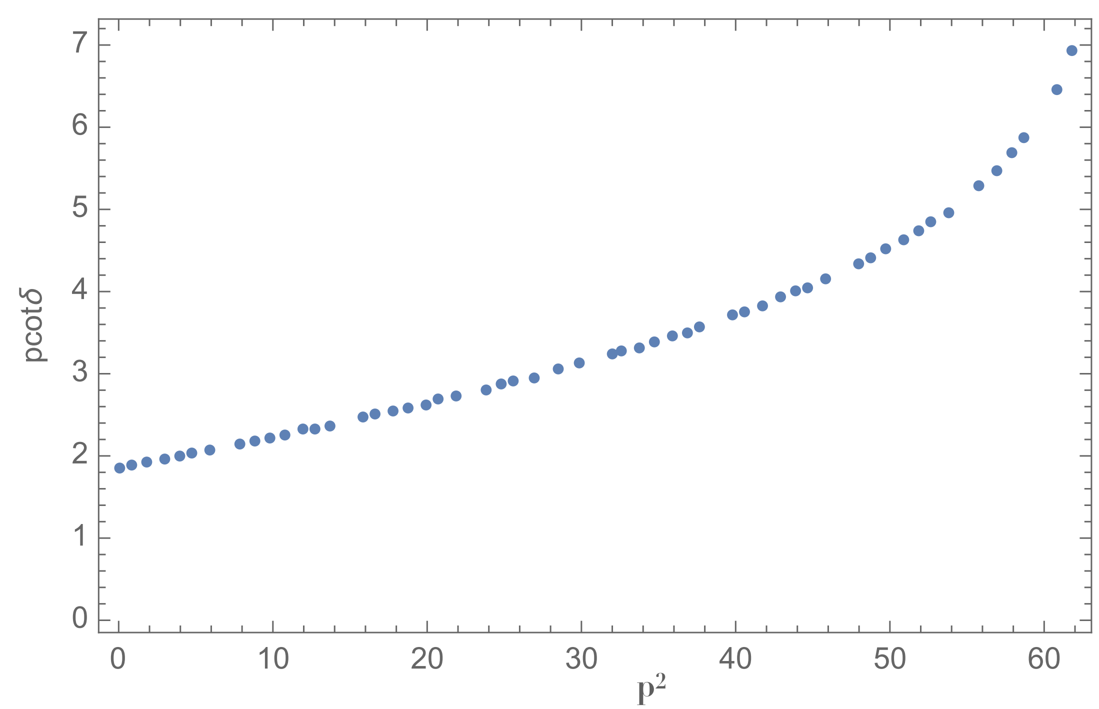
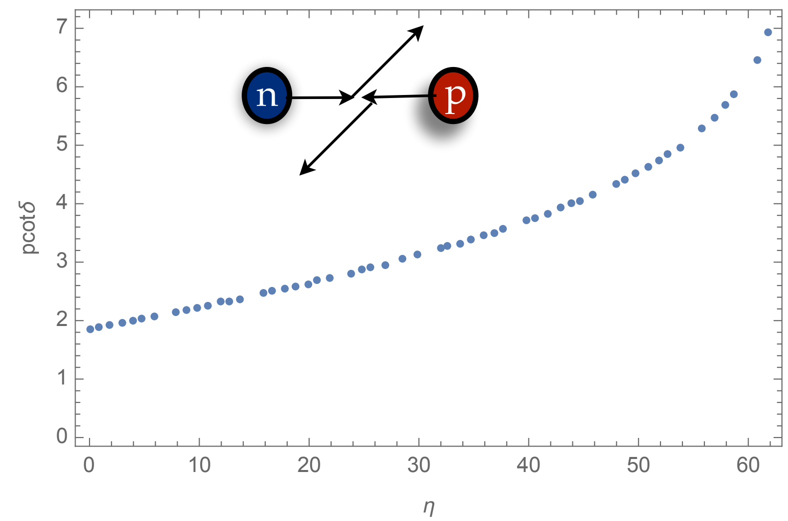
Endres, Kaplan, Lee, Nicholson (2011)

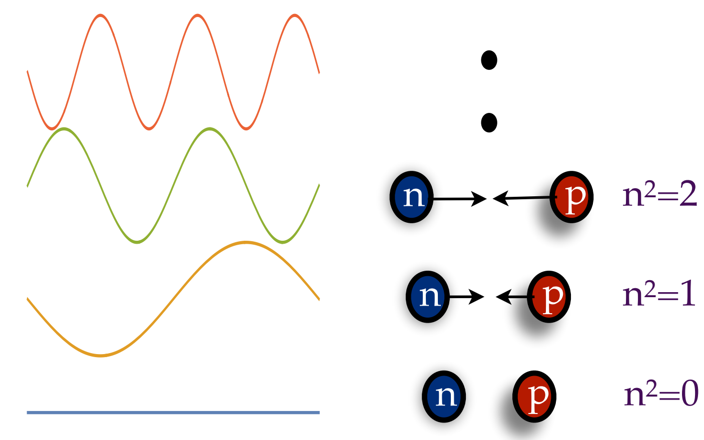


No bound state

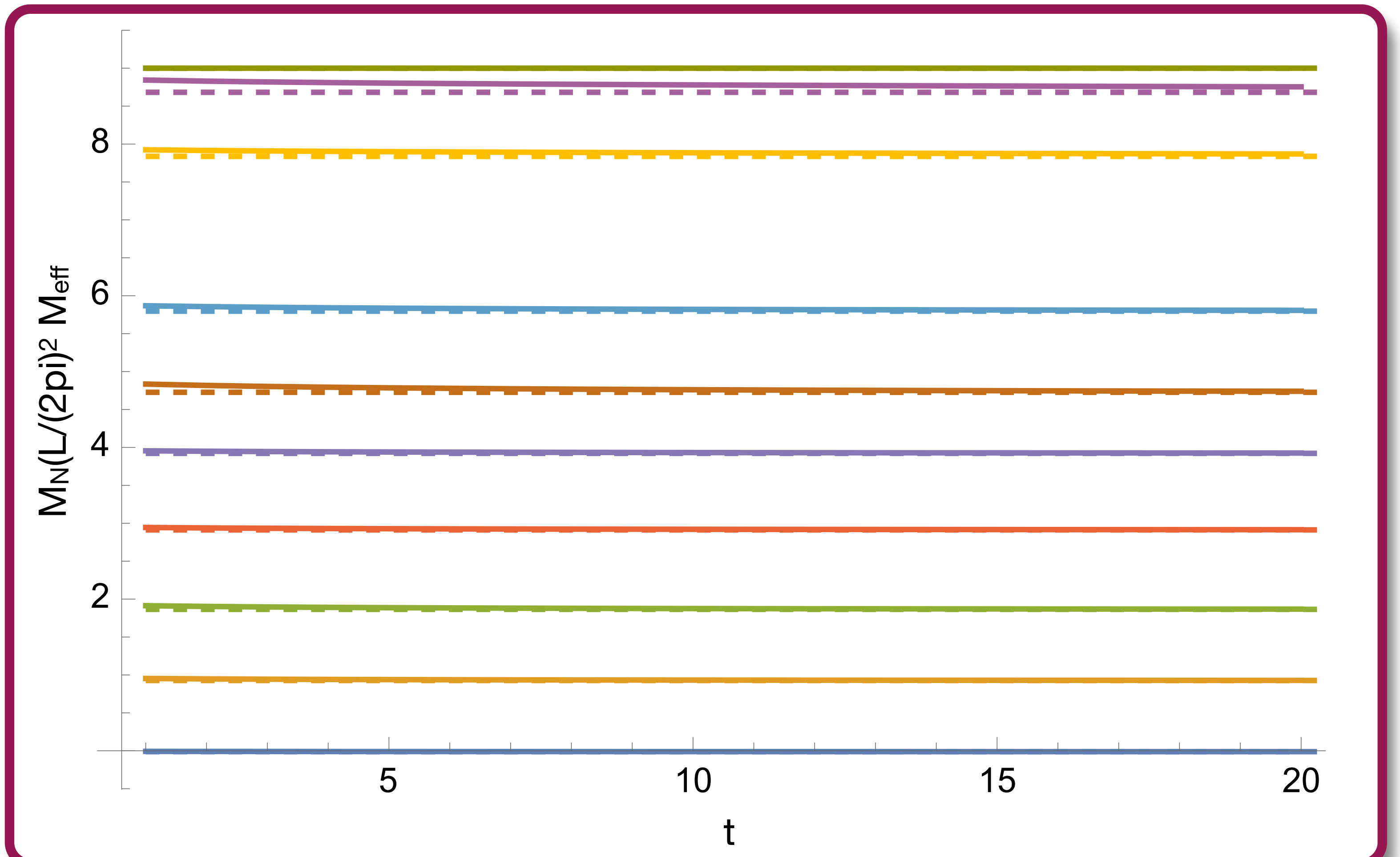
Physical:



Operators:

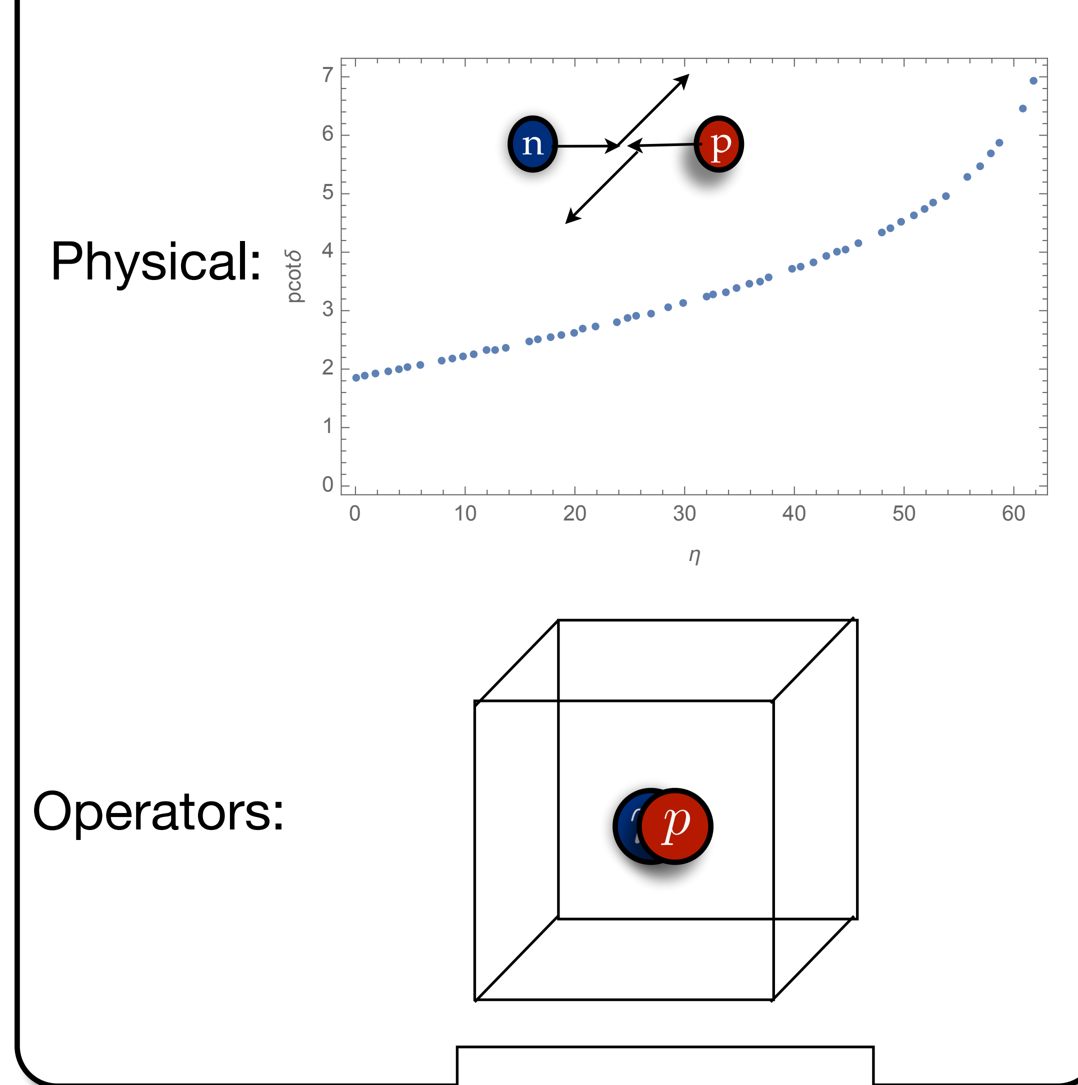


GEVP: 10 momentum ops

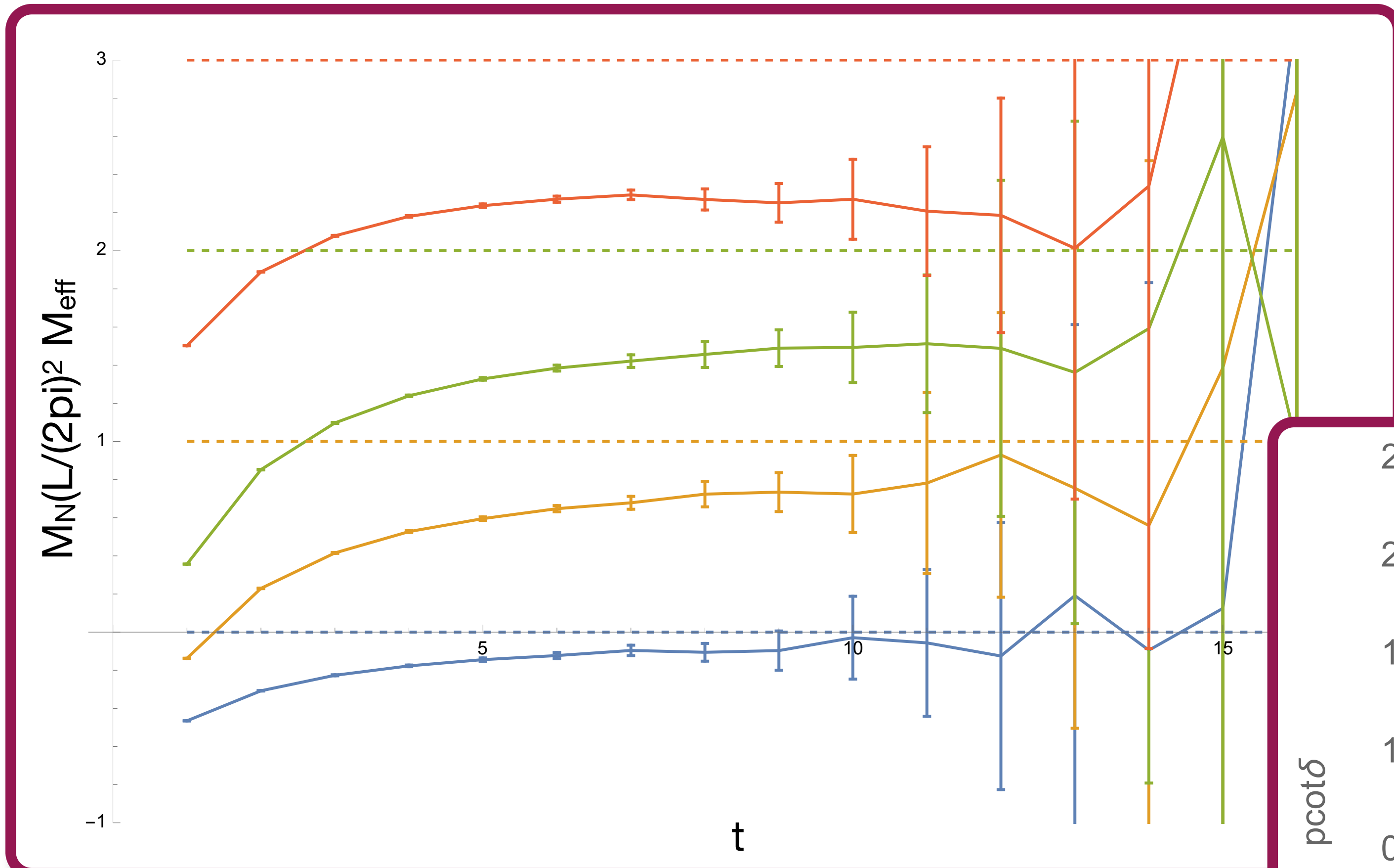


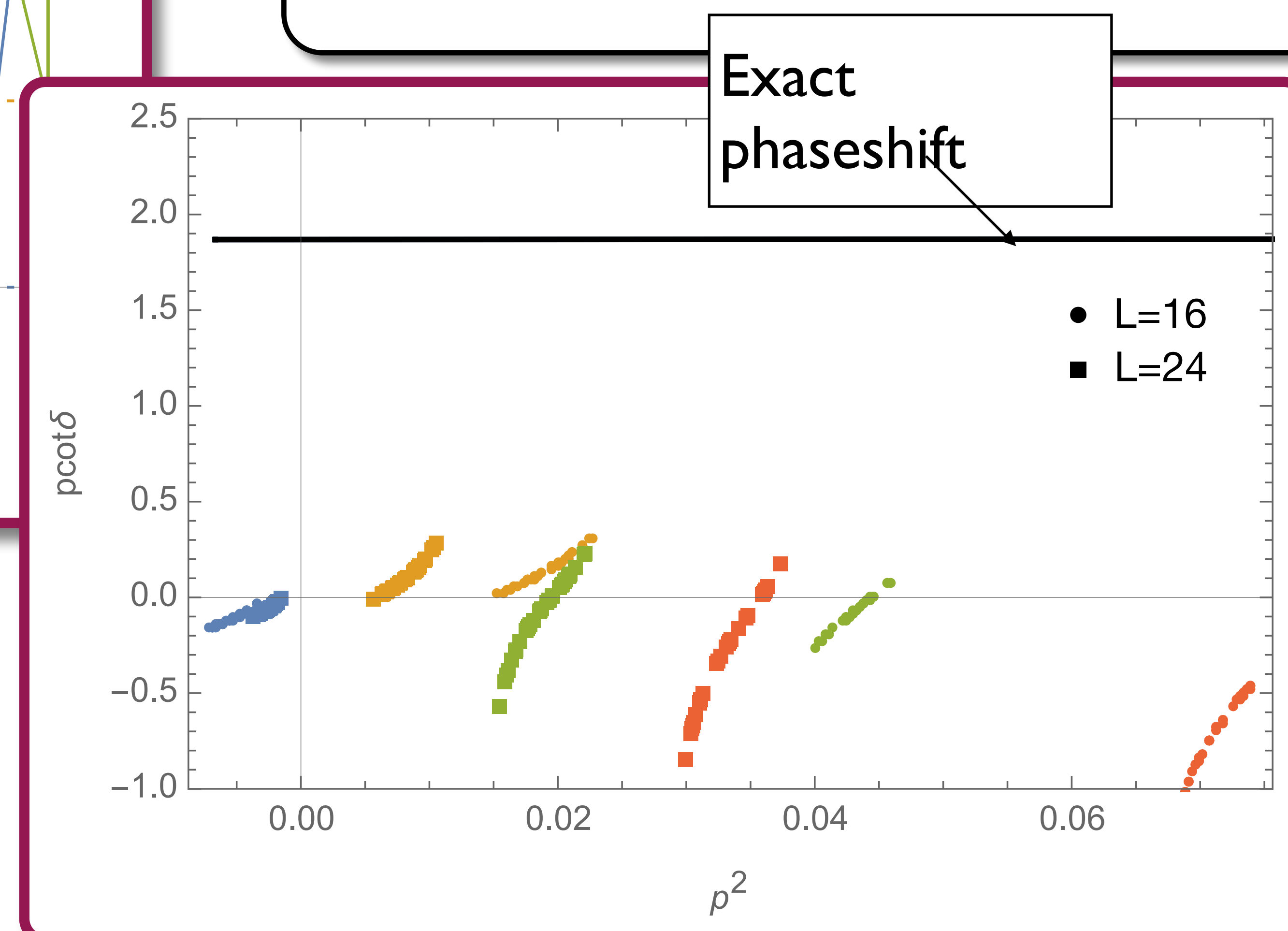
Dashed lines give exact spectrum

No bound state

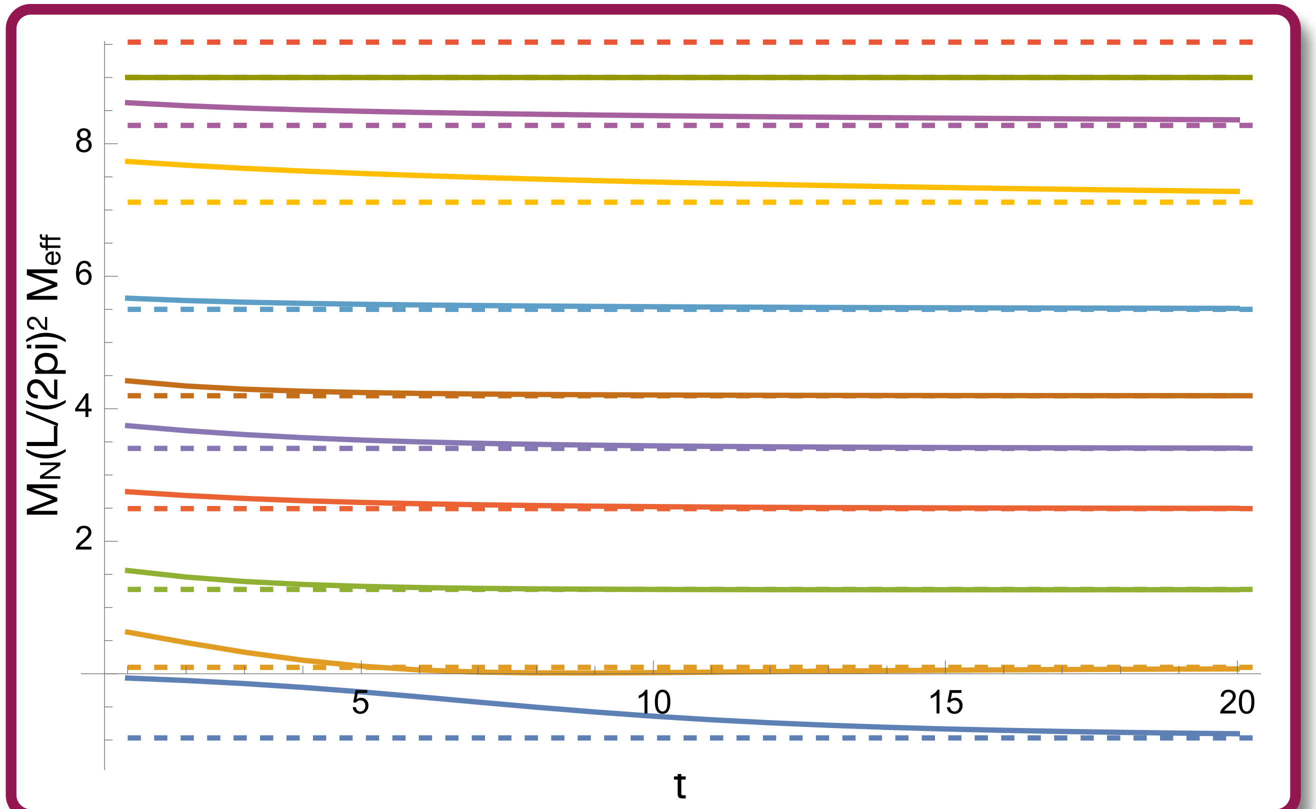


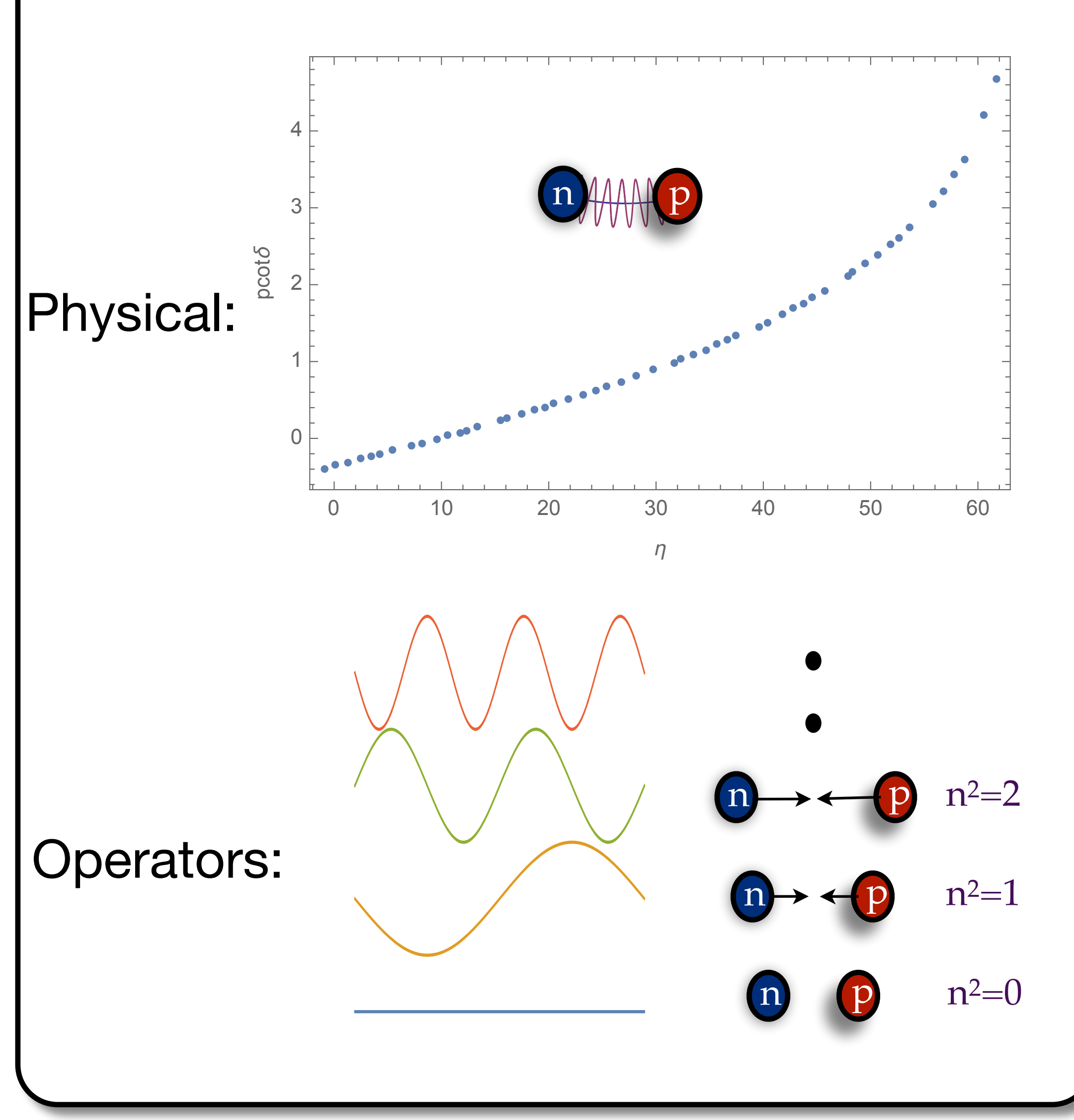
Off-diagonal: hexaquark -> momentum





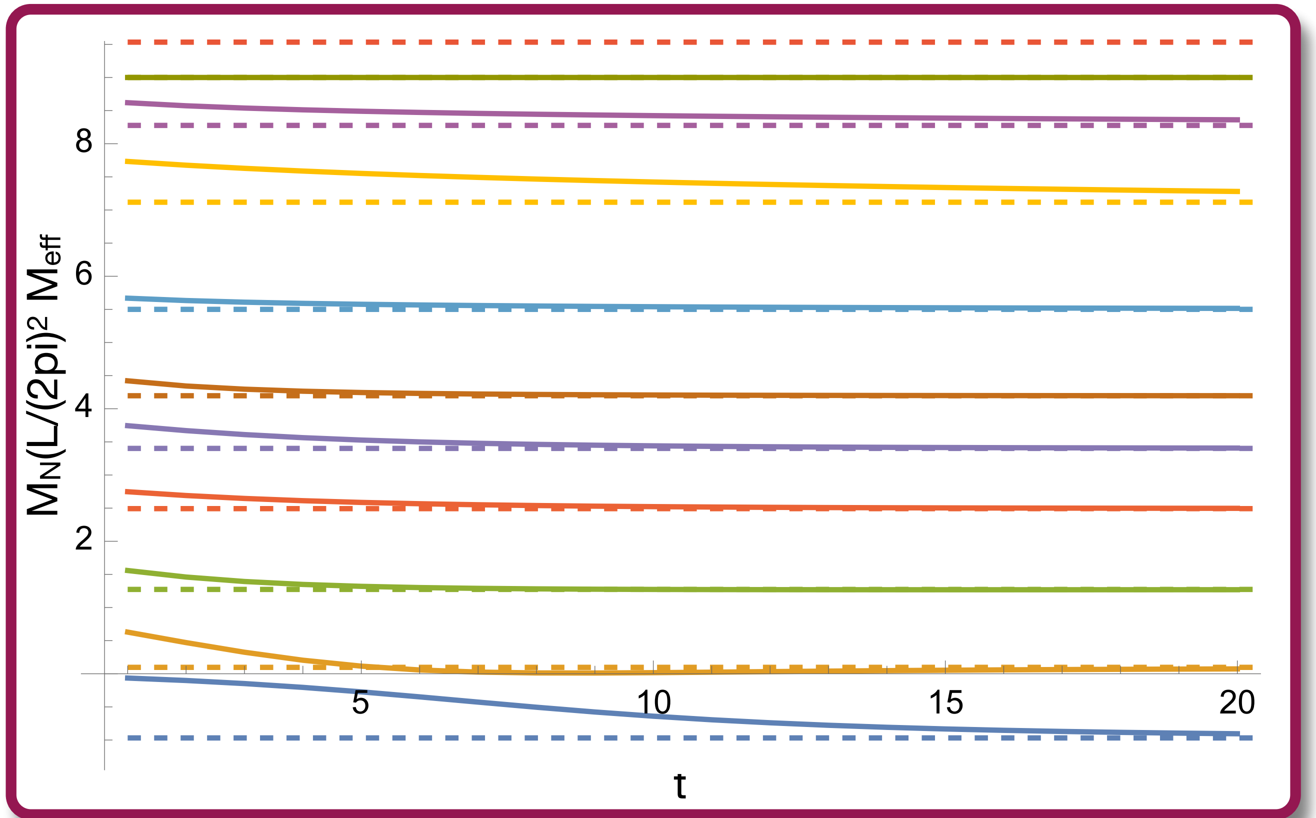
Bound state



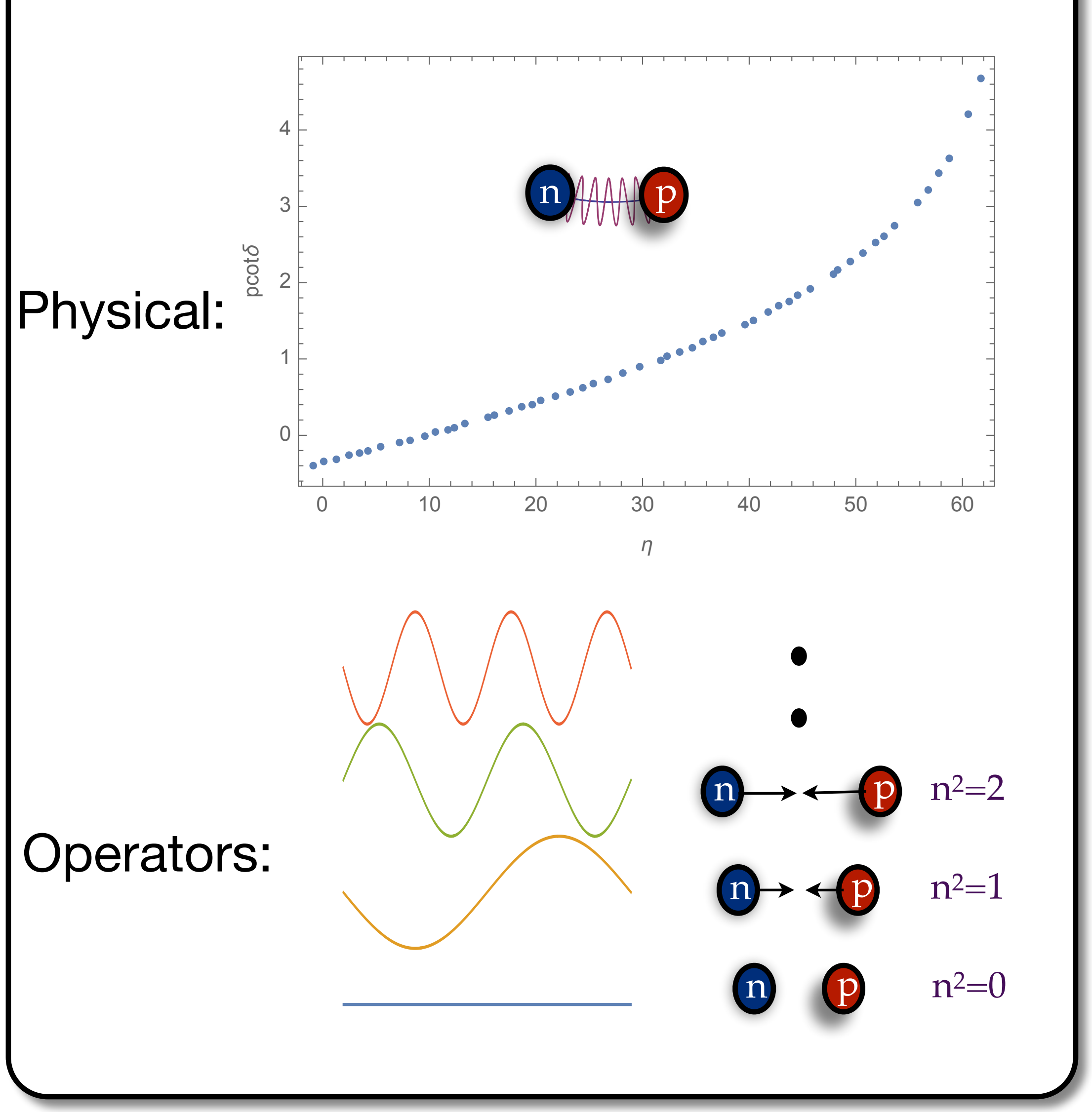


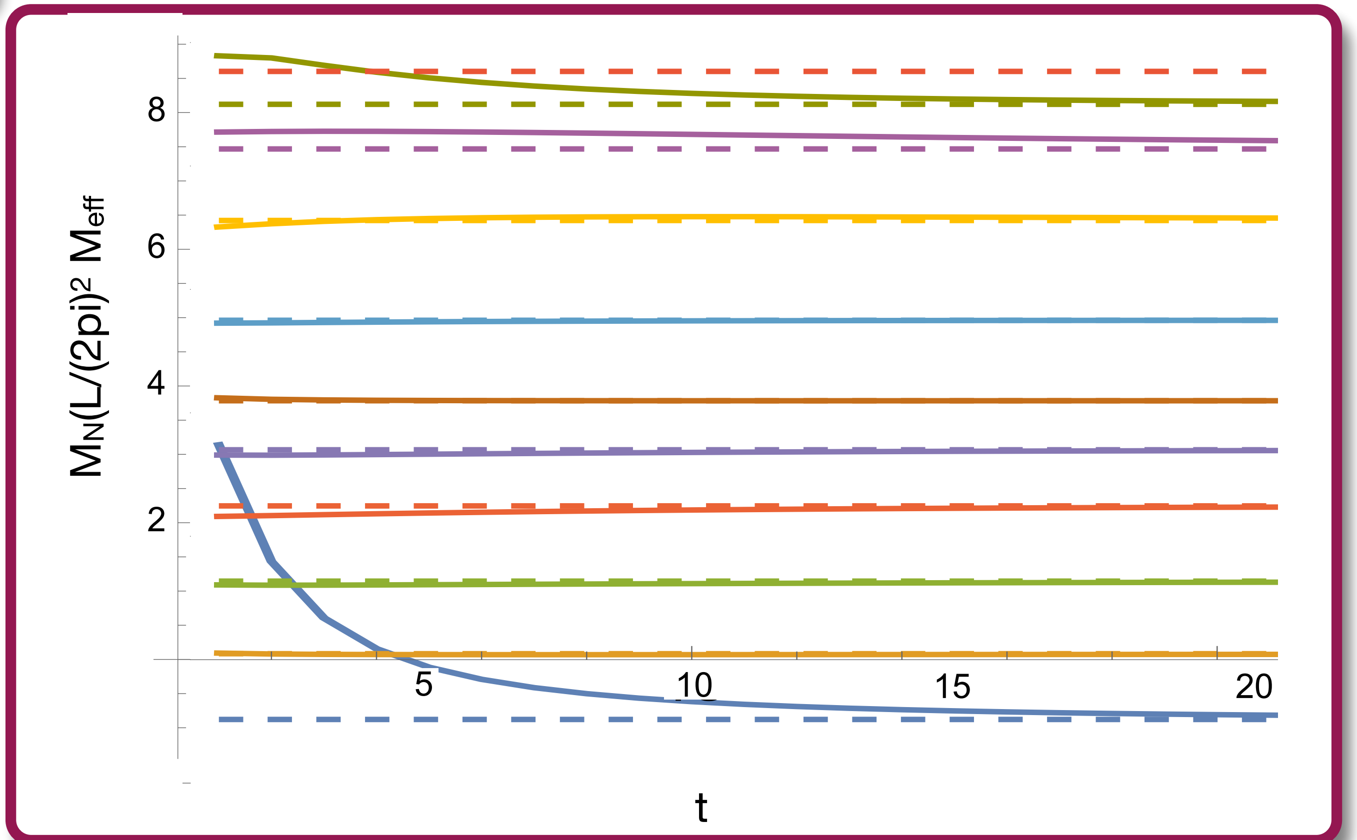
