Pushing the limits of the three-particle quantization condition with lattice QCD

Andrew Hanlon
Brookhaven National Laboratory

HU Berlin / NIC DESY Zeuthen
Joint Lattice Seminar

Based on arXiv:2106.05590

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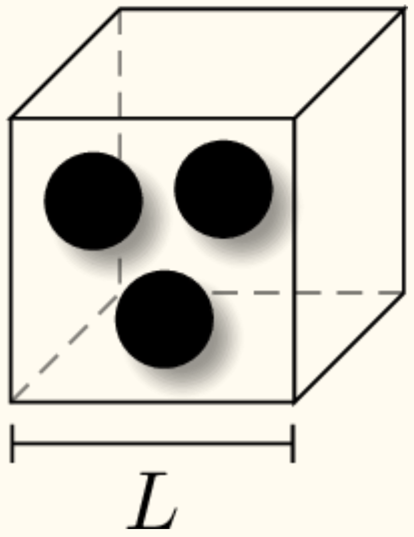
Brookhaven National Laboratory

Outline

1. Motivation
   - Test and push the limits of three-particle quantization condition
   - Study three-body interactions relevant for the Roper and neutron stars, etc.
2. Setup and technical details
   - Three-particle quantization condition
   - Ensembles, code, analysis
3. Results for pions and kaons
   - Three pion masses: 200, 280, 340 MeV
   - d-wave interactions constrained
   - Preliminary mixed flavor systems

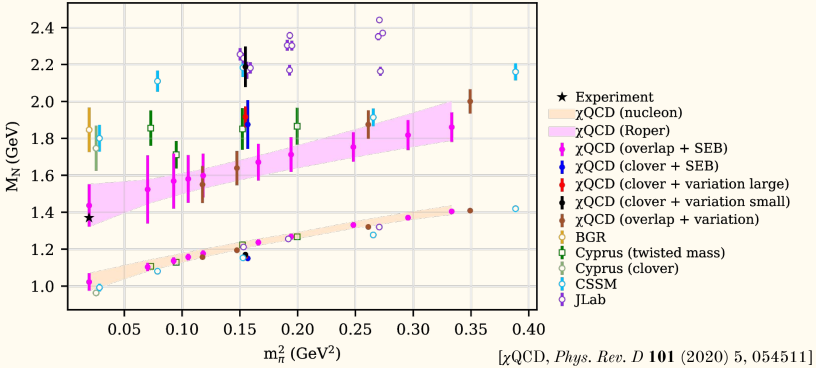


Motivation

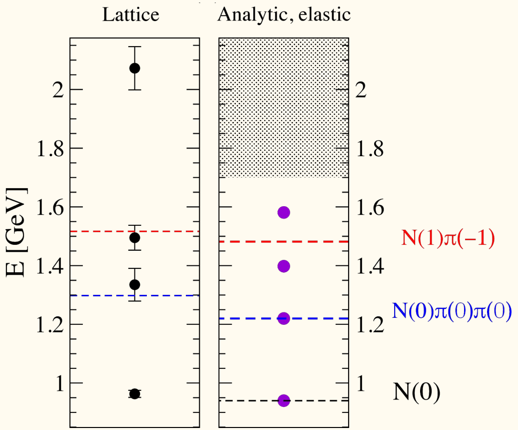
- Most QCD resonance decays involve three or more particles
  - $\omega(782) \to \pi\pi\pi$, $a_1(1260) \to \pi\pi\pi$, $N(1440) \to N\pi\pi$
- Many recent developments on the theoretical side (and their applications)
- Three competing formalisms (quantization conditions) to interpret three-particle finite-volume energies [Review arXiv:1901.00483]
  - Relativistic Field Theory (RFT) approach [Hansen, Sharpe, ...]
  - Finite-volume unitarity (FVU) approach [Mai, Döring, ...]
  - Non-relativistic effective field theory (NREFT) [Hammer, Pang, Rusetsky, ...]
- Provide real lattice data to test and push the limits of various three-particle formalisms

The Roper resonance

- Quark models predict the $N(1535)$-$1/2^-$ should lie below the $N(1440)$-$1/2^+$ (Roper)
- Various proposals for its solution (*e.g.* [Burkert, Roberts, *Rev. Mod. Phys.* **91** (2019) 1, 011003])
- Use lattice QCD to get an answer from first principles
- Claims from χQCD that chiral symmetry is essential at coarse lattice spacings
- Other suggestions that $N\pi\pi$ operators needed
- Formalism for interpreting $N\pi\pi$ energies needed

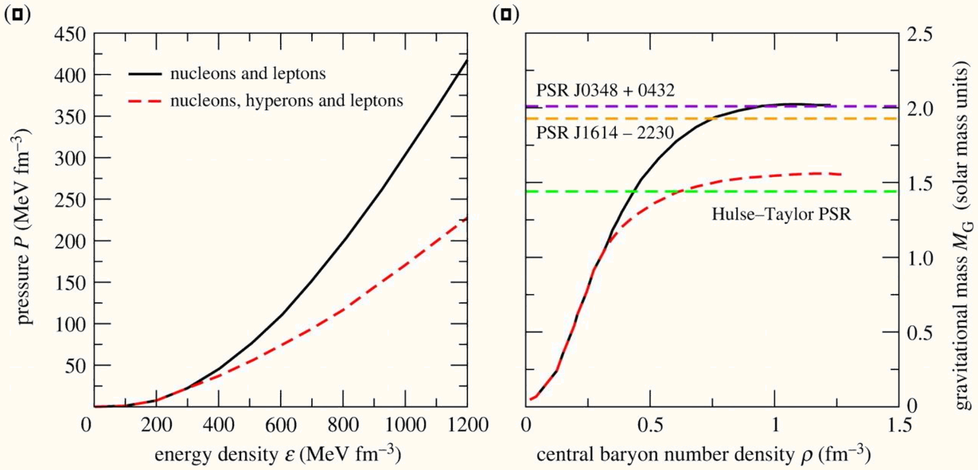


[χQCD, *Phys. Rev. D* **101** (2020) 5, 054511]

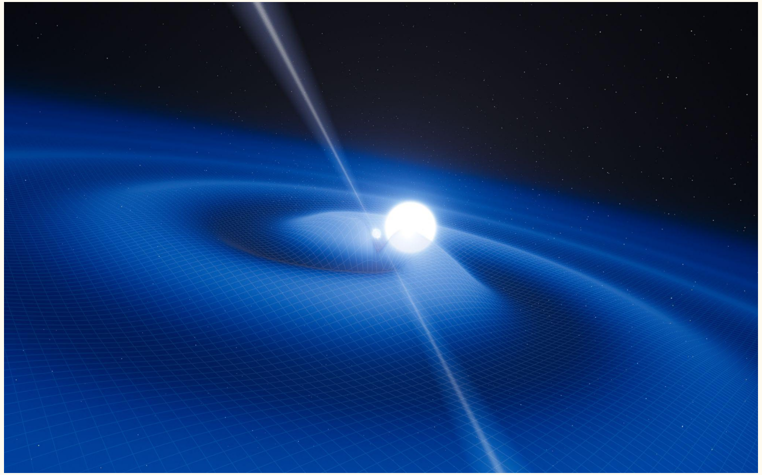


[C.B. Lang *et al.*, *Phys. Rev. D* **95** (2017) 1, 014510]

