# Two-nucleon interactions from lattice QCD with a variational method: where are the bound states?

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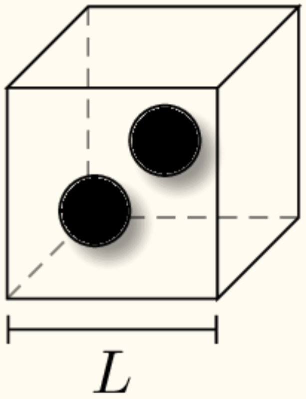
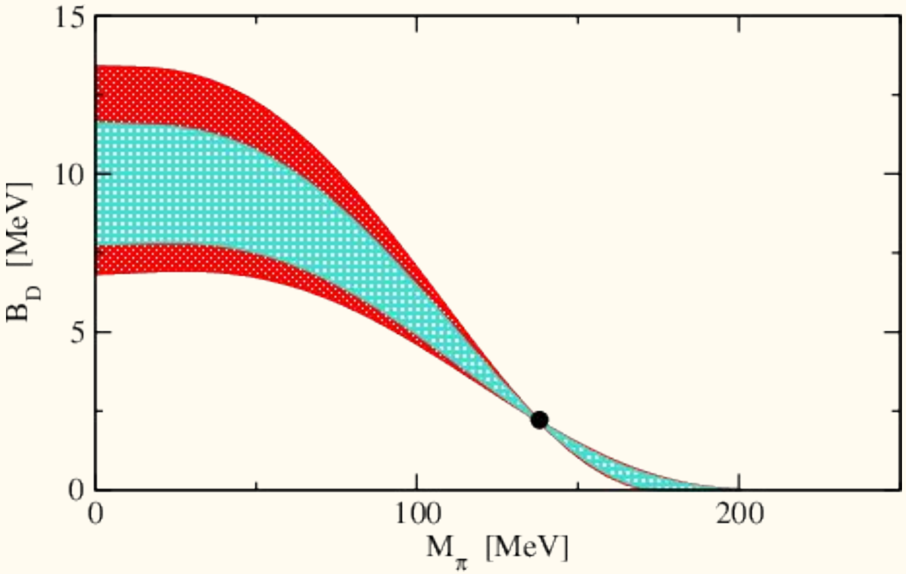
# Outline

1. History of two-baryon studies on the lattice
    - Disagreement in the literature on binding energies
2. Technical details
    - Variational method
    - Lüscher formalism
3. Recent results from sLapHnn and Mainz
    - sLapHnn - NN (I=0,1) systems at $m_\pi \sim 714$ MeV
    - Mainz - H dibaryon at $m_\pi \sim 420$ MeV with continuum limit



# Two-baryon systems

- Deuteron: only known stable dibaryon
  - Predicted to unbind for $m_\pi \sim 175$ MeV
- Jaffe prediction of a six-quark deeply bound (~80 MeV) flavor-singlet scalar
  - Upper bound of ~7 MeV on binding energy
- d*(2380) resonance
  - Possible dark matter candidate
- Nucleon-hyperon interactions in Neutron stars




Deuteron binding energy from ChPT

[E. Epelbaum, Ulf-G. Meißner,W. Glöckle, *Nucl.Phys.A* 714 (2003) 535-574]

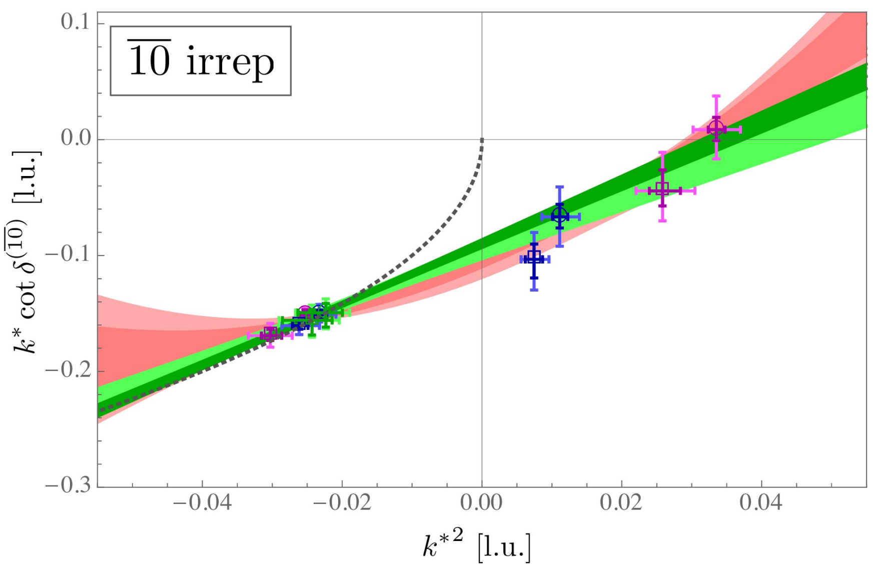
# Results from NPLQCD at $m_\pi \sim$ 806 MeV

Pole below threshold indicates a bound state

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

Nontrivial mass dependence required to reconcile EFT/ChPT prediction with bound state at large pion mass

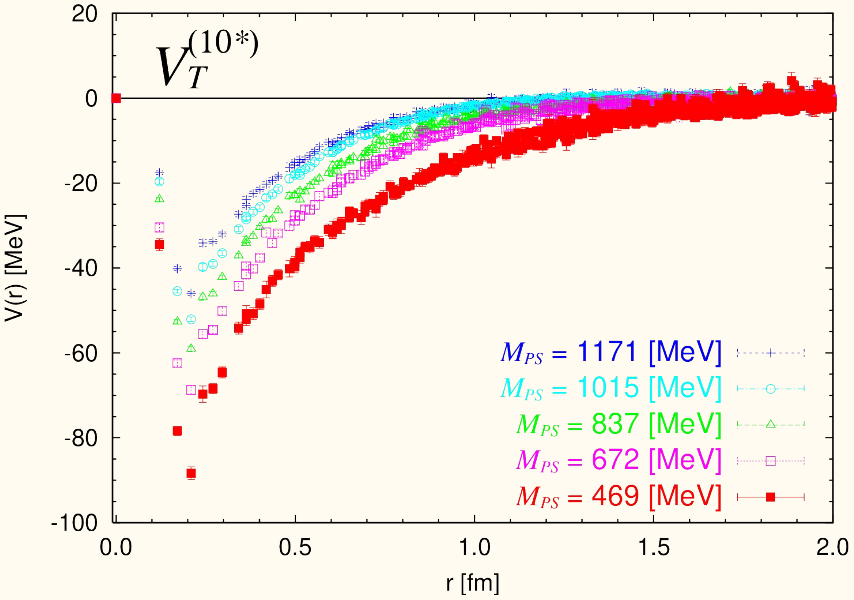
Bound state also at $m_\pi \sim$ 450 MeV