GEVP: 10 momentum ops

Bound state



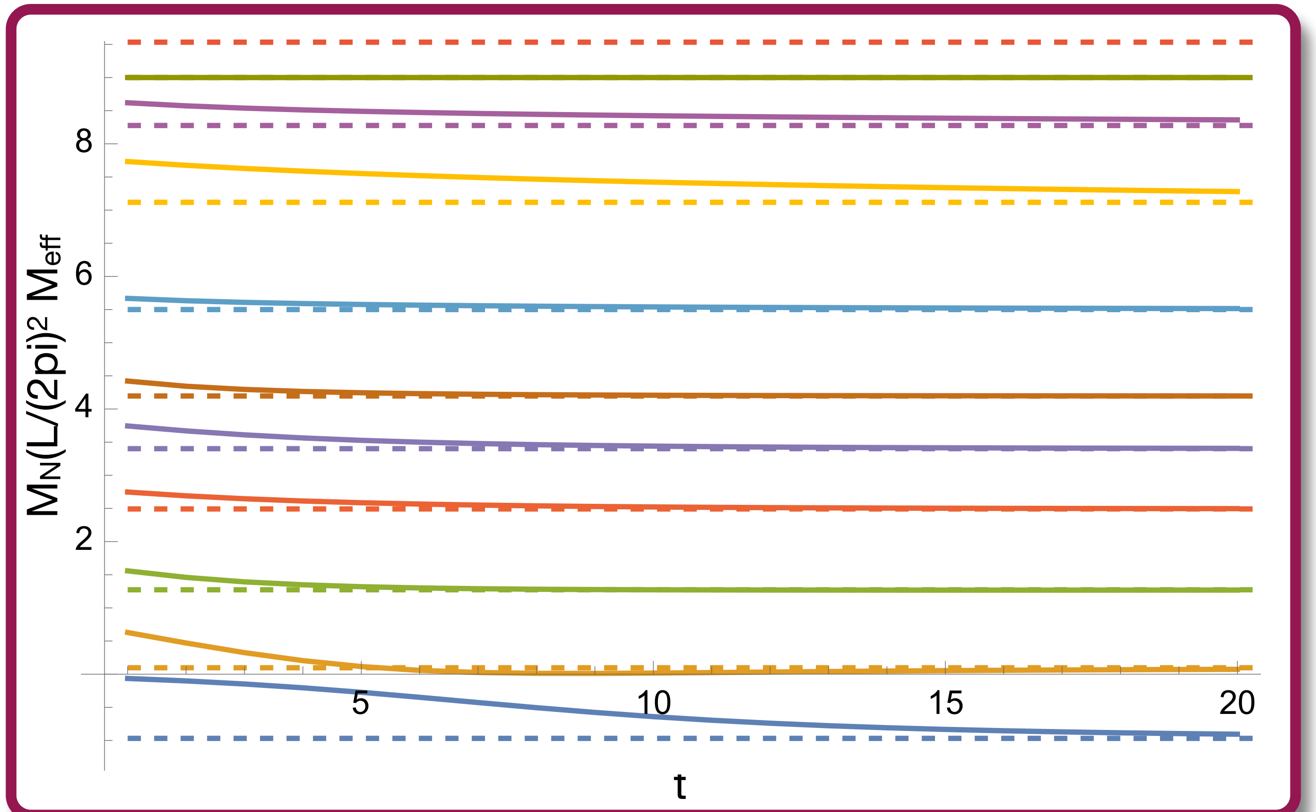
GEVP: 10 momentum ops

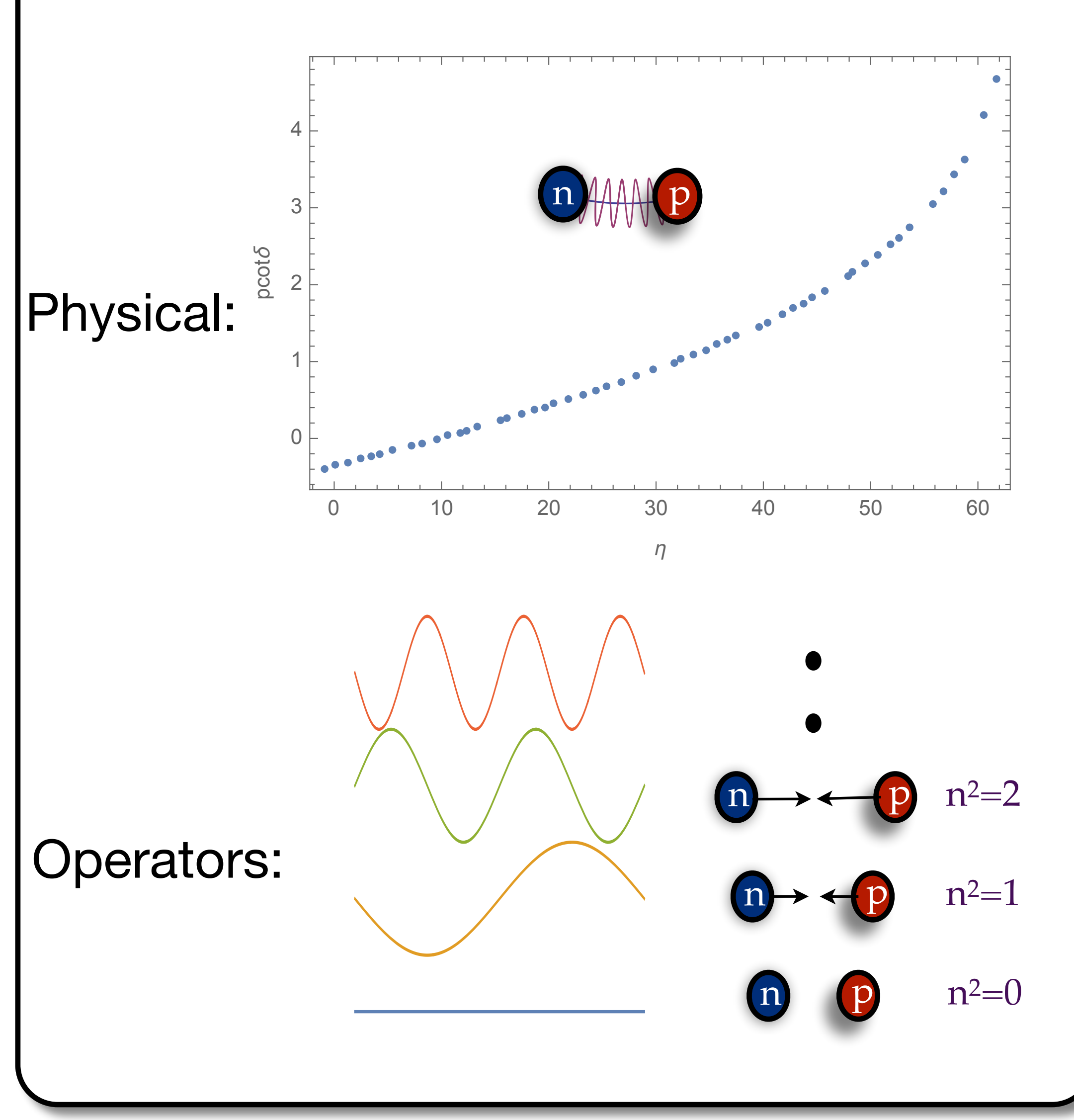




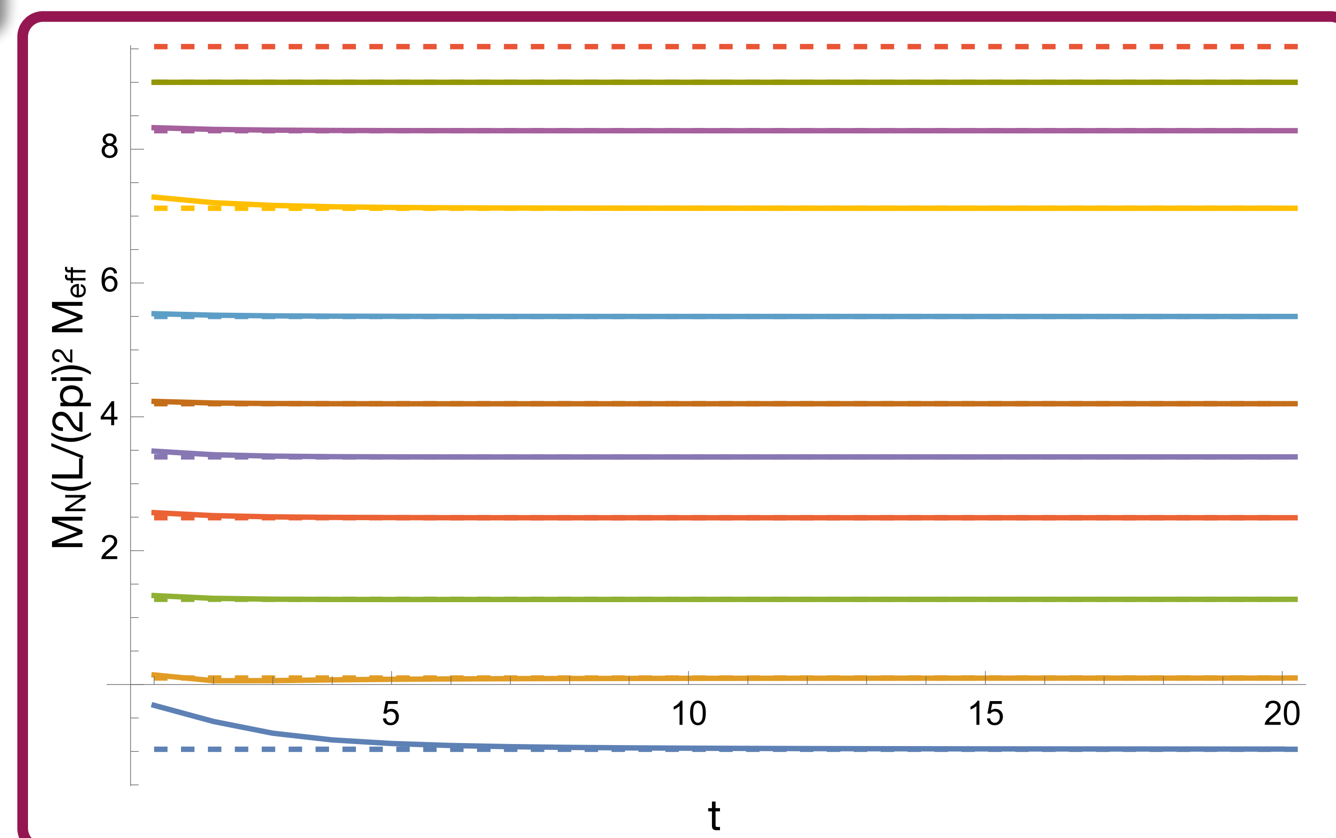
GEVP: 10 mom ops + hexaquark

Bound state



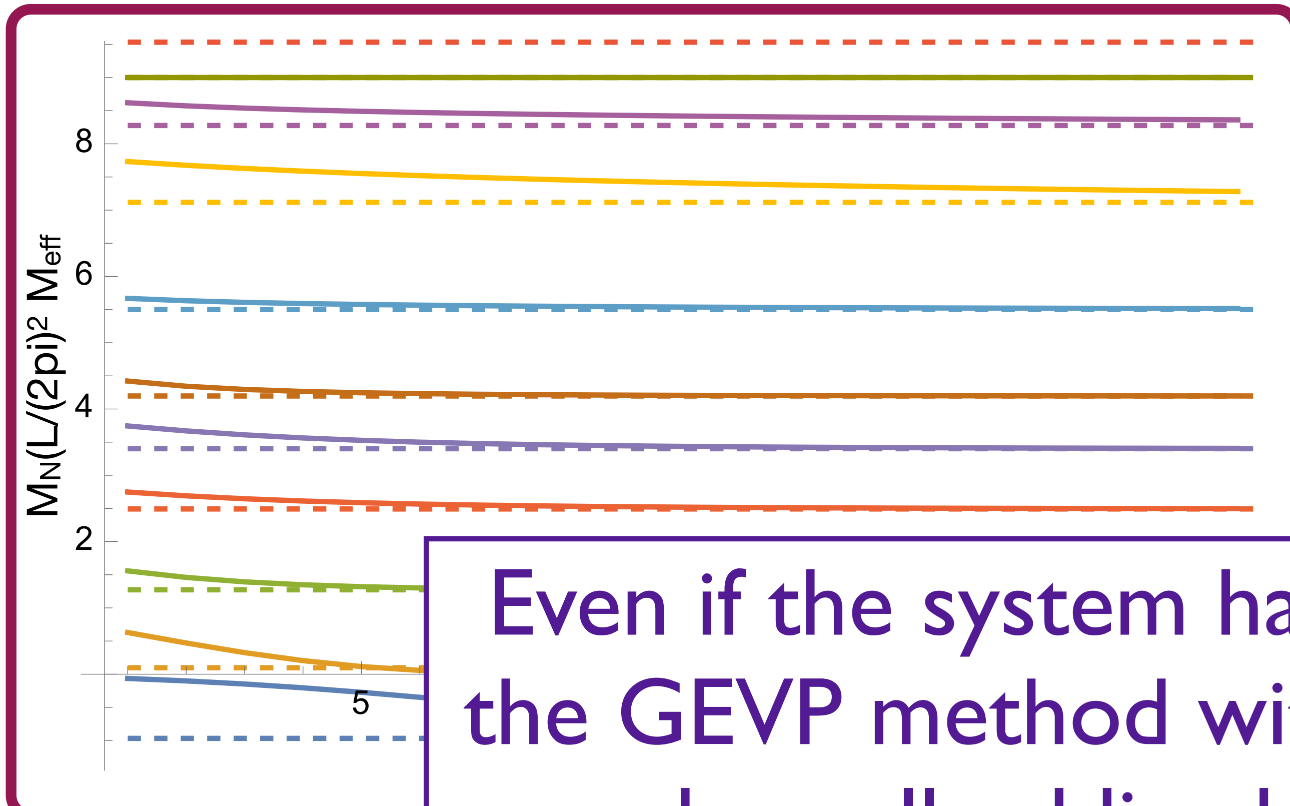


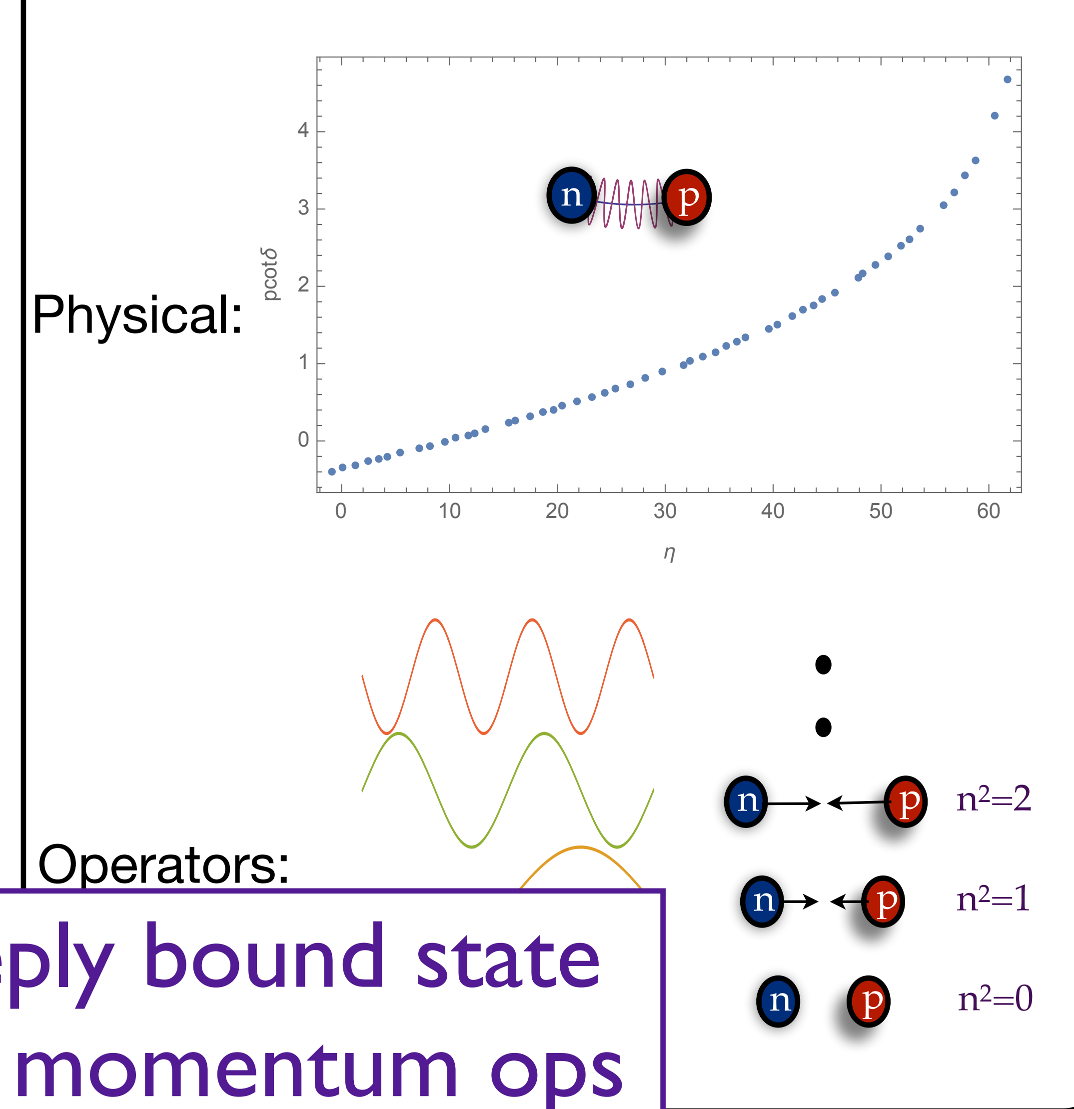
GEVP: 10 momentum ops



GEVP: 30 momentum ops

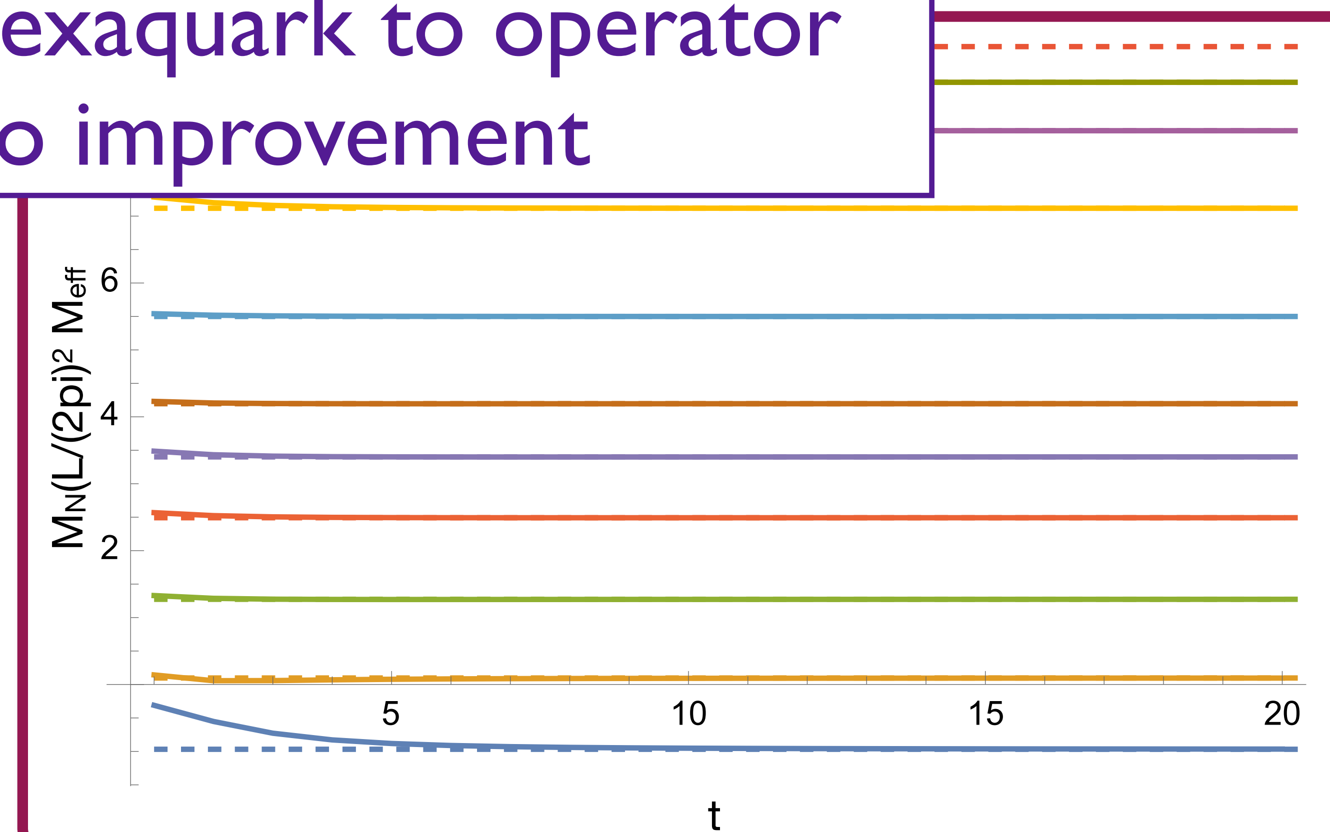
Bound state





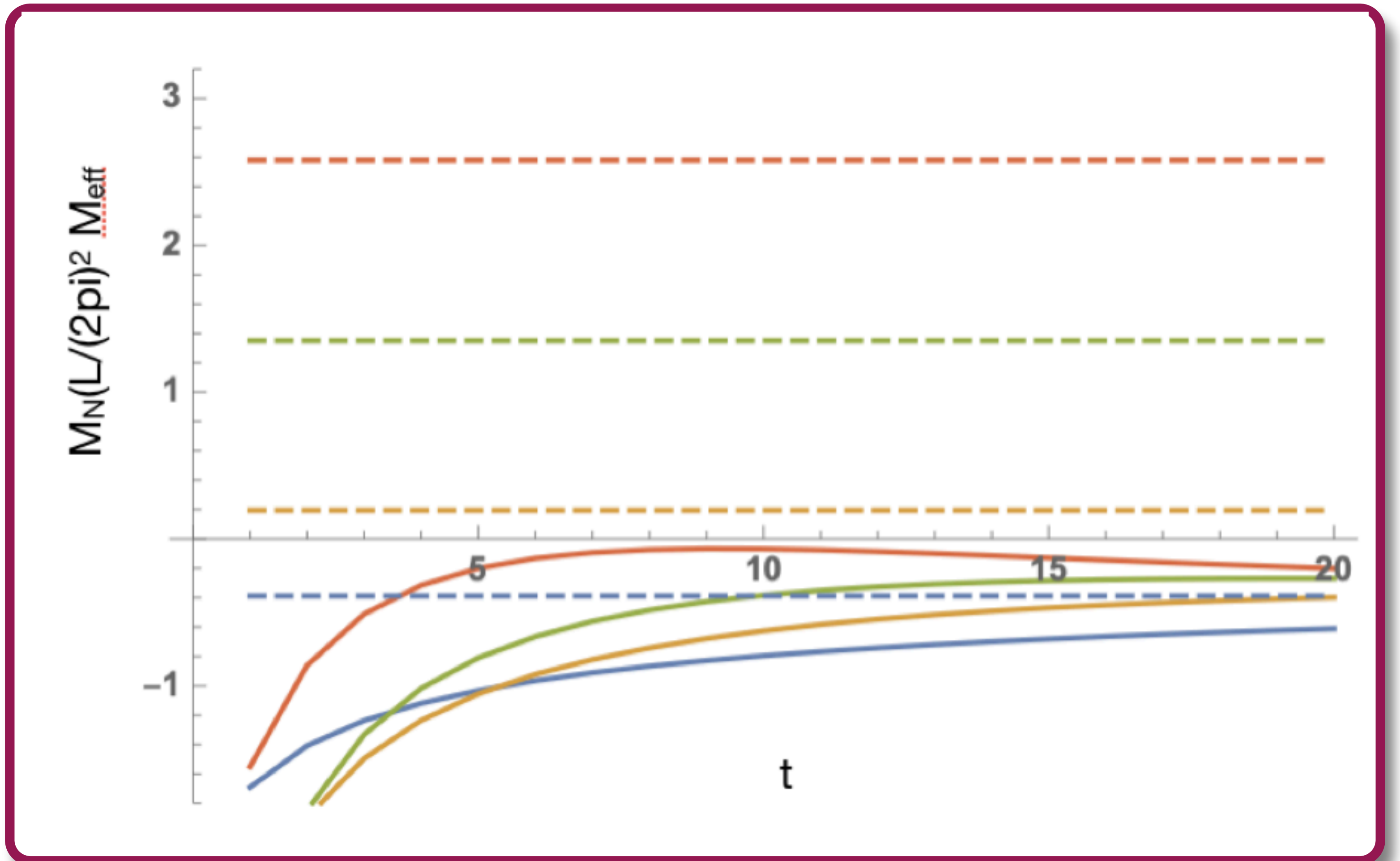