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
- Relieves Fermi pressure and leads to a softer equation of state, in contradiction with observation (‘hyperon’ puzzle)
- Two- and three-hadron interactions involving hyperons may supply the needed repulsion

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
- 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

Teasing out three-pion interactions

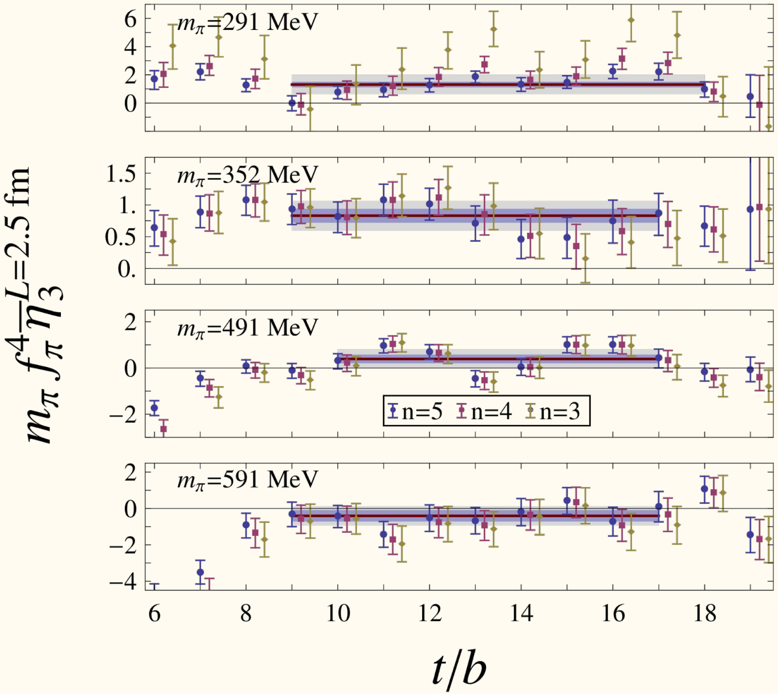
- Finite-volume energies from two-point correlators

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

- $1/L$ expansion to determine threshold three-pion interactions $\overline{\eta}_3^L$

$$\Delta E_n = \frac{4\pi\, a}{M\, L^3}\binom{n}{2}\left\{1-\frac{a\,\mathcal{I}}{\pi\, L}+\left(\frac{a}{\pi\, L}\right)^2\left[\mathcal{I}^2+(2n-5)\mathcal{J}\right]\right.$$
$$\left.-\left(\frac{a}{\pi\, L}\right)^3\left[\mathcal{I}^3+(2n-7)\mathcal{I}\mathcal{J}+\left(5n^2-41n+63\right)\mathcal{K}\right]\right\}$$
$$+\binom{n}{2}\frac{8\pi^2 a^3}{M\, L^6} r+\binom{n}{3}\frac{\overline{\eta}_3^L}{L^6}+\mathcal{O}\left(1/L^7\right)$$

- Very limited compared to full quantization conditions



[NPLQCD, *Phys. Rev. Lett.* **100** (2008) 082004]

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 - finite-volume energies

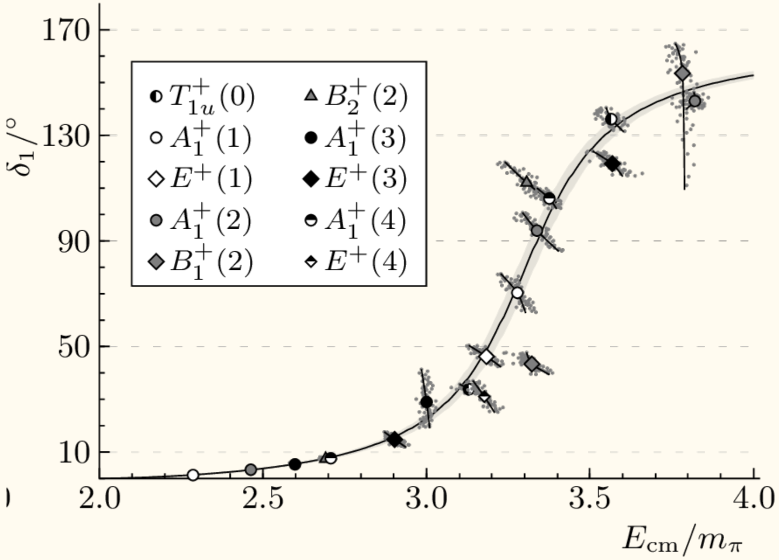
$\mathcal{K}_2$- 2-to-2 K-matrix

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

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



[C. Andersen, *et al.*, *Nucl.Phys.B* 939 (2019) 145]

Two- and Three-particle Quantization Conditions

Two-particle QC

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

- Equation in ℓm basis
- F is a purely kinematic known finite-volume function
- $\mathcal{K}_2(E_2^*)_{\ell' m';\ell m} = \delta_{\ell'\ell}\delta_{m'm}\mathcal{K}_2^{(\ell)}(E_2^*)$ is an infinite-volume quantity with algebraic relation to two-particle scattering amplitude

Three-particle QC

$$\det\left[F_3(E, \mathbf{P}, L)^{-1} + \mathcal{K}_{\mathrm{df},3}(E^*)\right] = 0$$

- Equation in $k\ell m$ basis (spectator - dimer)
- F_3 contains both kinematic functions and the two-particle K-matrix
- $\mathcal{K}_{\mathrm{df},3}$ is a real, analytic, infinite-volume quantity but is scheme-dependent
- Must solve integral equation to obtain three-particle scattering amplitude

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)

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

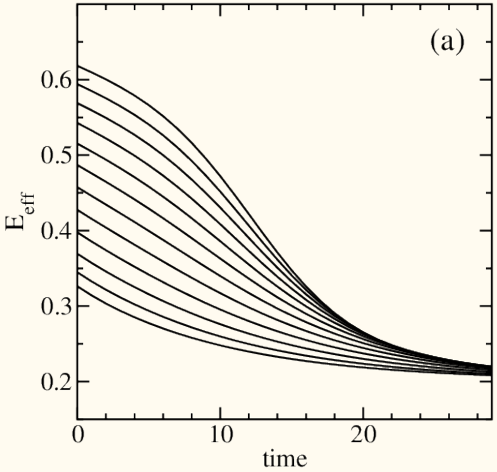
And use the eigenvectors to rotate $\hat{C}(t)$ at all other times