[NPLQCD Collaboration, *Phys.Rev.D* 96 (2017) 11, 114510]

# The HAL QCD Method

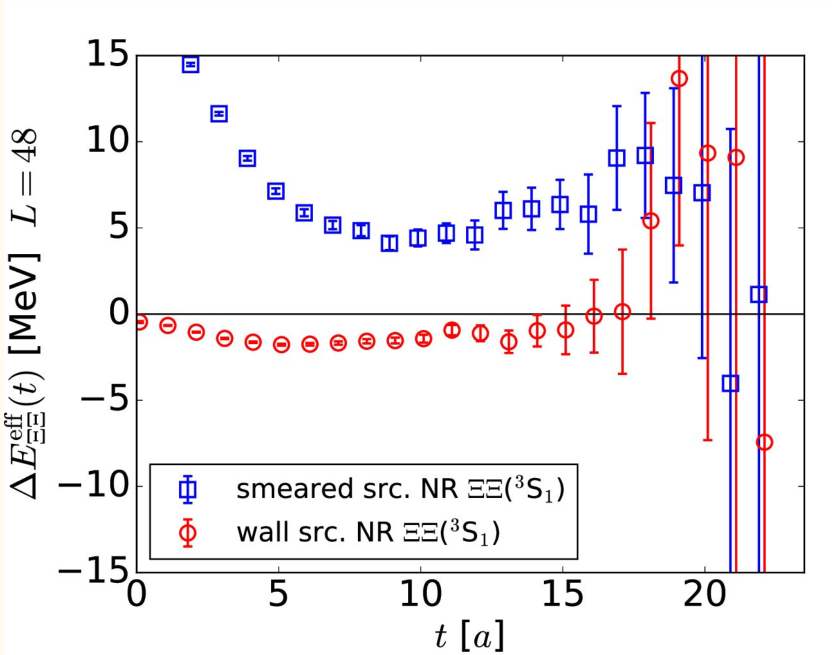
- Extract potentials from Nambu-Bethe-Salpeter wave function
- Obtain observables from solving Schrödinger equation
- No bound state for wide range of pion mass




[HAL QCD, *Nucl.Phys.A* 881 (2012) 28-43]

# What’s going wrong?

- Signal-to-noise ratio $\propto e^{-(m_B - 3m_\pi/2)t}$ makes this problem challenging
- Different methods
  - HAL QCD method vs. Lüscher method
- Possible systematics
  - Misidentified plateau for energies or incomplete operator basis (Lüscher method)
  - Truncation of derivative expansion (HAL QCD method)
  - Discretization effects




[Takumi Iritani et al., *JHEP 10*, 101 (2016)]

[*Nucl.Phys.B* 339, 222 (1990);
*JHEP 04*, 094 (2009)]

# Variational Method to Extract Excited States

Form $N \times N$ correlation matrix, which has the spectral decomposition

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

Solve the following eigenvector problem (equivalent to a generalized eigenvalue)

$$\hat{C}(\tau_D) = C(\tau_0)^{-1/2}\, C(\tau_D)\, C(\tau_0)^{-1/2}$$

And use the eigenvectors to rotate $\hat{C}(t)$ at all other times

If $\tau_0$ is chosen sufficiently large, then eigenvalues $\lambda_n(t, \tau_0)$ behave as

$$\lambda_n(t, \tau_0) \propto e^{-E_n t} + O(e^{-(E_N - E_n)t})$$

# Lüscher two-particle formalism

Compact formula for quantization condition

$$\det[\mathcal{M}^{-1}(E_L) + F^{(P)}(E_L, L)] = 0$$

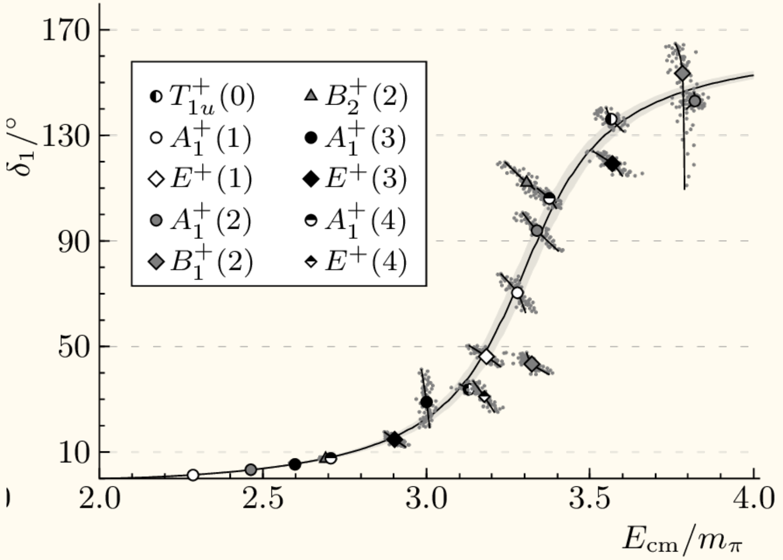
$E_L$ - finite-volume energies

$\mathcal{M}$ - 2-to-2 scattering amplitude

$F^{(P)}$ - known geometric function

Caveats: truncated at some max $\ell$, only valid above t-channel cut and below 3 (or 4) particle threshold, assumes continuum energies

$I = 1$ π-π $P$-wave scattering phase shift




[C. Andersen, J. Bulava, B. Hörz, C Morningstar, *Nucl.Phys.B* 939 (2019) 145]

PHYSICAL REVIEW C **103**, 014003 (2021)

# Two-nucleon $S$-wave interactions at the SU(3) flavor-symmetric point with $m_{ud} \approx m_s^{\rm phys}$: A first lattice QCD calculation with the stochastic Laplacian Heaviside method