Even if the system has a deeply bound state the GEVP method with only momentum ops works well; adding hexaquark to operator basis shows no improvement

GEVP: 1(

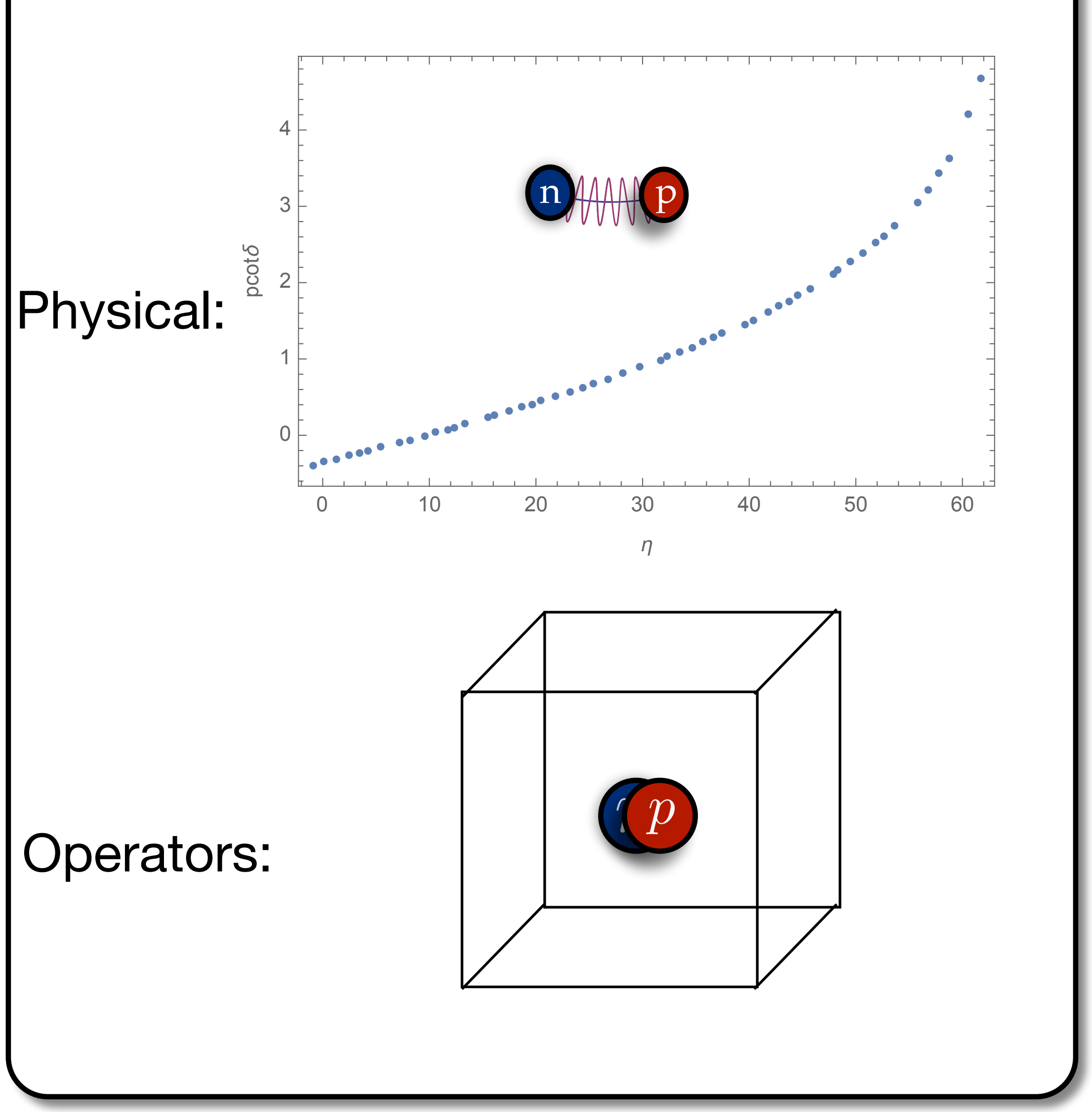


GEVP: 30 momentum ops

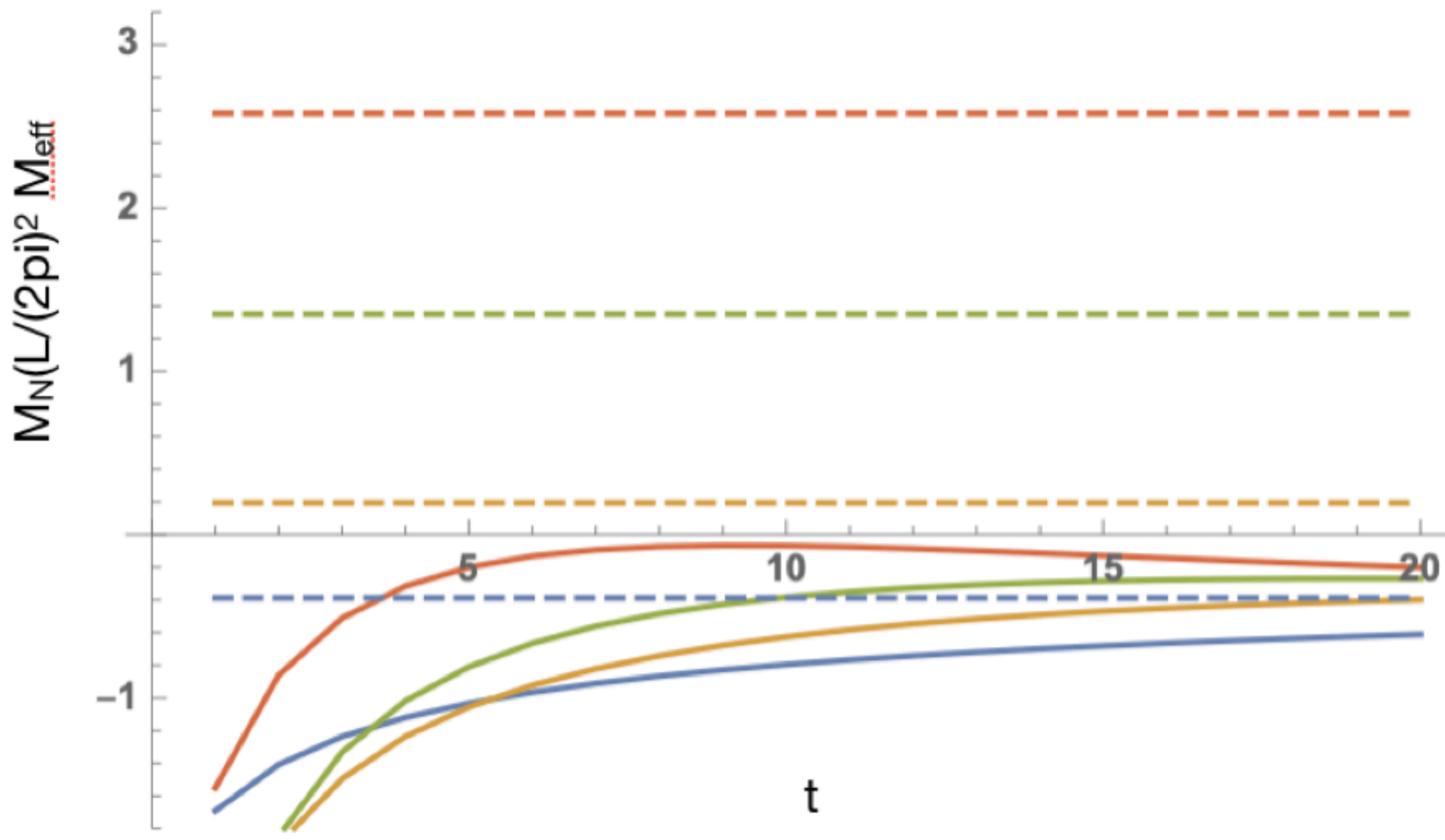
Bound state



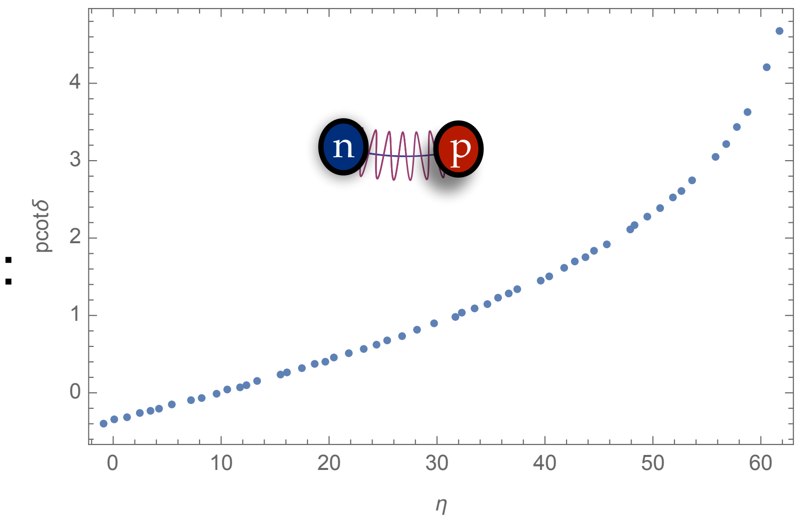
Off-diagonal: hexaquark -> momentum



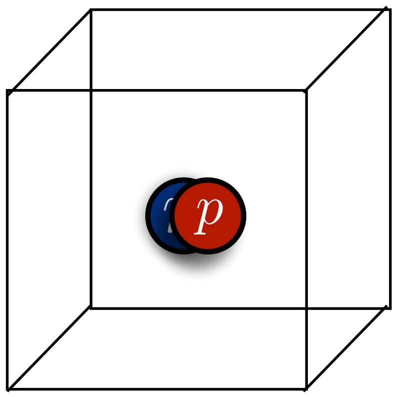
Bound state



Physical:

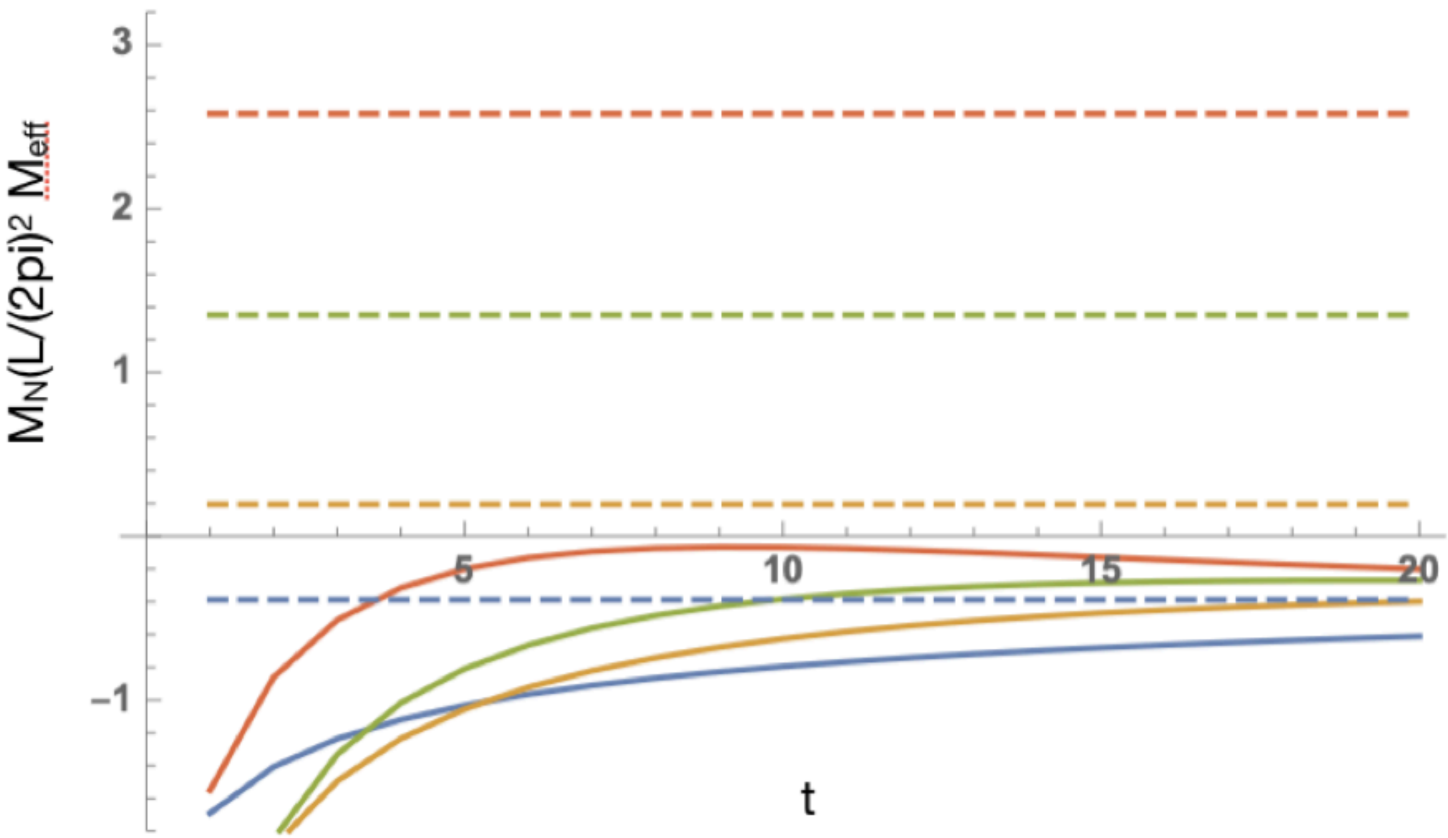


Operators:

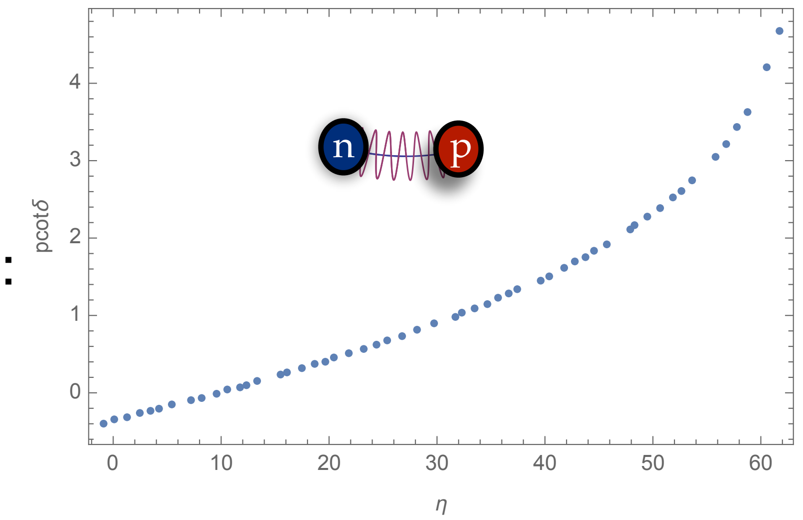


1. This is not the behavior seen in LQCD hexaquark calculations - they look more like the situation shown previously for a system with no physical bound state

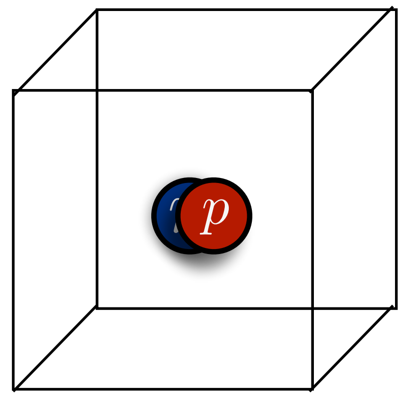
Bound state



Physical:



Operators:



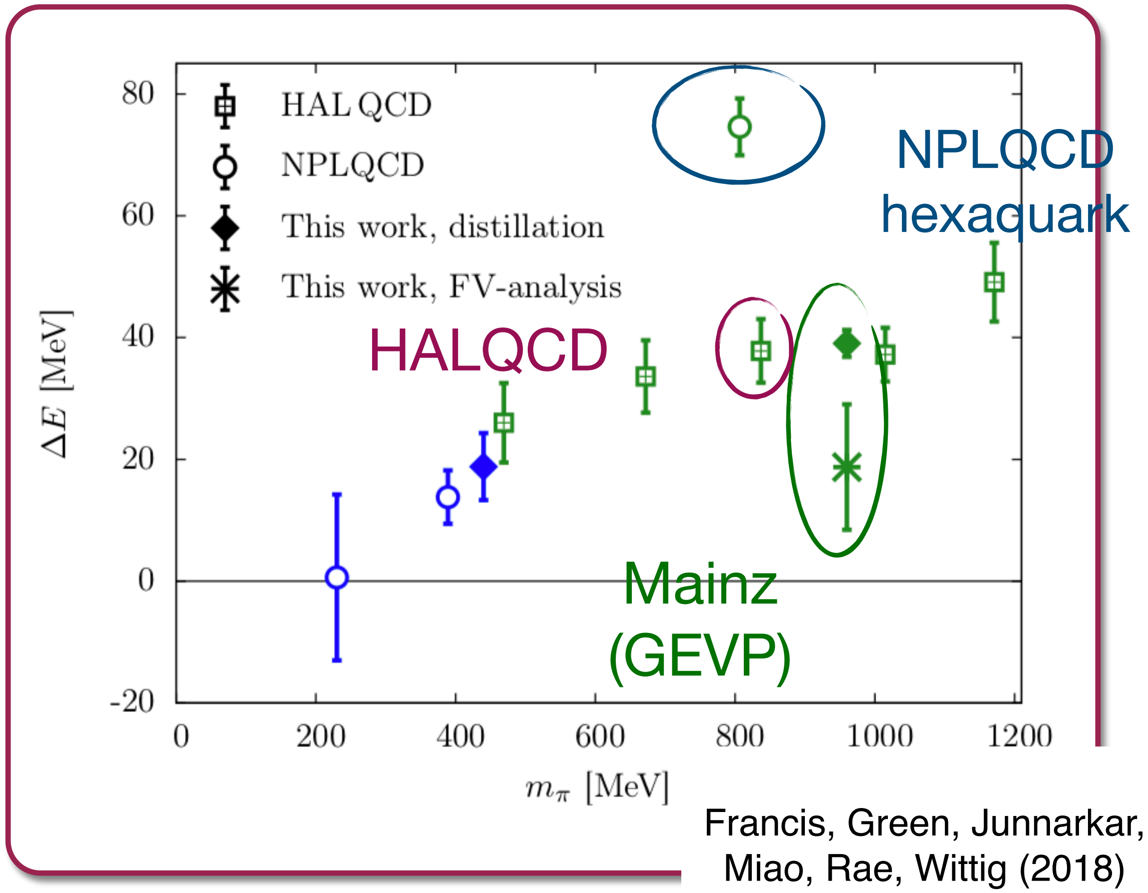
1. This is not the behavior seen in LQCD hexaquark calculations - they look more like the situation shown previously for a system with no physical bound state

2. Even if the system has a physical deeply bound state the hexaquark correlator approaches the ground state very slowly - momentum state variational far superior

More recent Baryon-baryon calculations: GEVP

More recent Baryon-baryon calculations: GEVP

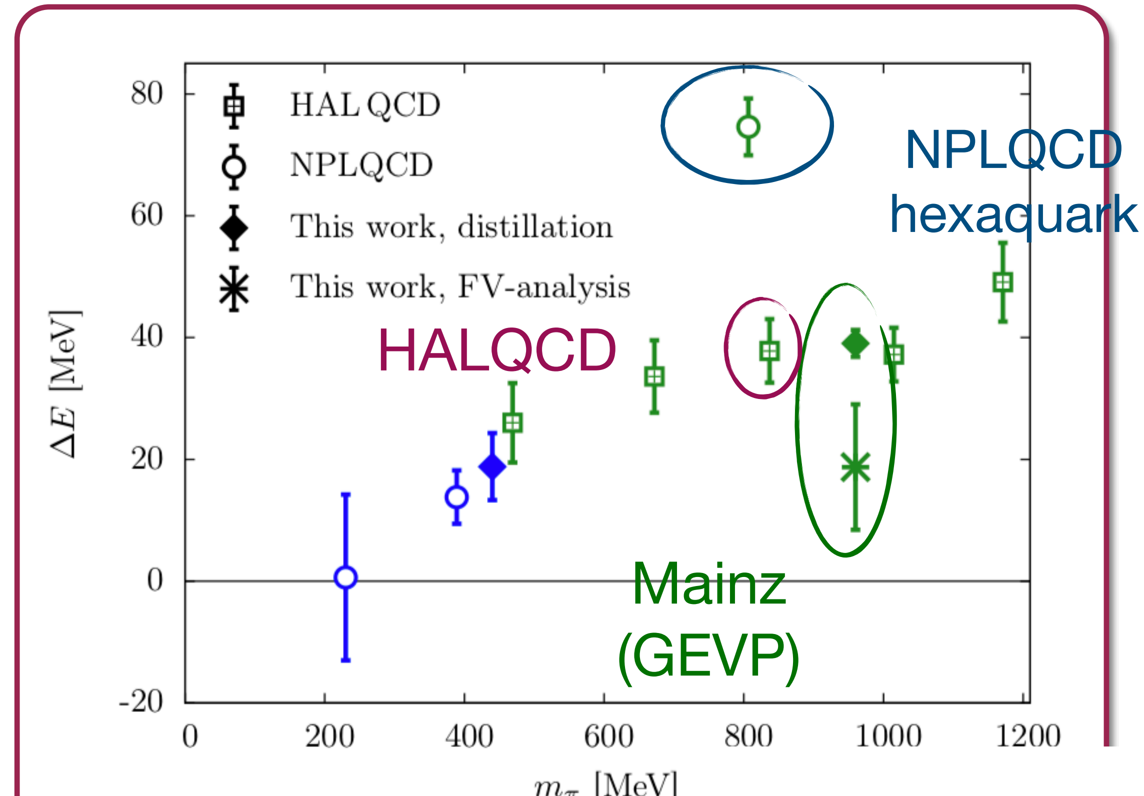
H-dibaryon



Francis, Green, Junnarkar, Miao, Rae, Wittig (2018)

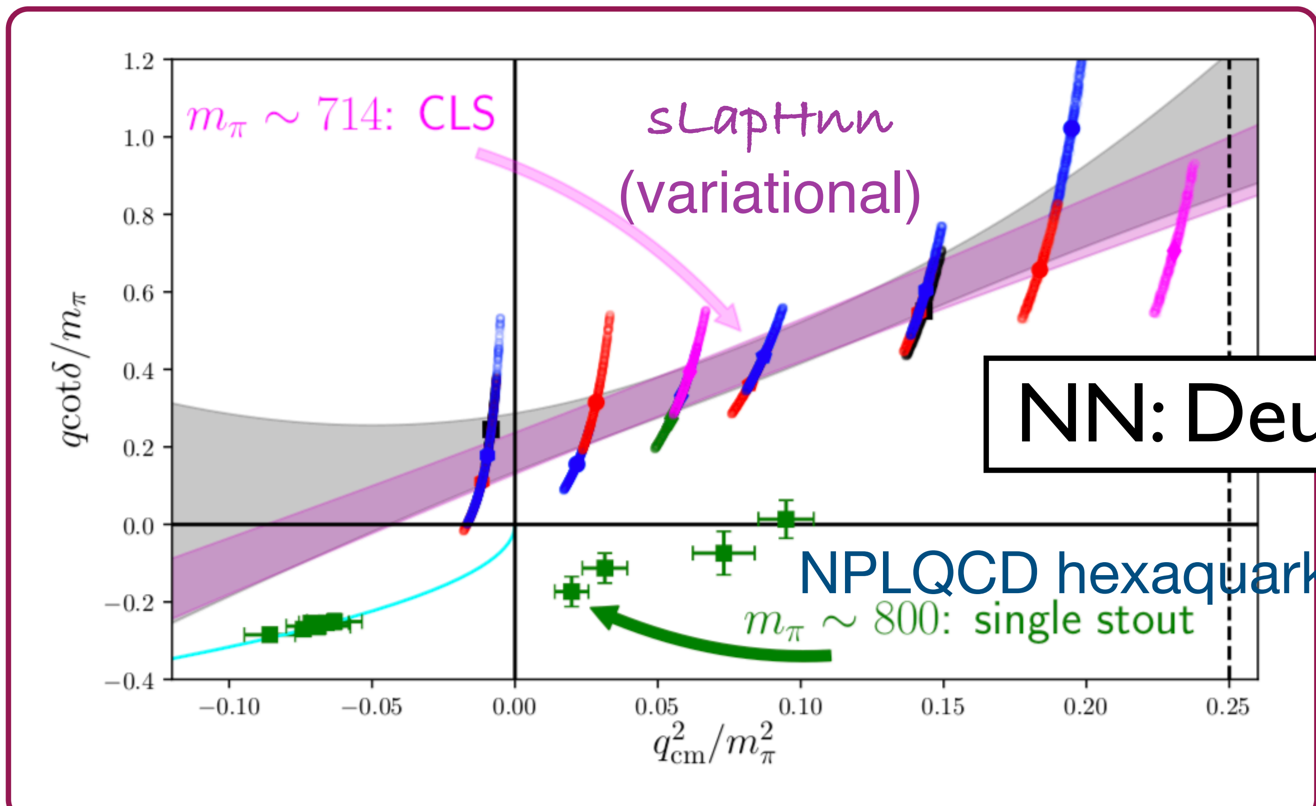
More recent Baryon-baryon calculations: GEVP

H-dibaryon

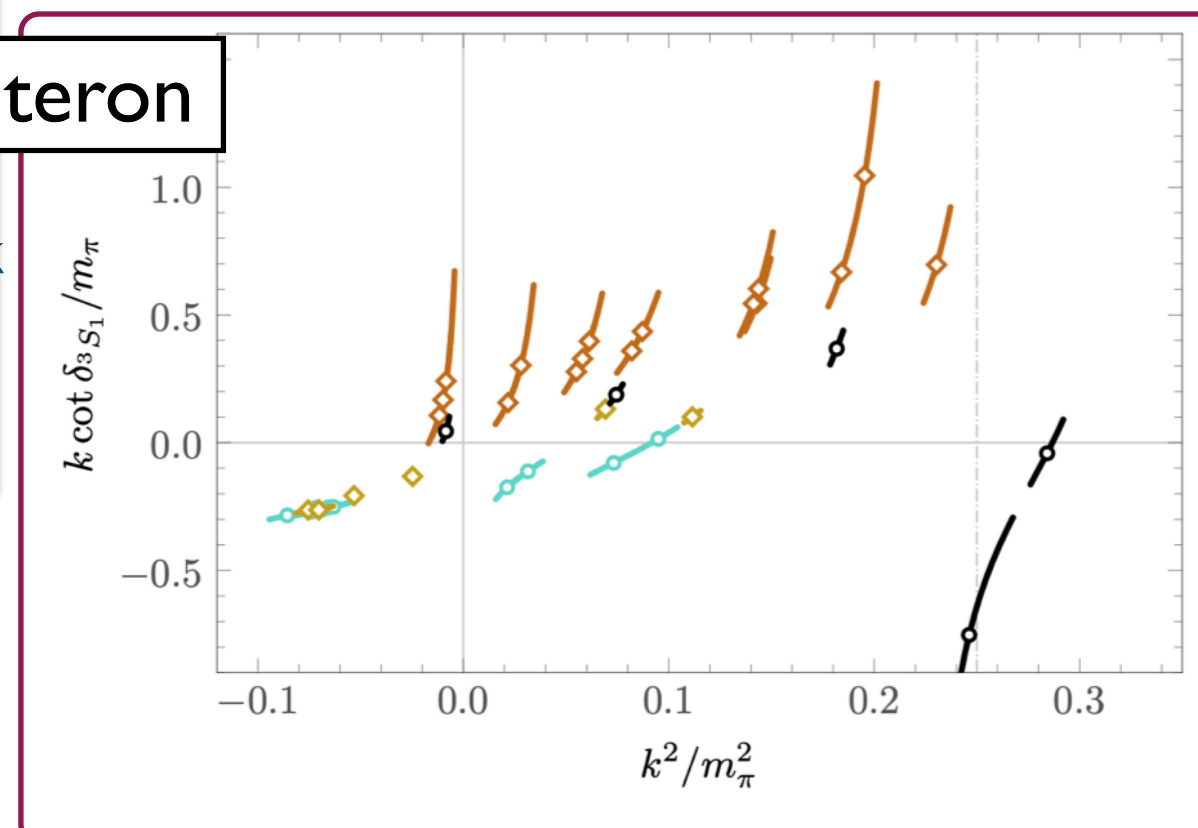


Francis, Green, Junnarkar, Miao, Rae, Wittig (2018)

NN: Deuteron



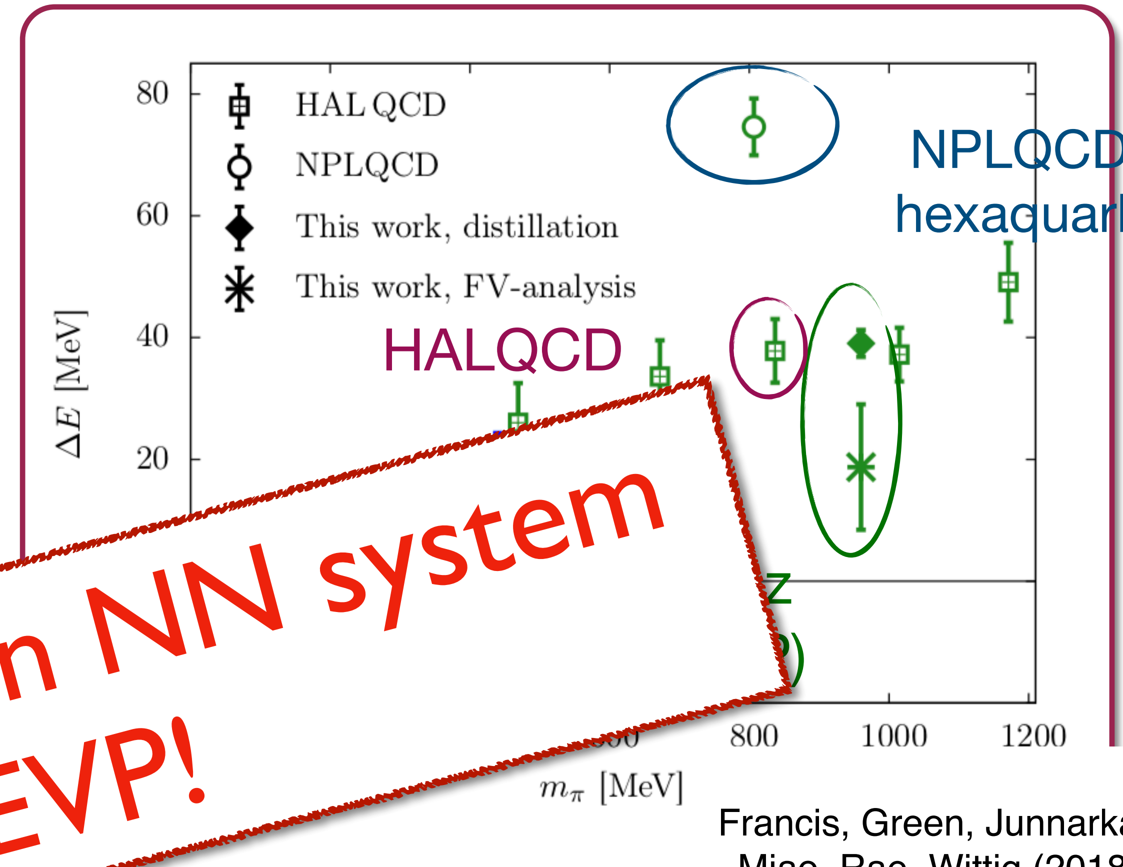
sLapHnn (2021)



