On the Reliability of Two-Baryon Interactions from Lattice QCD

Andrew Hanlon

KENT STATE UNIVERSITY

INT 26-1: Nuclear Hamiltonians for Advancing Nuclear Physics and Beyond

Institute for Nuclear Theory
May 19, 2026

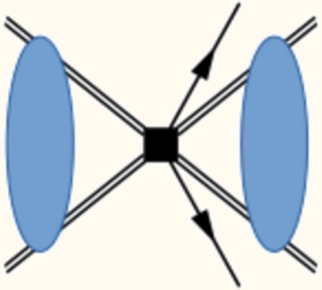
Why study BB interactions from lattice QCD?

- NN interactions known from experiment, and can be used to verify lattice results
- Pion mass dependence of NN interactions provides another lever arm for constraining LECs
- Interactions involving hyperons can be determined as well, which are not so simple to determine experimentally
- Paves the way towards three-baryon interactions, which are also difficult to constrain experimentally
- Needed for BSM matrix elements for NN, *e.g.* $0\nu\beta\beta$ decay
- Search for dibaryon bound states and resonances

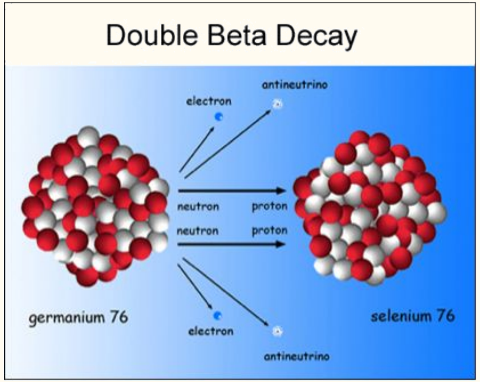
Lattice QCD→EFT→*Ab Initio* many-body theory

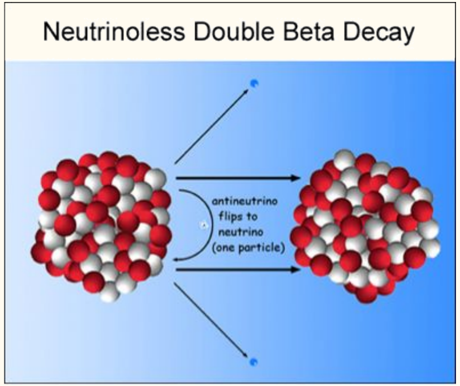
- Several research programs aim to calculate quantities involving large nuclei
  - Nuclear reactions
  - $0\nu\beta\beta$ decay
- Lattice QCD can constrain the LECs in EFTs, which can then be input to *ab initio* nuclear many-body calculations
- Recent discovery of leading-order short-range operator for $nn \rightarrow ppee$ within chiral EFT with unknown LEC g_ν^{NN}

[V. Cirigliano et al., 1802.10097]



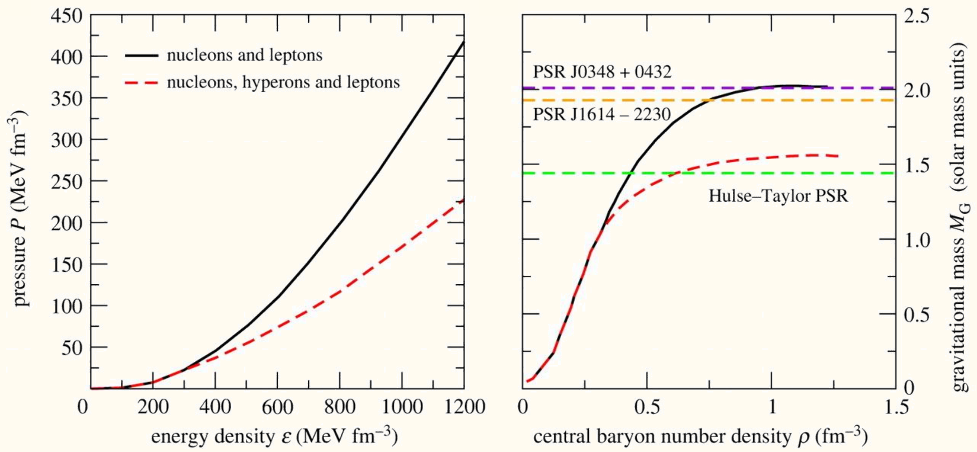
- Lattice QCD can provide multi-hadron matrix elements
- However, controlling power-law finite-volume effects requires reliable determination of multi-hadron interactions



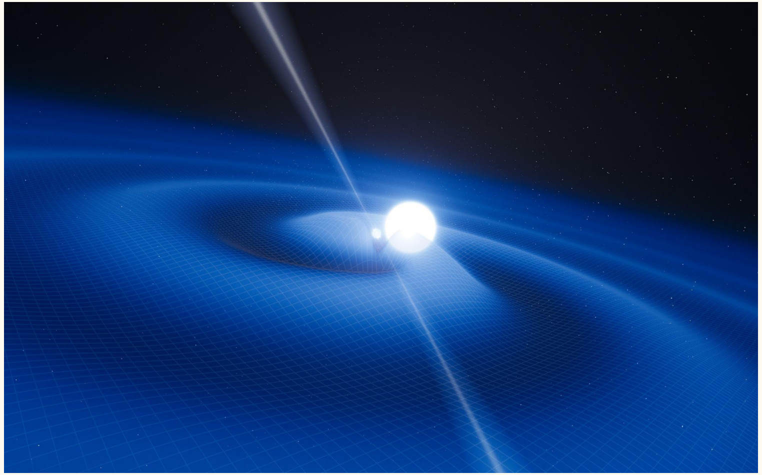


[Neutrinoless Double Beta Decay Experiments, PARTICLEBITES, https://www.particlebites.com/?p=1002]

Two and three-body forces in neutron stars



[D. Chatterjee, I. Vidaña *Eur. Phys. J. A.* **52** 2016] [I. Vidaña 2018 *Proc. R. Soc. A.* **474** 20180145]



[Artist's impression of the pulsar PSR J0348+0432 and its white dwarf companion, **Credit:** ESO/L. Calçada, https://www.eso.org/public/images/eso1319c/]

- High densities in neutron stars make hyperons energetically favorable
- Inclusion of hyperons leads to a softer equation of state, in contradiction with observation
- Two- and three-hadron interactions involving hyperons may supply the needed repulsion
- Constraints can be provided from lattice QCD

Lattice QCD

- Non-perturbative, *Euclidean* QCD
- "Impossible" integral becomes hard integral

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}[\psi, \overline{\psi}]\, \mathcal{D}[U]\, e^{-\overline{\psi} M[U] \psi} e^{-S_G[U]}\, \mathcal{O}[\psi, \overline{\psi}, U]$$
$$= \frac{1}{Z} \int \mathcal{D}[U]\, \det[M[U]]\, e^{-S_G[U]}\, \mathcal{O}[M^{-1}[U]]$$

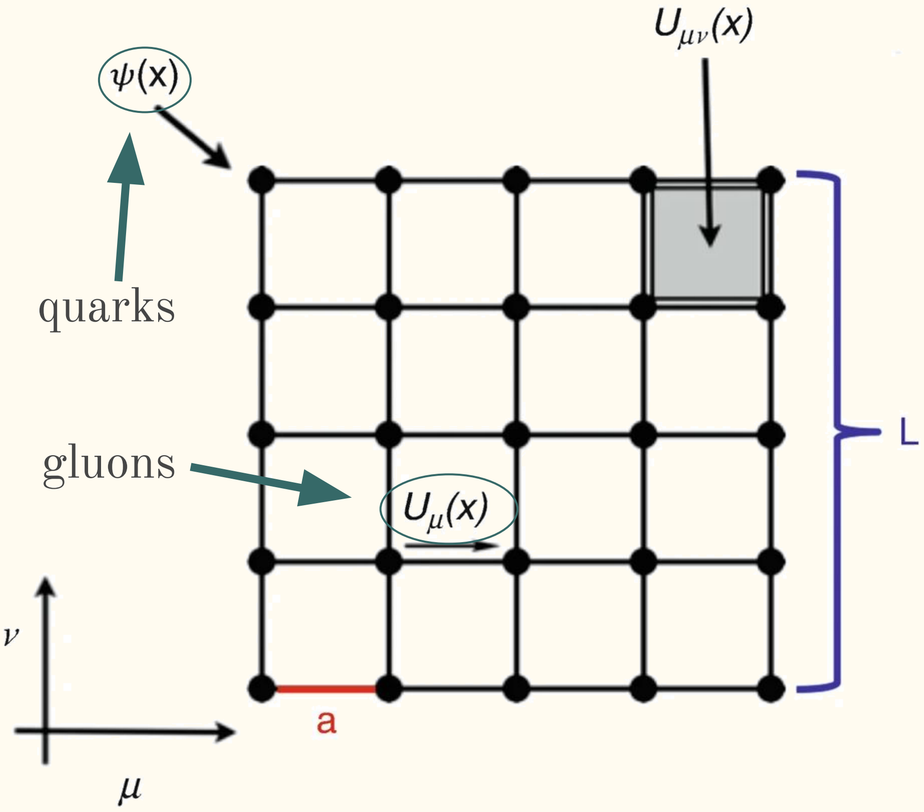
Probability Weight

- Generate "Gauge configurations" using Markov Chain Monte Carlo

$$U_\mu^{(0)}(x) \to U_\mu^{(1)}(x) \to U_\mu^{(2)}(x) \to \dots$$

- Estimate expectation value

$$\langle \mathcal{O} \rangle = \frac{1}{N_U} \sum_{n=1}^{N_U} \mathcal{O}[M^{-1}[U^{(n)}]] \pm \frac{\sigma_{\mathcal{O}}}{\sqrt{N_U}}$$



[Fig. from: The Deconfinement Transition of QCD, Claudia Ratti & Rene Bellwied]

Scattering in One Finite Dimension

- Given two spin-0 particles interacting via a symmetric potential of finite range R

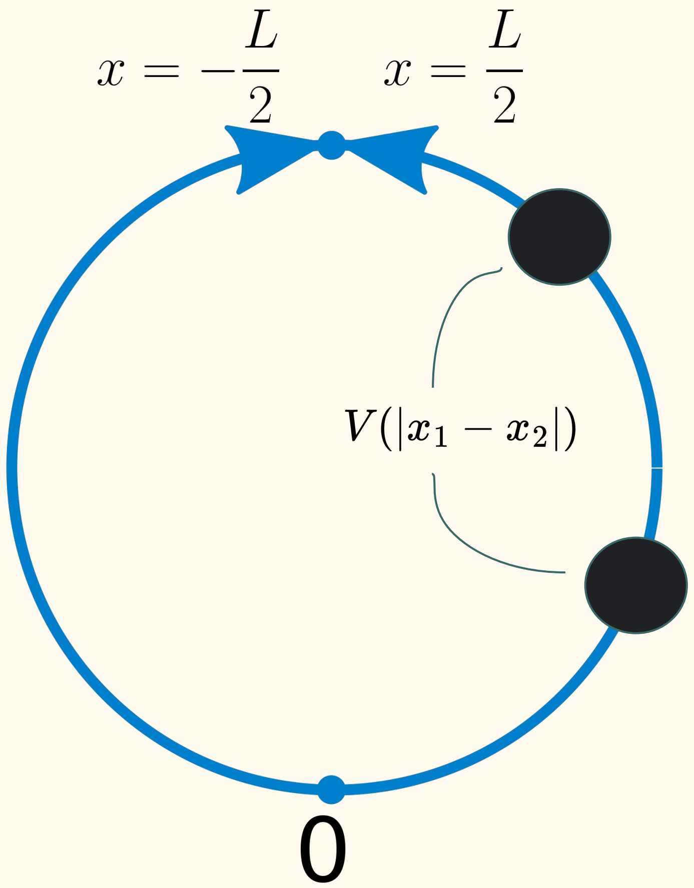
$$\psi_k(x) \to \cos[k|x| + \delta(k)]$$

one can use Schrödinger equation inside and outside potential region and match to find $\delta(k)$

- What if we restrict to a periodic, finite volume?
  - Matching at $|x| = \frac{L}{2}$ leads to quantization condition

$$kL + 2\delta(k) = 2\pi n$$

- Each energy of the system leads to constraint on phase shift at that energy



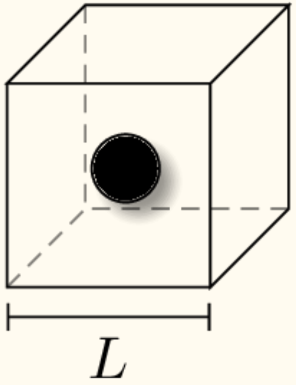
Volume Dependence of the Spectrum

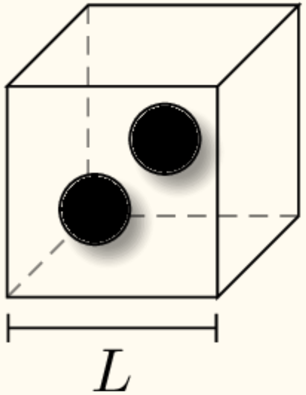
Single particle states have exponentially suppressed volume corrections

$$E_{\infty}^{(1)} - E_L^{(1)} \propto e^{-mL}$$

Volume dependence of two-particle states contains the scattering length

$$\Delta E^{(2)} \propto \frac{a_0}{L^3} + O\left(\frac{1}{L^4}\right)$$





For each two particle energy: $E_{\mathrm{cm}}^{(2)} = \sqrt{k^2 + m_1^2} + \sqrt{k^2 + m_2^2}$

the scattering phase shift, at that energy, depends on known functions through

$$\tan[\delta(k)] = -\tan[\phi^{\mathbf{P}}(k)]$$

[Lüscher ‘86, ‘91; generalizations]