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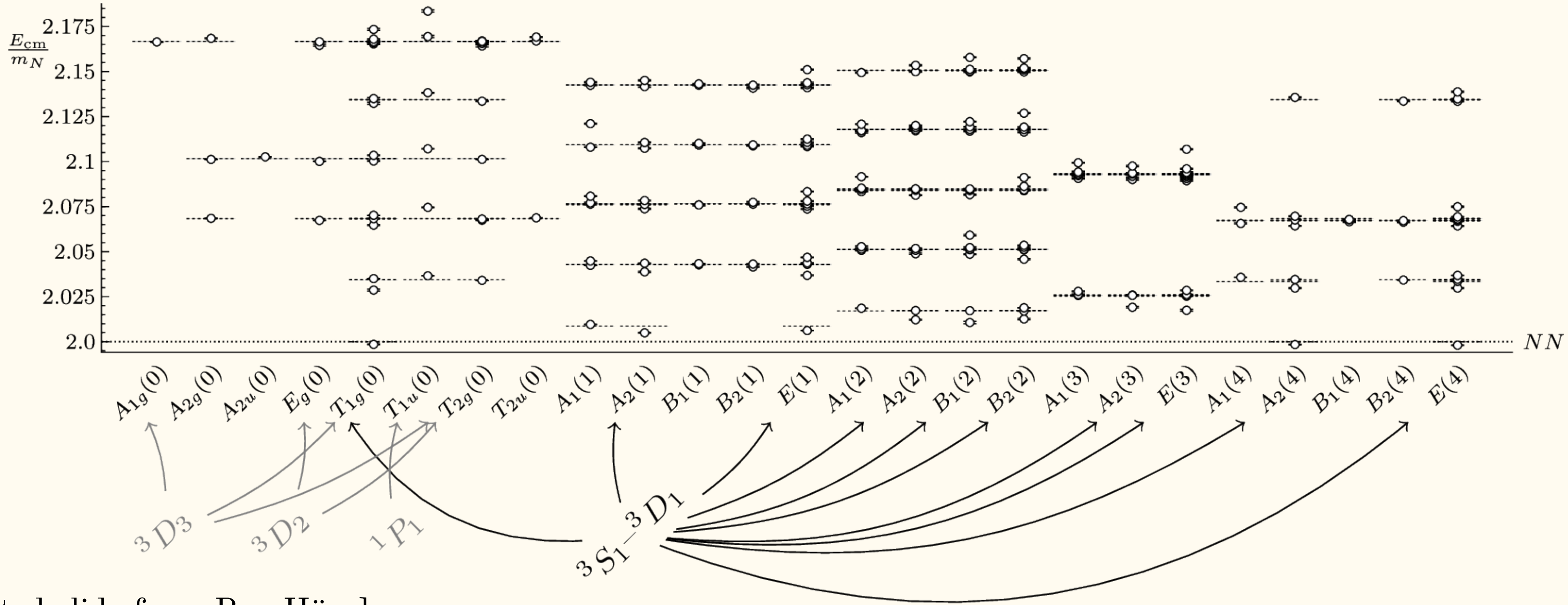
We report on the first application of the stochastic Laplacian Heaviside method for computing multiparticle interactions with lattice QCD to the two-nucleon system. Like the Laplacian Heaviside method, this method allows for the construction of interpolating operators which can be used to construct a set of positive-definite two-nucleon correlation functions, unlike nearly all other applications of lattice QCD to two nucleons in the literature. It also allows for a variational analysis in which optimal linear combinations of the interpolating operators are formed that couple predominantly to the eigenstates of the system. Utilizing such methods has become of paramount importance to help resolve the discrepancy in the literature on whether two nucleons in either isospin channel form a bound state at pion masses heavier than physical, with the discrepancy persisting even in the SU(3)-flavor-symmetric point with all quark masses near the physical strange quark mass. This is the first in a series of papers aimed at resolving this discrepancy. In the present work, we employ the stochastic Laplacian Heaviside method without a hexaquark operator in the basis at a lattice spacing of $a \approx 0.086$ fm, lattice volume of $L = 48a \approx 4.1$ fm and pion mass $m_\pi \approx 714$ MeV. With this setup, the observed spectrum of two-nucleon energy levels strongly disfavors the presence of a bound state in either the deuteron or dineutron channel.

# $NN\ I{=}0$ Finite-volume spectrum

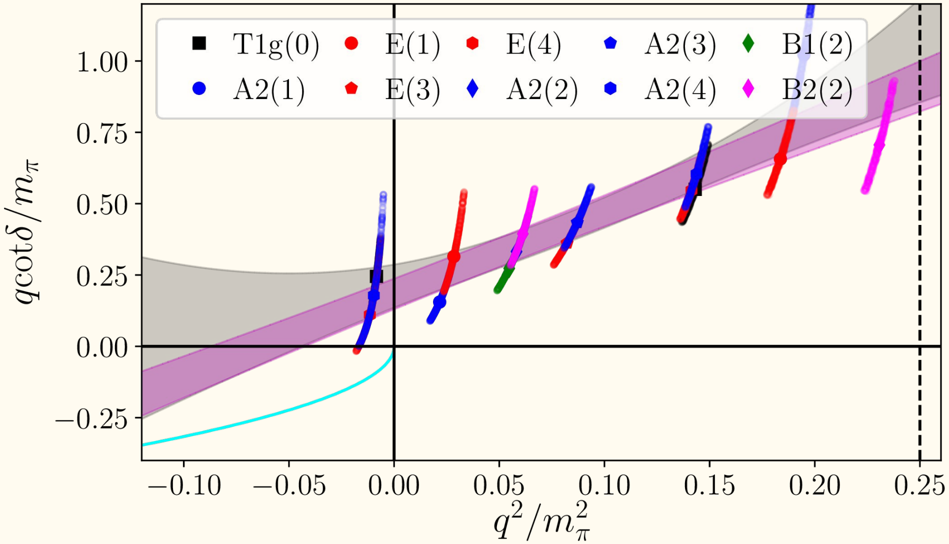
Lowest partial wave contributions




[Adapted slide from Ben Hörz]