NPLQCD GEVP (2022)

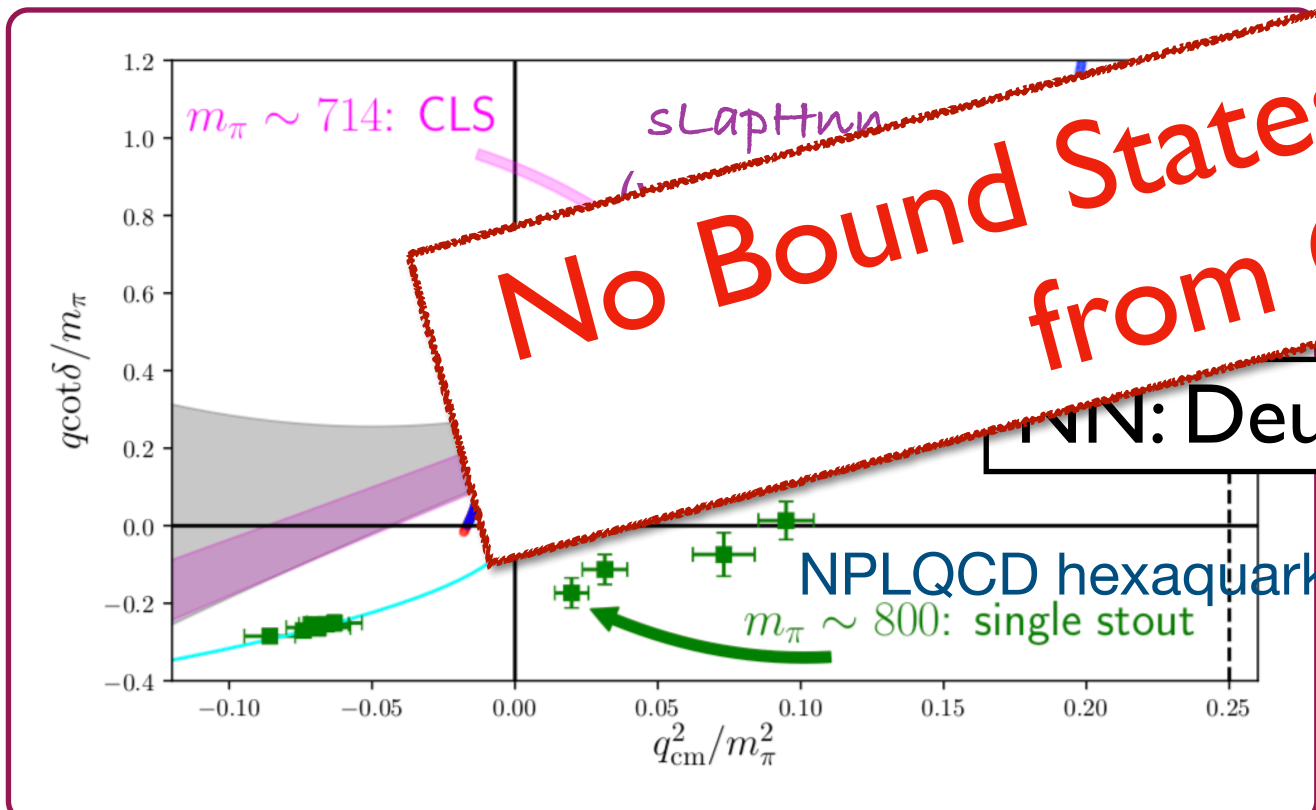
More recent Baryon-baryon calculations: GEVP

H-dibaryon



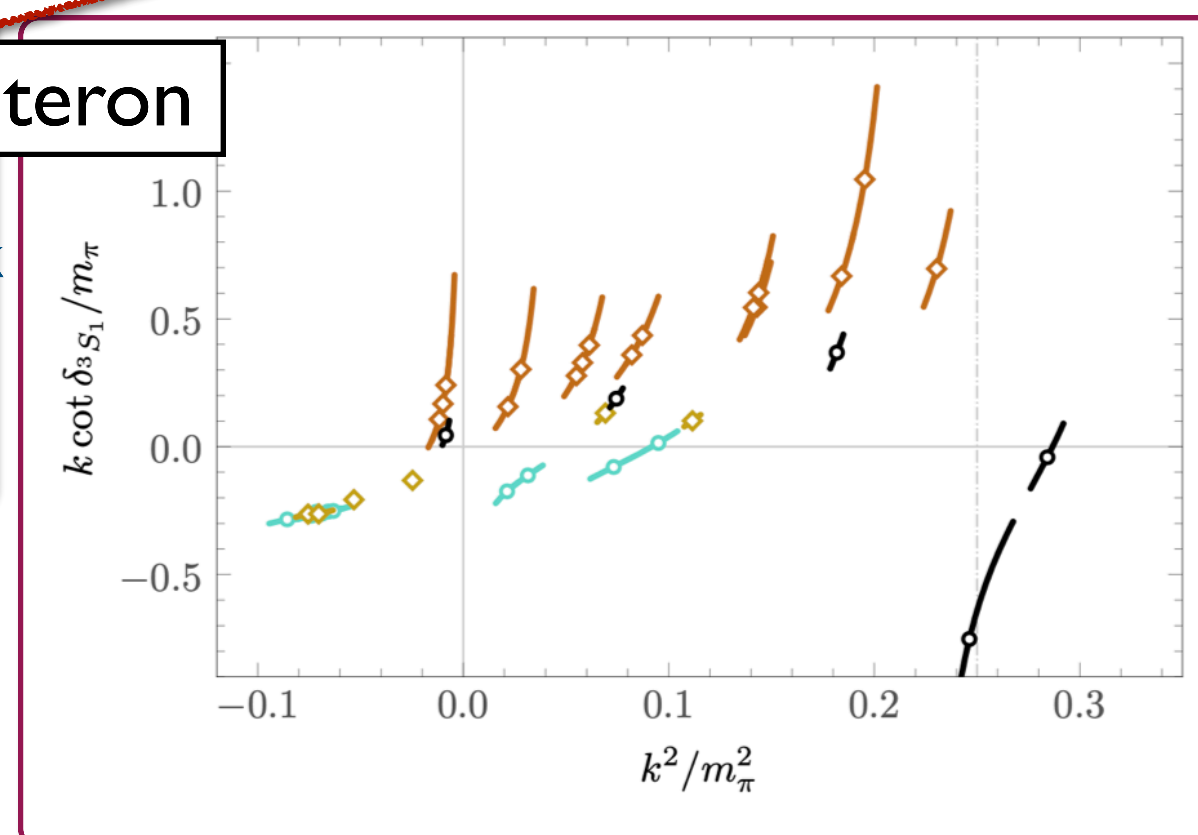
Francis, Green, Junnarkar, Miao, Rae, Wittig (2018)

No Bound States in NN system from GEVP!



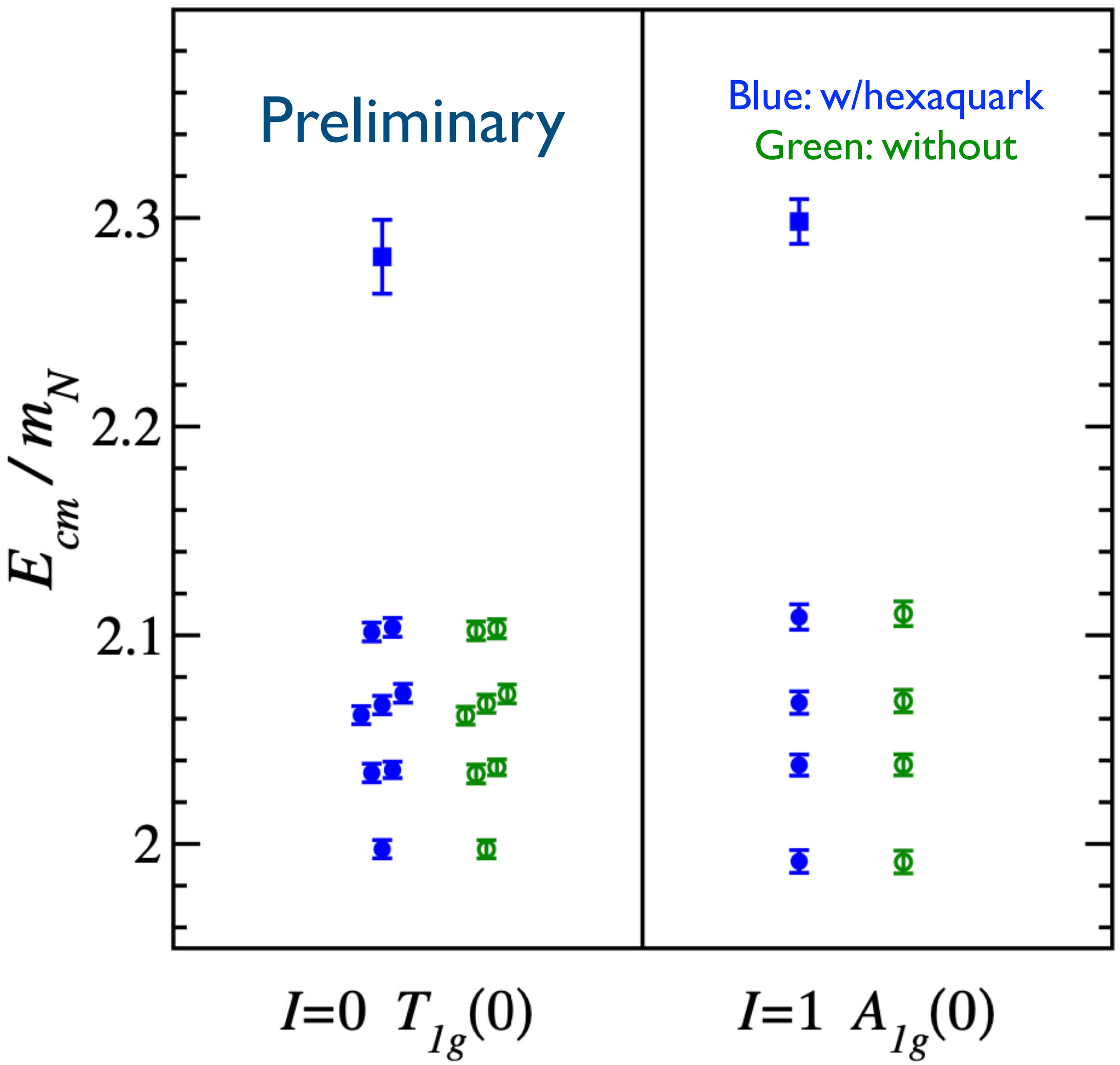
sLapHnn (2021)

NN: Deuteron

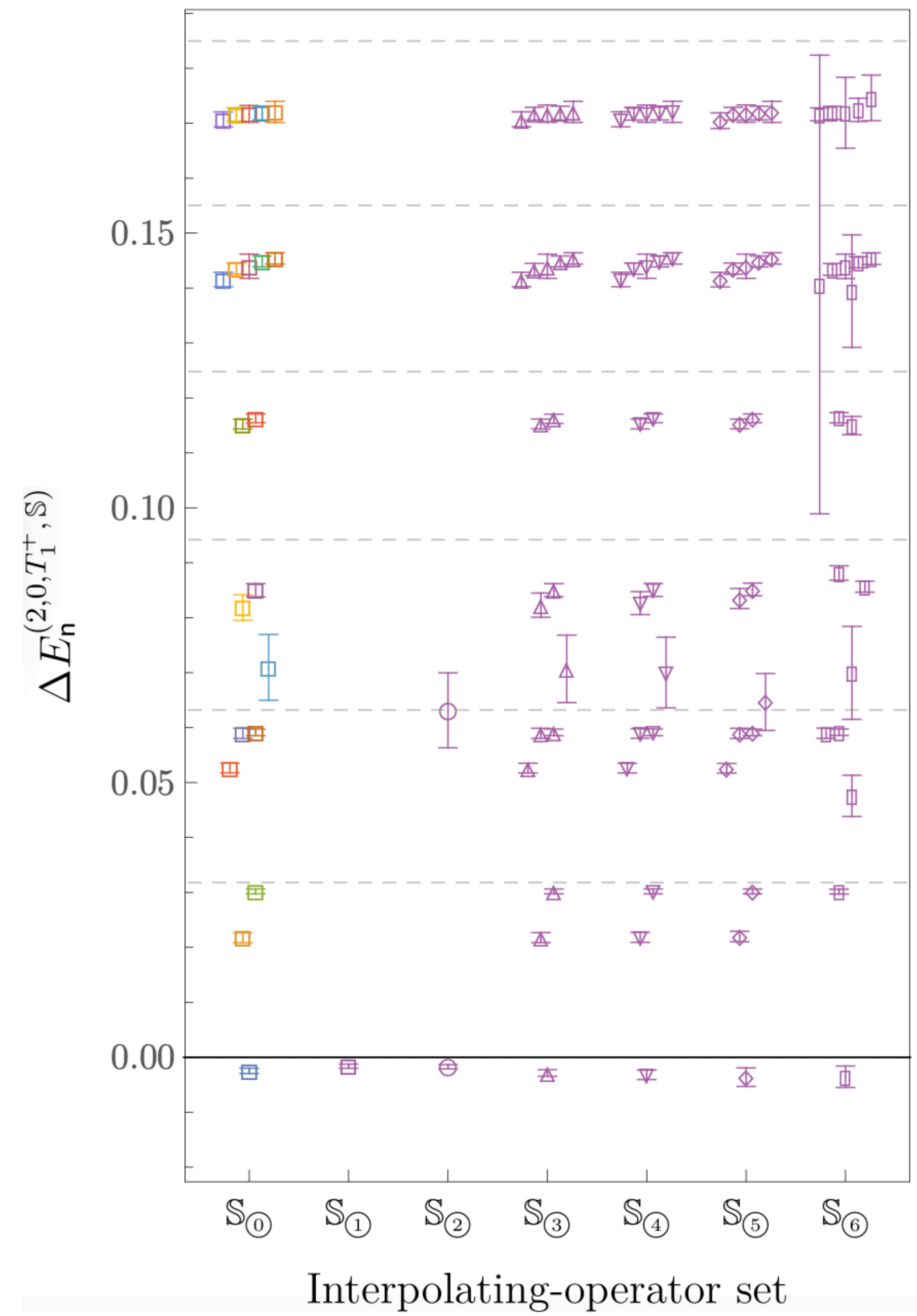


NPLQCD GEVP (2022)

Do we need the hexaquark operator in our GEVP basis?



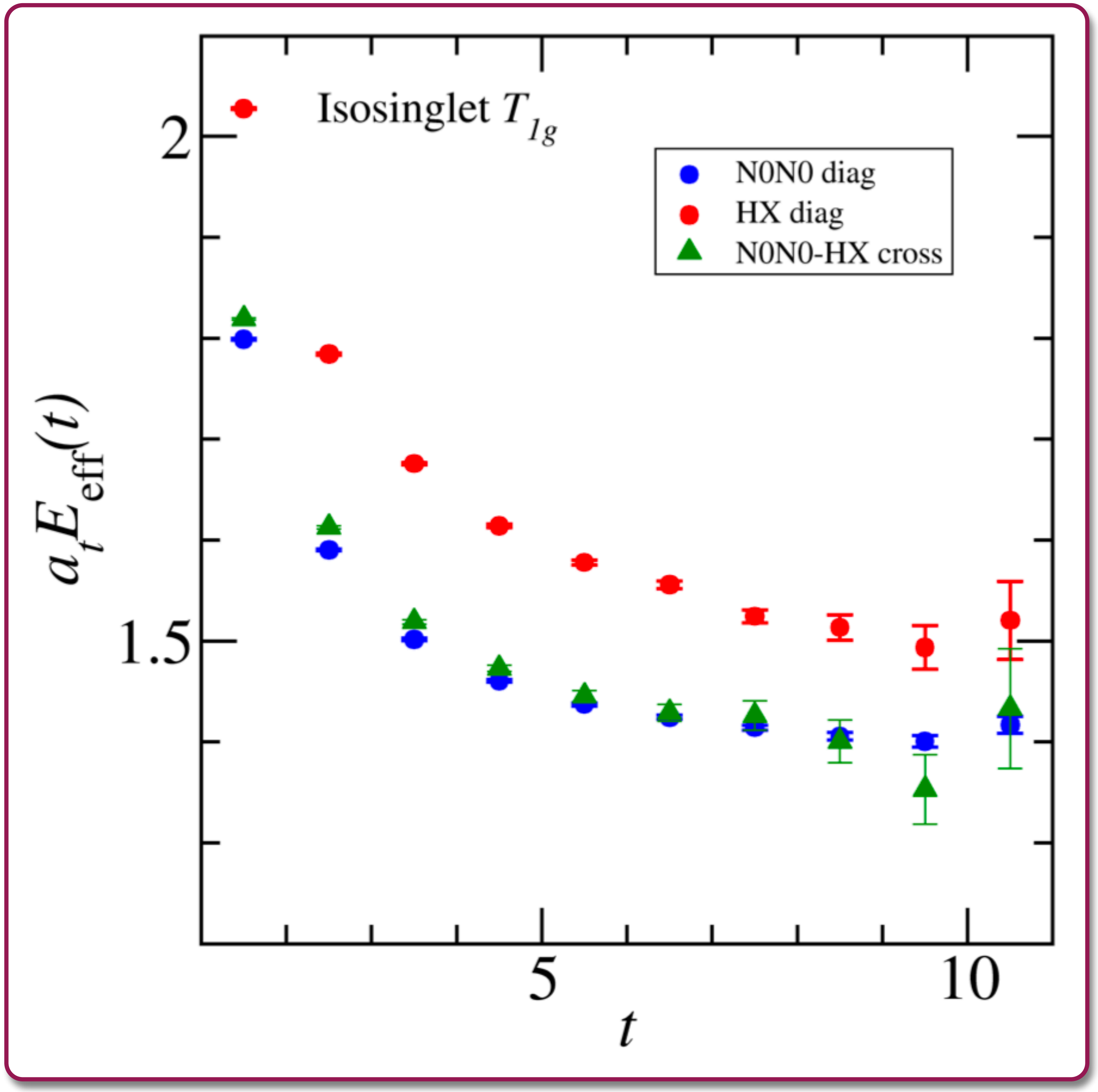
Ground state does not change when hexaquark is removed, or more/less momentum states used



