Two-nucleon interactions in the continuum from lattice QCD

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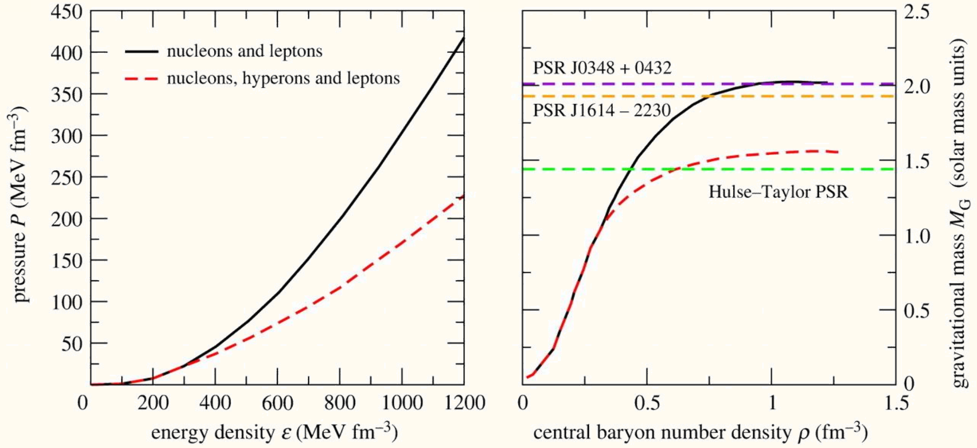
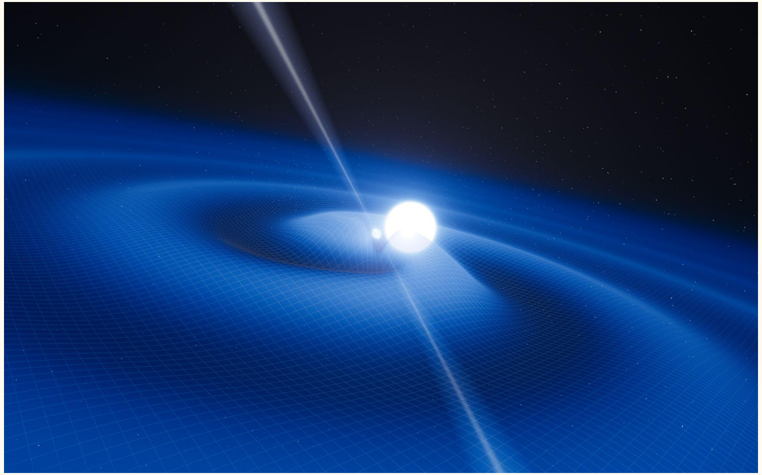
Outline

1. Examples of long-range science goals involving multi-baryon interactions
    - Neutron stars, $0\nu\beta\beta$ decay
2. Early NN results from lattice QCD
    - Quick review of formalism
    - Comparison of Lüscher and HAL QCD
3. Modern methods for spectroscopy
    - GEVP for controlling excited states and distillation for all-to-all quark propagation
4. Recent NN results from lattice QCD
    - Results at $m_\pi \sim 714$ MeV
    - Results in the continuum with $m_\pi \sim 420$ MeV

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]

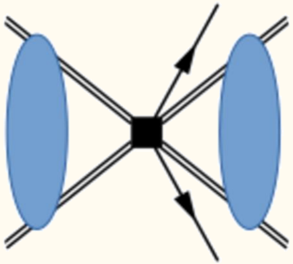


[Artist's impression of the pulsar PSR J0348+0432 and its white dwarf companion, **Credit:** ESO/L. Calçada, https://www.eso.org/public/images/eso1319c/]

- 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

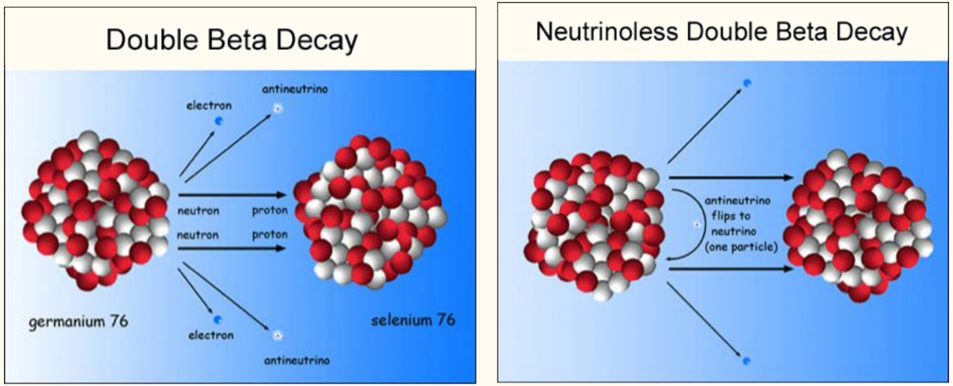
Lattice QCD→EFT→*Ab Initio* many-body theory

- Several research programs aim to calculate quantities involving large nuclei
  - νA scattering
  - $0\nu\beta\beta$ 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., *Phys. Rev. Lett.* 120, 202001 (2018)]

- 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]

Multi-hadron interactions from Lattice QCD

- Lattice simulations are necessarily performed in Euclidean space
  - Asymptotic temporal separation of Euclidean correlators in infinite-volume cannot constrain scattering amplitude away from threshold [Maiani, Testa, *Phys. Lett. B* **245** (1990) 585]
- Finite volume can be used as a tool, since the interactions leave imprints on the finite-volume energies
  - $1/L$ expansion of energy shifts can be used to access scattering parameters, but is a limited approach
  - Lüscher formalism (and its generalization) constrain the scattering amplitude at energies equal to the energies in finite-volume
- Recent promising alternative: extraction of spectral functions from finite-volume Euclidean correlators [J. Bulava, M. Hansen, *Phys. Rev. D* **100** (2019) 3, 034521]
  - Requires large n-point correlation functions
  - Inverse problem
  - Large lattices

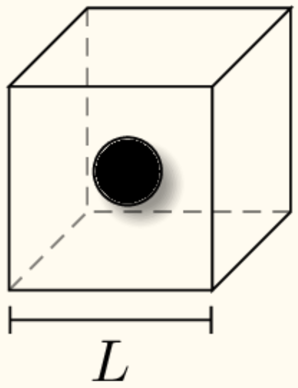
Volume Dependence of the Spectrum

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

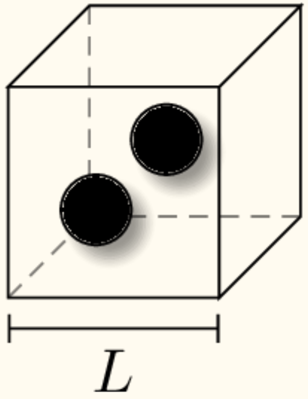
$$\Delta E^{(2)} \propto \frac{a_0}{L^3} + O\Big(\frac{1}{L^4}\Big)$$



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

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

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



[Lüscher ‘86, ‘91; generalizations]

Lüscher two-particle formalism

Compact formula for quantization condition

$$\det\left[F(E_2,\mathbf{P},L)^{-1}+\mathcal{K}_2(E_2^*)\right]=0$$

E_2 - finite-volume energies

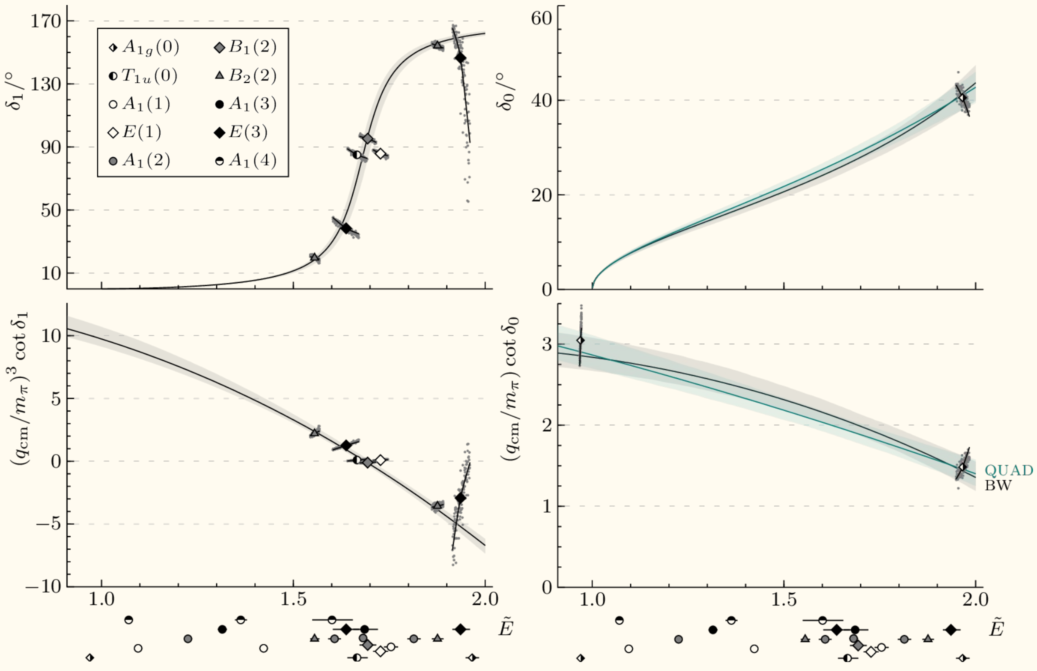
$\mathcal{K}_2$- 2-to-2 K-matrix

F - known geometric function

Caveats:

- truncated at some max ℓ
- only valid above t-channel cut and below 3 (or 4) particle threshold
- assumes continuum energies
- ignores exponentially small contributions

Example: s- and p-wave $I=1/2\ K\pi$ scattering



[R. Brett, J. Bulava, J. Fallica, **AH**, Ben Hörz, Colin Morningstar, *Nucl. Phys.* **B932**, 29-51 (2018)]

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

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

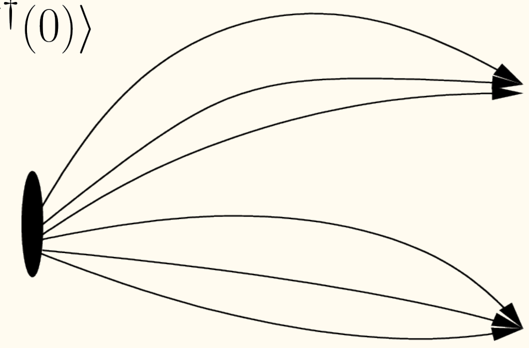
- Look for plateau in effective energy to indicate ground state saturation
    - Approach can be non-monotonic if sink and source operators are not the same

- 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

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



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

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

- Used point sources, and uses correlators of the form

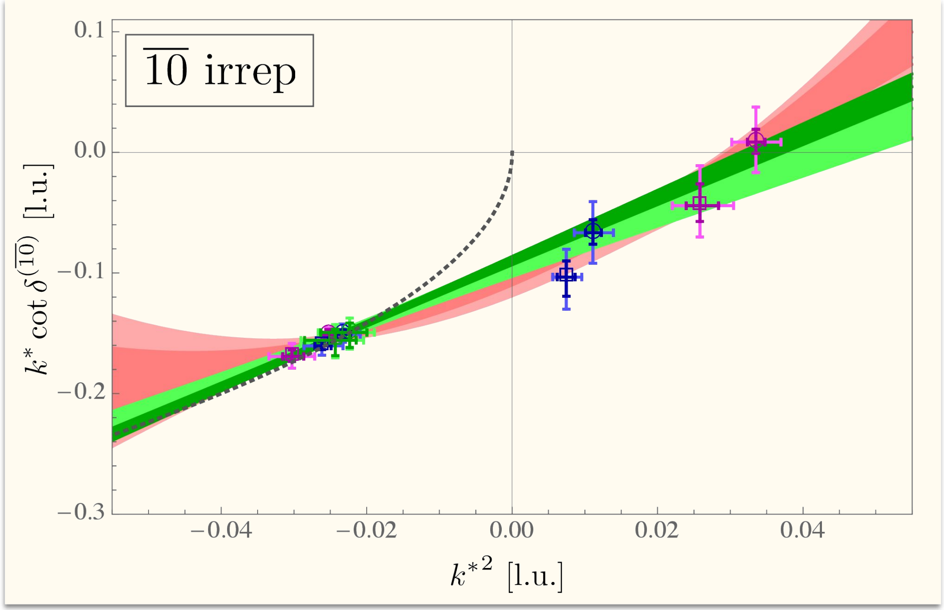
$$\langle BB(t) H^\dagger(0) \rangle$$

- 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, *Phys.Rev.D* 96 (2017) 11, 114510]

The HAL QCD Method

- Calculate NBS wave function

  $\phi_{\mathbf{k}}(\mathbf{r})e^{-W_{\mathbf{k}}t} = \langle 0|N(\mathbf{x}+\mathbf{r},t)N(\mathbf{x},t)|NN,W_{\mathbf{k}}\rangle,$

  where $W_{\mathbf{k}} = 2\sqrt{\mathbf{k}^2+m_N^2}$

- If $W_{\mathbf{k}} < W_{\mathrm{th}}$, then $\phi_{\mathbf{k}}(\mathbf{r})$ satisfies

  $$(E_{\mathbf{k}}-H_0)\phi_{\mathbf{k}}(\mathbf{r}) = \int \mathrm{d}^3r' U(\mathbf{r},\mathbf{r}')\phi_{\mathbf{k}}(\mathbf{r}')$$

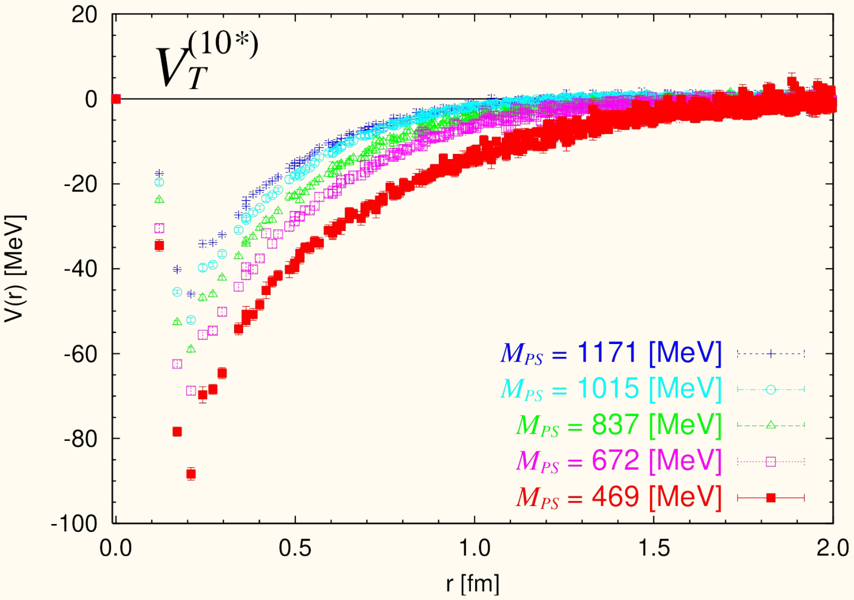
- Define potential via derivative expansion

  $$U(\mathbf{r},\mathbf{r}') = \sum_n V_n(\mathbf{r})\nabla^n\delta(\mathbf{r}-\mathbf{r}')$$

- Determine scattering observables from solving Schrödinger equation

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

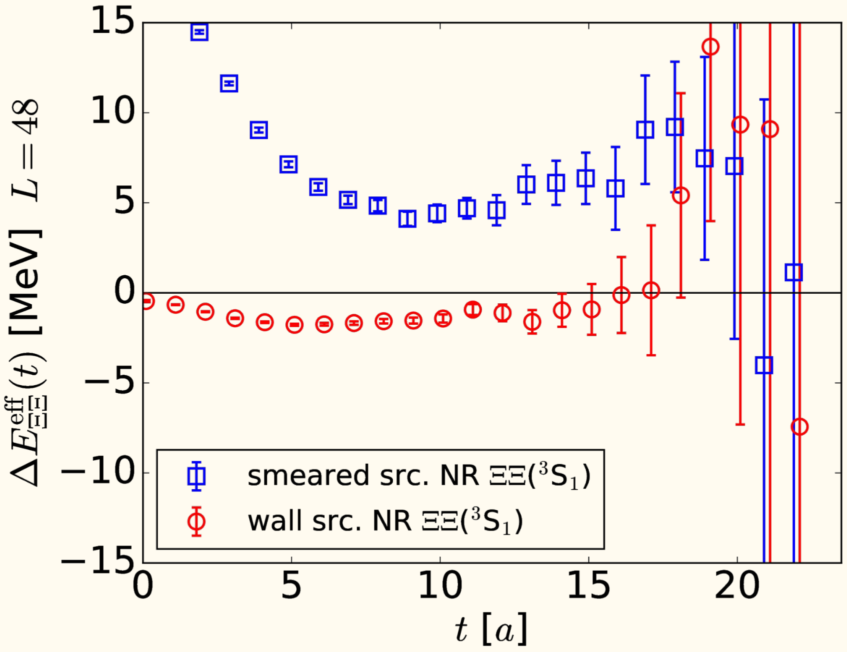
$$U(\mathbf{r},\mathbf{r}') = (V_c(\mathbf{r})+V_T(\mathbf{r})S_{12}+\mathcal{O}(\nabla^2))\delta(\mathbf{r}-\mathbf{r}')$$



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

What's going wrong?