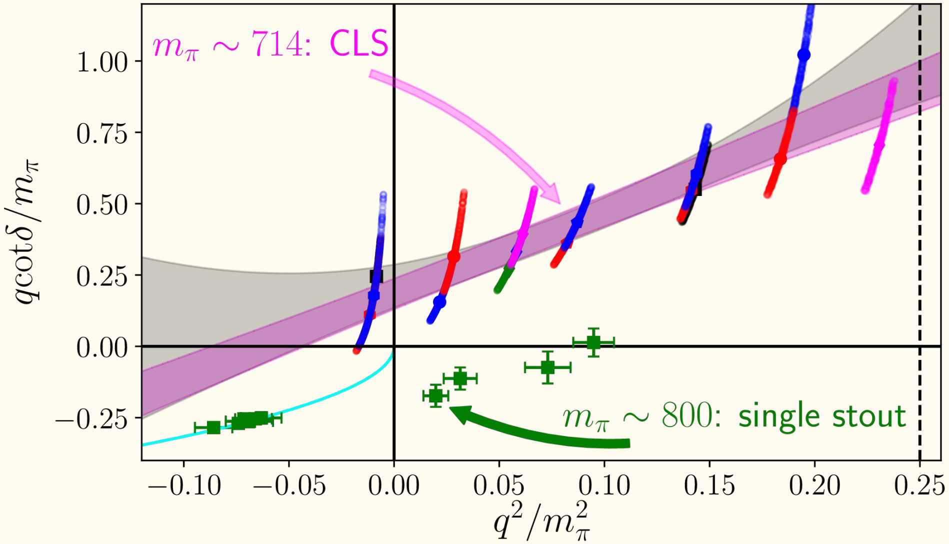
# $NN\ I{=}0\ {}^3S_1$ interaction

- All higher partial waves (including physical ${}^3S_1$ - ${}^3D_1$ mixing) ignored
- Fit to 2 (magenta) and 3 (gray) terms of effective range expansion
- Strongly disfavors a bound state



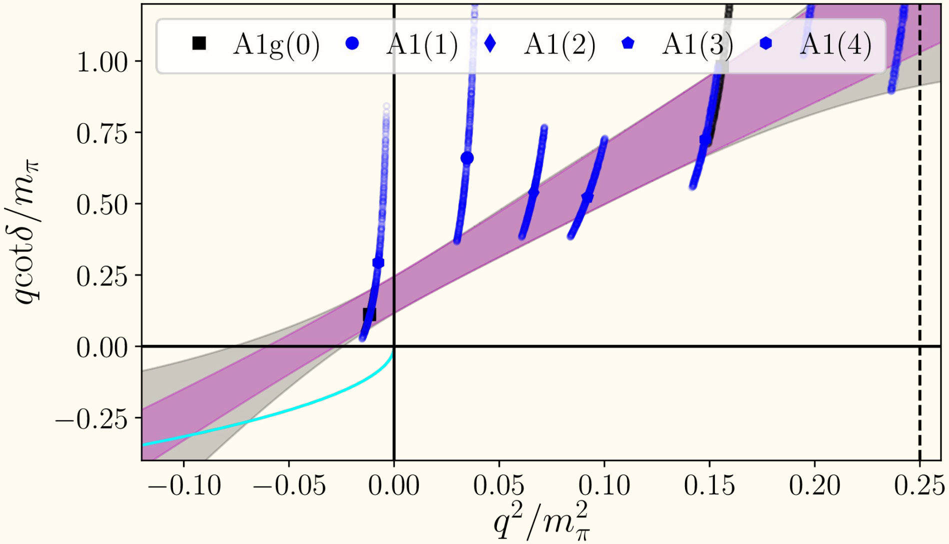
# Comparison to NPLQCD

- Comparison with NPLQCD shows strong tension
- Different action used, therefore discretization effects could be playing a role
- NPLQCD uses a hexaquark operator at the source



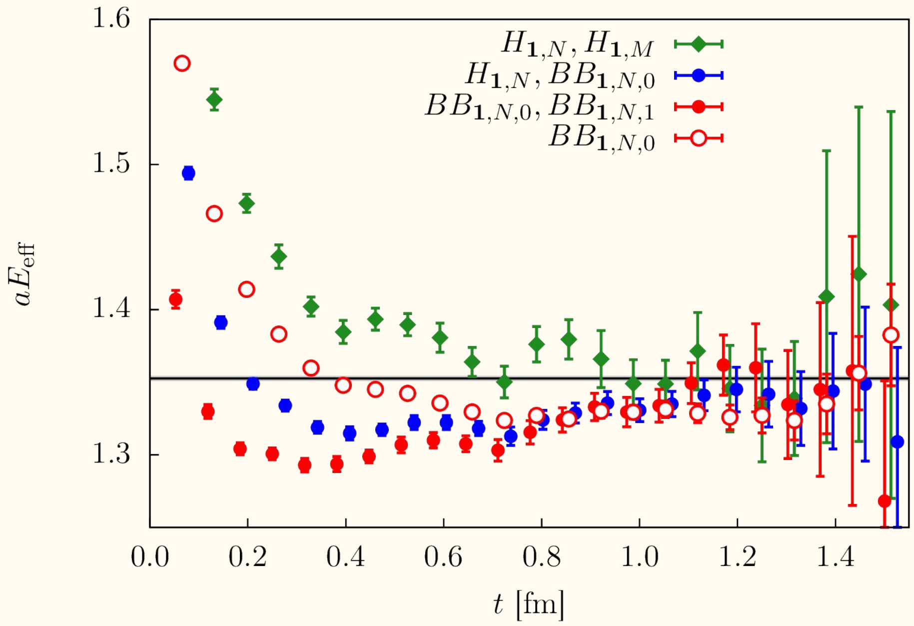
# $NN\ I{=}1\ {}^1S_0$ interaction

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



# Perhaps a deeply bound hexaquark?

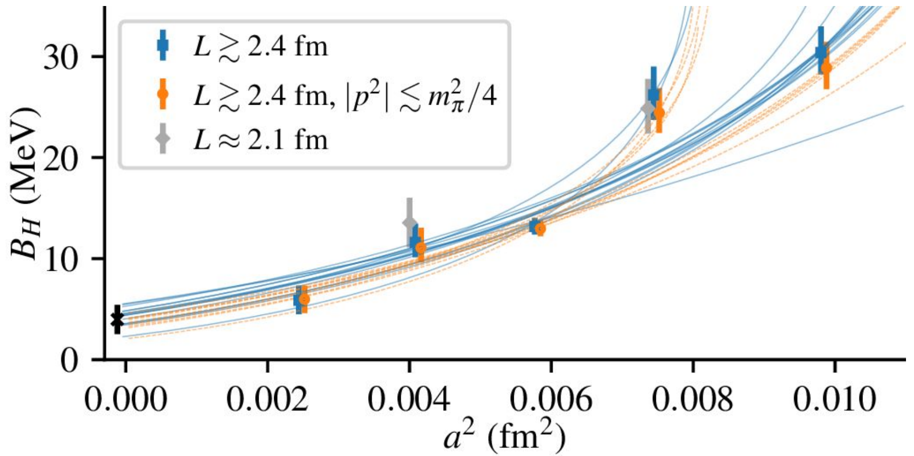
- No hexaquark operator was used in previous study
- Results from Mainz suggest the hexaquark might not be so important