Lowest partial wave truncation

- Two way equation:
  - Given energies ⇒ constraint on phase shift
  - Given phase shift ⇒ prediction of spectrum
- Assuming contributions from s-wave only

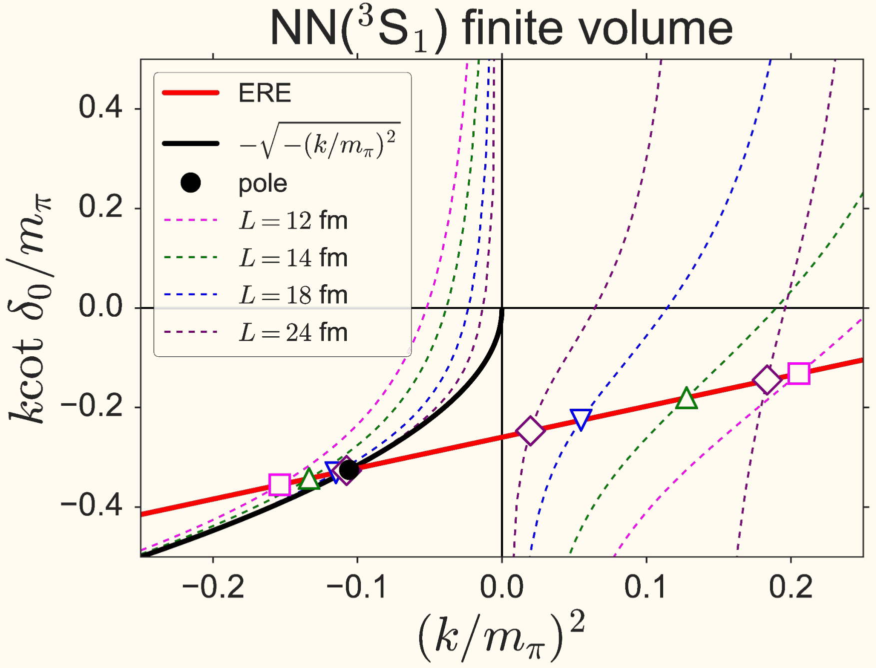
$$\boxed{k \cot \delta_0(k) = \frac{2}{\sqrt{\pi} L \gamma} Z_{00}^{\vec{P}L/(2\pi)}\left(1, \left(\frac{kL}{2\pi}\right)^2\right)}$$

$Z_{00}^{\vec{P}L/(2\pi)}$ - generalized zeta function

$\boldsymbol{k}$ - momentum of scattering particles

$\gamma = E/E_{\text{cm}}$ - Lorentz boost factor

Truncated at $\ell_{\max} = 0 \Rightarrow$ one-to-one mapping



[HAL QCD, 1703.07210]

Energies from two-point correlators

- In principle, one can extract all desired energies from two-point correlators

$$C(t) = \langle 0|\mathcal{O}_{\text{snk}}(t)\mathcal{O}^{\dagger}_{\text{src}}(0)|0\rangle$$
$$= \sum_{n=0}^{\infty} \langle 0|\mathcal{O}_{\text{snk}}|n\rangle\langle 0|\mathcal{O}_{\text{src}}|n\rangle^{*} e^{-E_n t}$$

- Correlator asymptotes to ground state at large time separation

$$E^{\text{eff}}(t) \equiv -\frac{1}{\Delta t}\ln\left(\frac{C(t+\Delta t)}{C(t)}\right)$$

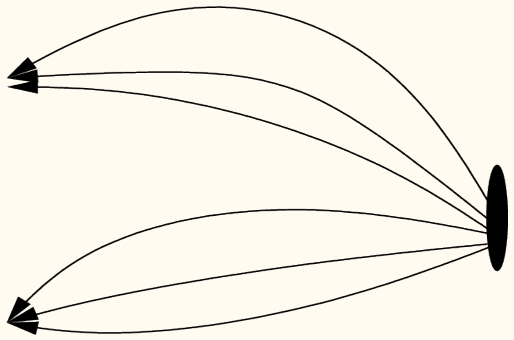
- Look for plateau in effective energy to indicate ground state saturation
  - Approach can be non-monotonic if sink and source operators are not the same

- Typical interpolator for two-baryon states

$$\mathcal{O} \sim \sum_{\vec{x}_1,\vec{x}_2} e^{-i\vec{p}_1\cdot\vec{x}_1} e^{-i\vec{p}_2\cdot\vec{x}_2}\, qqq(\vec{x}_1)qqq(\vec{x}_2)$$

- Use of point-to-all quark propagation requires a completely local operator at the source

$$\langle BB(t)H^{\dagger}(0)\rangle$$



[Figure: Mainz 1805.03966]

Early results at $m_\pi \sim$ 806 MeV

- Used point sources, and therefore uses correlators of the form

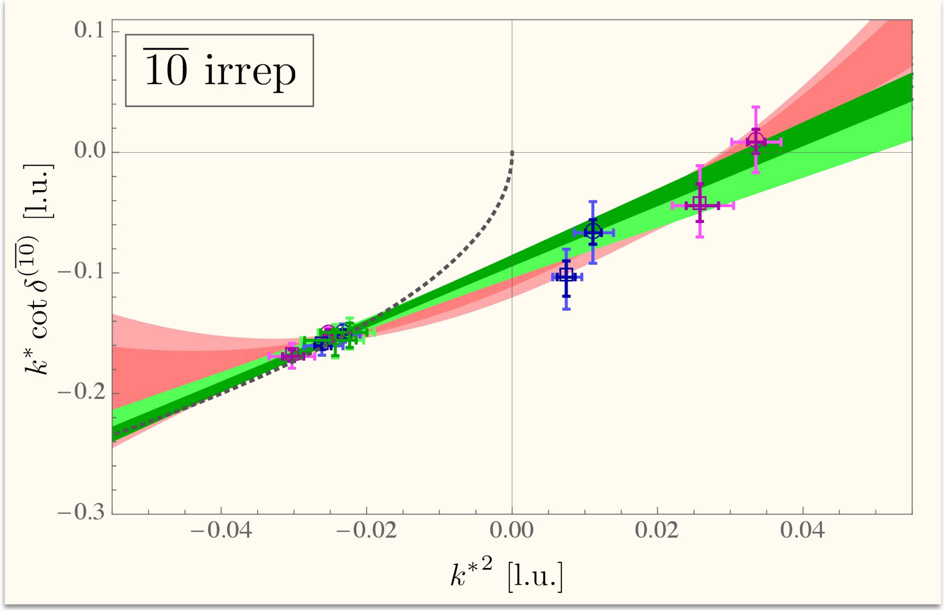
$$\langle BB(t) H^\dagger(0) \rangle$$

- Pole below threshold indicates a bound state

$$\mathcal{M} \propto \frac{1}{k^* \cot \delta_0(k^*) - ik^*}$$

- Bound state also at $m_\pi \sim$ 450 MeV

Deuteron



[NPLQCD Collaboration, 1706.06550]

The HAL QCD Method

- The ratio

$$R(t,\mathbf{r}) = \frac{\sum_{\mathbf{x}} \langle N(t,\mathbf{x}+\mathbf{r}) N(t,\mathbf{x}) N^\dagger(0) N^\dagger(0)\rangle}{\sum_{\mathbf{x}} \langle N(t,\mathbf{x}) N^\dagger(0)\rangle}$$

is related to the Nambu-Bethe-Salpeter wave function and satisfies

$$\left[\frac{\partial_t^2}{4M_N} - \partial_t - \frac{\nabla^2}{M_N}\right] R(t,\mathbf{r}) = \int d^3r'\, U(\mathbf{r},\mathbf{r}') R(t,\mathbf{r}')$$

- The potential is defined via a derivative expansion

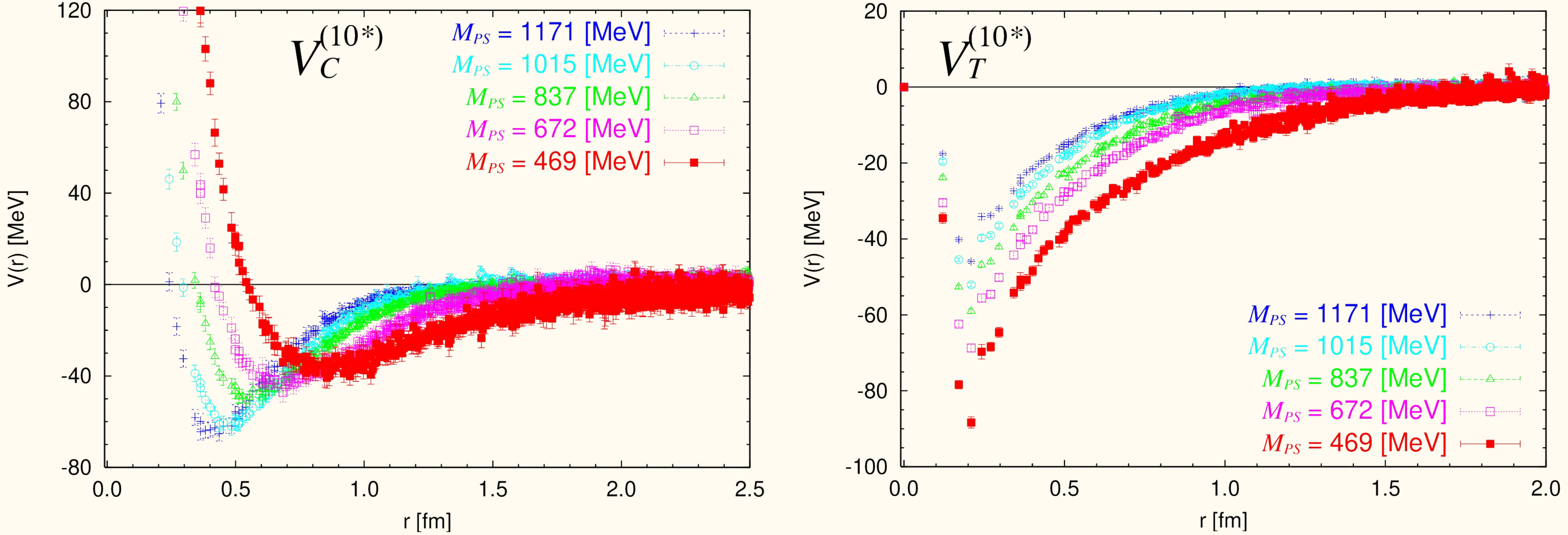
$$U(\mathbf{r},\mathbf{r}') = \sum_n V_n(\mathbf{r}) \nabla^n \delta(\mathbf{r}-\mathbf{r}') = [V_c(\mathbf{r}) + \cdots]\delta(\mathbf{r}-\mathbf{r}')$$

- Given the (local) potential, the Schrödinger equation gives the scattering information
- Importantly, $R(t,\mathbf{r})$ must have negligible contributions from inelastic states, but contributions from elastic states do not cause any issues

[HAL QCD, 1203.3642, 2003.10730]

The HAL QCD Method

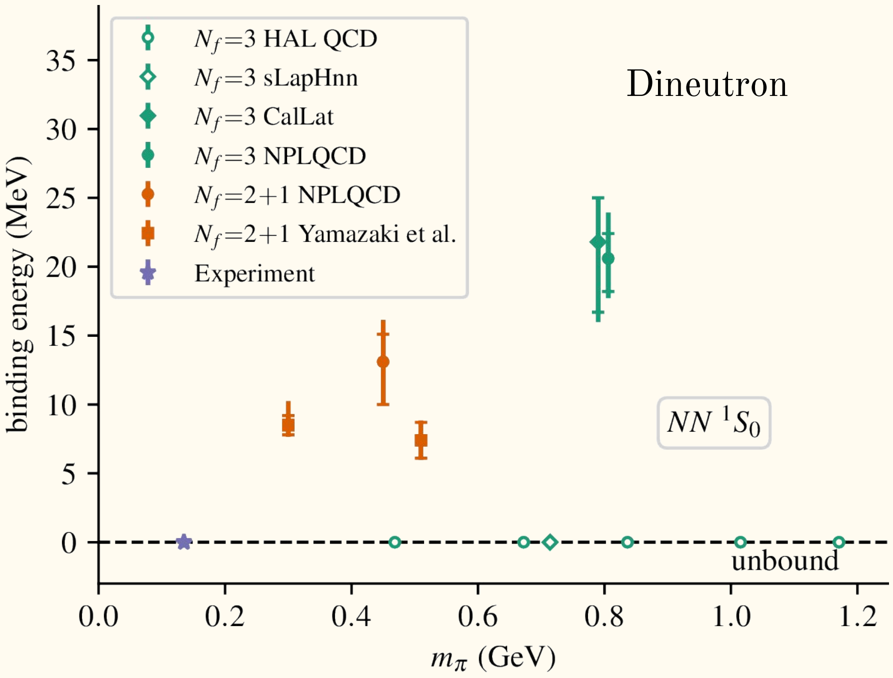
$NN\ I{=}0\ {}^3S_1$ - no bound state supported for heavy pions!