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



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

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)

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

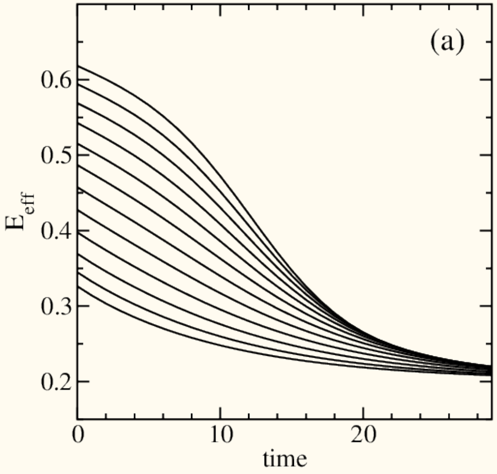
And use the eigenvectors to rotate $\hat{C}(t)$ at all other times

If τ_0 is chosen sufficiently large, then eigenvalues $\lambda_n(t, \tau_0)$ behave as

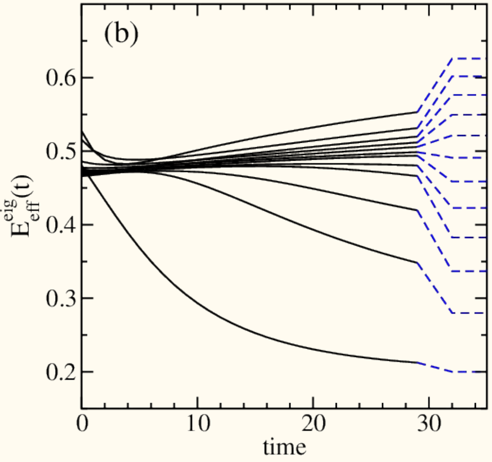
$$\lambda_n(t, \tau_0) \propto e^{-E_n t} + O(e^{-(E_N - E_n)t})$$

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

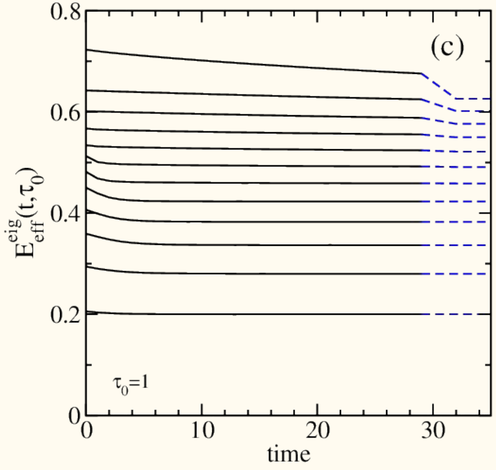
Correlator matrix toy model



Diagonal elements of C(t)



Eigenvalues of C(t)



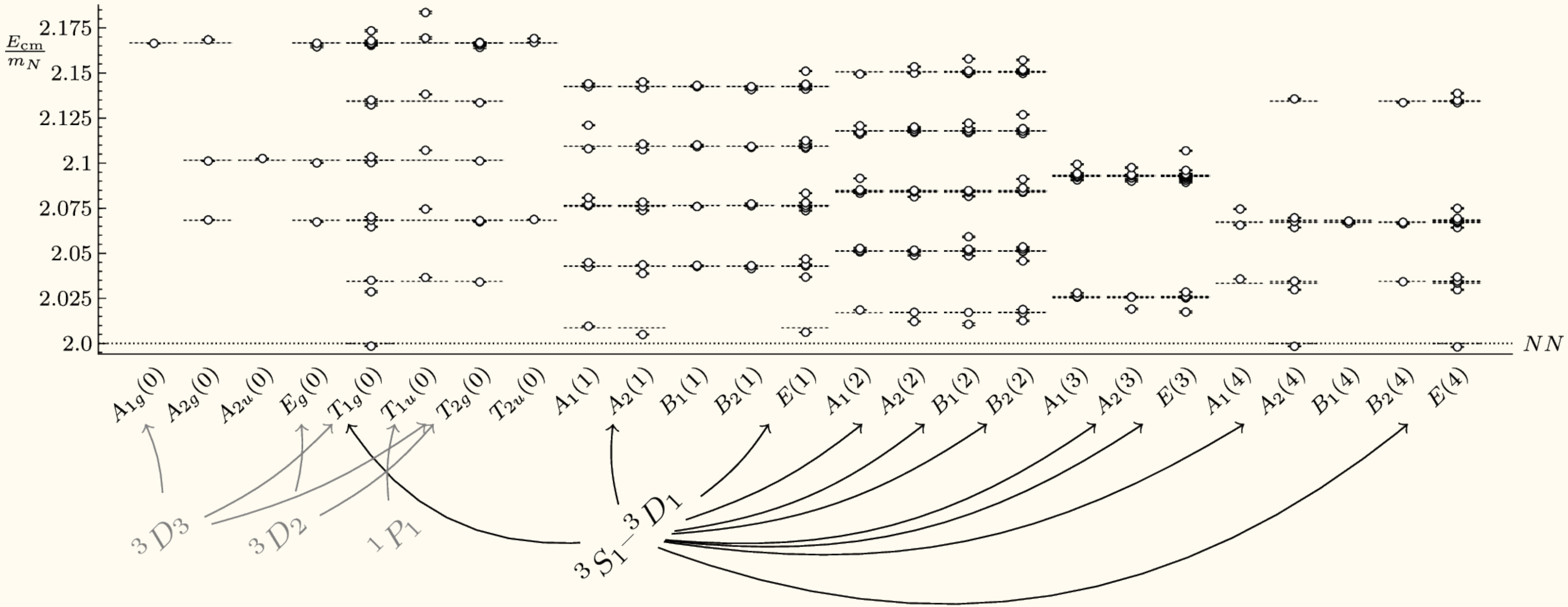
Generalized eigenvalues of C(t)

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

[Plots courtesy of Colin Morningstar]

NN $I=0$ Finite-volume spectrum

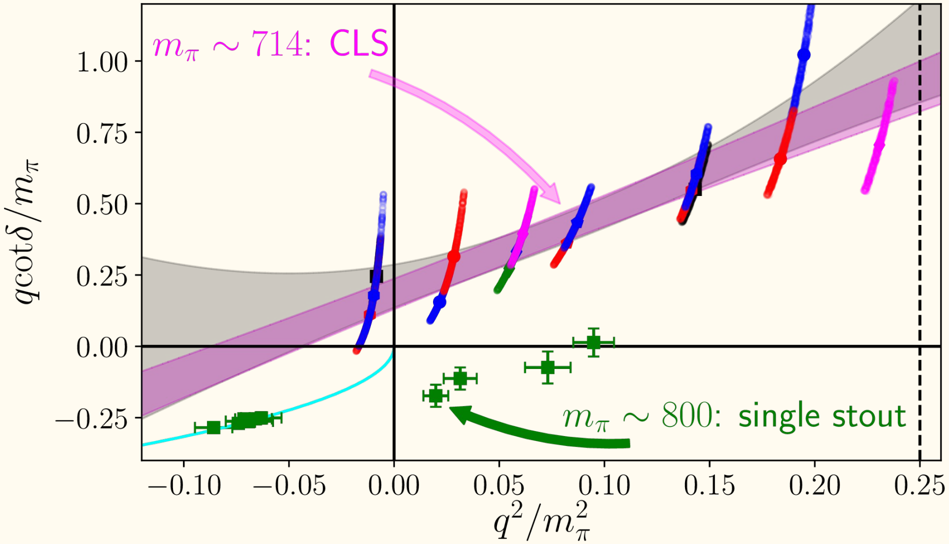
Lowest partial wave contributions to each irrep. Open circle for each interacting NN energy. Non-interacting levels denoted by horizontal dashed lines.



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., *Phys.Rev.*C 103 (2021) 1, 014003]

$NN\ I{=}0\ ^3S_1$ comparison to NPLQCD

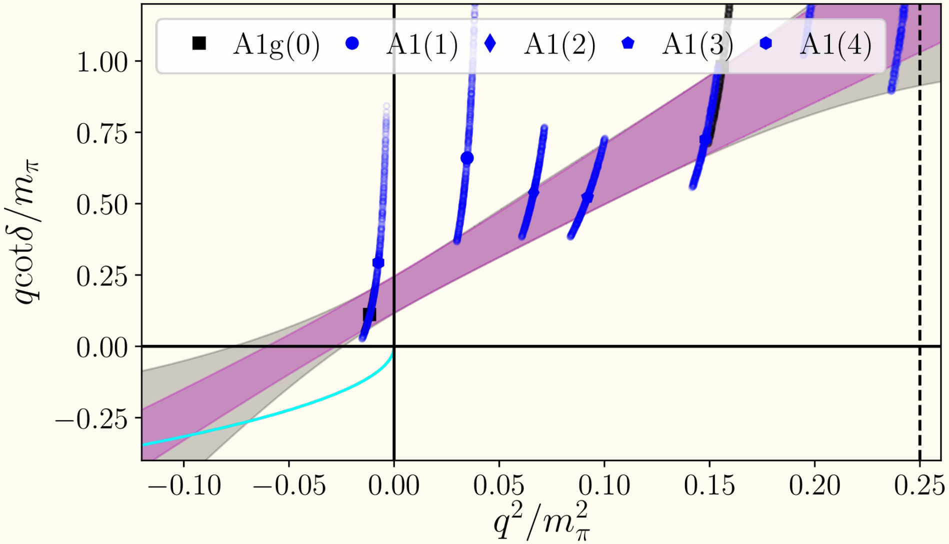
- Comparison with NPLQCD shows strong tension
- Different action used, therefore discretization effects could be playing a role
- NPLQCD uses a hexaquark operator at the source



[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., *Phys.Rev.*C 103 (2021) 1, 014003]

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

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



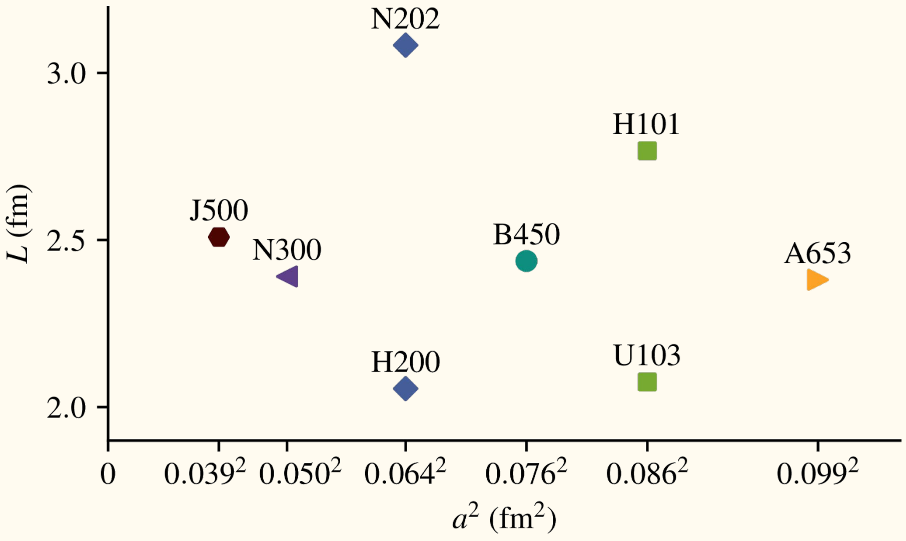
[B. Hörz, D. Howarth, E. Rinaldi, **AH**, et al., *Phys.Rev.*C 103 (2021) 1, 014003]