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

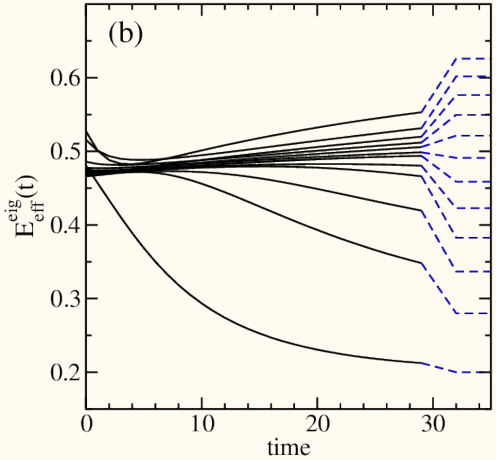
$$\lambda_n(t, \tau_0) \propto e^{-E_n t} + O(e^{-(E_N - E_n)t})$$

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

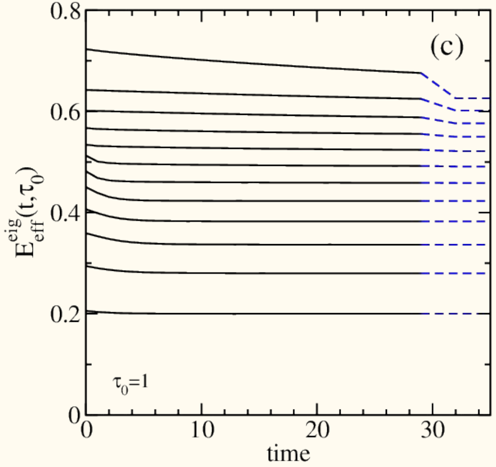
Correlator matrix toy model



Diagonal elements of C(t)



Eigenvalues of C(t)



Generalized eigenvalues of C(t)

$$E_n = E_{n-1} + \frac{0.08}{\sqrt{n}}, \qquad n = 1, 2, \ldots, 199\ , \qquad E_0 = 0.20,$$

$$Z_j^{(n)} = \frac{(-1)^{j+n}}{1 + 0.05(j-n)^2}$$

[Plots courtesy of Colin Morningstar]

Constraining interaction with excited states

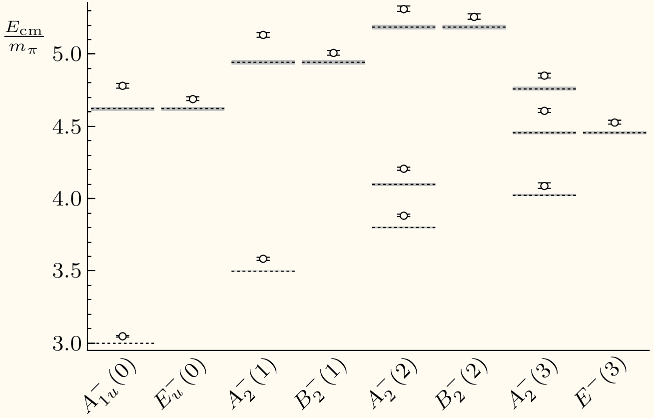
- First application of quantization condition using excited-state energies

$$\pi\pi\pi^{(\mathbf{P},\Lambda)} = c^{(\mathbf{P},\Lambda)}_{\mathbf{p}_1,\mathbf{p}_2,\mathbf{p}_3}\pi_{\mathbf{p}_1}\pi_{\mathbf{p}_2}\pi_{\mathbf{p}_3}$$

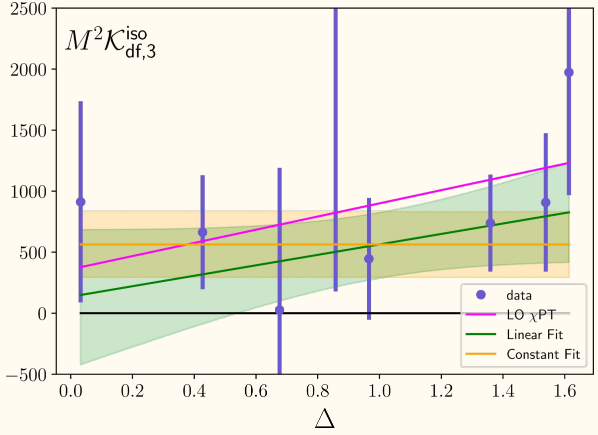
- Threshold expansion up to linear order

$$\mathcal{K}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso}}_{\mathrm{df},3} = \mathcal{K}^{\mathrm{iso},0}_{\mathrm{df},3} + \mathcal{K}^{\mathrm{iso},1}_{\mathrm{df},3}\Delta\,, \qquad \Delta = \frac{E^2_{\mathrm{cm}} - 9m^2_\pi}{9m^2_\pi}$$

- Three-pion energy shifts dominated by two-body interactions

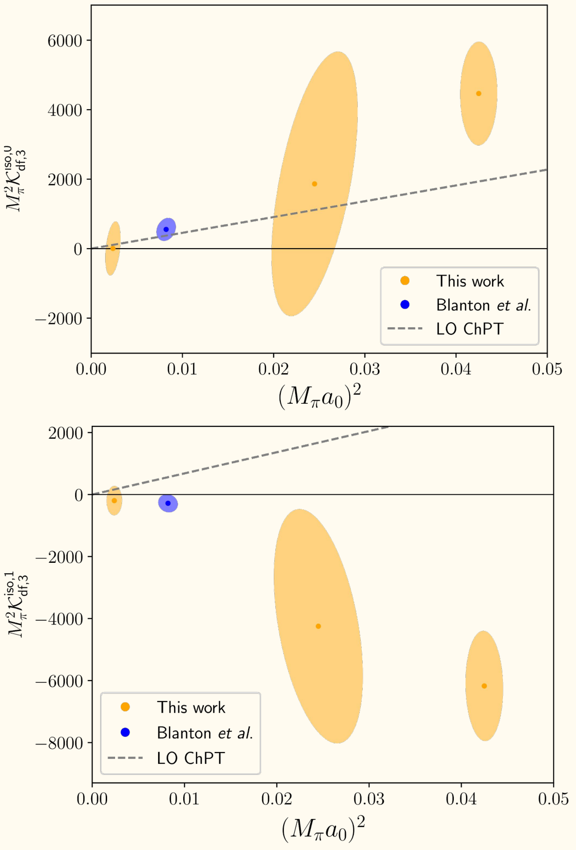


[B. Hörz, AH, *Phys. Rev. Lett.* **123** (2019) 14, 142002]