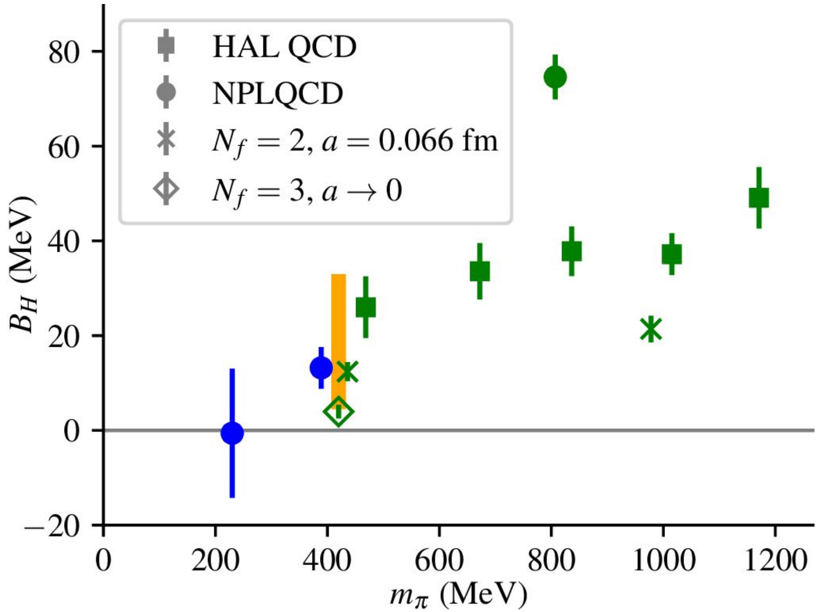



[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

# Discretization effects?

- $H$ dibaryon binding energy has strong dependence on the lattice spacing
- Could explain large disagreements from various groups

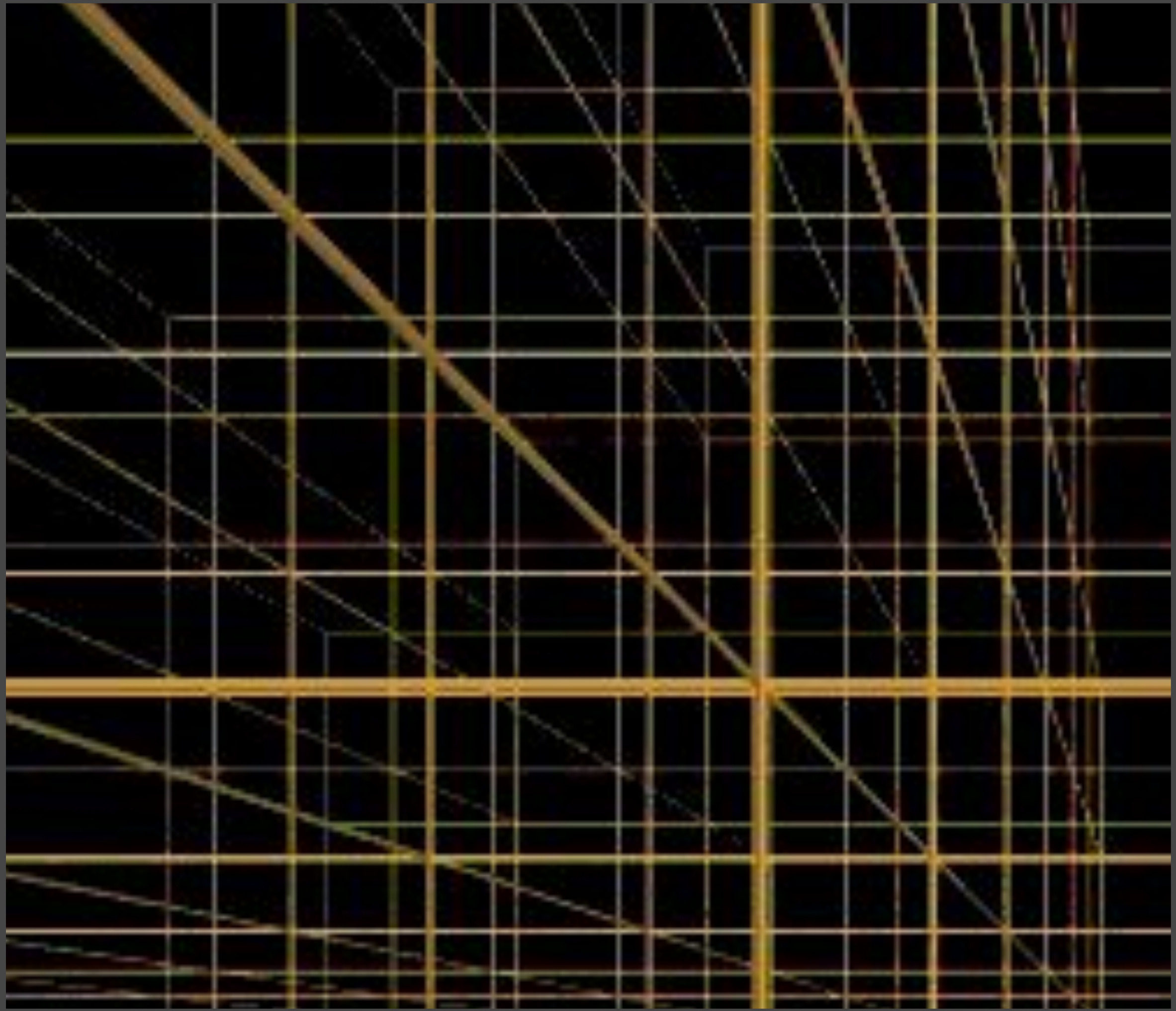


# Conclusions and Outlooks

- Status of baryon-baryon calculations from lattice QCD
  - More work is needed to understand the disagreement in the literature
  - If discretization effects are pervasive - huge efforts will be required
- Future work on baryon-baryon systems
  - Move away from SU(3)-symmetric point
  - Include coupled-channel analysis
  - Investigate role of hexaquark and other methods
  - Try other actions
- Discrepancy must be resolved before going beyond these simple systems