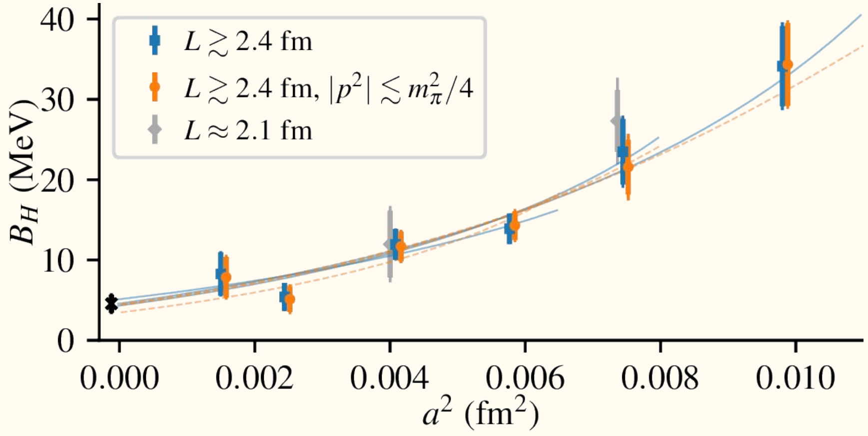
Mainz efforts toward two-baryon interactions

Eight SU(3)-symmetric ($m_\pi \sim 420$ MeV) ensembles with Wilson-clover fermions generated by CLS

Study of H dibaryon found significant discretization effects!

[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]





Extraction of energy shifts

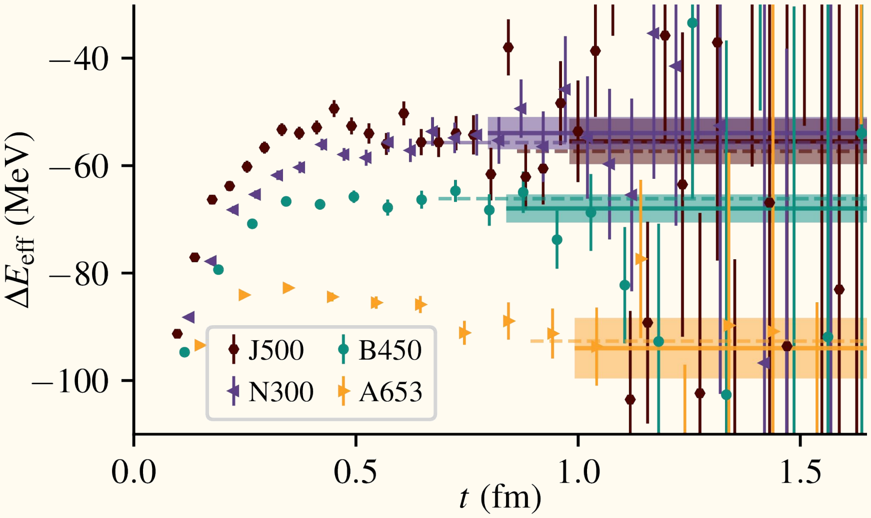
- Fit ratio of diagonalized correlator

$$R_n(t) \equiv \frac{v_n^\dagger(\tau_0,\tau_D)C(t)v_n(\tau_0,\tau_D)}{\prod_i C^{(\mathrm{sh})}(\mathbf{p}_i^2,t)}$$

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

- Leads to partial cancellation of correlated fluctuations and residual excited states
- Should wait until single-baryon correlators have plateaued
- Use alternative spectrum for systematics

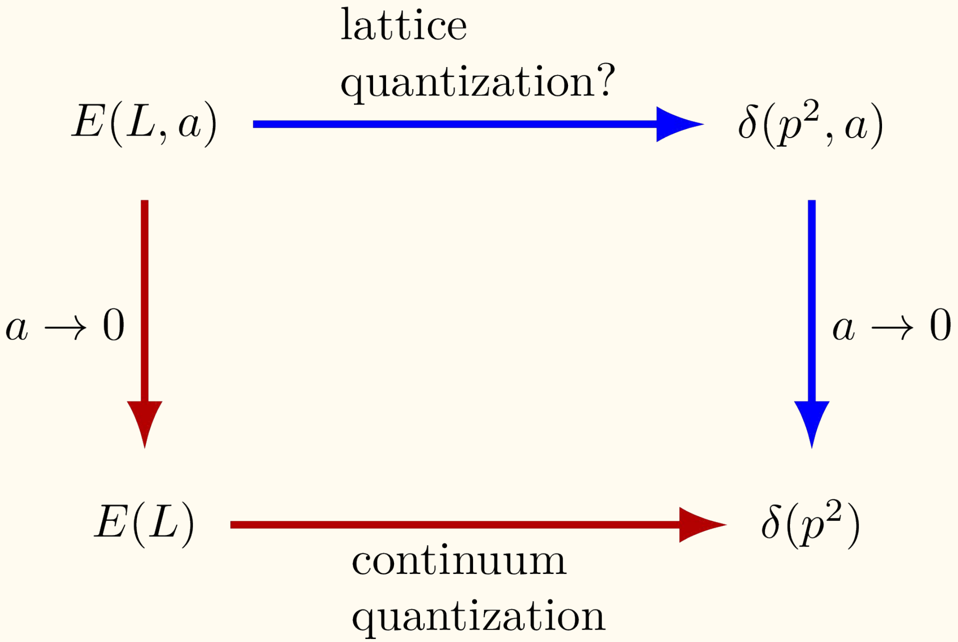
Effective energy difference for ground state in (0,0,1)
Discretization effects apparent already!



[J. R. Green, **ADH**, P. M. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

Towards NN interactions in the continuum

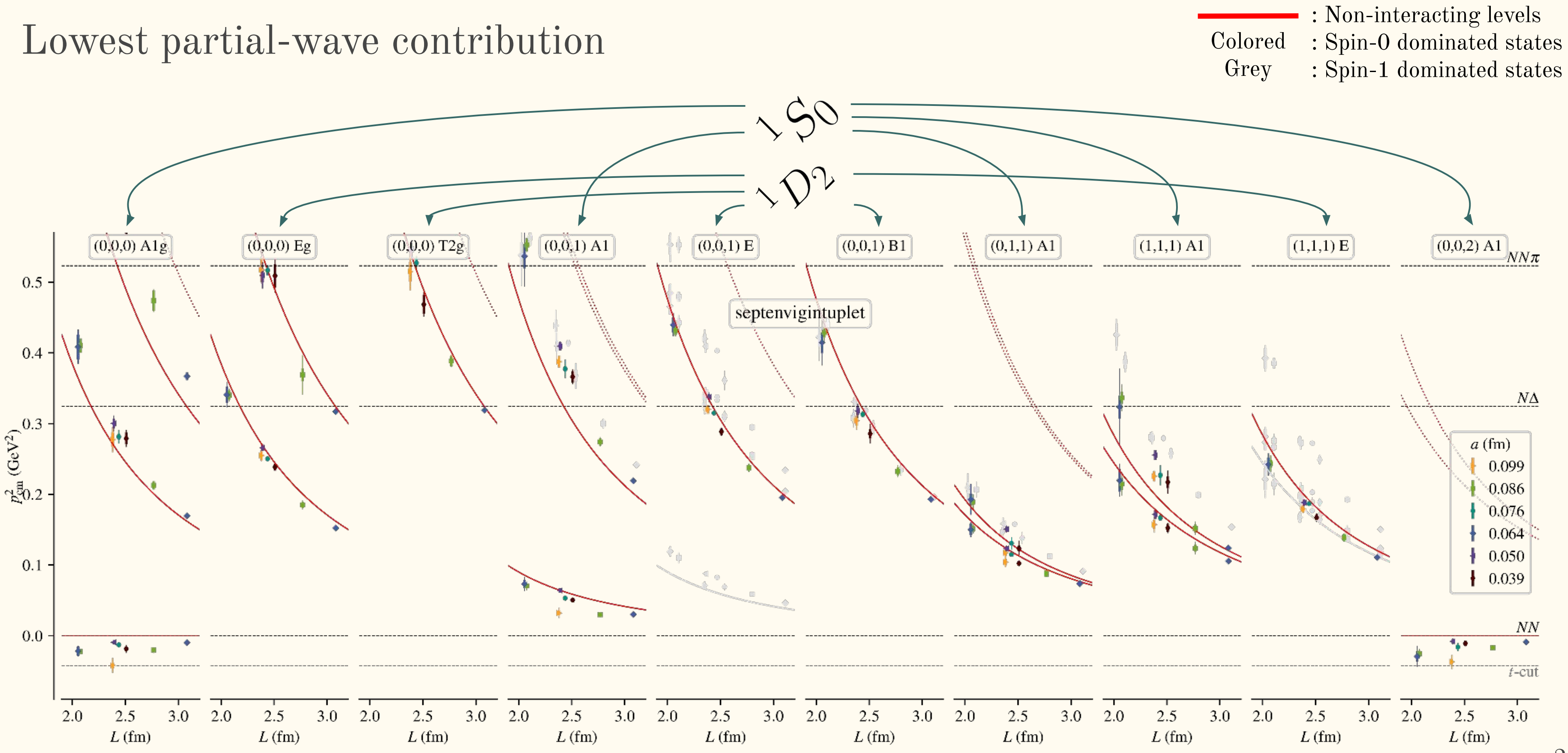
- All results should be considered preliminary!
- Red path more theoretically sound approach, but practically difficult
- Blue path much simpler: modify fit parameters to include lattice spacing dependence