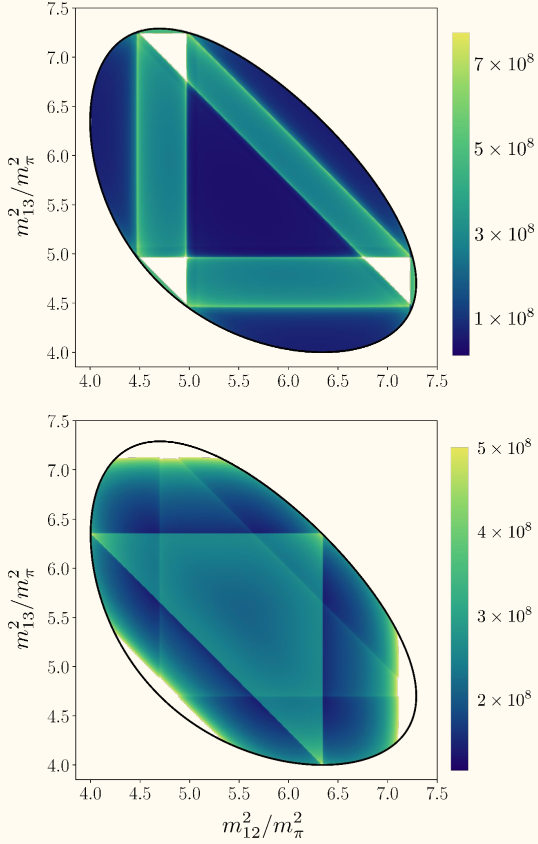


[T. Blanton *et al.*, *Phys. Rev. Lett.* **124** (2020) 3, 032001]

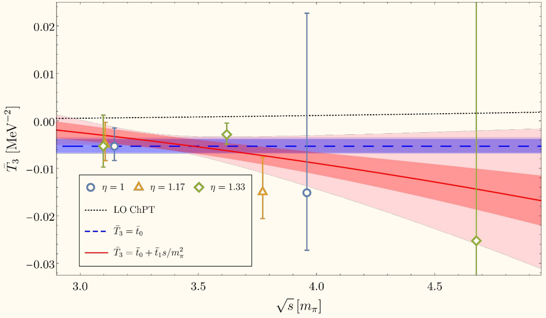
Other three-pion results



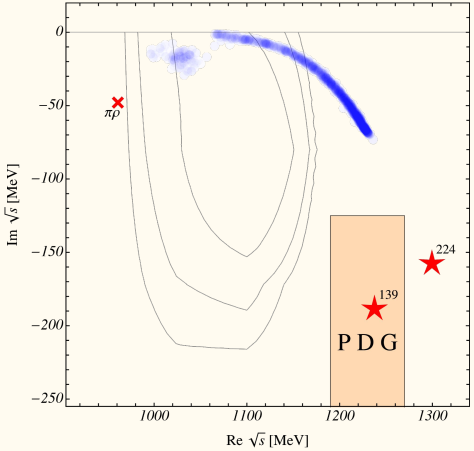
[ETMC, *Eur. Phys. J. C* **81** (2021) 5, 436]



[HadSpec, *Phys. Rev. Lett.* **126** (2021) 012001]



[Brett, *et al.*, *Phys. Rev. D* **104** (2021) 1, 014501]



[GWQCD, *Phys. Rev. Lett.* **127** (2021) 22, 222001]

Interactions of two and three mesons including higher partial waves from lattice QCD

Tyler D. Blanton, ADH, Ben Hörz, Colin Morningstar, Fernando Romero-López, Stephen R. Sharpe
JHEP **10** (2021) 023 · arXiv:2106.05590

Project Members

- Tyler Blanton (Postdoc, University of Maryland)
- Zachary Draper (Graduate student, University of Washington)
- Ben Hörz (Industry, Intel)
- Colin Morningstar (Carnegie Mellon University)
- Fernando Romero-López (Postdoc, MIT)
- Stephen R. Sharpe (University of Washington)

Procedure

1. Calculate matrices of two-point correlation functions
    a. Use stochastic LapH for quark propagation
    b. Construct operators to transform in irreps of little group
    c. Optimize contractions (https://github.com/laphnn/contraction_optimizer)
        i. Common subexpression elimination

2. Extract finite-volume energies from correlation matrices
    a. Solve Generalized EigenValue Problem (GEVP) for correlator matrices
    b. Fit ratio of rotated correlators to single-exponential to extract shifts from non-interacting
    c. Reconstruct energies and boost to center-of-momentum frame

3. Obtain K-matrices from spectrum
    a. Adjust K-matrix parameters until lattice energies match predictions from quantization condition

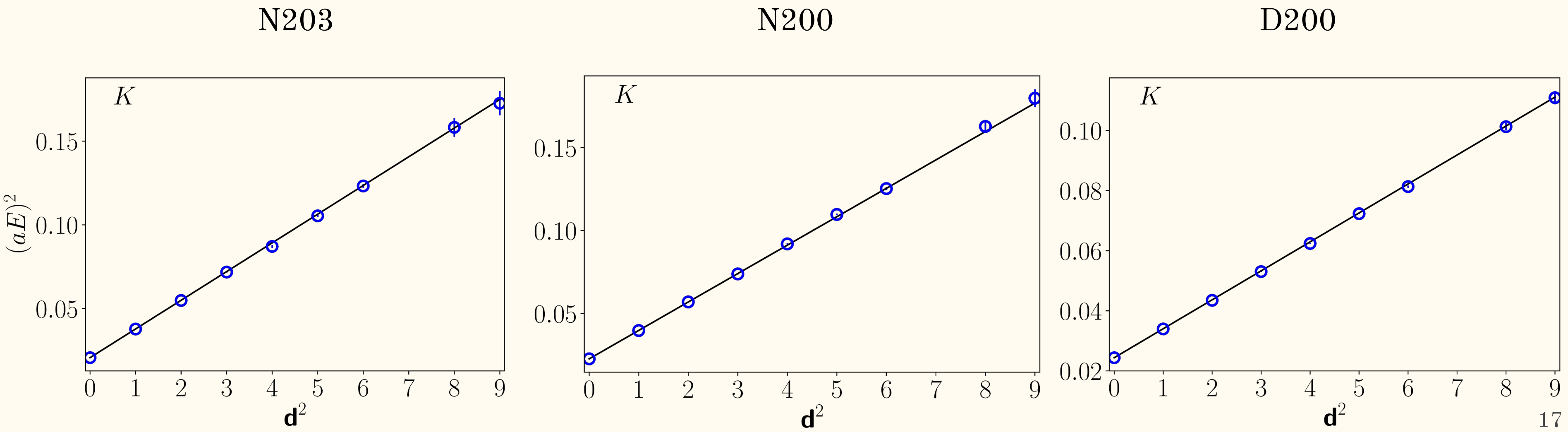
Lattice setup

- $N_F = 2 + 1$ *O(a)*-improved Wilson-clover fermions generated by CLS
- Three pion masses allow study of chiral dependence
  - Trace of bare quark masses held fixed
- One lattice spacing, $a = 0.06426(76)$ fm
- Consider constituent momenta up to and including $\boldsymbol{d}^2 = L^2/(2\pi)^2\, \boldsymbol{P}^2 = 9$