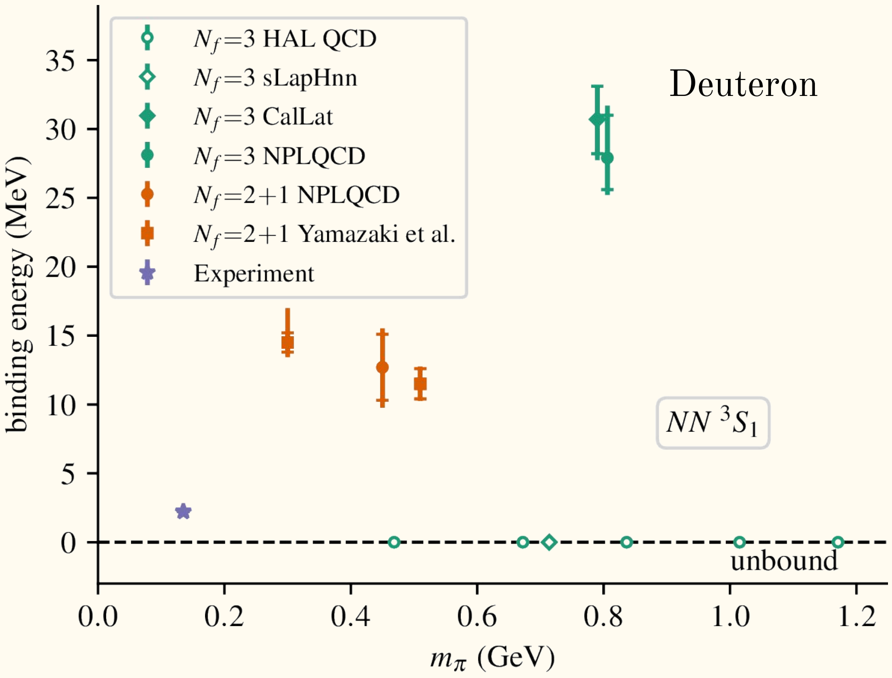


$$U(\mathbf{r},\mathbf{r}') = (V_c(\mathbf{r}) + V_T(\mathbf{r})S_{12} + \mathcal{O}(\nabla^2))\delta(\mathbf{r}-\mathbf{r}')$$

[HAL QCD, 1112.5926]

NN Comparison from Lattice QCD

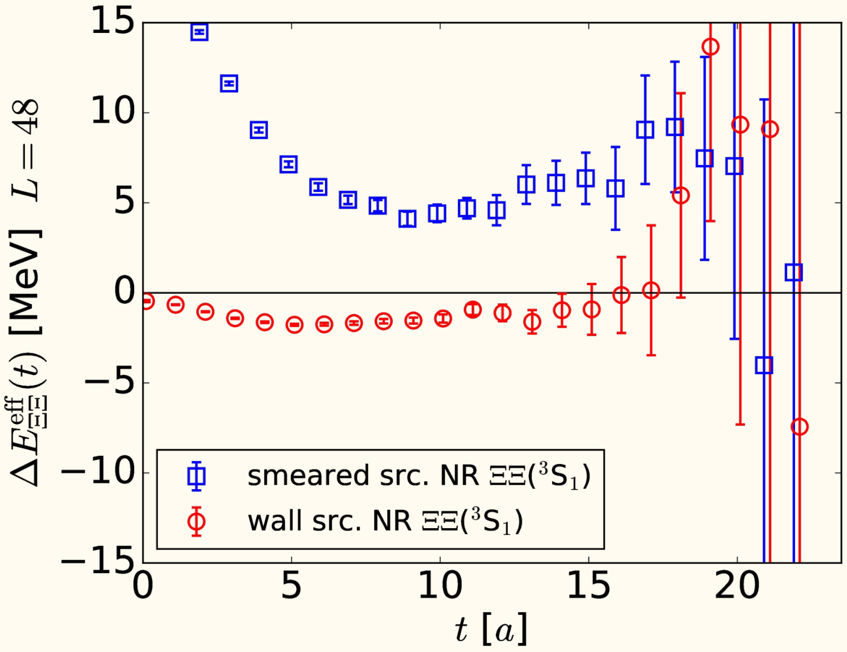




[Figures: J. Green, 2502.15546]

What's going wrong?

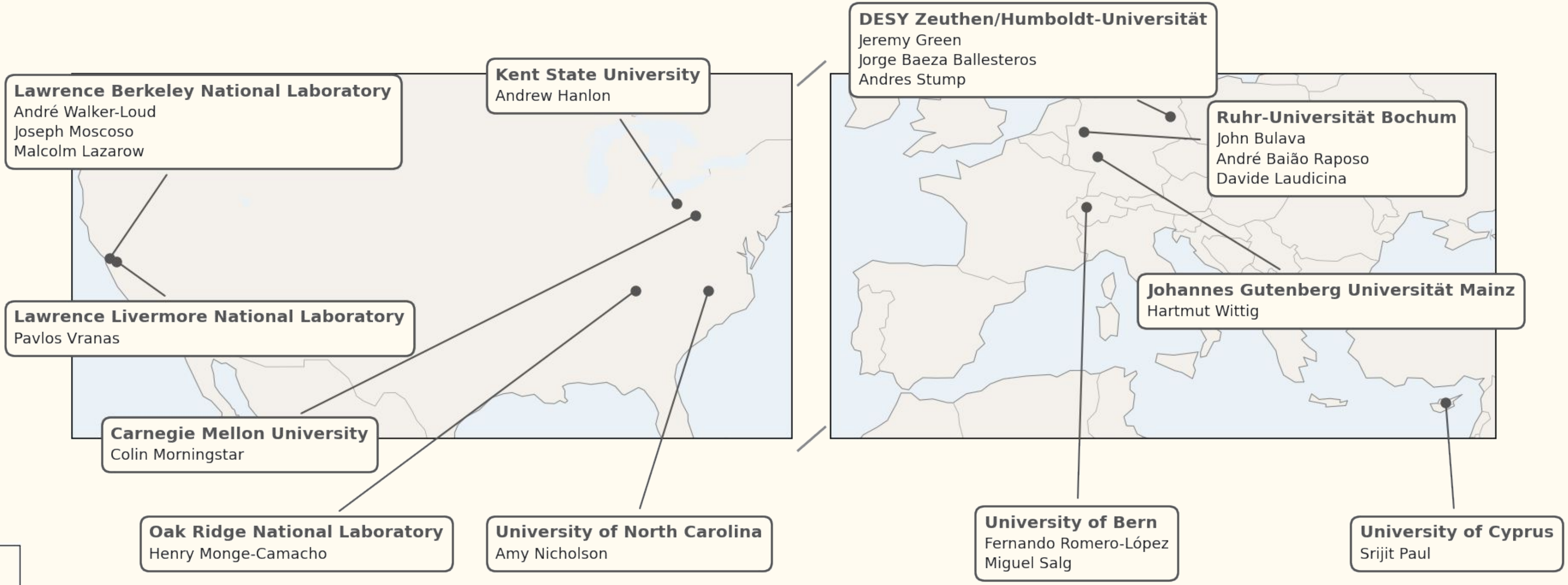
- Different methods
  - HAL QCD method vs. Lüscher
- Signal-to-noise ratio $\propto e^{-(m_B - 3m_\pi/2)t}$ makes this problem challenging
  - Ground-state saturation typically won't occur until ~ 4-10 fm
- Possible systematics
  - Truncation of derivative expansion (HAL QCD method)
  - Misidentified plateau for energies or incomplete operator basis (Lüscher method)
  - Discretization effects (both)



[HAL QCD, 1607.06371]

The Baryon Scattering (BaSc) Collaboration

Merging of Mainz, CalLat, *et al.* to address this problem



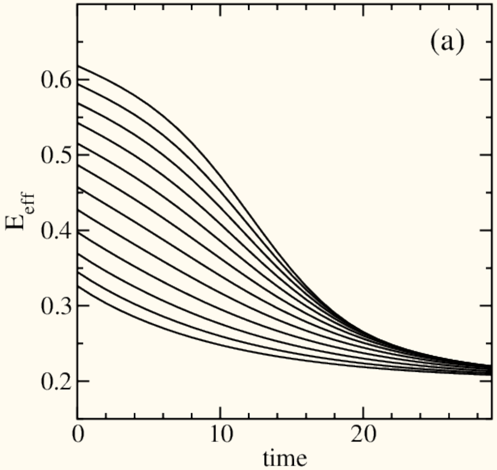
Correlator matrix toy model

Better to use a matrix of correlators:

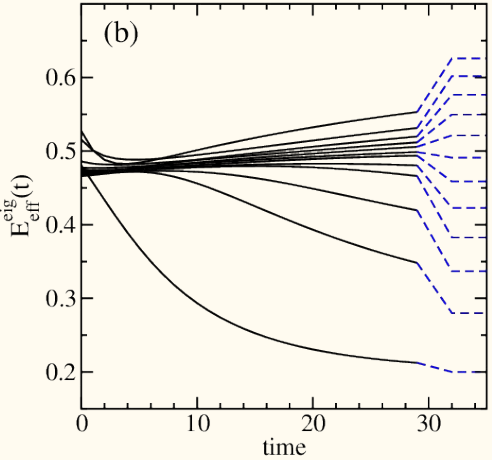
$$C_{ij}(t) = \langle \mathcal{O}_i(t)\, \mathcal{O}_j^\dagger(0) \rangle = \sum_{n=0}^{\infty} Z_i^{(n)}\, Z_j^{(n)*}\, e^{-E_n t}$$

Toy Model:

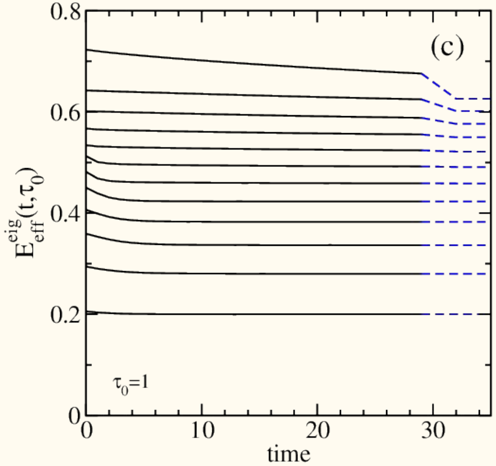
$$E_n = E_{n-1} + \frac{0.08}{\sqrt{n}}, \qquad n = 1, 2, \ldots, 199\ , \qquad E_0 = 0.20, \qquad Z_j^{(n)} = \frac{(-1)^{j+n}}{1 + 0.05(j-n)^2}$$



Diagonal elements of C(t)



Eigenvalues of C(t)



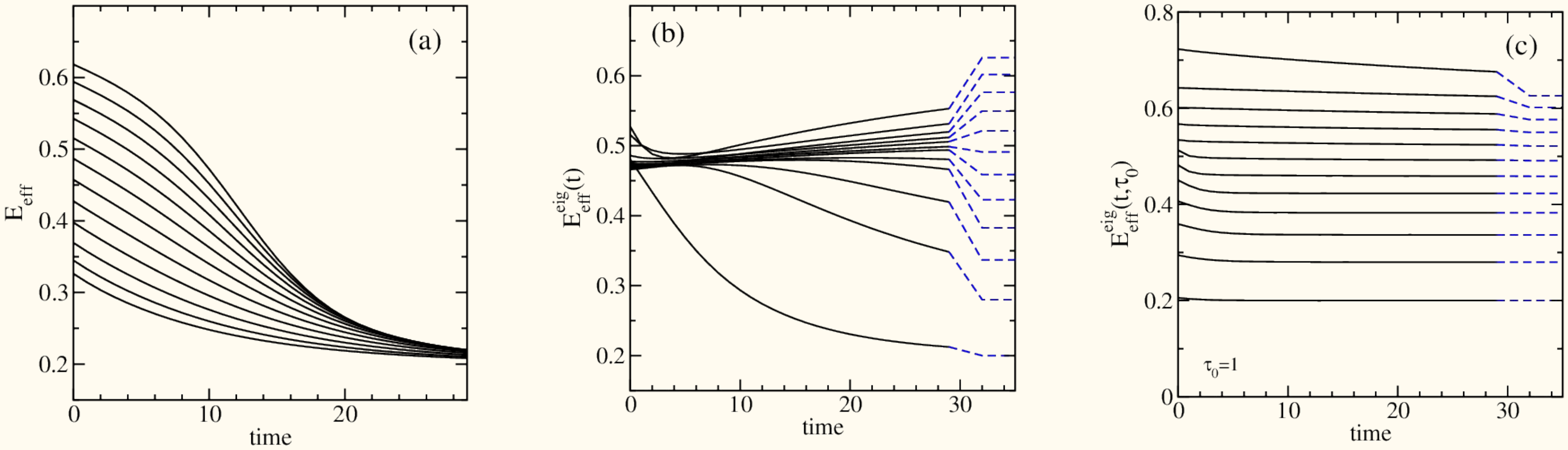
Generalized eigenvalues of C(t)

[Plots courtesy of Colin Morningstar]

Correlator matrix toy model

$$C_{ij}(t) = \langle \mathcal{O}_i(t)\mathcal{O}_j^\dagger(0)\rangle = \sum_{n=0}^{\infty} Z_i^{(n)} Z_j^{(n)*} e^{-E_n t}, \quad i,j = 1,2,\ldots,N$$