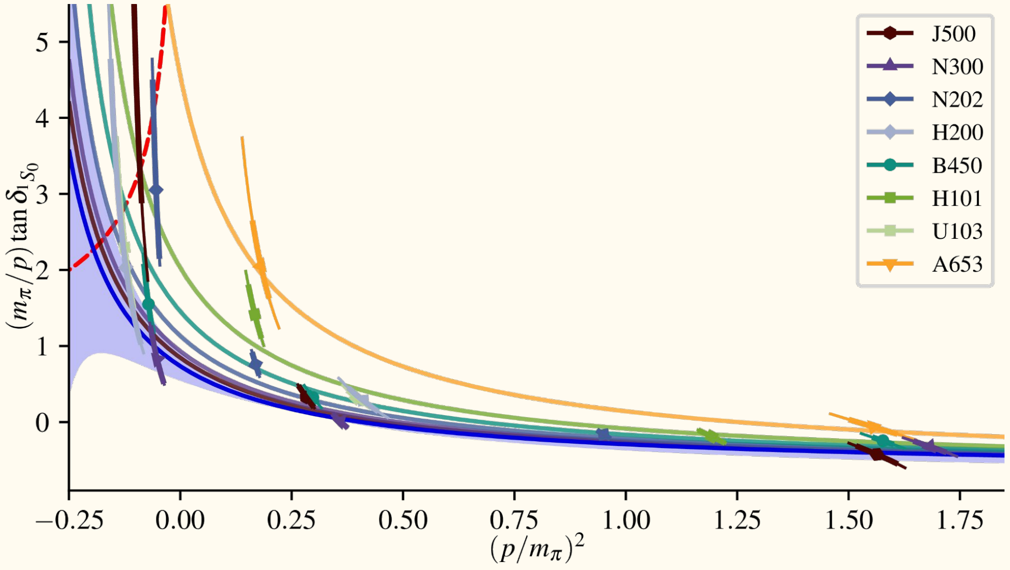
[Ch. 16 of *Few Body Syst*. 63 (2022) 4, 67]

NN I=1 (27-plet) Spectrum

Lowest partial-wave contribution



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



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

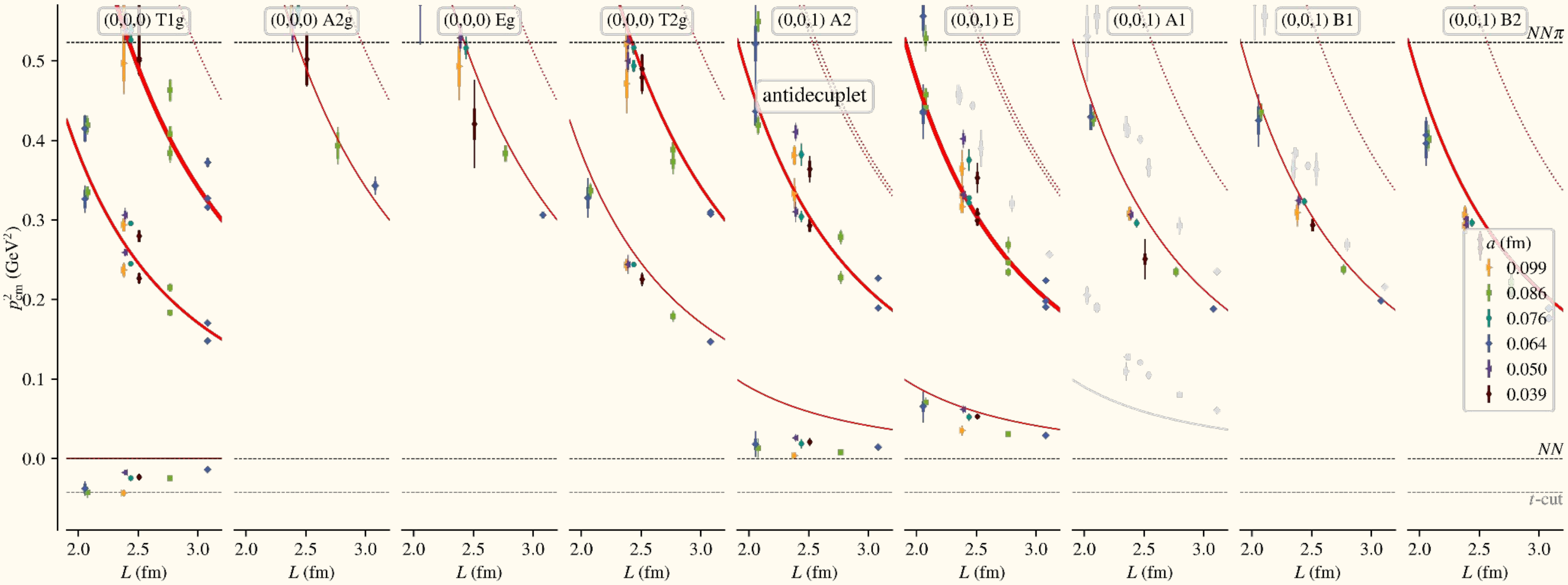
- Assumes only S-wave contributes
- Fit all levels in $A_{1g}(0)$ and $A_1(1)$ that are above t-channel cut and below inelastic threshold to

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

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

NN I=0 (Antidecuplet) Spectrum

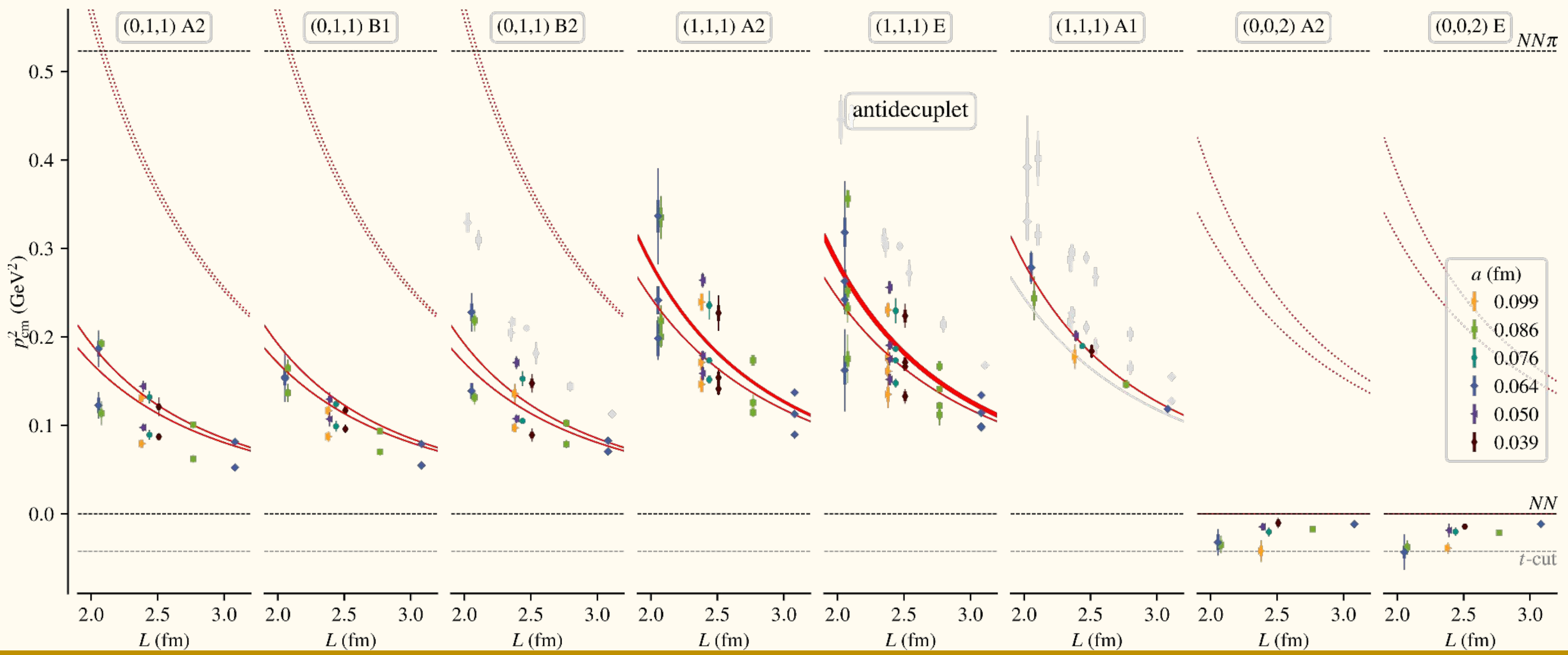
Initially focus on spin-1 states, as the quantization condition factorizes in spin