	$(L/a)^3 \times (T/a)$	M_π [MeV]	M_K [MeV]	$N_{\rm cfg}$	$t_{\rm src}$	$N_{\rm ev}$
N203	$48^3 \times 128$	340	440	771	32, 52	192
N200	$48^3 \times 128$	280	460	1712	32, 52	192
D200	$64^3 \times 128$	200	480	2000	35, 92	448

Single-Meson Energies

- Single-exponential fits to correlators of momentum-projected kaon operators
- Continuum dispersion relation works well up to $\boldsymbol{d}^2 = 9$
- No sign of cutoff effects here
- Similar situation for pions

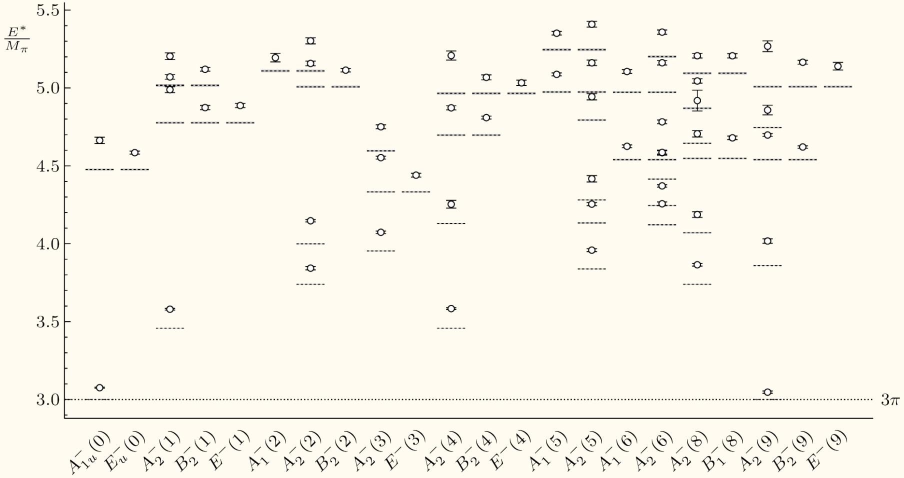


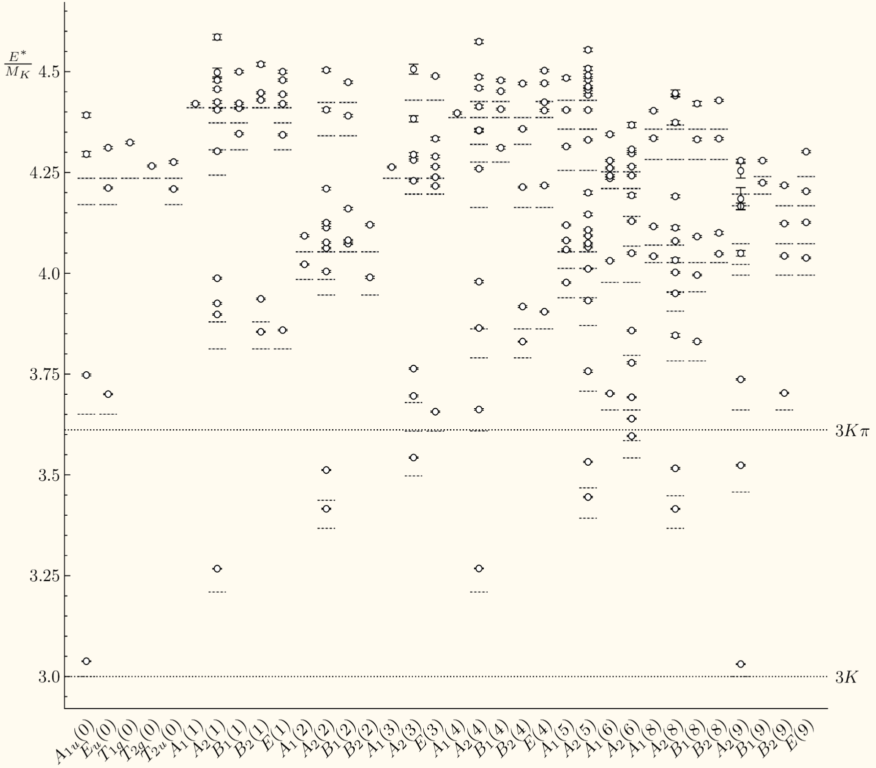
Spectrum results on N200

Single-exponential fits to

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

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





Parameterizations

- Parameterization of two-particle K-matrix
  - For s-wave, use the effective range expansion or a form that explicitly includes the Adler zero
  - Use the d-wave scattering length
- Parameterization of $\mathcal{K}_{\mathrm{df},3}$ given by threshold expansion to quadratic order

$$\mathcal{K}_{\mathrm{df},3} = \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},0} + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},1}\Delta + \mathcal{K}_{\mathrm{df},3}^{\mathrm{iso},2}\Delta^2 + \underbrace{\mathcal{K}_A\Delta_A + \mathcal{K}_B\Delta_B}_{\text{Two-particle d-wave contributions}}$$