Diagonal elements of C(t) | Eigenvalues of C(t) | Generalized eigenvalues of C(t)



$$C_{ii}(t) = A_i e^{-E_0 t}[1 + \mathcal{O}(e^{-\Delta_{10} t})]$$

$$\lambda_n(t) = A_n e^{-E_n t}[1 + \mathcal{O}(e^{-\Delta_{nm} t})]$$

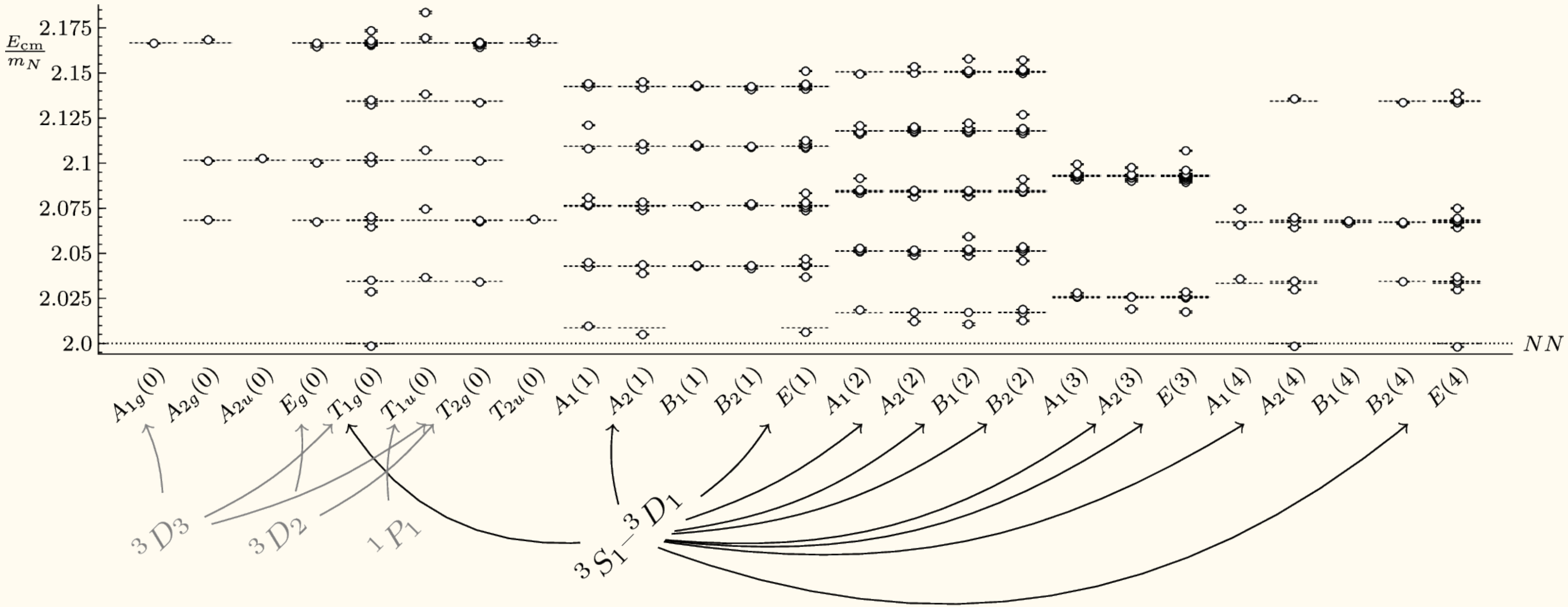
$$\lambda_n(t,\tau_0) = A_n e^{-E_n t}[1 + \mathcal{O}(e^{-\Delta_{Nn} t})]$$

[Plots courtesy of Colin Morningstar]

[B. Blossier *et al.*, 0902.1265]

NN I=0 Finite-volume spectrum, $m_\pi \sim 714$ MeV

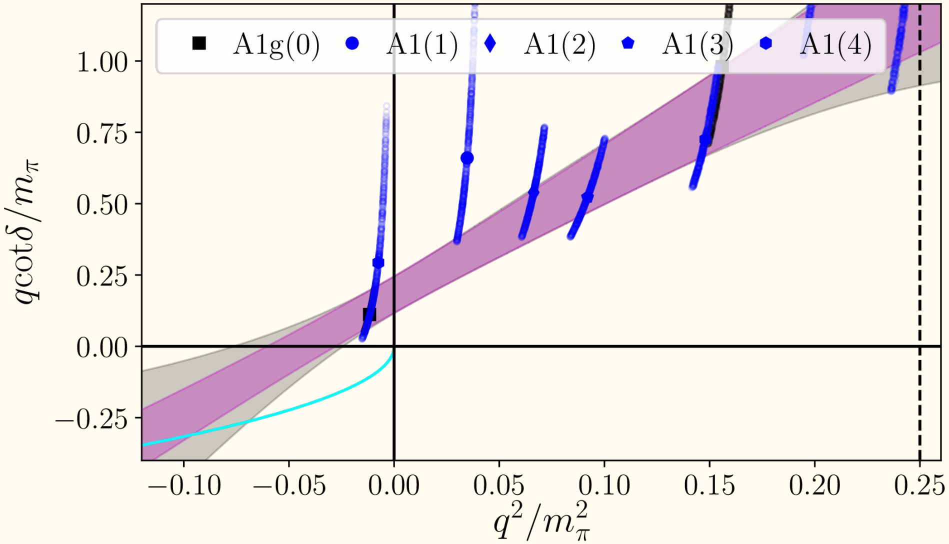
Lowest partial wave contributions to each irrep. Open circle for each interacting NN energy. Non-interacting levels denoted by horizontal dashed lines.



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., 2009.11825]

NN I=1 $^1S_0$ interaction

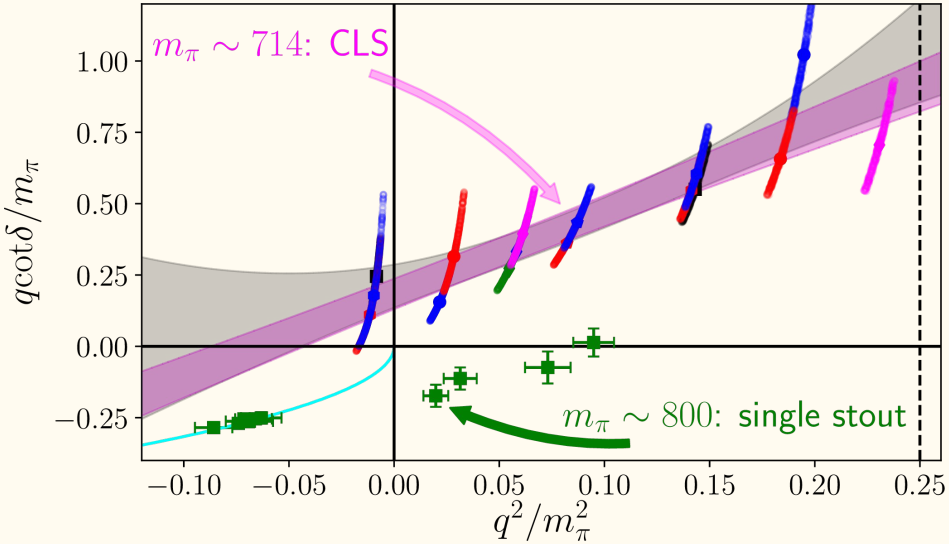
- All higher partial waves ignored
- Fit to 2 (magenta) and 3 (gray) terms of effective range expansion
- Strongly disfavors a bound state



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., 2009.11825]

NN $I=0$ $^3S_1$ interaction

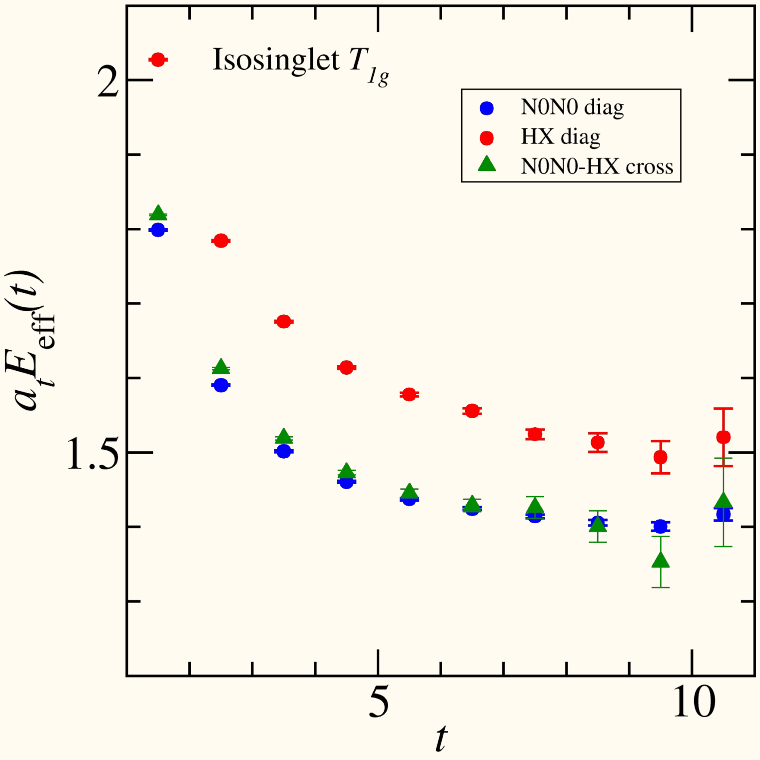
- Comparison with early results that used $\langle BB(t)H^\dagger(0)\rangle$ correlators
  [NPLQCD, Phys.Rev.D 96 (2017) 11, 114510]
- Earlier results use smeared action
- Different lattice spacings,
  $a \sim 0.086$ fm vs. $a \sim 0.145$ fm
- Perhaps the use of a hexaquark operator is playing a role?



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., 2009.11825]

Hexaquark?

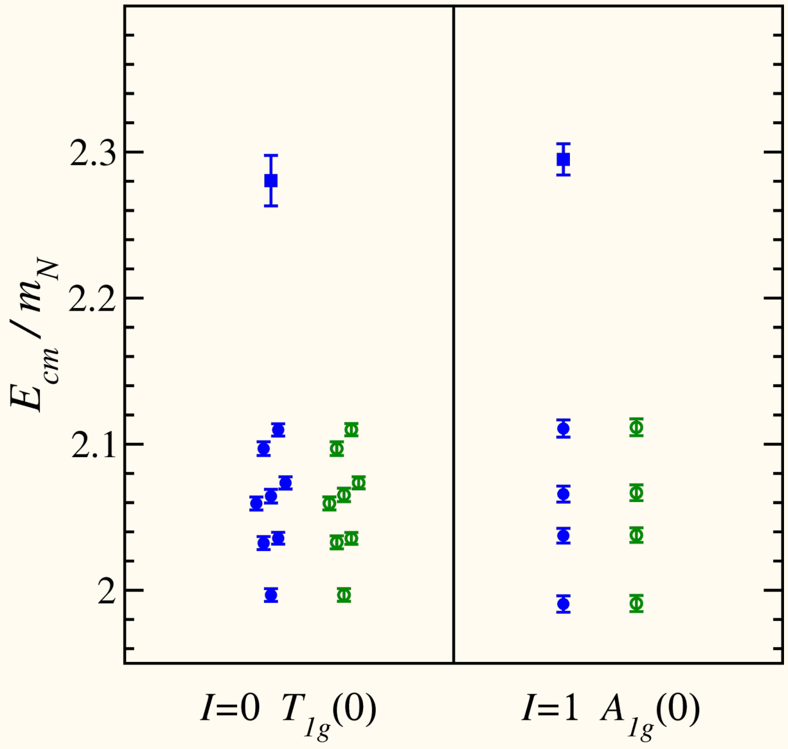
- In a recent update to the $m_\pi \sim$ 714 MeV NN results, hexaquark operators were studied
- $\langle BB(t)\, H(0)^\dagger \rangle$ correlator consistent with single $\langle BB(t)\, BB(0)^\dagger \rangle$



[BaSc, 2505.05547]

Hexaquark?