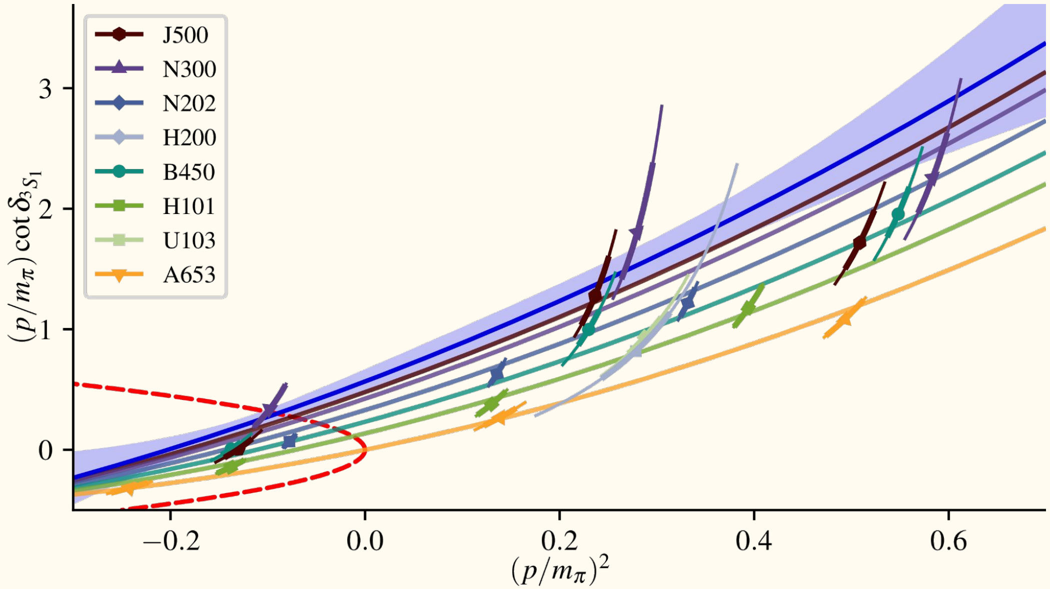
NN $I=0$ (Antidecuplet) Spectrum (cont.)

Initially focus on spin-1 states, as the quantization condition factorizes in spin

: Non-interacting levels
Colored : Spin-1 dominated states
Grey : Spin-0 dominated states



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

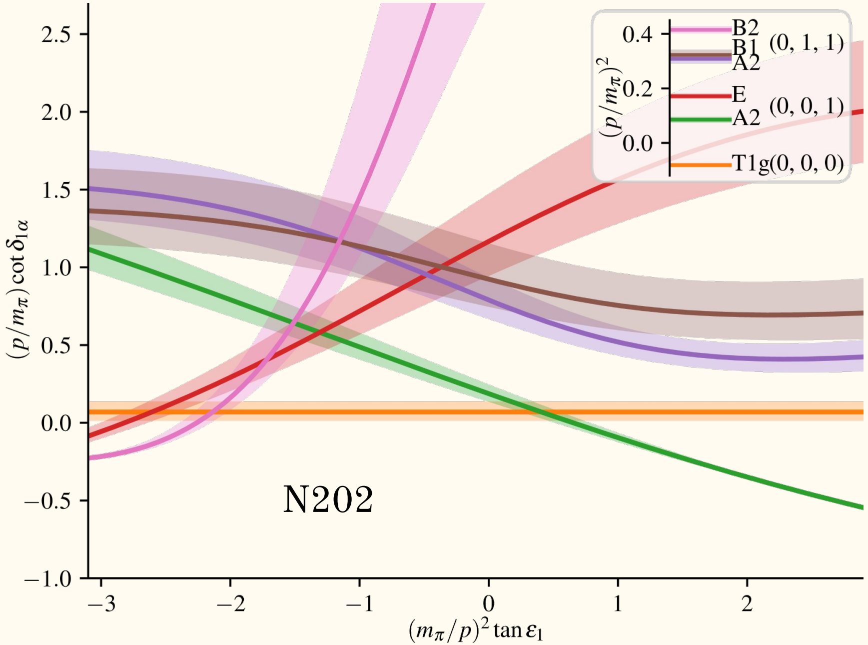
$$p\cot\delta(p) = c_0 + c_1 p^2$$

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

$^3S_1$-$^3D_1$ Mixing

Blatt-Biedenharn parametrization:

$$\tilde{K}^{-1} = \begin{pmatrix}1 & 0\\ 0 & p^2\end{pmatrix}\begin{pmatrix}\cos\epsilon_1 & -\sin\epsilon_1\\ \sin\epsilon_1 & \cos\epsilon_1\end{pmatrix}\begin{pmatrix}p\cot\delta_{1\alpha} & 0\\ 0 & p\cot\delta_{1\beta}\end{pmatrix}\begin{pmatrix}\cos\epsilon_1 & \sin\epsilon_1\\ -\sin\epsilon_1 & \cos\epsilon_1\end{pmatrix}\begin{pmatrix}1 & 0\\ 0 & p^2\end{pmatrix}$$



Assuming $\delta_{1\beta} = 0$, then the quantization condition

$$\det[\tilde{K}^{-1} - B] = 0$$

leads to

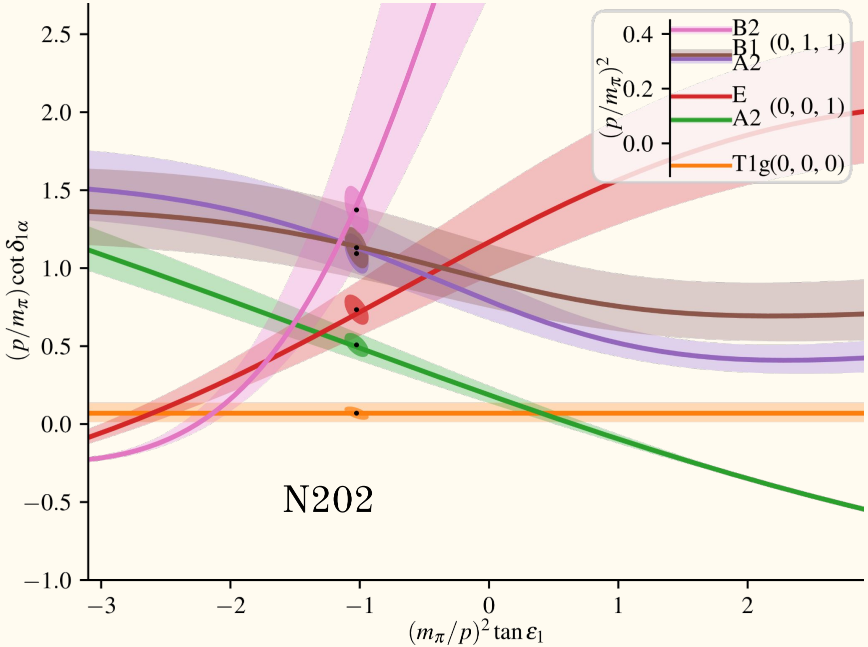
$$p\cot\delta_{1\alpha} = \frac{B_{00} + (B_{01} + B_{10})x + B_{11}x^2}{1 + p^4x^2},$$

where $x = p^{-2}\tan\epsilon_1$.