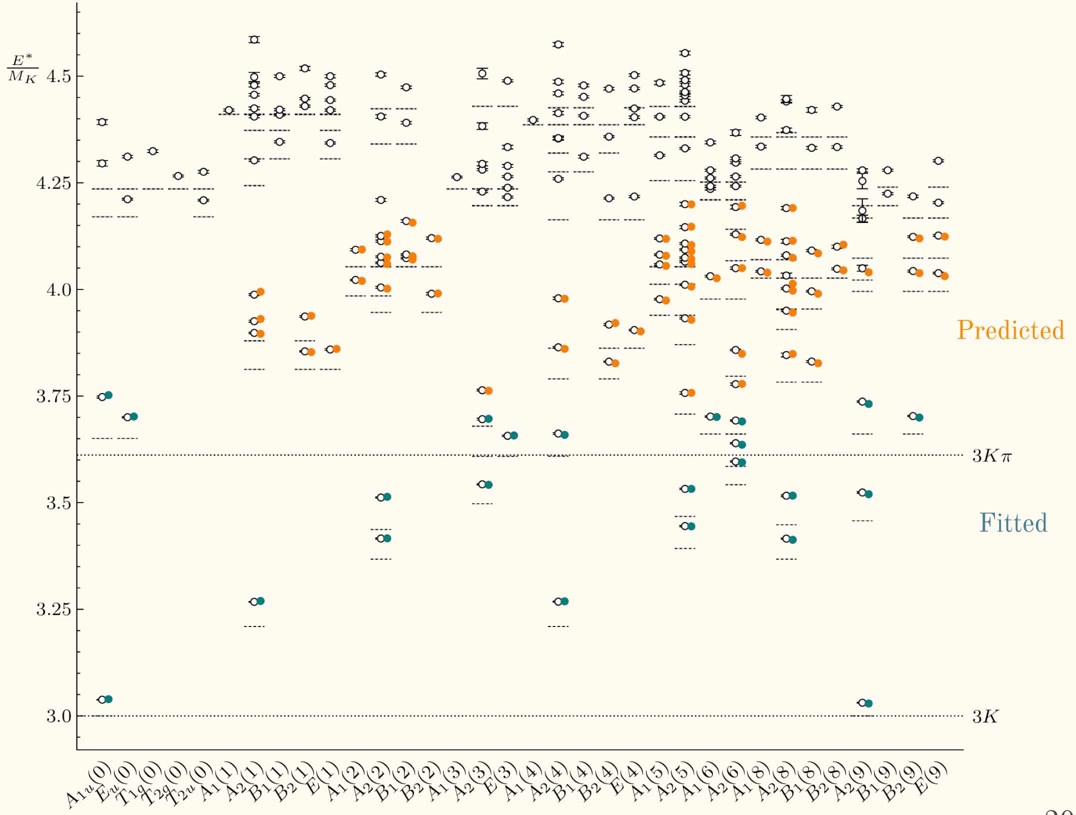
(see arXiv:1901.07095 for details)

- Parameters $\{p_n\}$ determined from minimum of

$$\chi^2(\{p_n\}) = \sum_{ij}\left(E_i - E_i^{\mathrm{QC}}(\{p_n\})\right) C_{ij}^{-1}\left(E_j - E_j^{\mathrm{QC}}(\{p_n\})\right)$$

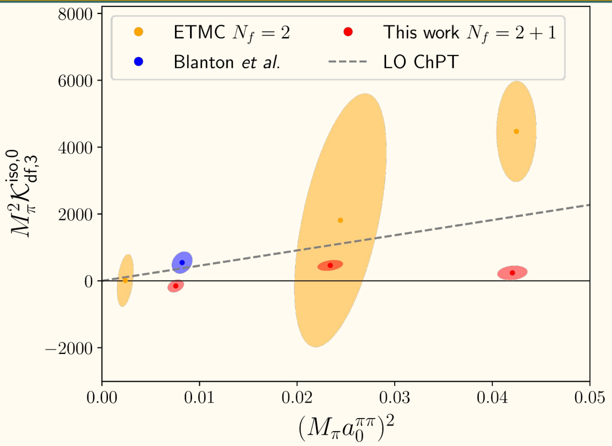
Testing the Limits of the Formalism

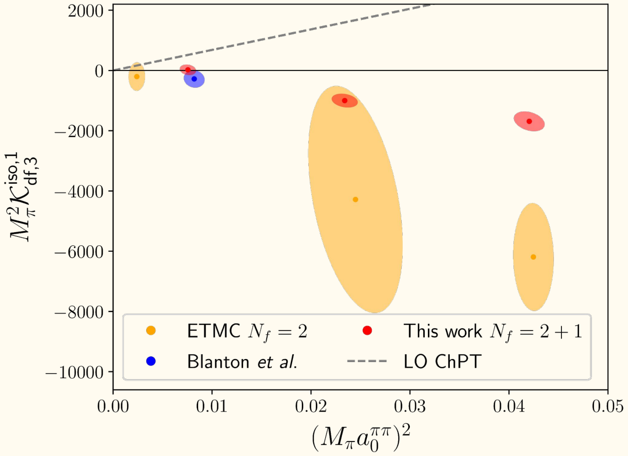
- QC is valid up to first threshold with more than three particles (depending on allowed transitions)
- Transition to 3Kπ expected to be NNLO in ChPT, leading to suppressed coupling near threshold
- Fits describe data well above rigorous applicability of QC



Comparisons to other groups

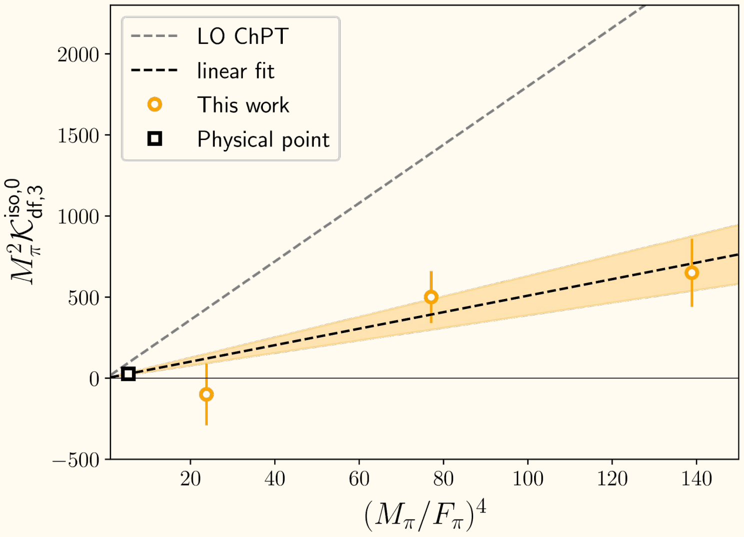
- Comparison to other results using RFT approach
- Some tension with older result on subset of data
- Difficult to make comparisons with FVU, due to scheme dependence