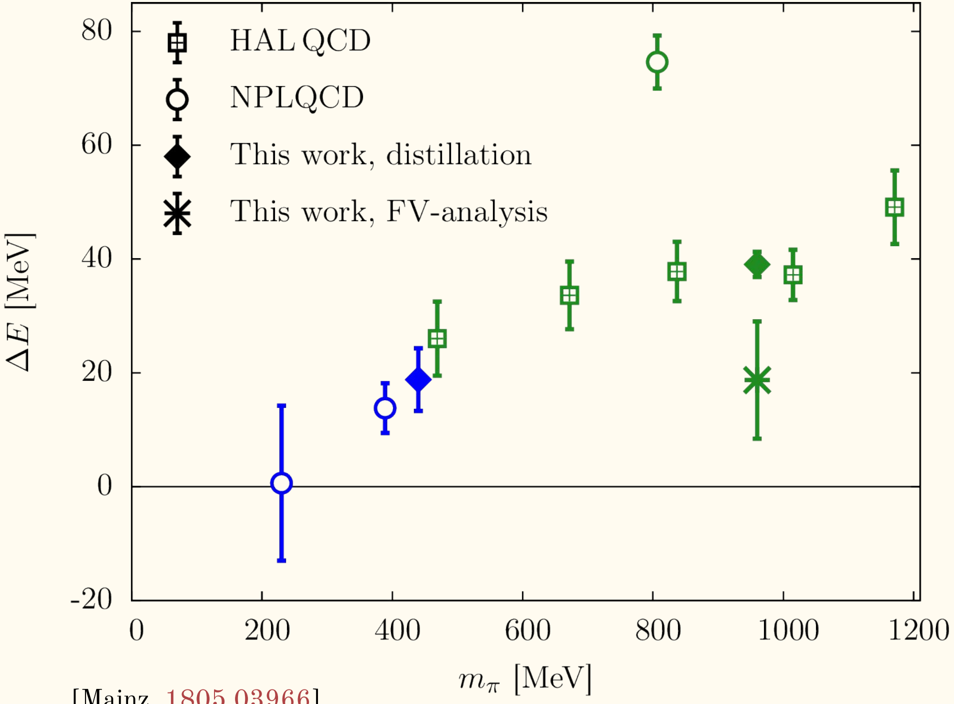
- In a recent update to the $m_\pi \sim 714$ MeV NN results, hexaquark operators were studied
- $\langle BB(t)\, H(0)^\dagger \rangle$ correlator consistent with single $\langle BB(t)\, BB(0)^\dagger \rangle$
- The spectrum for zero total momentum with (blue) and without (green) a hexaquark operator
- Inclusion of the hexaquark leads to an extra very high-lying level, but the spectrum is otherwise consistent when not using a hexaquark operator



[BaSc, 2505.05547]

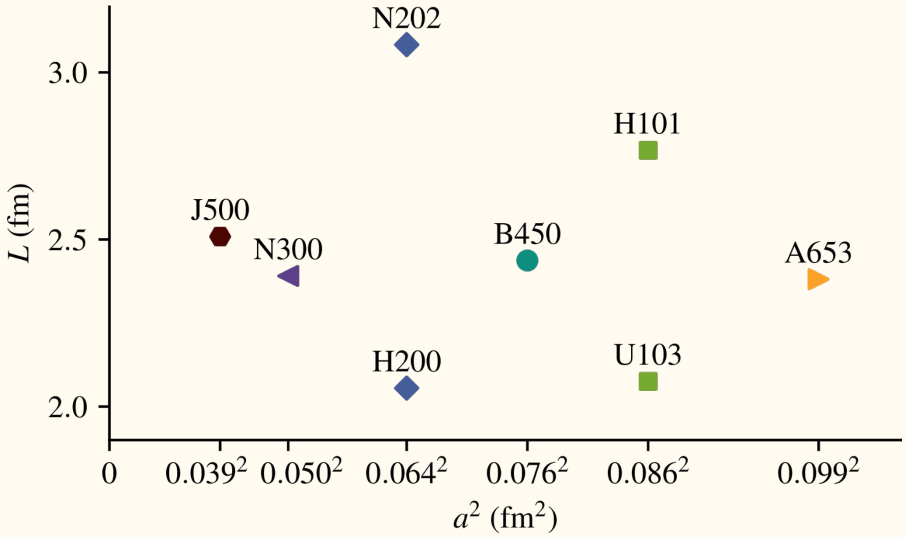
What about ΛΛ interactions?

- Disagreements also exist for the binding of lambda baryons too



[Mainz, 1805.03966]

- Mainz effort to better understand systematics



[Mainz, 2103.01054]

Extraction of energy shifts

- Fit ratio of diagonalized correlator

$$R_n(t) \equiv \frac{v_n^\dagger(\tau_0,\tau_D)\,C(t)\,v_n(\tau_0,\tau_D)}{C_\Lambda^{\vec{p}_1}(t)\,C_\Lambda^{\vec{p}_2}(t)}$$

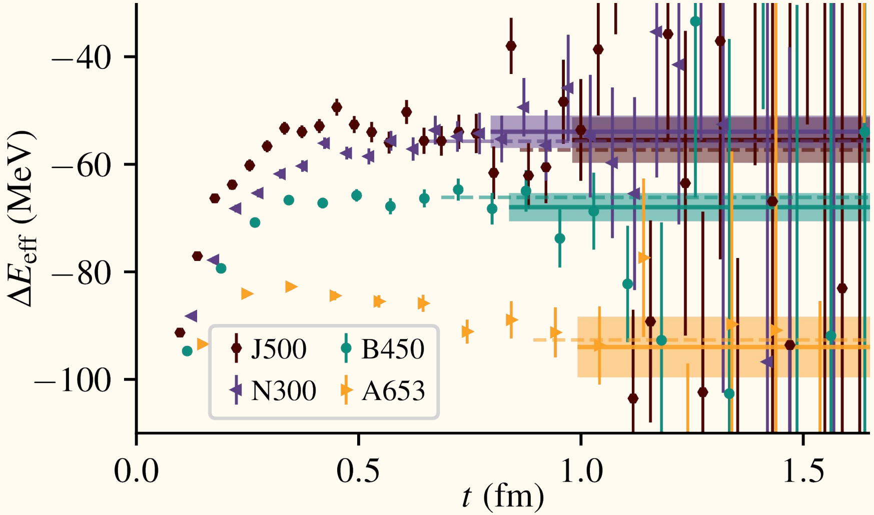
$$\lim_{t\to\infty} R_n(t) \propto e^{-\Delta E_n t}$$

- Leads to partial cancellation of correlated fluctuations and residual excited states

- Should wait until numerator and denominator have individually plateaued

- Use alternative spectrum for systematics

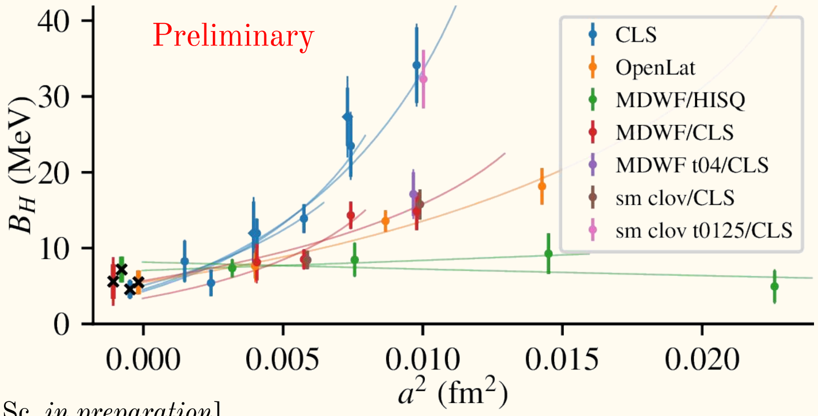
Effective energy difference for *Λ(1)Λ(0)* (singlet) ground state, using ensembles with similar volumes.



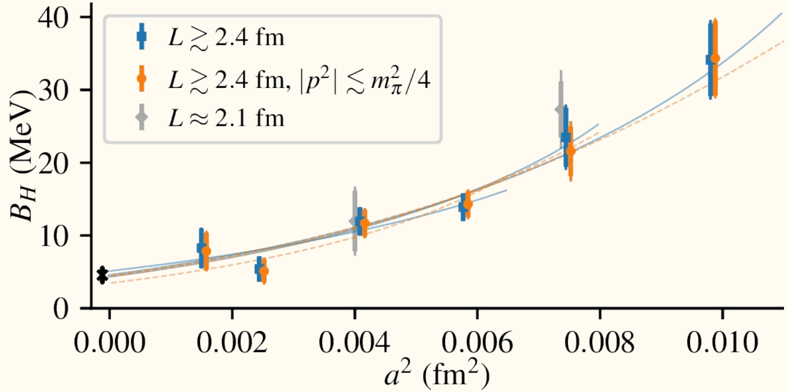
[Mainz, 2103.01054]

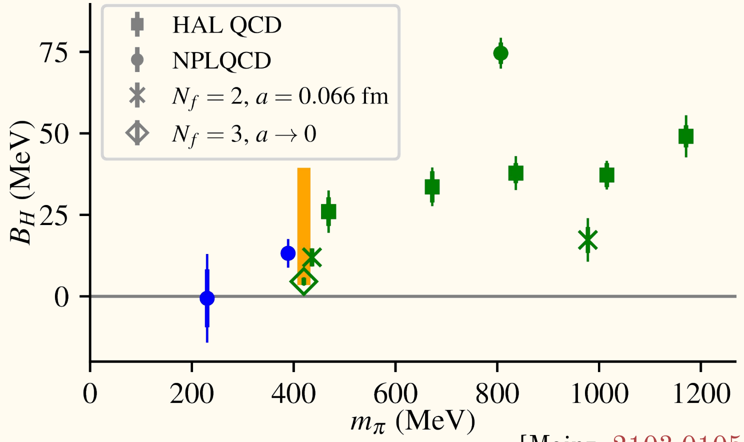
The H dibaryon binding energy summary

- From the phase shift, the binding energy of two Λ baryons can be determined
- Large dependence on the lattice spacing was found
- Does this explain the discrepancy?
- Other actions seems less affected



[BaSc, *in preparation*]

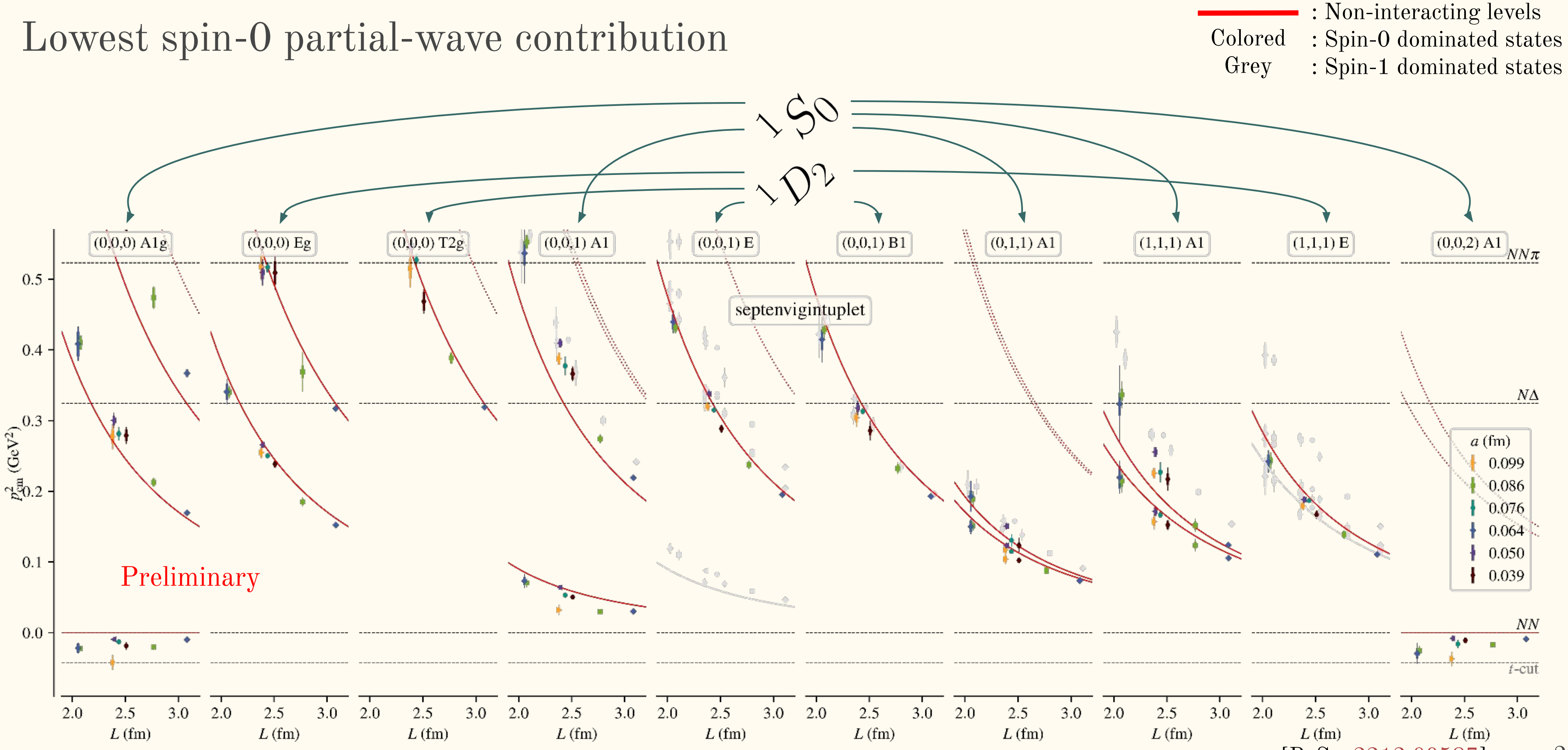




[Mainz, 2103.01054]

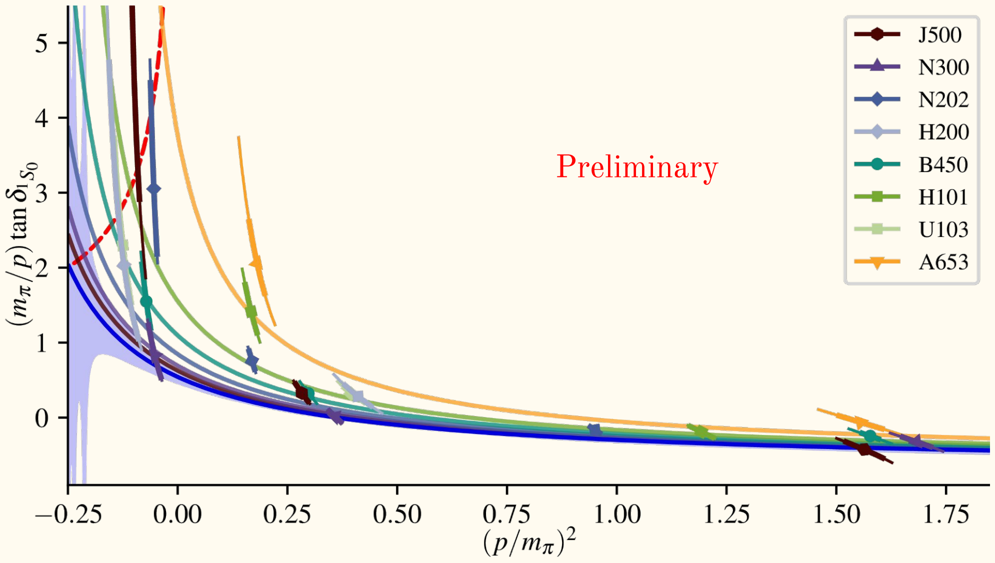
NN I=1 (27-plet) Spectrum

Lowest spin-0 partial-wave contribution



[BaSc, 2212.09587]