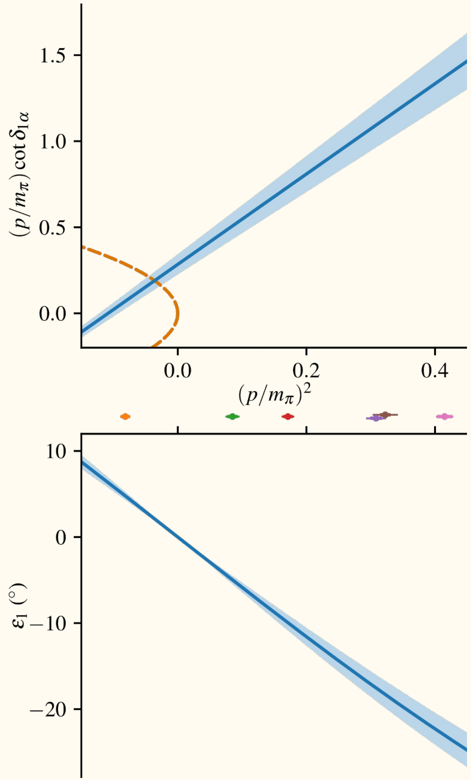
$^3S_1$-$^3D_1$ Mixing

Fit to spectrum using

$$p \cot \delta_{1\alpha} = c_1 + c_2 p^2, \quad p^{-2} \tan \epsilon_1 = c_3.$$

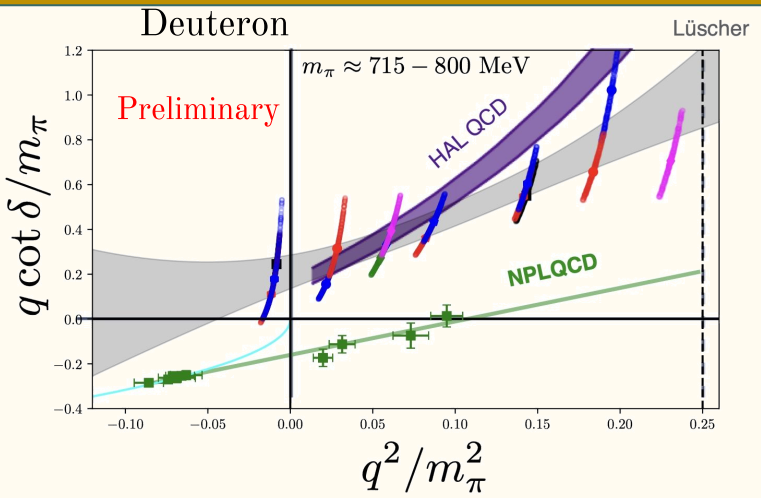


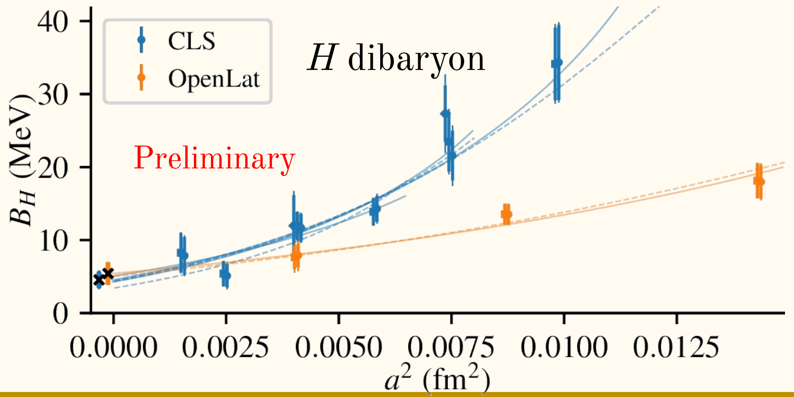
ϵ_1 has opposite sign to experiment

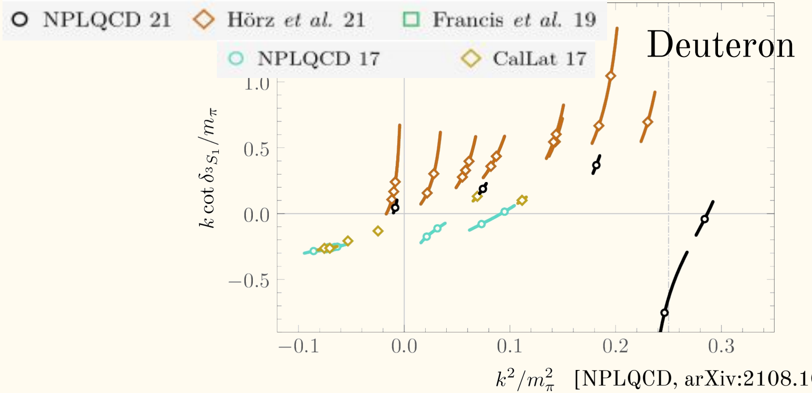


Results beginning to converge?

- *NN* results in continuum see only virtual bound state [Mainz]
- GEVP results see no bound state, while asymmetric correlators do[NPLQCD]
- Agreement between Lüscher and HAL QCD method on same ensemble [sLapHnn]
- Continuum *H*-dibaryon binding energy in agreement from two actions [BaSc: Mainz+sLapHnn]







[NPLQCD, arXiv:2108.10835]

Conclusions and Outlooks

Conclusions

- Only studies which use local hexaquark operators at the source see deep bound states
- Discretization effects are important
  - Exponentiated-clover action appears less affected
- Convergence of results using GEVP

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
- How important is including a local hexaquark?
- Need to push calculations toward the physical point to make connections with chiral EFT

Collaborators

Mainz:

Jeremy Green (DESY)
Parikshit Junnarkar (Darmstadt)
Nolan Miller (Mainz)
M. Padmanath (Mainz)
Srijit Paul (Edinburgh)
Hartmut Wittig (Mainz)

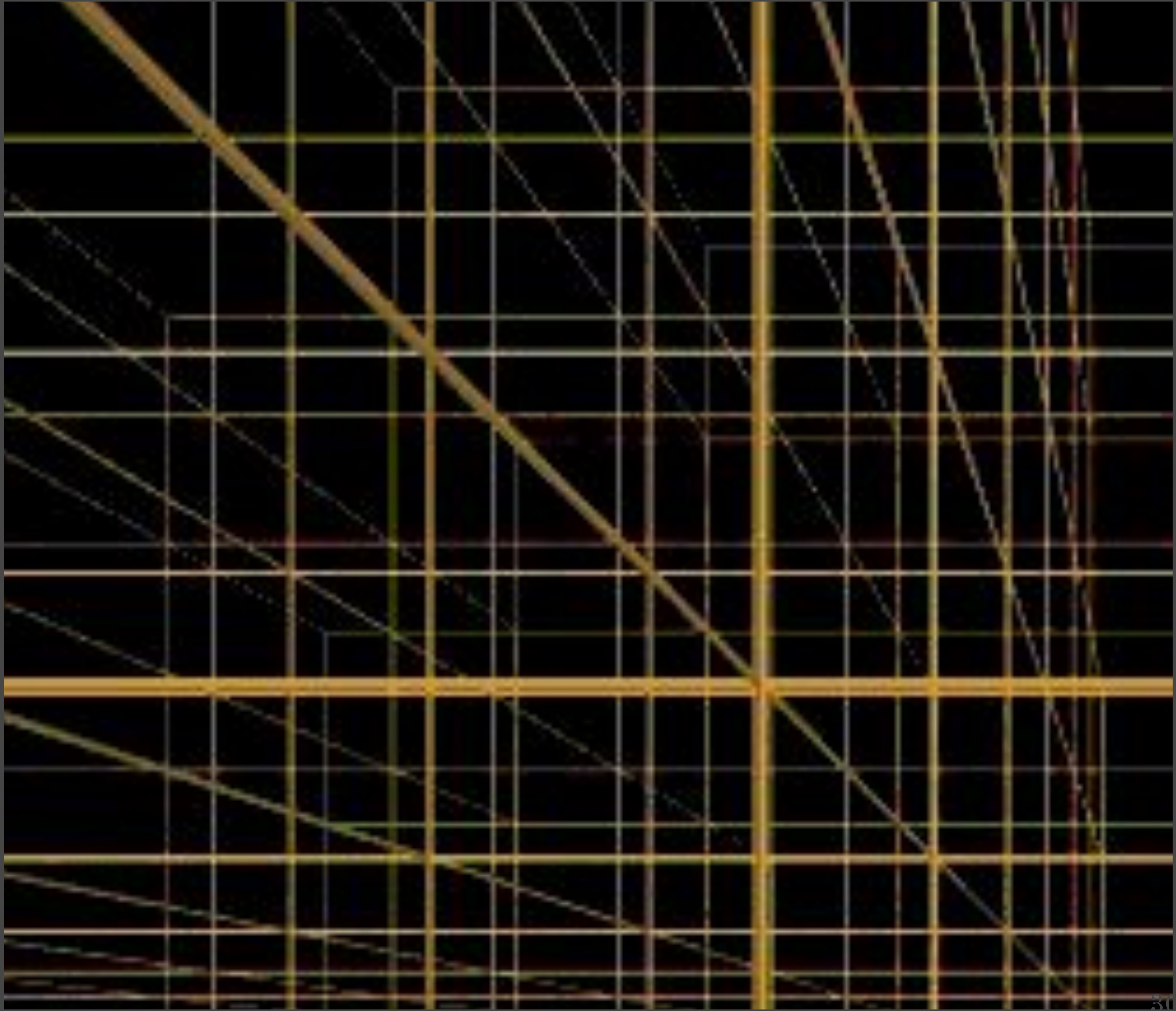
BaSc: Mainz + sLapHnn

sLapHnn:

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

Thanks!

Questions?



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

Extra Slides

Nonperturbative formulation of QCD on a Lattice

- Finite lattice spacing a (UV regulator)

$$\int \mathrm{d}^4x \to a^4 \sum, \quad \int_{-\infty}^{\infty} \mathrm{d}p \to \int_{-\pi/a}^{\pi/a} \frac{\mathrm{d}p}{2\pi}$$

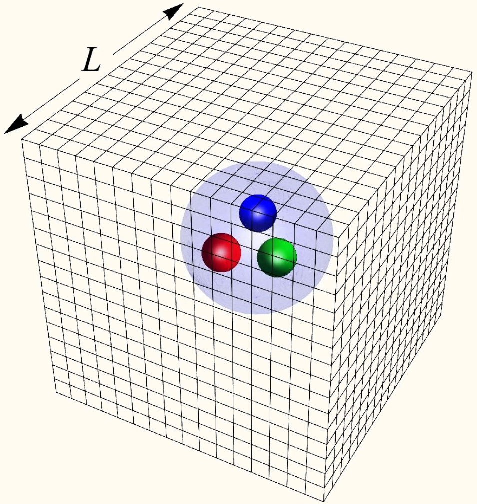
- Finite volume L (IR regulator)

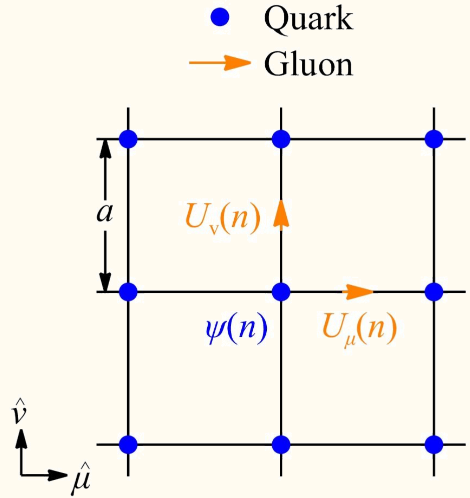
$$\vec{P} = \frac{2\pi}{L}\vec{n}, \; n_i \in \mathbb{Z}$$