# Thanks!



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

# Backup Slides

# Interpolating operators

Must design operators to create states of interest

Start from momentum-projected octet baryon operators

$$B_\alpha(\boldsymbol{p},t)[rst] = \sum_{\boldsymbol{x}} e^{-i\boldsymbol{p}\cdot\boldsymbol{x}} \epsilon_{abc}(s^a C\gamma_5 P_+ t^b) r^c_\alpha$$

Form spin-zero and spin-one basis of two-baryon operators

$$[B_1 B_2]_0(\boldsymbol{p}_1,\boldsymbol{p}_2) = B^{(1)}(\boldsymbol{p}_1) C\gamma_5 P_+ B^{(2)}(\boldsymbol{p}_2), \quad [B_1 B_2]_i(\boldsymbol{p}_1,\boldsymbol{p}_2) = B^{(1)}(\boldsymbol{p}_1) C\gamma_i P_+ B^{(2)}(\boldsymbol{p}_2),$$

Particular linear combinations of these are needed for definite flavor and irrep of lattice symmetry group

# Energies from 2-point correlation functions

In principle, one can extract all desired energies from 2-point correlators

$$C(t) = \langle 0|\mathcal{O}(t+t_0)\mathcal{O}^\dagger(t_0)|0\rangle = \sum_{n=0}^{\infty} |\langle 0|\mathcal{O}|n\rangle|^2 e^{-E_n t}$$

Correlator asymptotes to ground state at large time separation

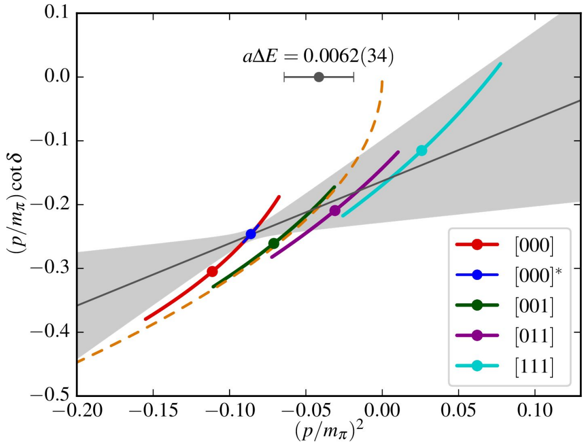
Numerically difficult due to signal-to-noise ratio $\propto e^{-(m_B - 3m_\pi/2)t}$

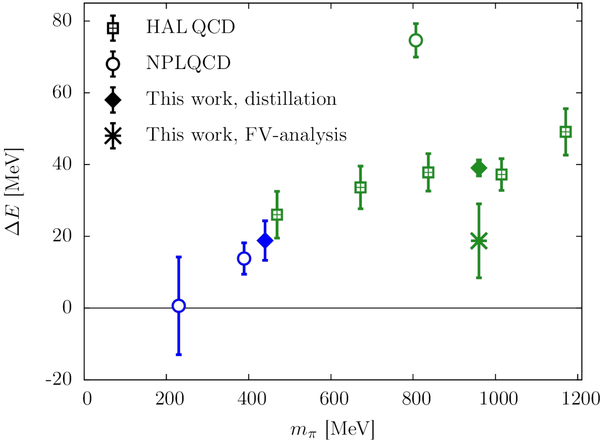
Smearing of the quark fields in interpolating operators reduces excited state contamination

$$\tilde{q}(\vec{y}, t) = \mathcal{S}^{(t)}(\vec{y}, \vec{x}) q(\vec{x}, t)$$

# Mainz joins the party

- First two-baryon calculation using distillation and a variational approach
- A bound dineutron is found to be unlikely
- H-dibaryon binding energy has tension with other results
- Quenched strange quark




[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

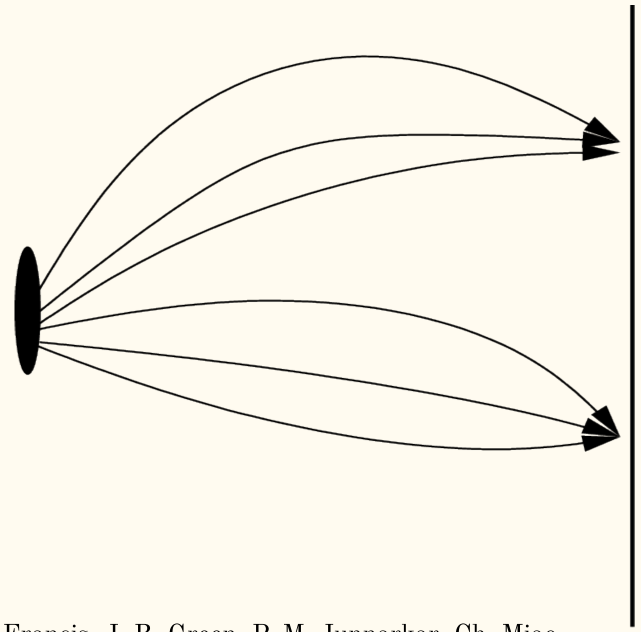
# Disadvantages of point sources

Source operator must be a local operator (hexaquark)

Non-hermitian correlator matrix means non-monotonic decay of effective energy

Plateau identification more difficult

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



[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

[*Phys.Rev.D* 80, 054506 (2009)]

# Quark Propagation with Distillation

A particular smearing kernel, Laplacian-Heaviside (LapH) smearing, turns out to be particularly useful

$$\mathcal{S}^{(t)}_{ab}(\vec{x},\vec{y}) = \Theta(\sigma_s + \Delta^{(t)}_{ab}(x,y)) \approx \sum_{k=1}^{N_{\mathrm{LapH}}} v^{(k)}_a(\vec{x},t) v^{(k)}_b(\vec{y},t)^*$$