NN I=1 ${}^1S_0$ interaction



Results in the continuum and at each lattice spacing indicate a virtual bound state

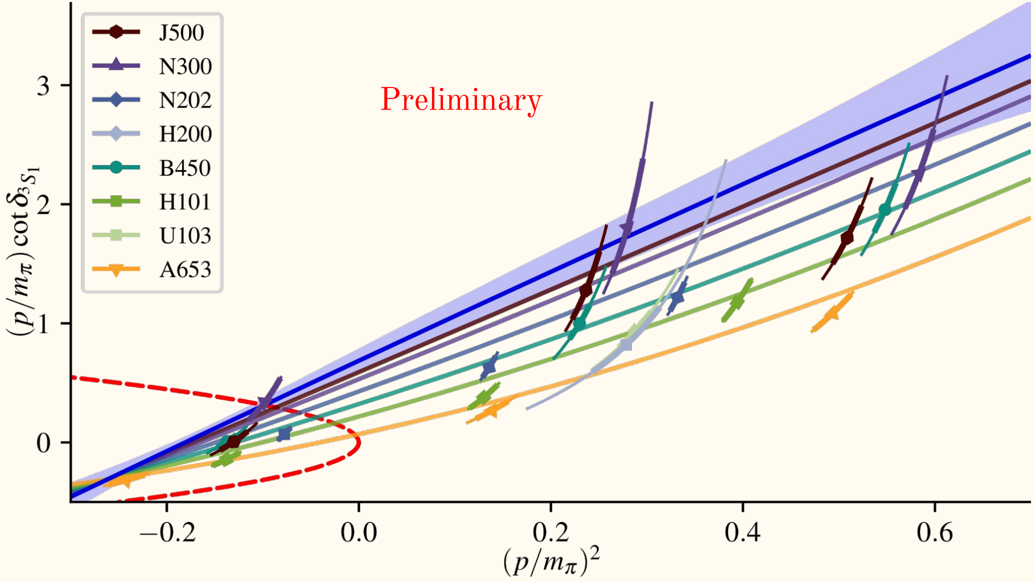
- Assumes only S-wave contributes
- Fit all levels in $A_{1g}(0)$ and $A_1(1)$ that are above t-channel cut and below inelastic threshold to

$$p\cot\delta(p) = \frac{c_0 + c_1 p^2}{1 + c_2 p^2}$$

where $c_i = c_{i0} + c_{i1}a^2$

[BaSc, 2212.09587]

NN $I{=}0$ $^3S_1$ Interaction



Fits for each lattice spacing and continuum prefer virtual bound state
(largest lattice spacing nearly a true bound state)

- Use levels up to second moving frame that contribute to S-wave
- Average over helicity in moving frames to suppress higher partial waves
  [R. Briceño et al., *Phys.Rev.*D 88 (2013) 11, 114507]
- Fit levels to
  $$p\cot\delta(p) = c_0 + c_1 p^2$$
  where $c_i = c_{i0} + c_{i1}a^2$

[BaSc, 2212.09587]

Conspiracy fit model

- Ratio fits from previous work also do not have monotonic effective energies

- Inspired by the benefits of the ratio fit, we utilize the conspiracy fit model which modifies the non-interacting model

$$C^{\text{free}}_{N_1N_2}(t) = \left[\sum_{n=0}^{N_1-1} A_n^{(1)} e^{-E_n^{(1)}t}\right]\left[\sum_{m=0}^{N_2-1} A_m^{(2)} e^{-E_m^{(2)}t}\right]$$

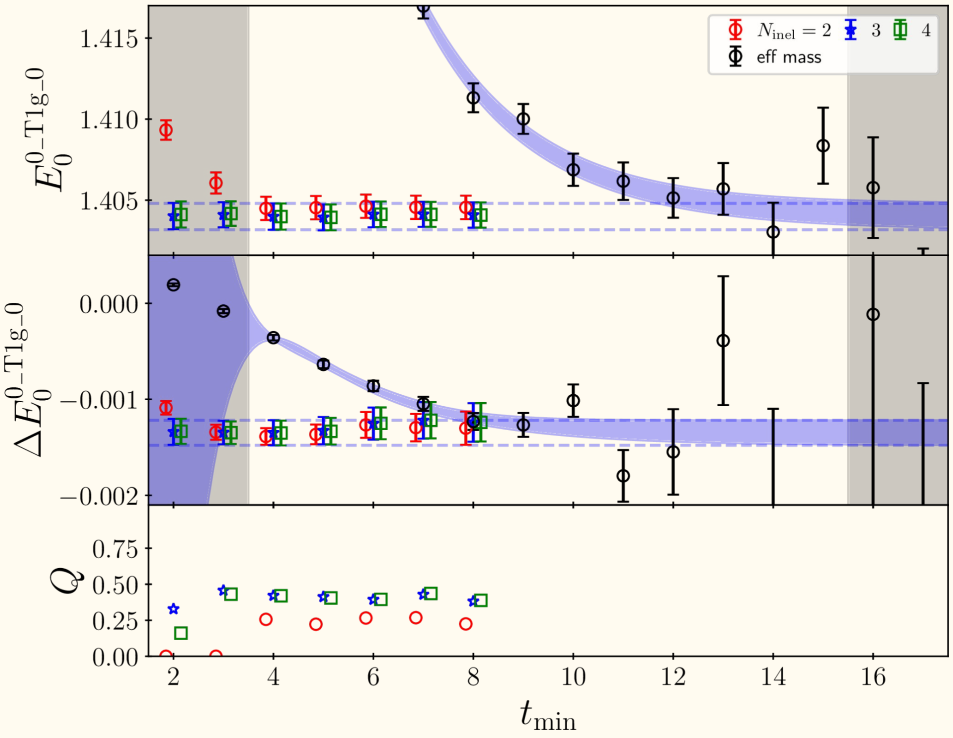
with a small shift in each exponential

$$E^{N_1^n N_2^m} = E_n^{(1)} + E_m^{(2)} + \delta_{nm}$$

where $E_n^{(1)}$ and $E_m^{(2)}$ are the single nucleon energies

- Perform global fit to single- and two-nucleon correlators

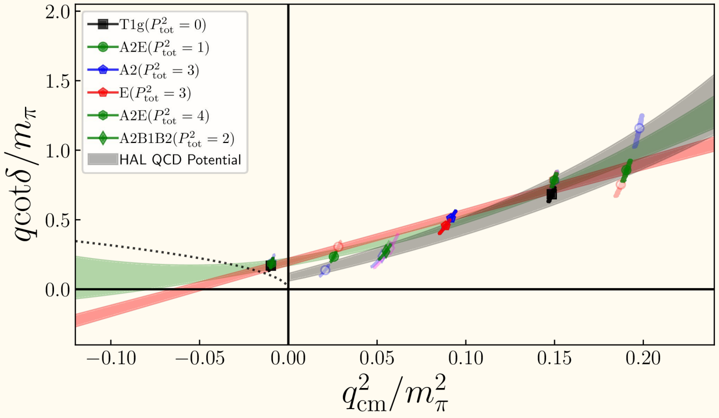
P=0, g.s. energy (deuteron), m$_\pi$~ 714 MeV

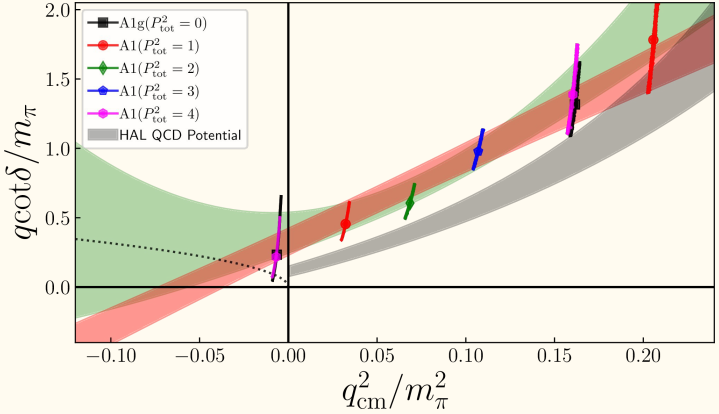


[BaSc, 2505.05547]

Updated results at $m_\pi \sim 714$ MeV

- Reanalysis with updated statistics
- Bound deuteron ruled out by $> 5\sigma$
- Bound di-neutron excluded at $\lesssim 3\sigma$
- Applied the HAL QCD potential method on the same ensemble, which shows qualitative agreement
- Discretization or derivative truncation errors could be causing the disagreement

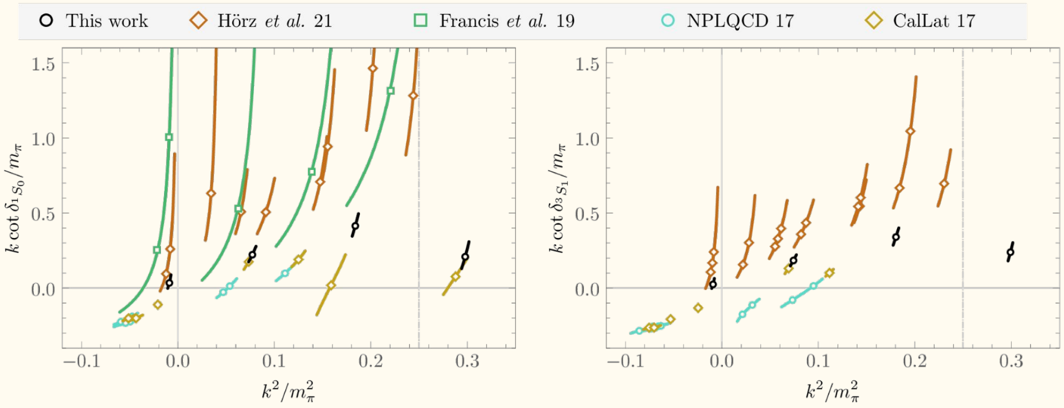


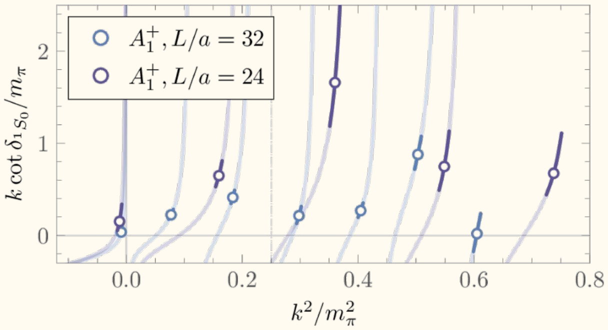


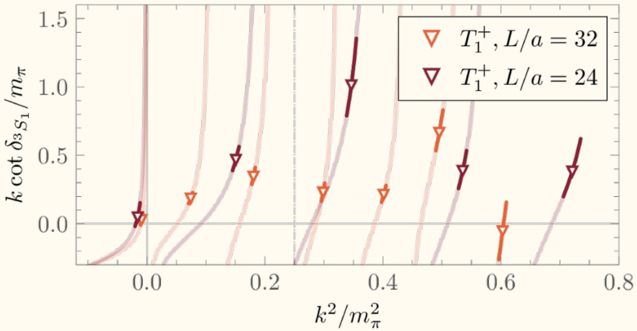
[BaSc, 2505.05547]

NN results beginning to converge

- *NN* results in continuum see only virtual bound state
- Qualitative agreement between Lüscher and HAL QCD on same ensemble
- GEVP results from all collaborations see no bound states at heavy pion masses

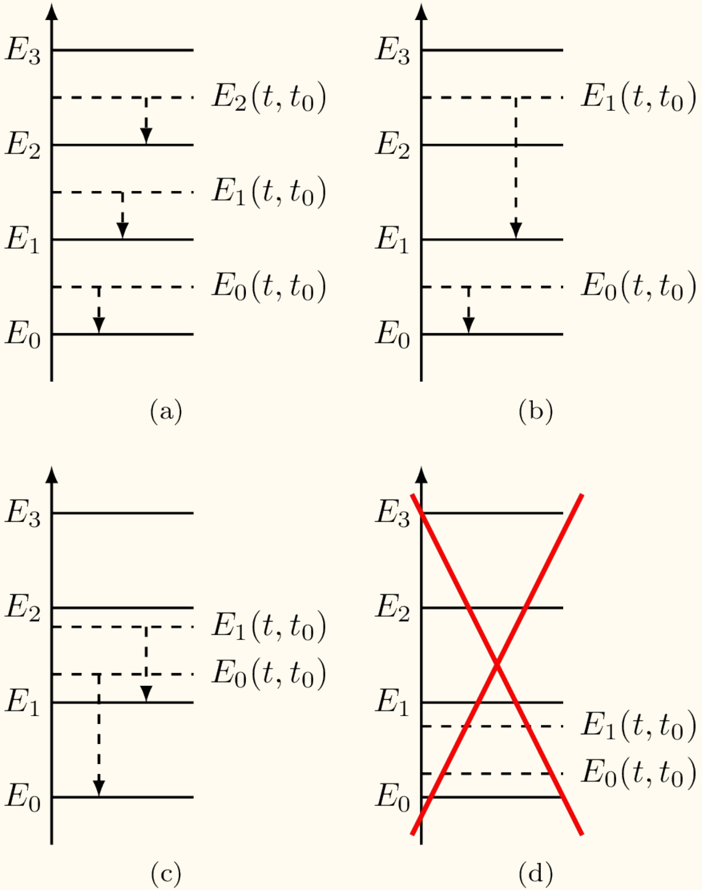






[NPLQCD, 2108.10835, 2404.12039]