- Path Integral becomes finite-dimensional integral (still large), use Monte Carlo
- Generally performed at higher than physical pion mass
- Steps of calculation
    a. Generate gauge ensembles
    b. Calculate quark propagators
    c. Contractions to observables
    d. Analysis of correlators
    e. Extrapolate to physical point

$$\langle O \rangle = \frac{1}{\mathcal{Z}} \int DU \prod_f^{N_f} \mathrm{Det}[\not{D}[U] + m_f] e^{-S_G[U]} O[U]$$

$$= \frac{1}{N_{\mathrm{cfg}}} \sum_{i=1}^{N_{\mathrm{cfg}}} O[U_i] + \mathcal{O}\left(\frac{1}{\sqrt{N_{\mathrm{cfg}}}}\right)$$

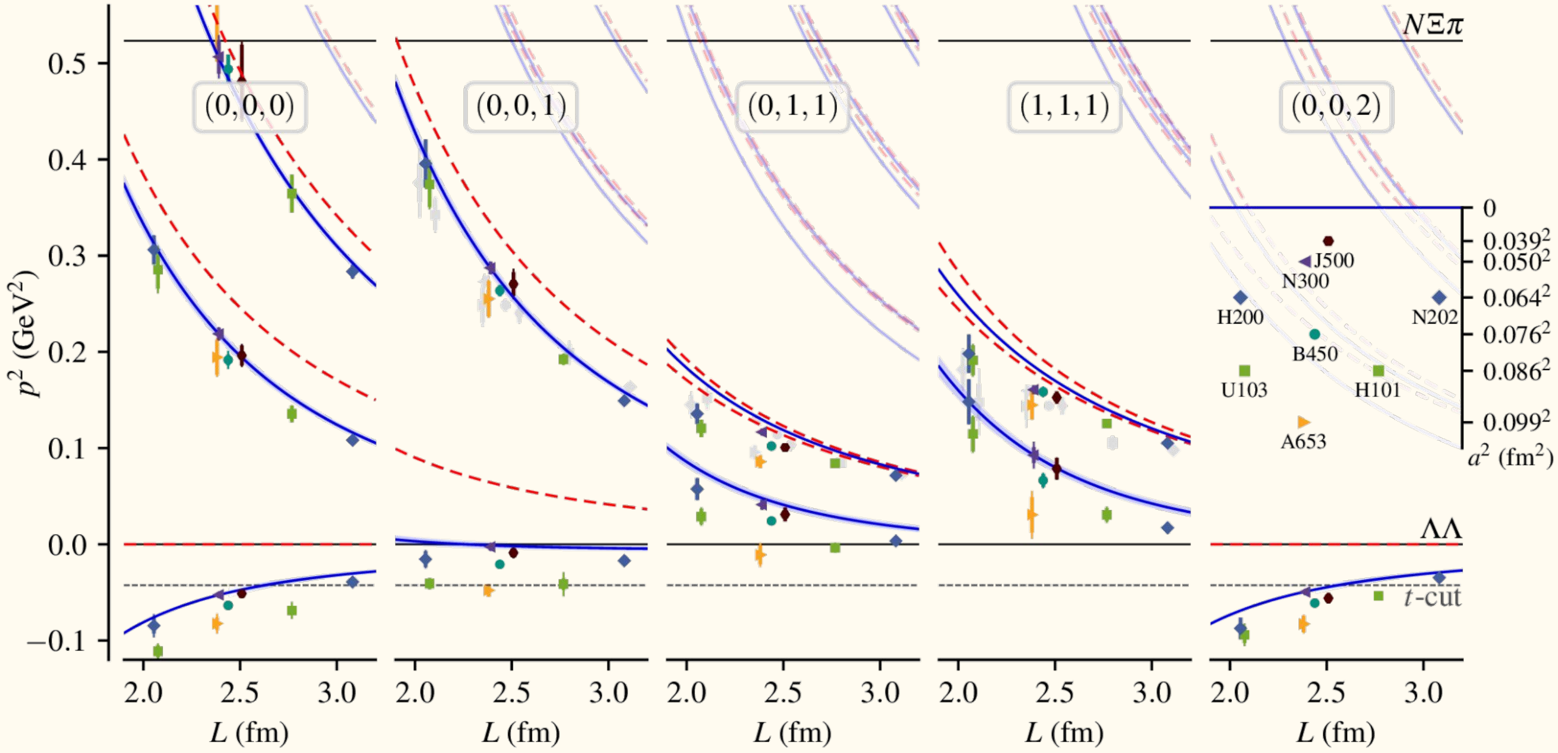




[Z. LI, L. LIU, *Nuclear Physics Review*, 2021, 38(2): 129-135]

H-dibaryon (ΛΛ, I=0, S=-2), $m_\pi \sim$ 420 MeV

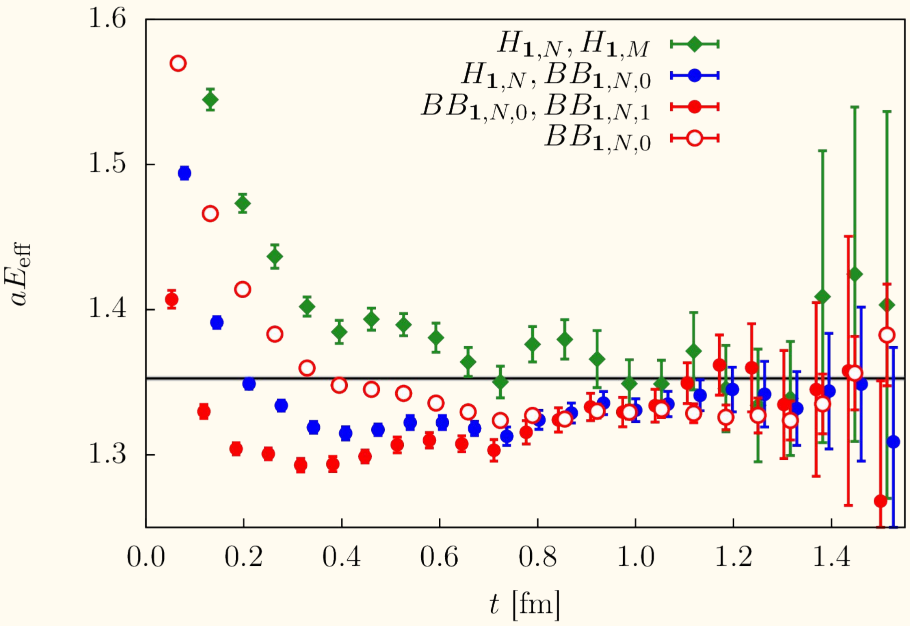
Clear trend as the lattice spacing is lowered



[J. Green, **ADH**, P. Junnarkar, H. Wittig, *Phys.Rev.Lett.* 127 (2021) 24, 242003]

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]

Quark Propagation with Distillation

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

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

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 Δ

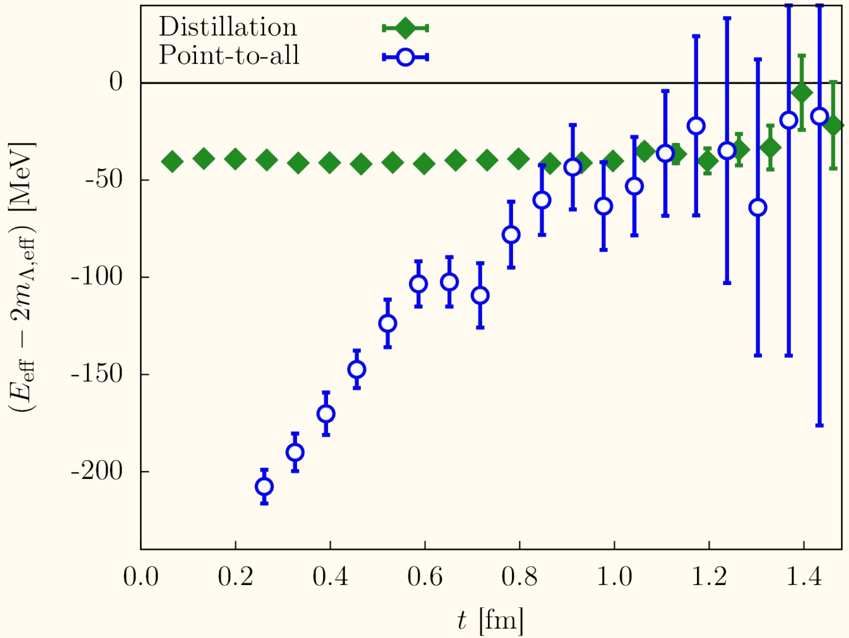
Only need the elements of the much smaller matrix (perambulators)

$$\tau_{kk'}(t,t') = V^\dagger M^{-1} V = v_a^{(k)}(x)^* M_{ab}^{-1}(x,y) v_b^{(k')}(y)$$

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

Distillation vs. Smeared Point Sources

- Distillation is a method for computing all-to-all quark propagators efficiently
- Individually momentum-projected two-baryon operators used in distillation
- Smeared point sources require local hexaquark at the source.
- Better quality data with less inversions
- Number of needed eigenvectors scales with the physical volume
  - Better cost scaling with stochastic version of distillation
- Contraction costs more expensive with distillation (local hexaquark not included)



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