Smearing of the quark fields results in smearing of quark propagator

$$\mathcal{S} M^{-1} \mathcal{S} = V(V^\dagger M^{-1} V) V^\dagger$$

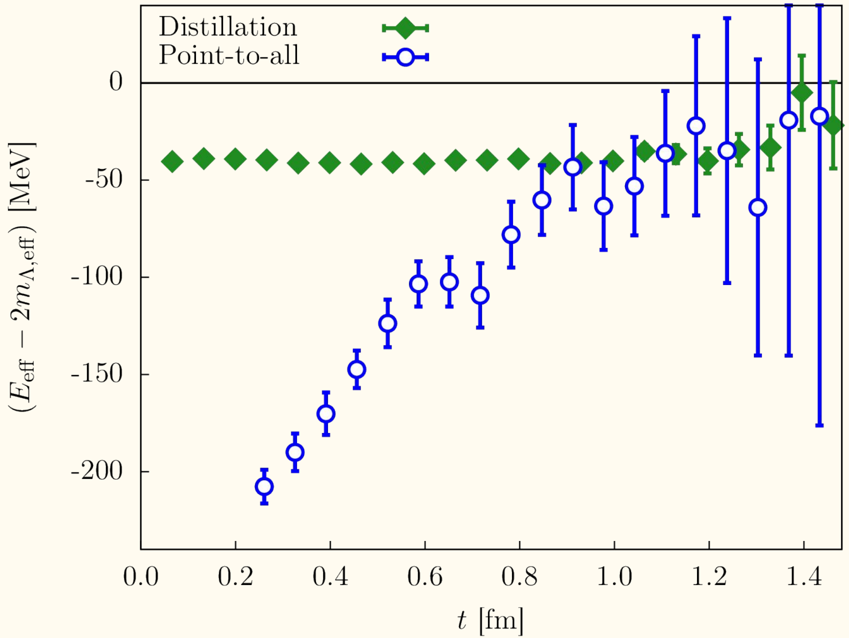
where the columns of $V$ are the eigenvectors of $\Delta$

Only need the elements of the much smaller matrix (perambulators)

$$\tau_{kk'}(t,t') = V^\dagger M^{-1} V = v^{(k)}_a(x)^* M^{-1}_{ab}(x,y) v^{(k')}_b(y)$$

# Distillation vs. Smeared Point Sources

- Distillation used two baryon operators at both source and sink
- Smeared point sources required hexaquark at the source.
- Better quality data with less inversions




[A. Francis, J. R. Green, P. M. Junnarkar, Ch. Miao, T. D. Rae, H. Wittig, *Phys.Rev.D* 99 (2019) 7, 074505]

[Lüscher '86, '91; generalizations]

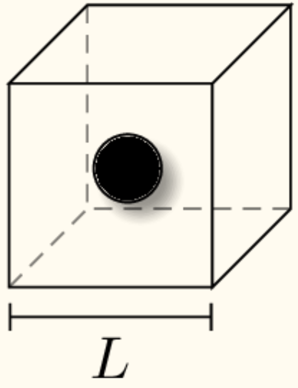
# Volume Dependence of the Spectrum

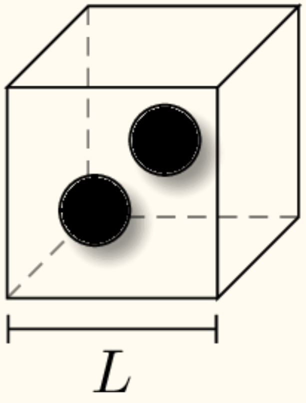
Single particle states have exponentially suppressed volume corrections

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

Volume dependence of two-particle states contains the scattering length

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




In general, the scattering phase shift depends on known functions of the finite-volume spectrum

$$\tan[\delta(p)] = -\tan\left[\phi^{\boldsymbol{P}}(p)\right]$$

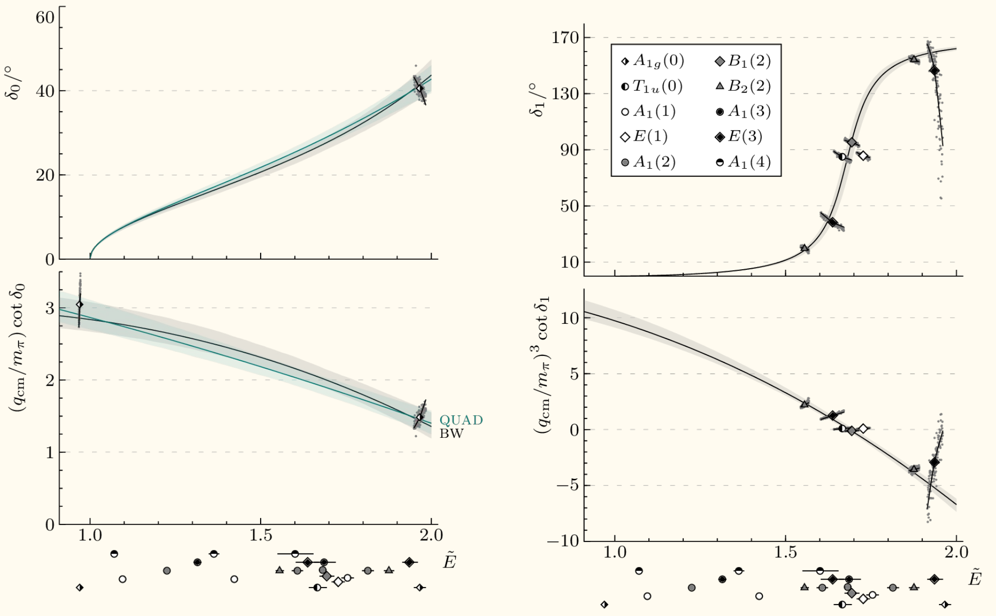
$$E_{\mathrm{cm}} = \sqrt{E^2 - \boldsymbol{P}^2} = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2}$$

# Including higher partial waves

Several partial waves can contribute!

- The $K^*(892)$ is described by a Breit-Wigner parameterization for $\ell = 1$
- The $K_0^*(700)$ is described by the effective range expansion for $\ell = 0$
- The contribution from $\ell = 2$ found to be negligible

$I = 1/2$ K-π $S$- and $P$-wave phase shift



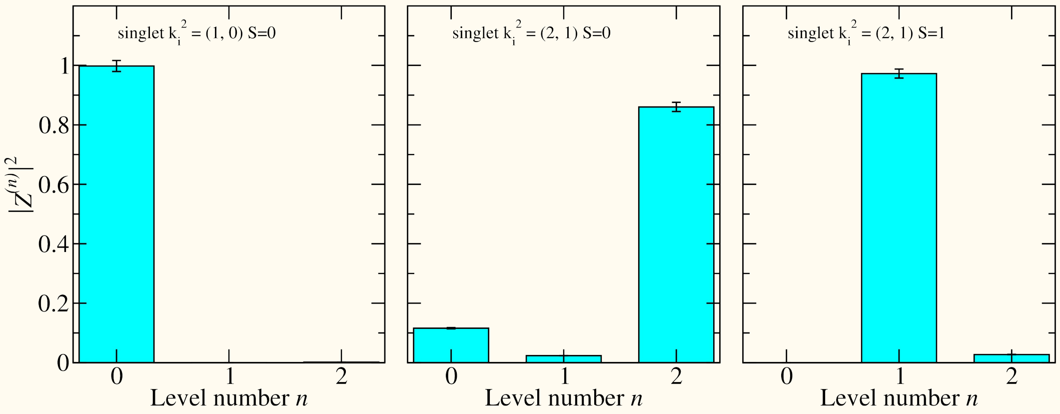

[Brett, Bulava, Fallica, AH, Hörz, Morningstar, *Nucl.Phys.B* 932 (2018) 29]