NPLQCD GEVP: arXiv:2108.10835

Off-diagonal hexaquark correlators

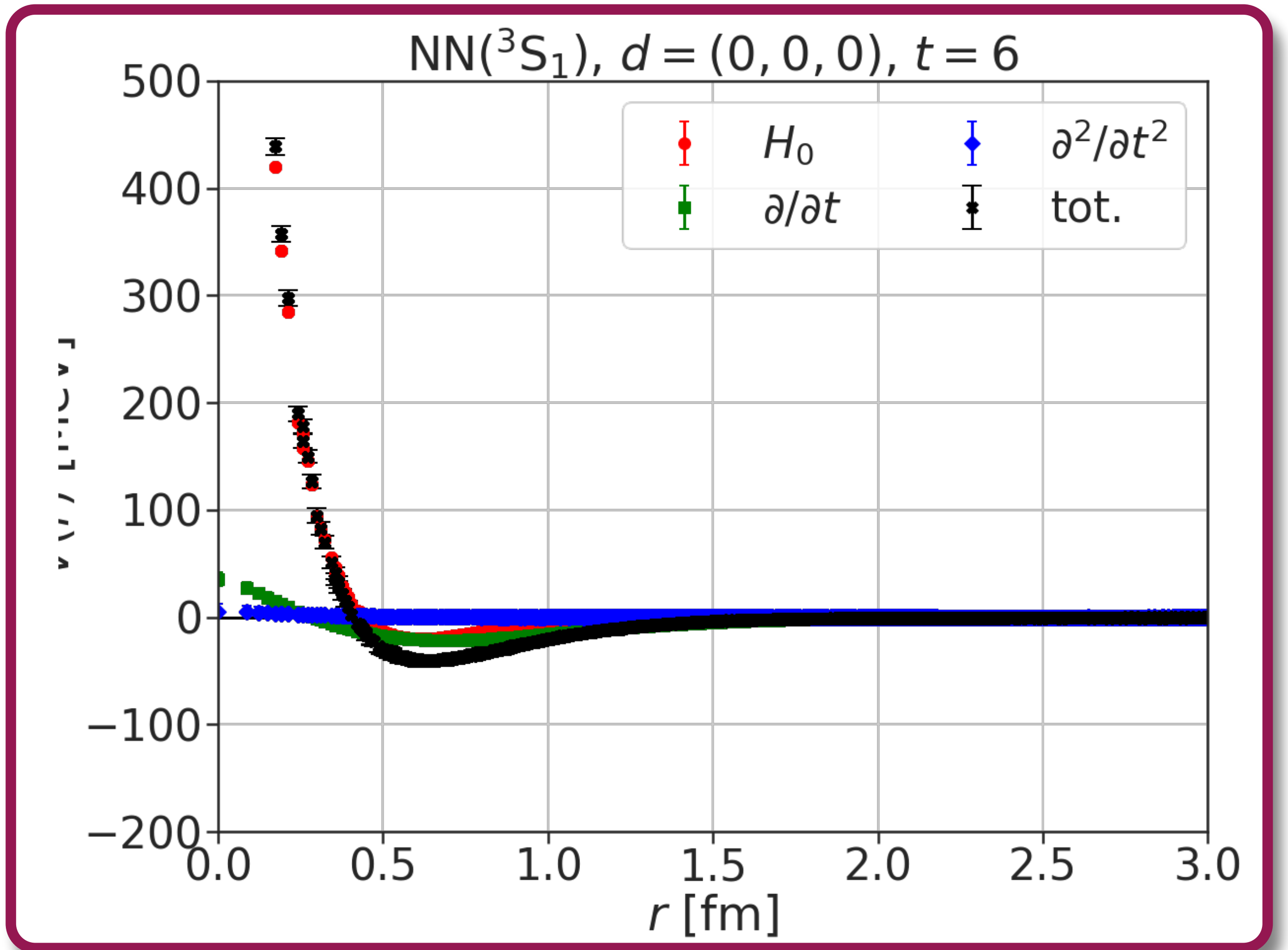
On the CLS C103 ensemble, we see no difference in g.s. energy using off-diagonal hexaquark correlator; previously some of us did find deep bound state using hexaquark ops on same configs as NPLQCD - is the deep bound state an artifact of particular quark smearings or discretizations?

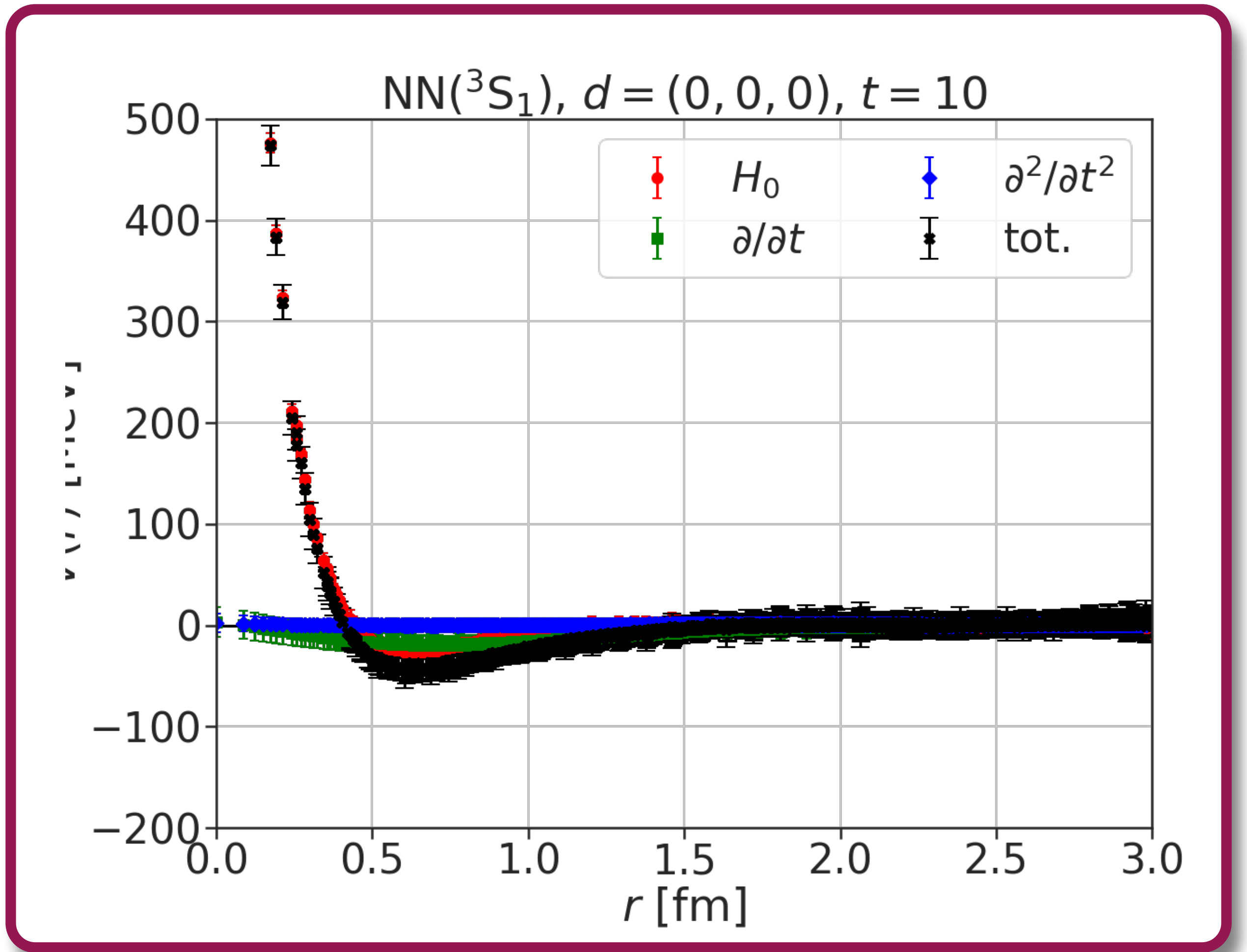


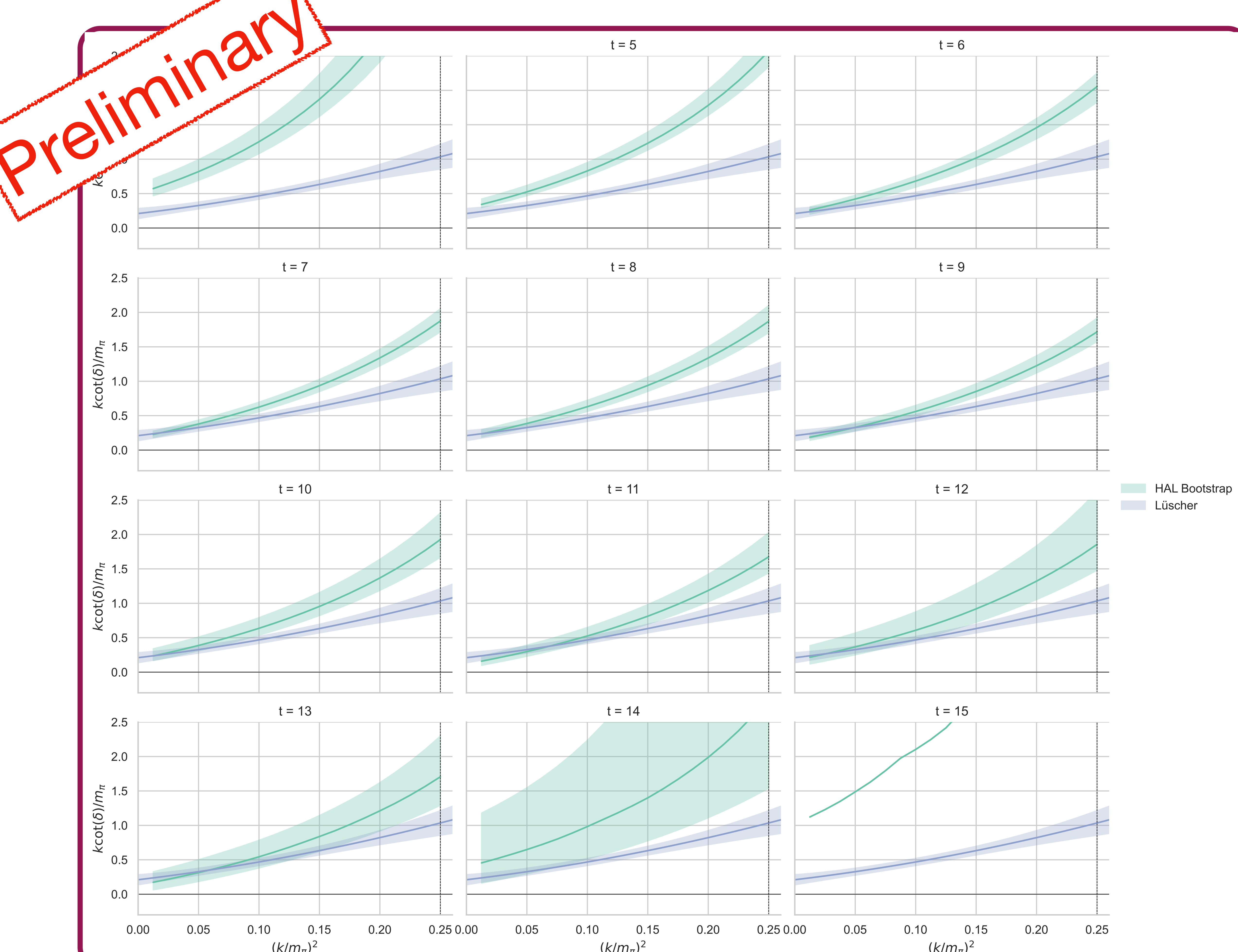
Preliminary

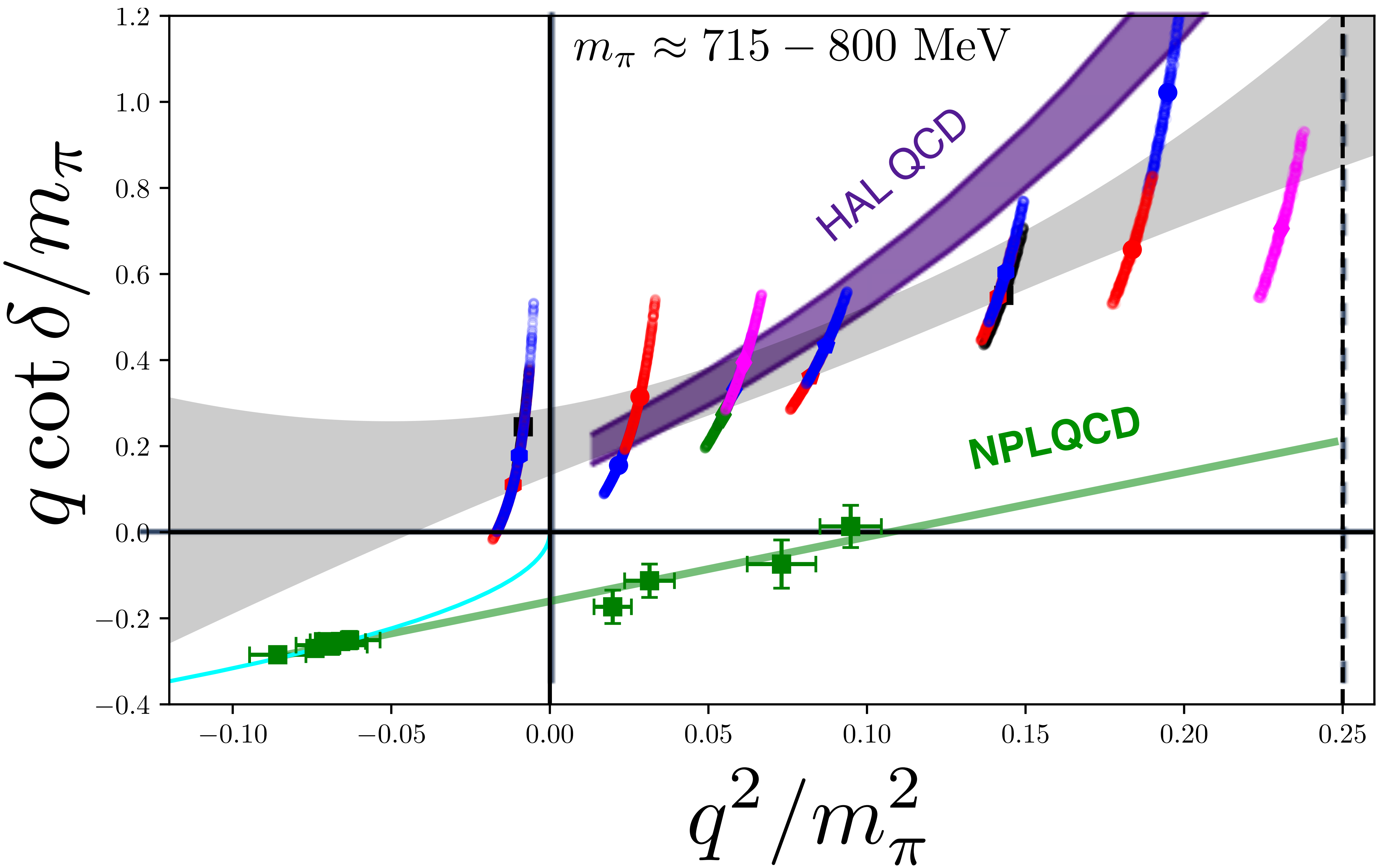
HALQCD Potential Method

CLS ensemble: $m_\pi \sim 714$ MeV, a ≈ 0.086 fm, L = 48
Wall quark sources

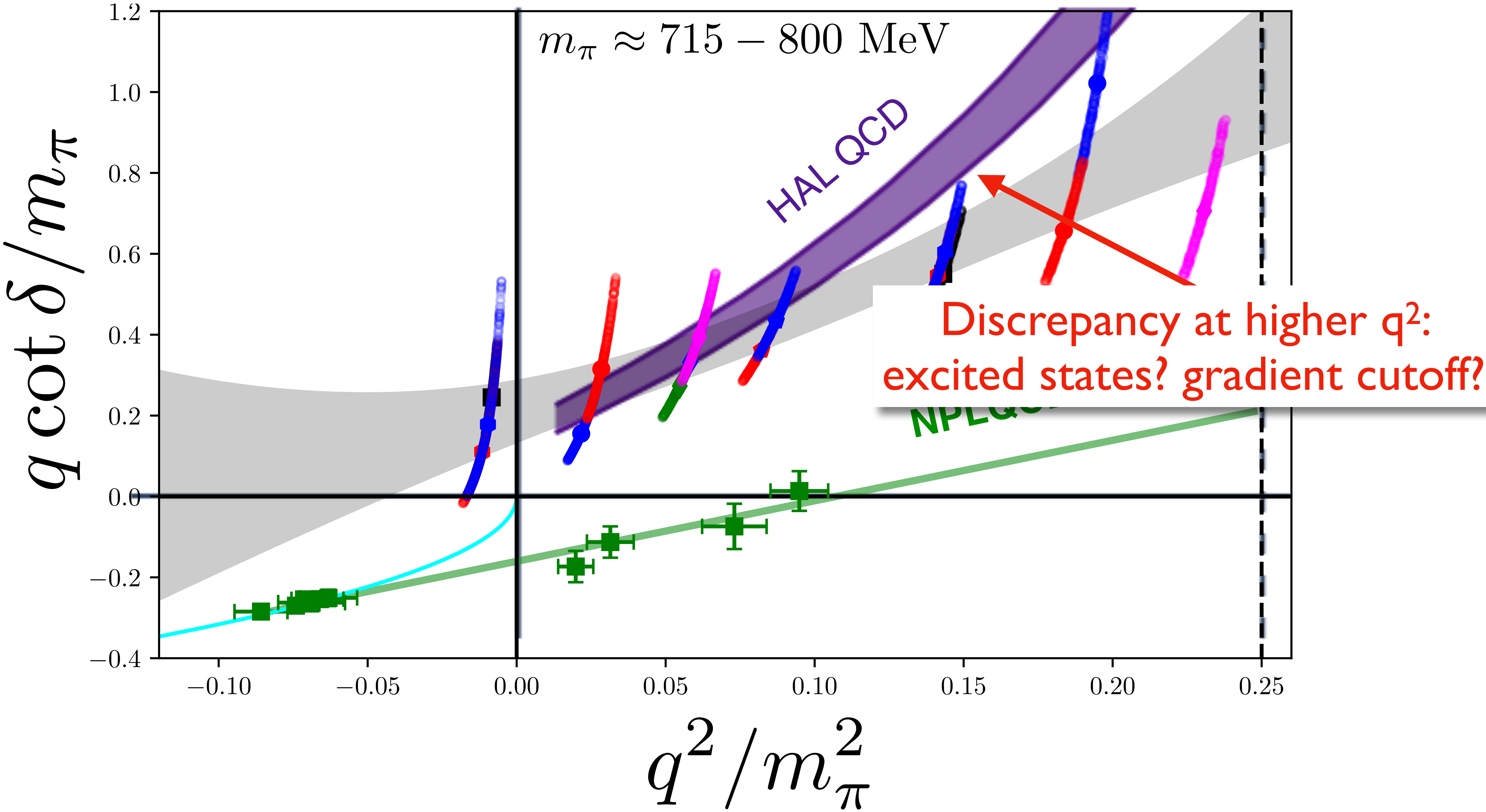




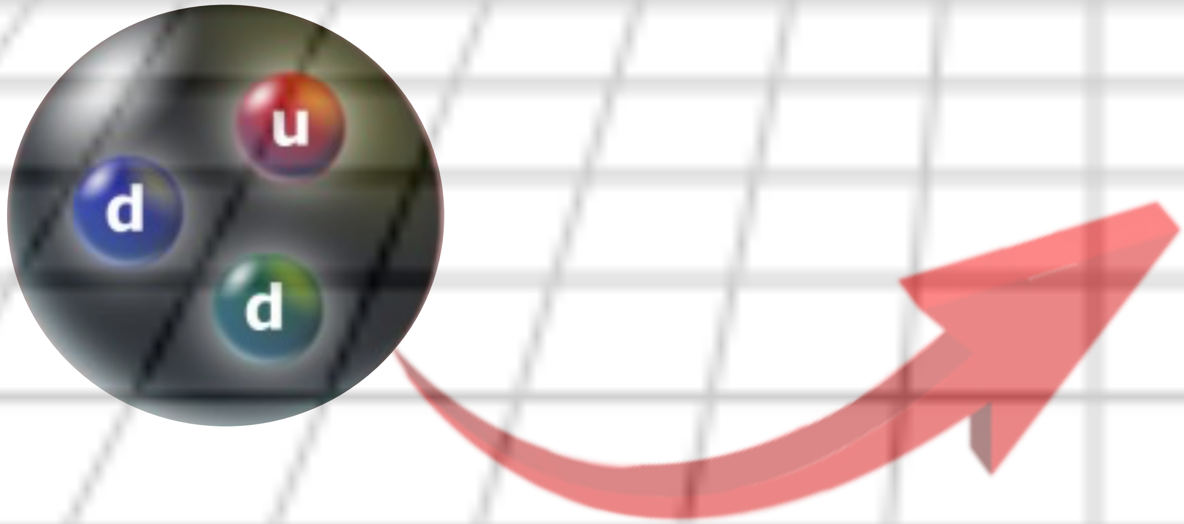

Preliminary
t = 5
t = 6
t = 7
t = 8
t = 9
t = 10
t = 11
t = 12
t = 13
t = 14
t = 15
$k\cot(\delta)/m_\pi$
$(k/m_\pi)^2$
HAL Bootstrap
Lüscher