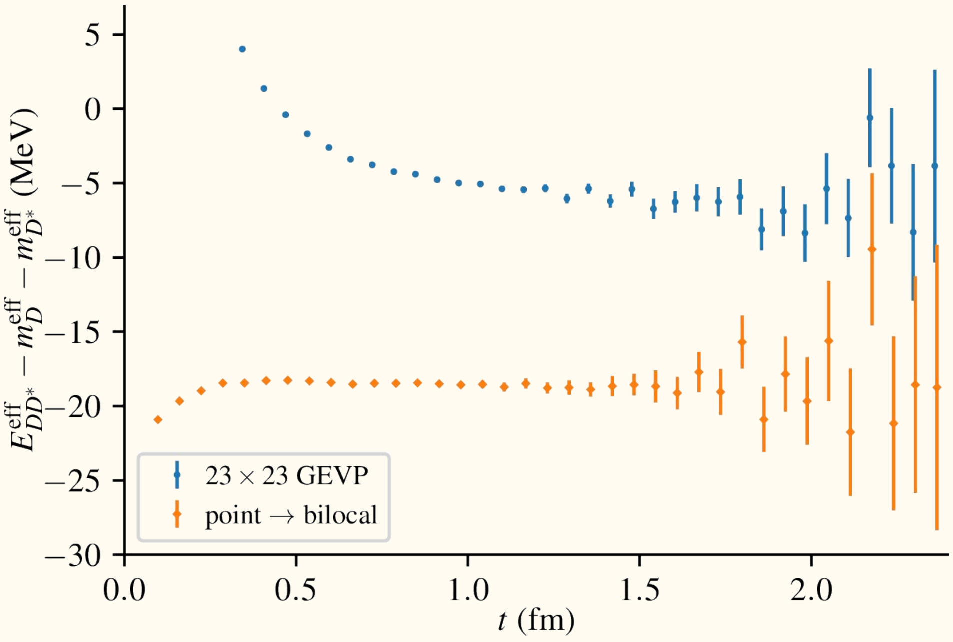
Variational Bounds?



- Effective energy of principal correlators (GEVP) approach true spectrum from above as Euclidean time separation is increased, hence "variational bound" is misleading
    - No cancellation of terms in spectral decomposition
    - Less likely to be misled by a false plateau
- Asymmetric correlators do not have this, desirable, property

[NPLQCD, 2404.12039]

Variational Bounds?

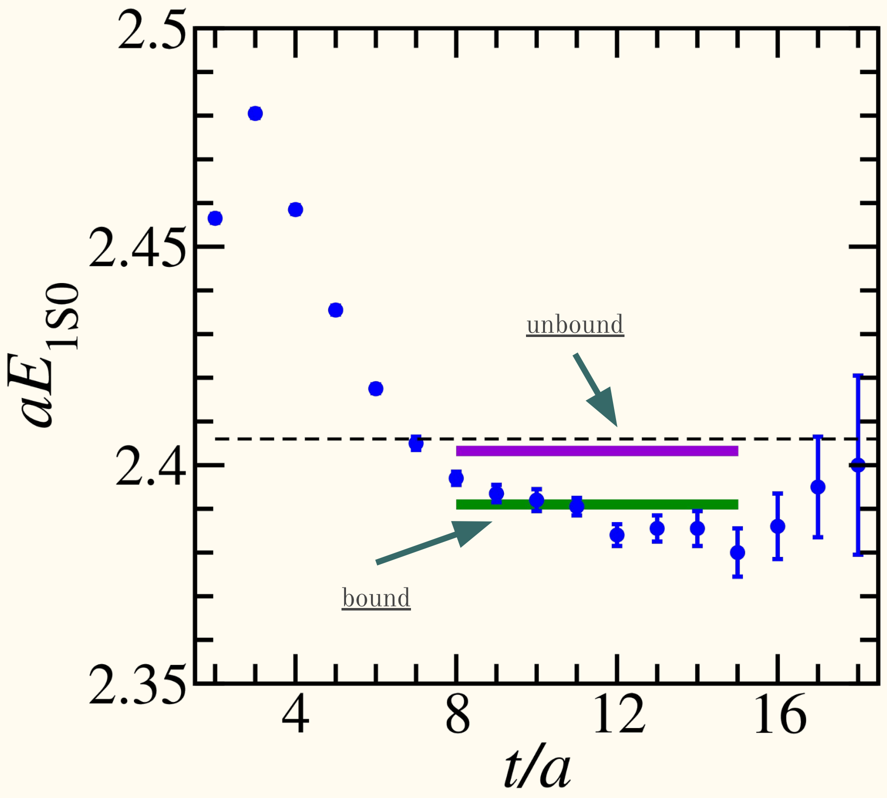


[J. Green, 2602.23244]

- Effective energy of principal correlators (GEVP) approach true spectrum from above as Euclidean time separation is increased, hence "variational bound" is misleading
  - No cancellation of terms in spectral decomposition
  - Less likely to be misled by a false plateau
- Asymmetric correlators do not have this, desirable, property
- Asymmetric correlator plateau can look convincing
  - GEVP increases gap to next contributing state
  - Gap for single correlator, $\Delta E^{-1} \approx 6\,\text{fm}$, suggesting no ground state saturation for asymmetric correlator.

Energy extraction systematic

- Identification of asymptotic regime for asymmetric correlators is more challenging
- The coefficients in the spectral decomposition are not guaranteed to be positive when using asymmetric correlator
- Therefore, the effective energy is not a monotonic function of the time separation

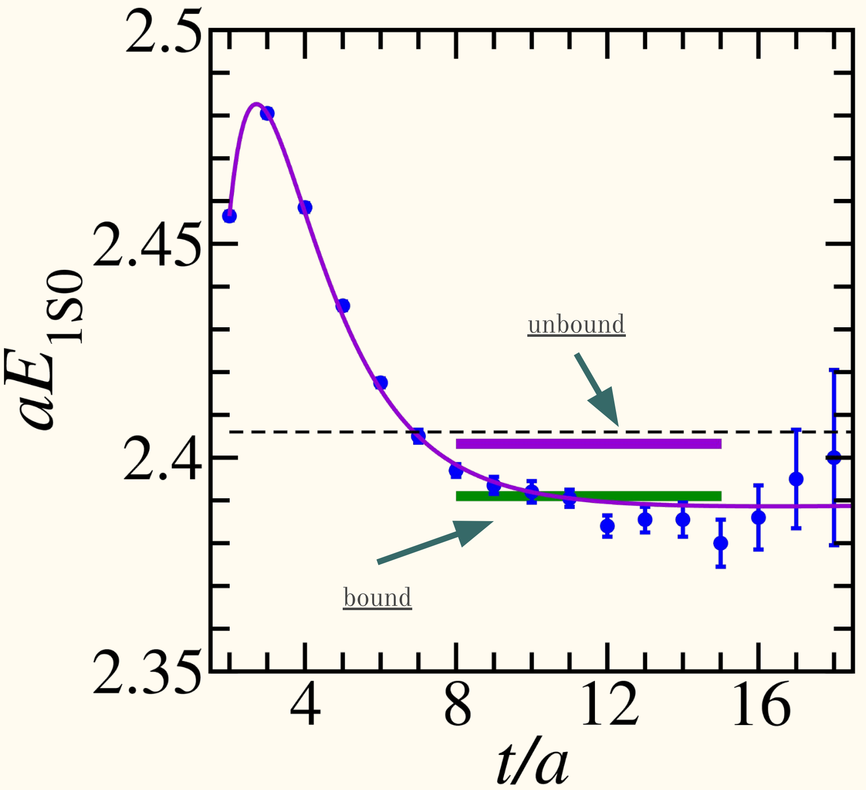


[Data: NPLQCD, 1705.09239]

Energy extraction systematic

- Identification of asymptotic regime for asymmetric correlators is more challenging
- The coefficients in the spectral decomposition are not guaranteed to be positive when using asymmetric correlator
- Therefore, the effective energy is not a monotonic function of the time separation
- A simple model of the correlator demonstrates this

$$C(t) = e^{-E_0 t}\Big(1 + A_1 e^{-\Delta_1 t} + A_2 e^{-\Delta_2 t} + A_3 e^{-\Delta_3 t} + A_4 e^{-\Delta_4 t}\Big)$$



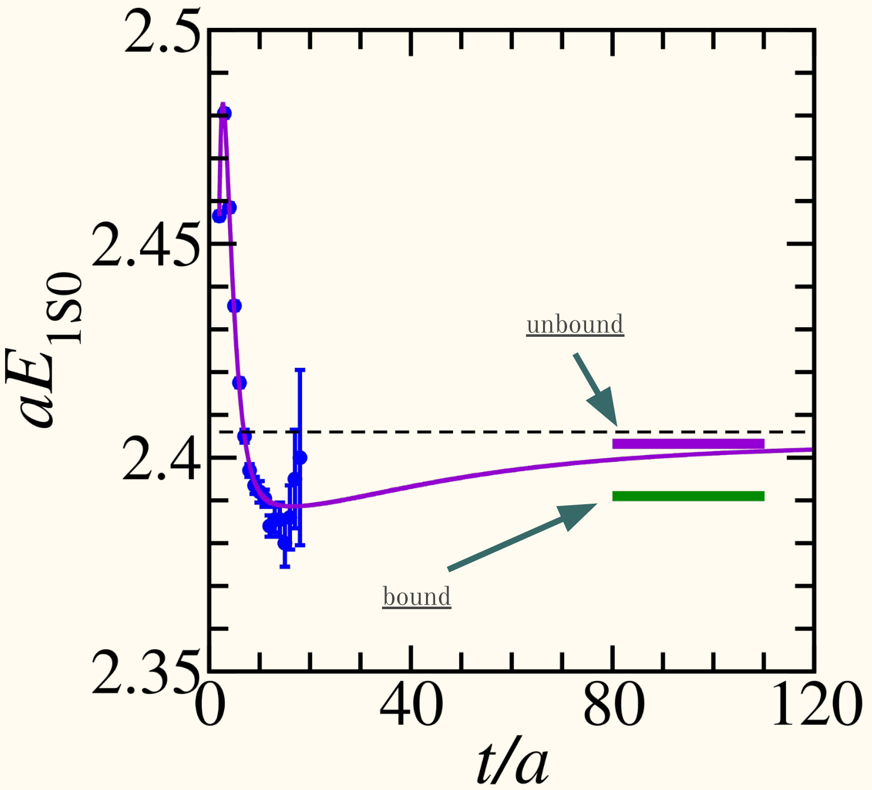
[Data: NPLQCD, 1705.09239]

[BaSc, 2505.05547]

Energy extraction systematic

- Identification of asymptotic regime for asymmetric correlators is more challenging
- The coefficients in the spectral decomposition are not guaranteed to be positive when using asymmetric correlator
- Therefore, the effective energy is not a monotonic function of the time separation
- A simple model of the correlator demonstrates this

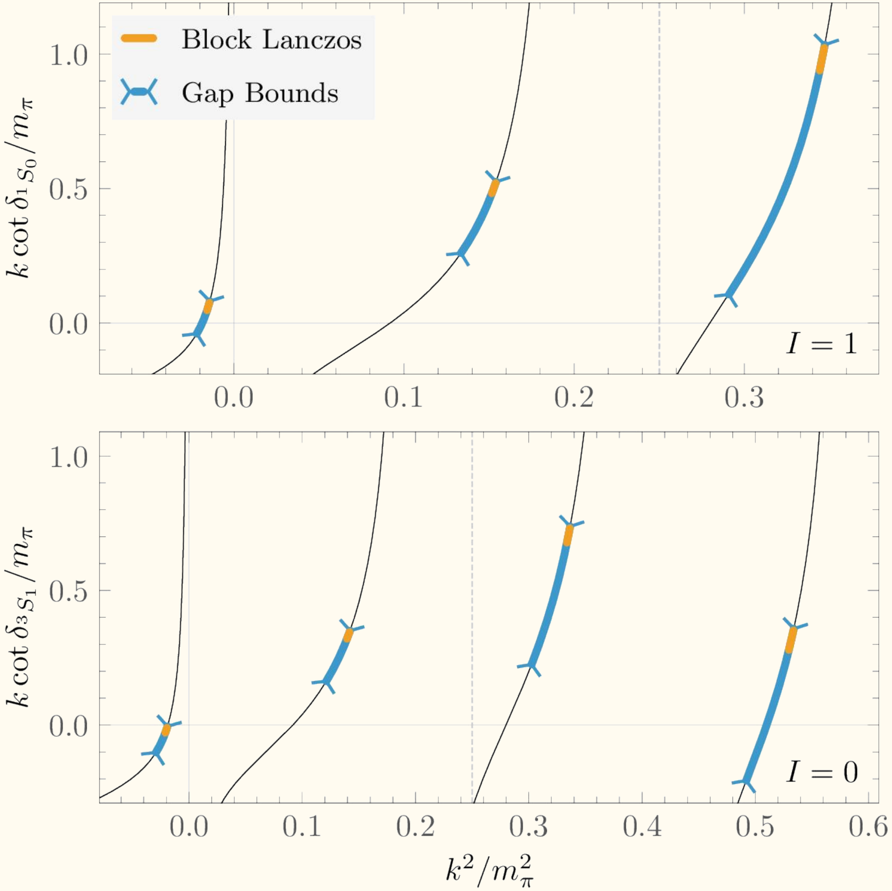
$$C(t) = e^{-E_0 t}\Big(1 + A_1 e^{-\Delta_1 t} + A_2 e^{-\Delta_2 t} + A_3 e^{-\Delta_3 t} + A_4 e^{-\Delta_4 t}\Big)$$