# What about the higher partial waves?

Including multiple channels and partial waves is possible

Simplest to only consider S-wave

- At rest, next contribution is from $^1G_4$
- Leading contributions in flight: $^3P_1$ and $^1D_2$
- Quantization condition factorizes in spin if scattering amplitude is diagonal in spin

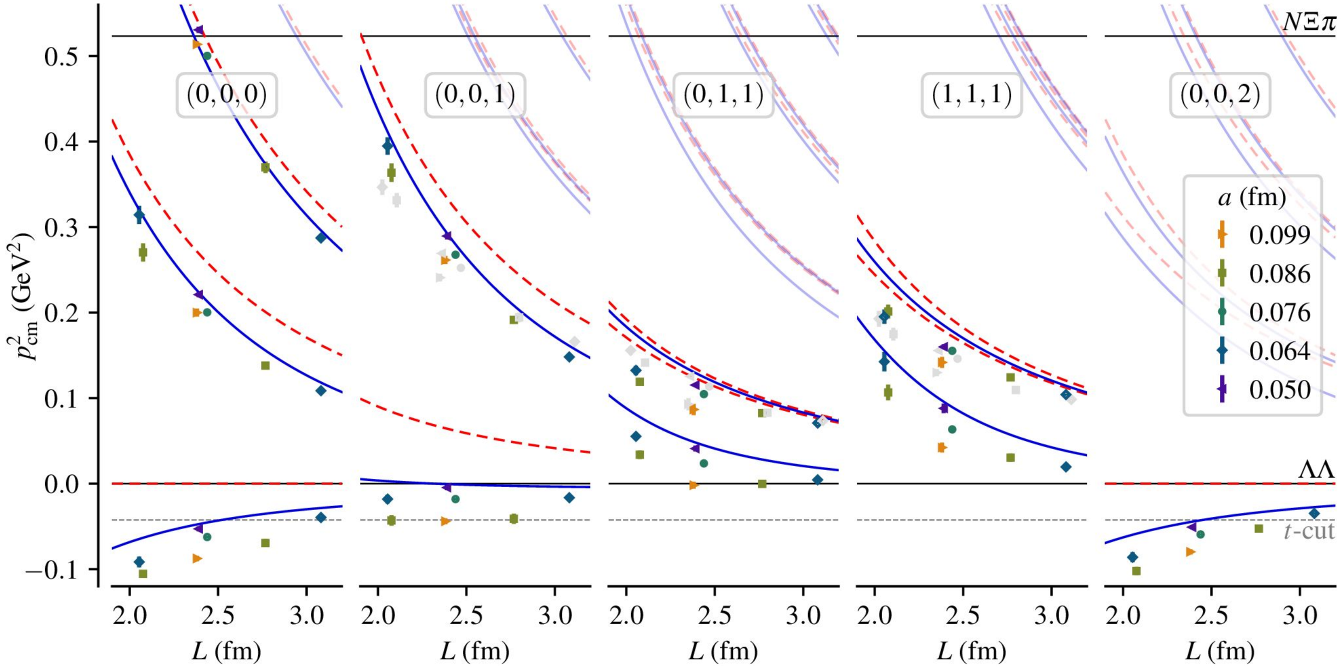



When studying $J^P = 1^+$ channel, physical $^3S_1$-$^3D_1$ mixing could be relevant

[J. Green, AH, P. Junnarkar, H. Wittig, arXiv:2103.01054]

# $H$-dibaryon spectrum ($\Lambda\Lambda$, $I$=0, $S$=-2)

Clear trend as the lattice spacing is lowered

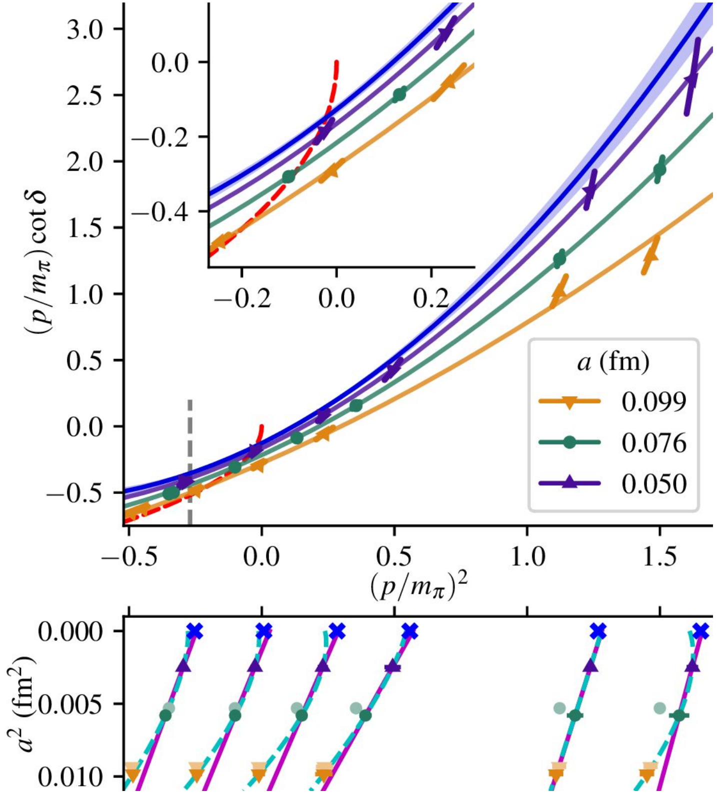


# Combined phase shift fits

- Perform combined fits to the data

$$p\cot\delta(p) = \sum_{i=0}^{N-1} c_i\, p^{2i} \qquad c_i = c_{i0} + c_{i1} a^2.$$

- *Alternatively*, extrapolate energies to the continuum




[J. Green, AH, P. Junnarkar, H. Wittig, arXiv:2103.01054]