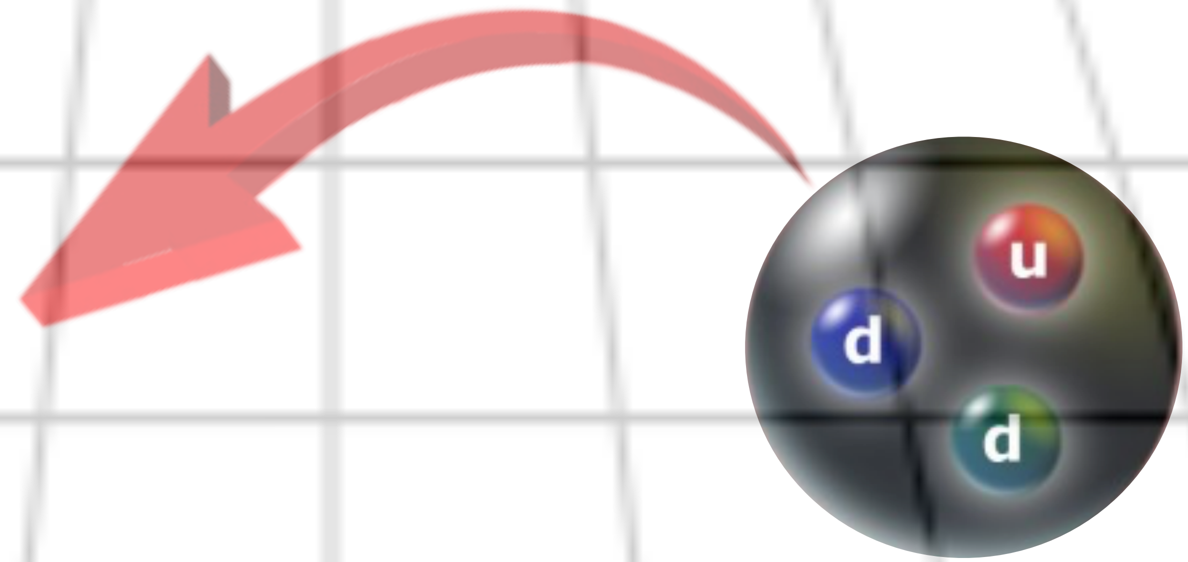
$m_\pi \approx 715 - 800$ MeV
HAL QCD
NPLQCD
$q \cot \delta / m_\pi$
q^2/m_π^2
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.10
−0.05
0.00
0.05
0.10
0.15
0.20
0.25



$m_\pi \approx 715 - 800$ MeV
HAL QCD
NPLQC
Discrepancy at higher q²: excited states? gradient cutoff?
$q \cot \delta / m_\pi$
q^2 / m_π^2
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
−0.10
−0.05
0.00
0.05
0.10
0.15
0.20
0.25

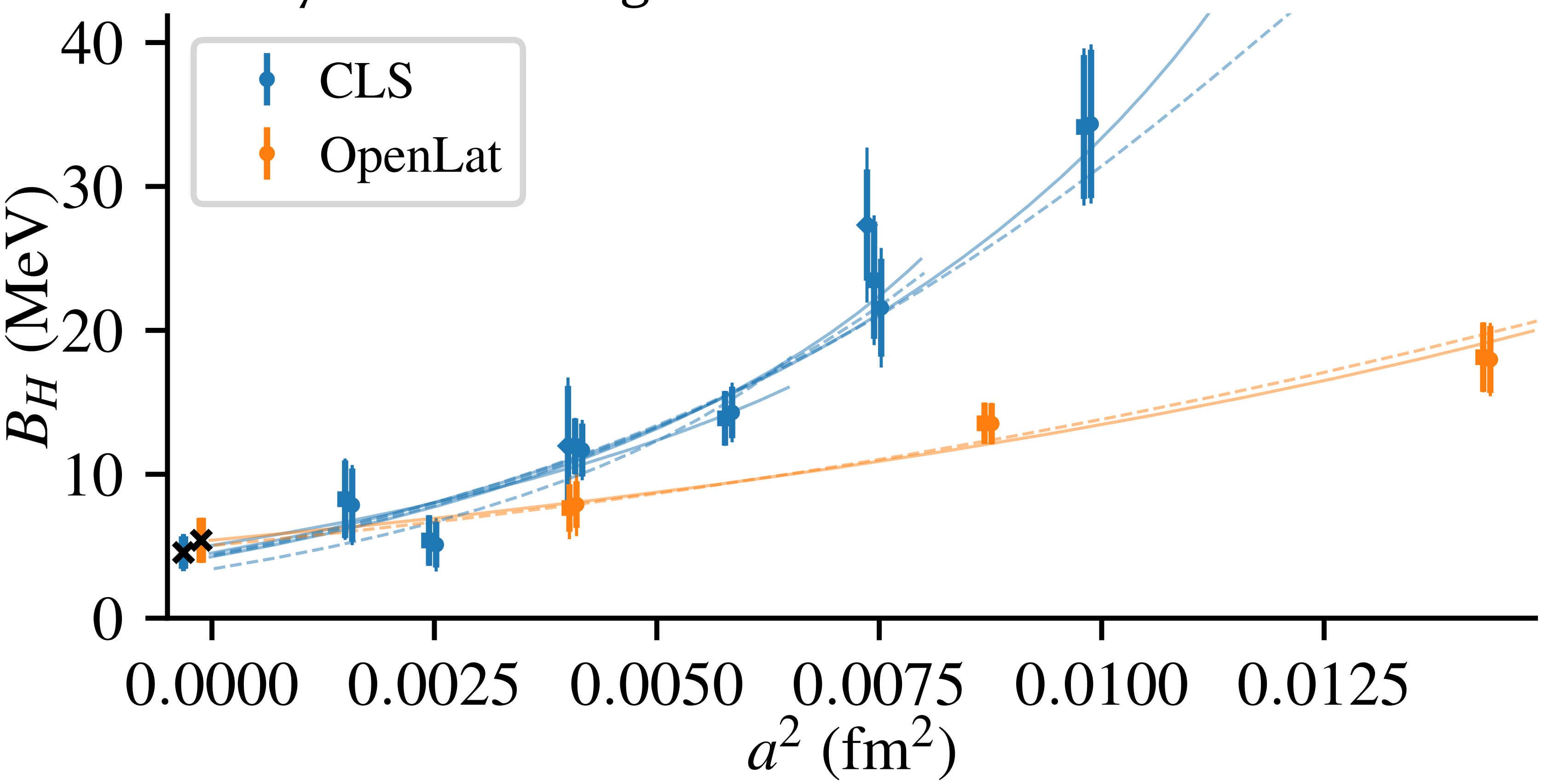


More progress



H dibaryon: $a \to 0$ universality (PRELIMINARY)

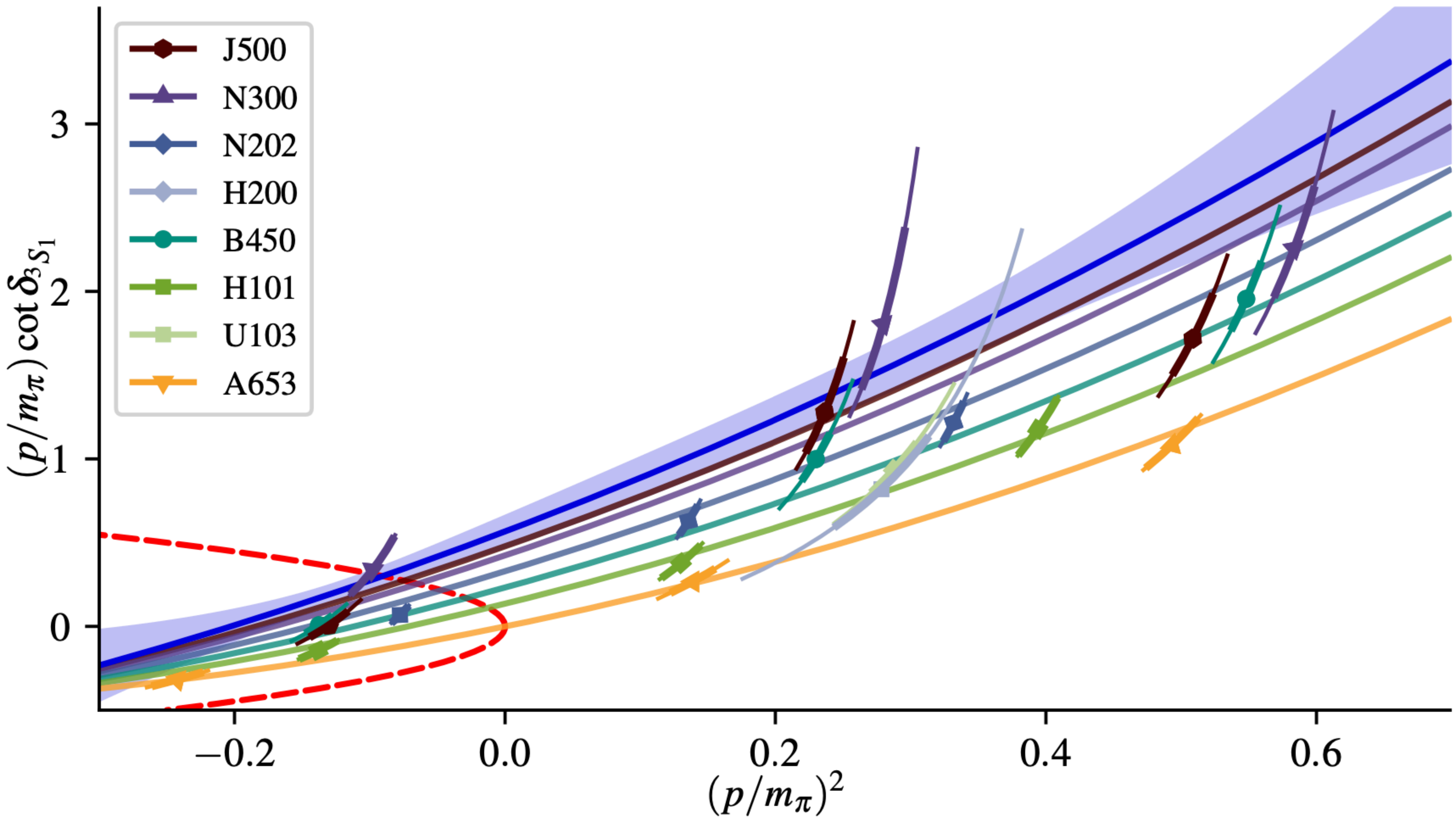
BaSc: Baryon Scattering collaboration — combined effort of “Mainz” and sLapHnn



Three exp-clover ensembles with $L \approx 3$ fm.

Second action at SU(3) point: exponentiated clover (OpenLat).
Smaller lattice artifacts than standard clover (CLS).

$m_\pi = m_K = m_\eta \approx 420$ MeV.



Jeremy R. Green,
Andrew D. Hanlon, Parikshit M. Junnarkar, Hartmut Wittig

NN scattering from LQCD

- **Controversy between methods: working to benchmark at m_π ~ 800 MeV**
- **Preponderance of evidence now shows that there is no bound state at heavy pion mass**
- **Hexaquark and off-diagonal correlators are not necessary, and can be misleading**
- **Preliminary results show that the HALQCD potential method agrees well with Lüscher at low momenta**
    - **Possible systematics at higher q^2**
- **Discretization effects appear to be non-negligible**

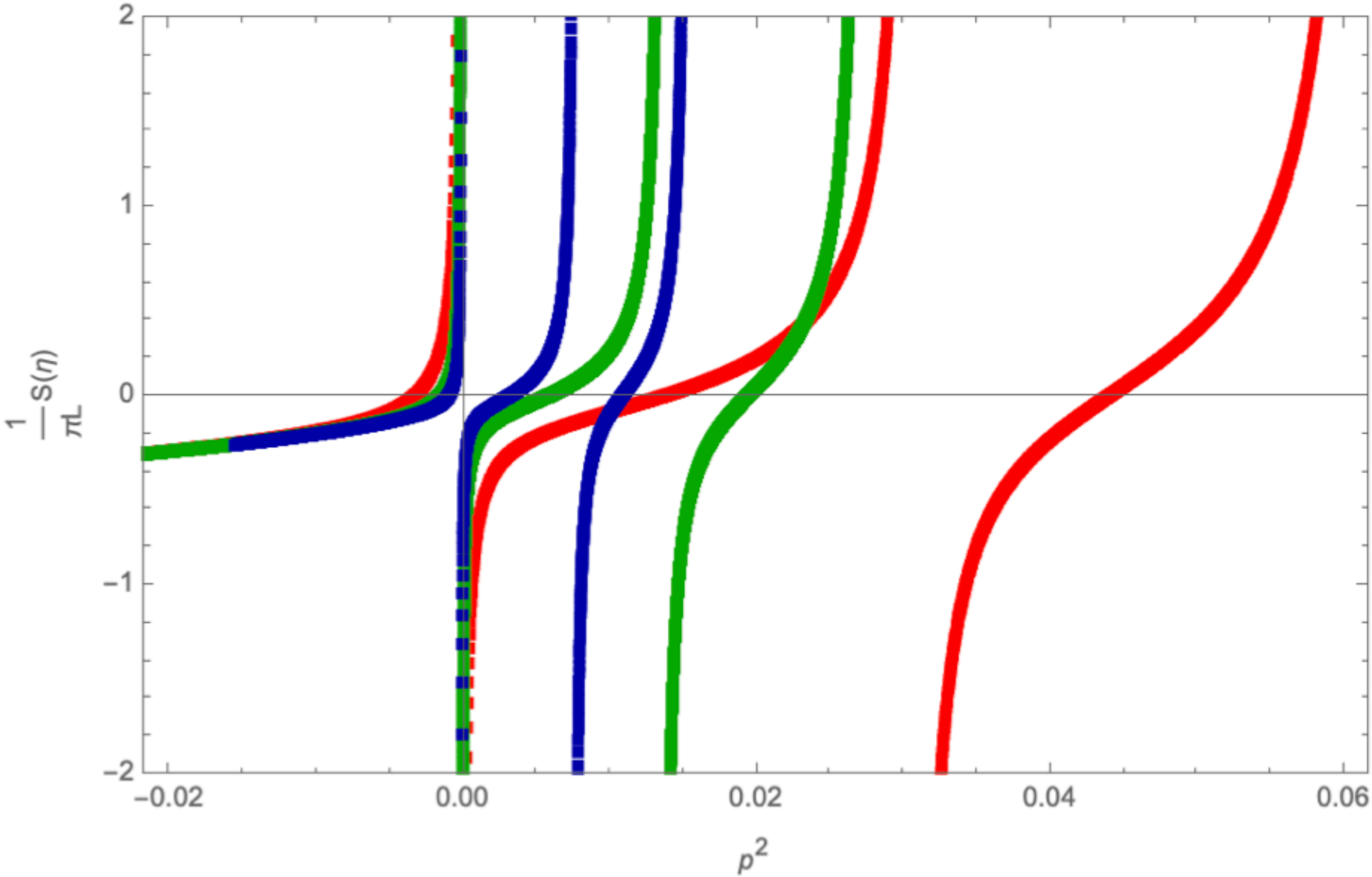
Ben Hörz (Intel)
Dean Howarth (LLNL)
Enrico Rinaldi (RIKEN)
Andrew Hanlon (BNL)
Chia Cheng Chang (RIKEN/LBNL)
Christopher Körber (Bochum/LBNL)
Evan Berkowitz (Jülich)
John Bulava (DESY)
M.A. Clark (NVIDIA)
Wayne Tai Lee (Columbia)
Kenneth McElvain (LBNL)
Colin Morningstar (CMU)
Amy Nicholson (UNC)
Pavlos Vranas (LLNL)
André Walker-Loud (LBNL)

OLCF
OAK RIDGE LEADERSHIP COMPUTING FACILITY

NERSC

TACC
TEXAS ADVANCED COMPUTING CENTER

U.S. DEPARTMENT OF ENERGY
INCITE
LEADERSHIP COMPUTING



2
1
0
−1
−2
$\frac{1}{\pi L} S(\eta)$
−0.02
0.00
0.02
0.04
0.06
p^2