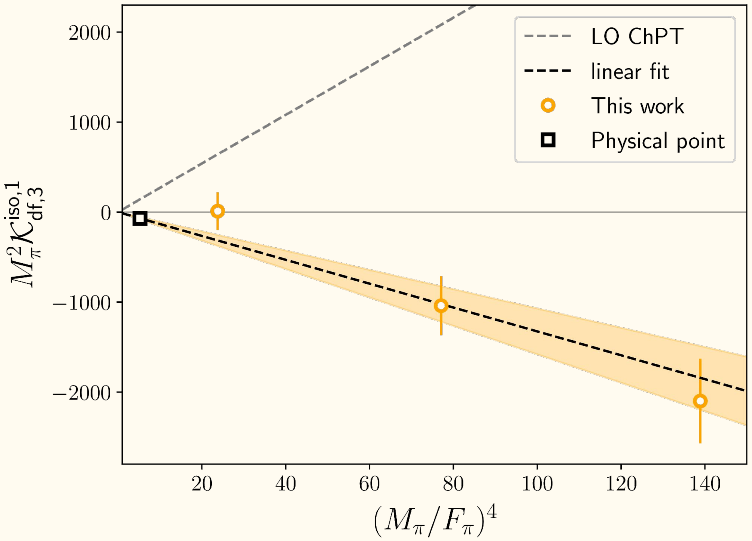




Inclusion of d-wave terms

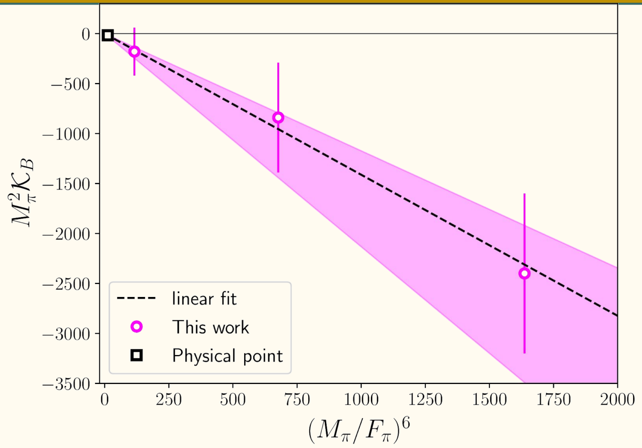
- $\mathcal{K}_B$ and d-wave in $\mathcal{K}_2$ essential for good fit quality
- Better chiral behavior
- Integral equations for d-wave not known

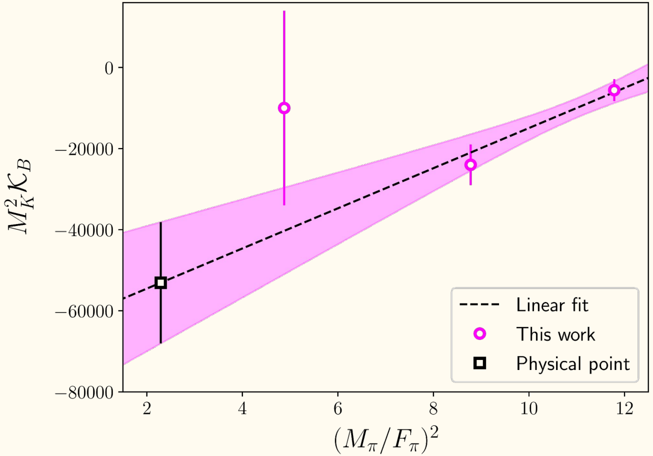




Chiral dependence

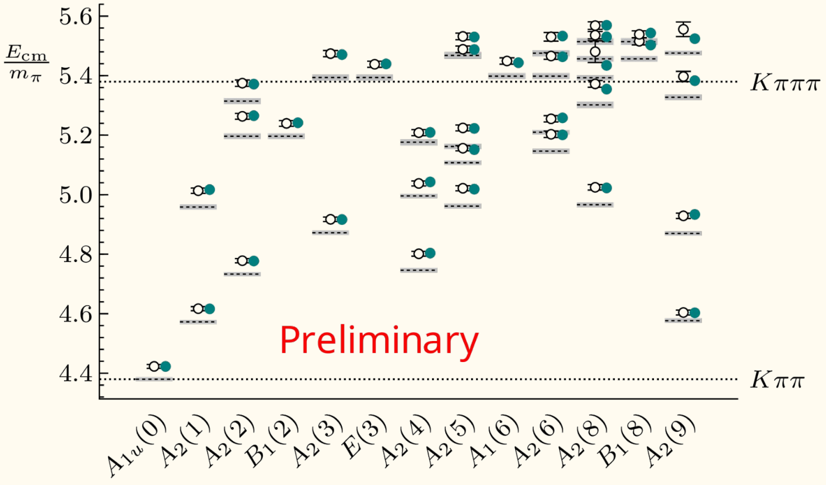
- Evidence for significant d-wave contributions
- Only $\mathcal{K}_B$ contributes to non-trivial irreps, making it easier to constrain
- Can only appear at NLO in ChPT
- Larger error on D200 from large $M_K L$, leading to suppression of energy shifts

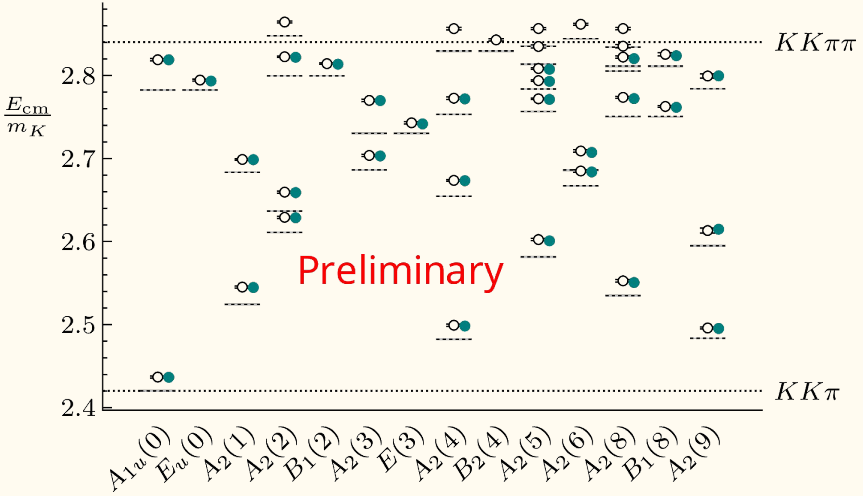




Mixed flavor systems

- Formalism for mixed flavor systems recently developed
  [T. Blanton, *et al.*, *JHEP* **02** (2022) 098]
- Preliminary results on D200, shows good description of data