[Data: NPLQCD, 1705.09239]

[BaSc, 2505.05547]

Two-sided bound from Lanczos algorithm



- New method utilizes the Lanczos algorithm to determine eigenvalues of transfer matrix

  [M. Wagman, 2406.20009]

  - Residual bounds give two-sided range where *some* energy is guaranteed to lie

- Applied to *NN* system with $m_\pi \sim 800$ MeV
  - Not conclusive on question of bound or unbound

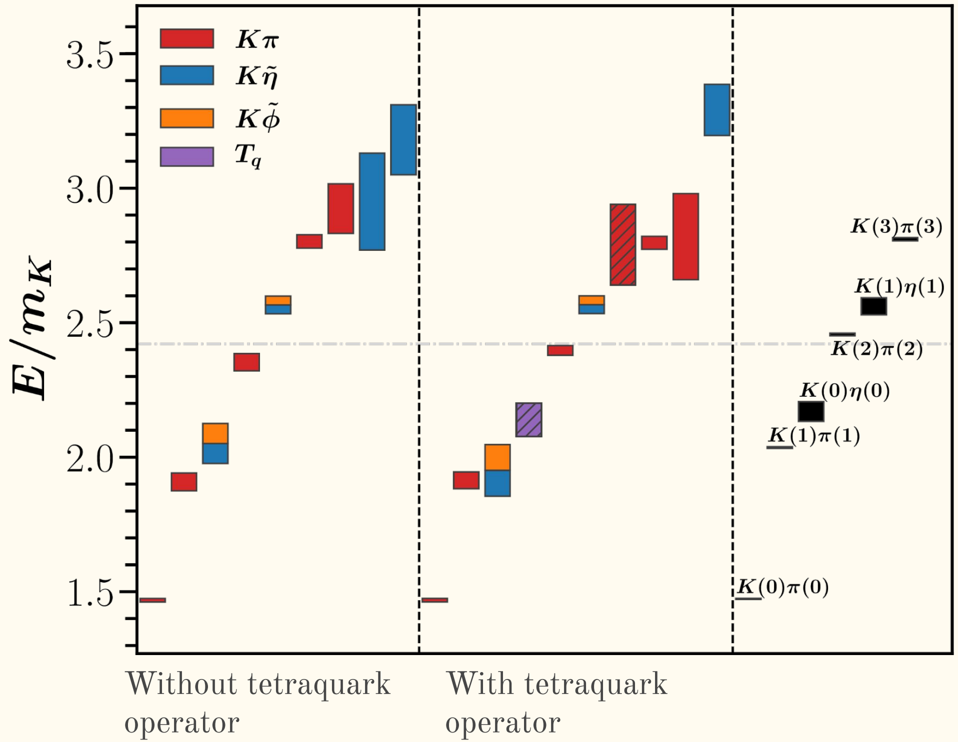
  [NPLQCD, 2601.22273, 2601.22272]

- Rigorous approach to error estimates for energies

- Does not solve the issue of missing states with poor overlap on operators

Missing Levels?

- How often do levels get missed?
  - Sometimes the operators used have small overlap onto some states
  - Recent example in the I=1/2, $K\pi$ system
  - Missing operators typically affects the accuracy of found energies

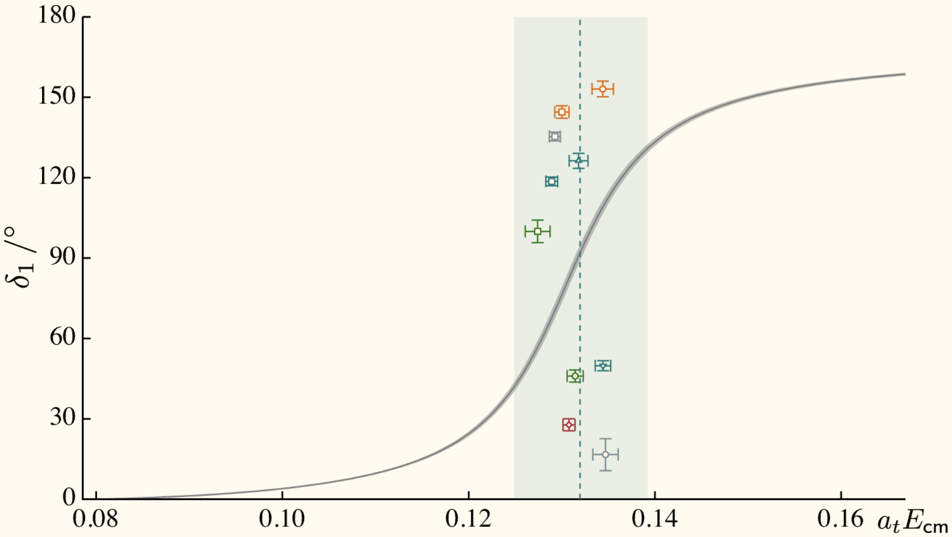


[**ADH** *et al.*, 2603.19192]

Missing Levels?

- How often do levels get missed?
  - Sometimes the operators used have small overlap onto some states
  - Recent example in the $I{=}1/2$, $K\pi$ system
  - Missing operators typically affects the accuracy of found energies

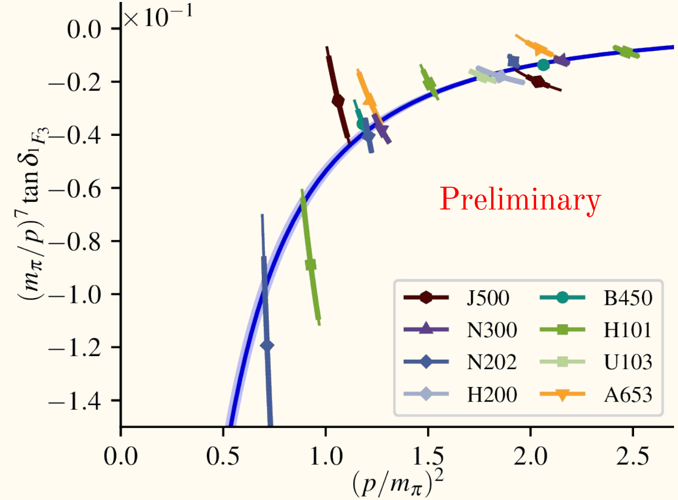
- The use of only $\bar{\psi}\Gamma\psi$ -like operators in ρ system, completing gets the spectrum wrong.
  - However, the quantization condition is signaling that the spectrum is wrong

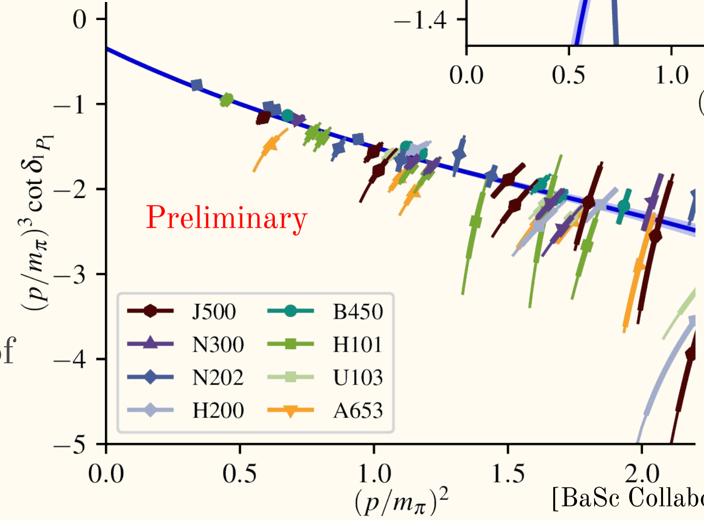


[Hadron Spectrum, 1507.02599]

Missing Levels?

- How often do levels get missed?
  - Sometimes the operators used have small overlap onto some states
  - Recent example in the *I*=*1/2*, $K\pi$ system
  - Missing operators typically affects the accuracy of found energies
- The use of only $\overline{\psi}\Gamma\psi$ -like operators in ρ system, completing gets the spectrum wrong.
  - However, the quantization condition is signaling that the spectrum is wrong
- Consistency with the Lüscher quantization condition is a highly non-trivial validation of the spectrum
  - For example, higher partial waves in *NN (I=0)* on the right





[BaSc Collaboration, *in preparation*]

Conclusions and Outlooks

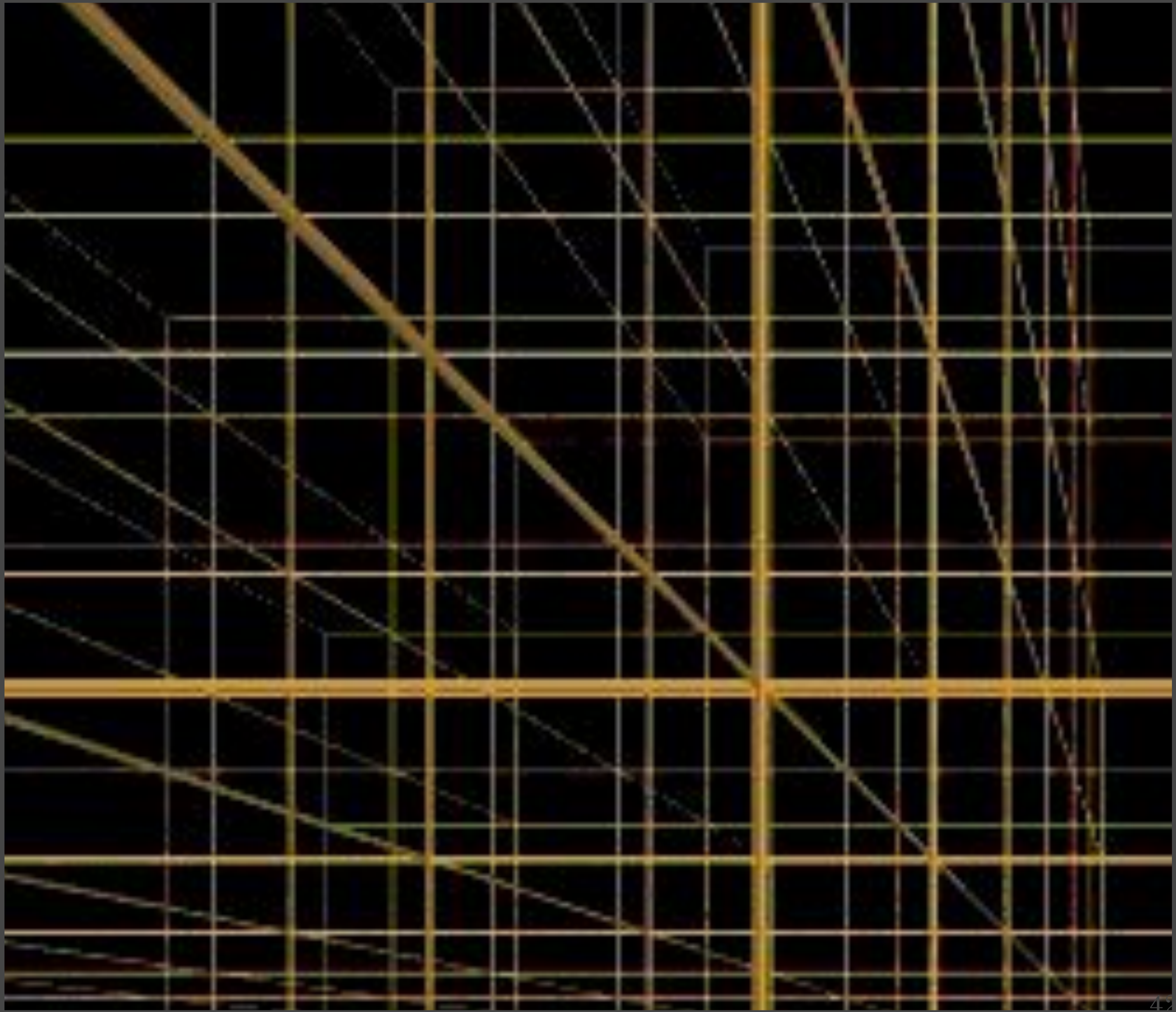
Conclusions

- Lots of evidence gathered that we can reliably determine *NN* spectrum
- Discretization effects can be important
- No sign of missing operators in dibaryon systems
- Results are converging from different groups/methods

Work for the future

- Reliable multi-nucleon matrix elements must wait for resolution of controversy
- Understand discretization effects from EFT?
- Other actions may be better for discretization effects
- Need to push calculations toward the physical point to make connections with chiral EFT
- Three nucleons..? The formalism is ready.. [Z. Draper *et al.*, 2303.10219]

Thanks!



Math grid tessellation (https://gifer.com/)