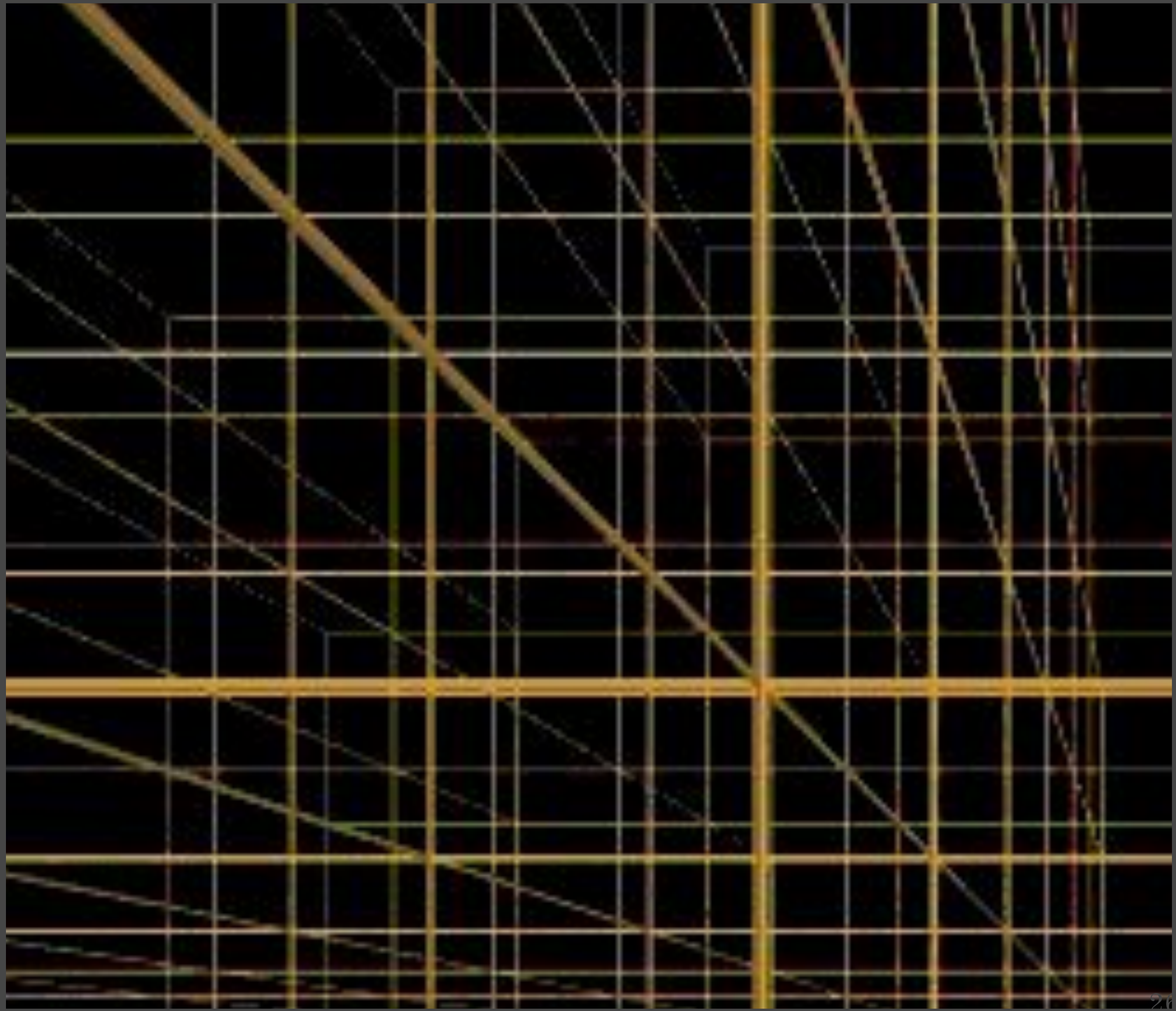




Conclusions and Outlooks

- Three-particle quantization condition for simple systems
  - Hundreds of energies extracted
  - d-wave terms in two- and three-particle K-matrix improve fit quality (substantially at times)
  - First calculation showing strong indication that non-zero three-particle interactions are needed
  - Mixed-flavor systems working well
- Future work
  - Systems with non-maximal isospin, resonances, and/or bound states
    - RFT formalism worked out [Hansen, Romero-López, Sharpe, *JHEP* **07** (2020) 047]
    - Application to $a_1(1260)$ [GWQCD, Phys. Rev. Lett. 127 (2021) 22, 222001]
  - Integral equations for d-wave
  - Inclusion of baryons (Roper and neutron stars)
  - 4 particles?

Thanks!



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

Extra Slides

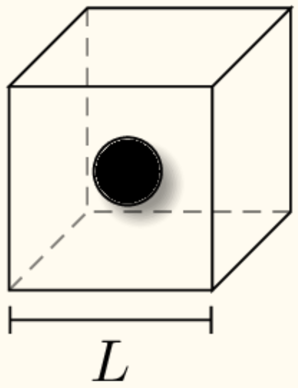
Volume Dependence of the Spectrum

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

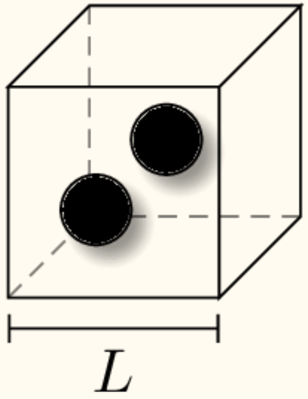
$$\Delta E^{(2)} \propto \frac{a_0}{L^3} + O\left(\frac{1}{L^4}\right)$$



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

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

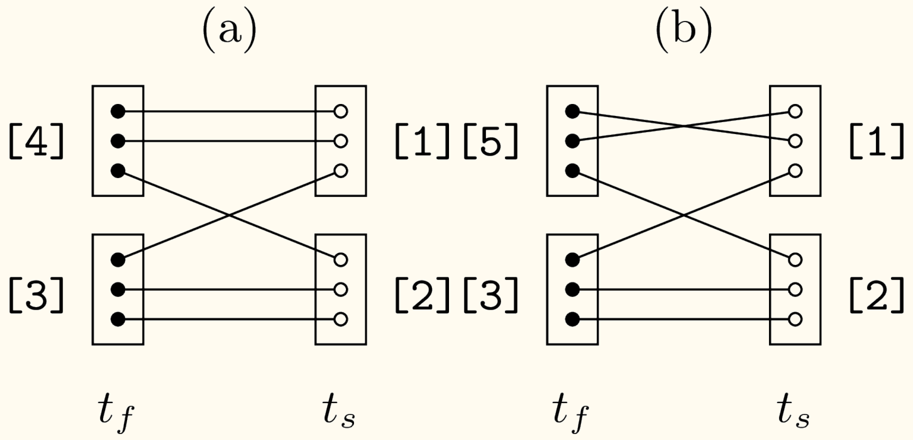
$$E_{\rm cm} = \sqrt{E^2 - \boldsymbol{P}^2} = \sqrt{p^2 + m_1^2} + \sqrt{p^2 + m_2^2}$$



[Lüscher '86, '91; generalizations]

Contractions Optimization

- The growing number of Wick contractions as more particles are considered is a technical challenge
- First, for each diagram consider optimal sequence for contractions of two tensors at a time
- Then, if two contraction steps are equally good, choose the one that appears the most across all diagrams (Common subexpression elimination)
- Contraction cost reduced by more than an order of magnitude for $I=3$ three-pion system



contraction step	removed indices	step complexity
[2] – [3]	2	N_{dil}^4
[1] – [4]	2	N_{dil}^4
[1] – [3]	1	N_{dil}^5
[2] – [4]	1	N_{dil}^5

https://github.com/laphnn/contraction_optimizer

Quark Propagation with Distillation

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

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 Δ

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

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