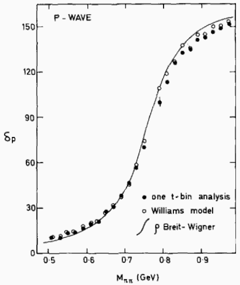
Progress towards nucleon-nucleon interactions with stochastic LapH

Ben Hörz (LBNL)

Frontiers in Lattice QCD and related topics
Yukawa Institute for Theoretical Physics, Kyoto University
Apr 17, 2019

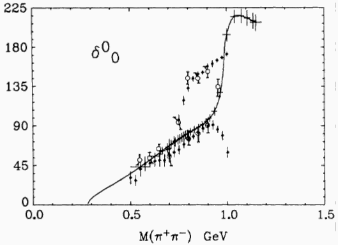
[Estabrooks, Martin 1975]



1. What can we learn about the QCD spectrum from first principles?
2. Lattice QCD as a tool for nuclear physics

Hadron interactions from Lattice QCD

[Protopopescu et al. 1973]



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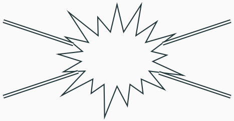

nucleon-nucleon interactions

nucleon-hyperon interactions
$N\Sigma, N\Lambda$

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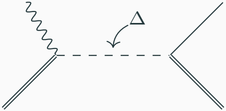


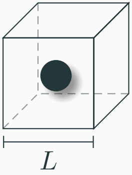
$\langle N\pi | J_\mu | N \rangle$

multi-hadron state

1. What can we learn about the QCD spectrum from first principles?
2. Lattice QCD as a tool for nuclear physics

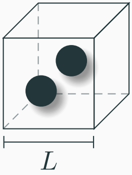
[NuSTEC White Paper: Status and Challenges of Neutrino-Nucleus Scattering 1706.03621]

> However better knowledge of contributions from heavier resonances is also important for higher energy experiments like NOvA and DUNE and seriously lacking.
> The most important challenges are
>
> - improving our knowledge of the axial part of nucleon-Δ transition matrix elements, either via a new hydrogen and/or deuterium experiment or via lattice-QCD calculations;
> - describing nonresonant contributions to pion production channels. Understanding the range



single particle in a periodic box
$\rightsquigarrow \Delta E \propto \mathrm{e}^{-mL}$

two spinless particles in a periodic box
$\rightsquigarrow \Delta E \propto a_0/L^3 + O(L^{-4})$ [Lüscher '86, '91]



$\Rightarrow$ 'The Lüscher method'

Review of formalism and results

Scattering processes and resonances from lattice QCD

Raúl A. Briceño,[1,*] Jozef J. Dudek,[1,2,†] and Ross D. Young[3,‡]

[1] *Thomas Jefferson National Accelerator Facility, 12000 Jefferson Avenue, Newport News, Virginia 23606, USA*

[2] *Department of Physics, College of William and Mary, Williamsburg, Virginia 23187, USA*

[3] *Special Research Center for the Subatomic Structure of Matter (CSSM), Department of Physics, University of Adelaide, Adelaide 5005, Australia*

(Dated: June 21, 2017)

The vast majority of hadrons observed in nature are not stable under the strong interaction, rather they are *resonances* whose existence is deduced from enhancements in the energy dependence of scattering amplitudes. The study of hadron resonances of-

[Briceño, Dudek, Young 1706.06223]

see also [Hansen, Sharpe 1901.00483]

2-particle channel
partial wave
(total angular mom.)

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

E_L – FV spectrum
$\mathcal{M}$ – 2-to-2 scatt. ampl.
F – known functions

Two-particle Quantization Condition

2-particle channel
partial wave
(total angular mom.)

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

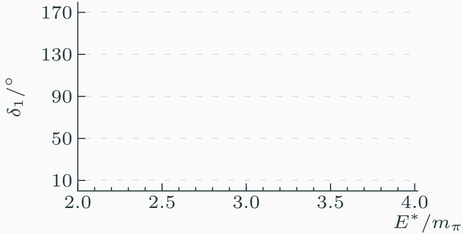
E_L – FV spectrum
$\mathcal{M}$ – 2-to-2 scatt. ampl.
F – known functions

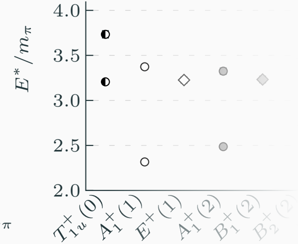
group theory worked out and publicly available on Github

[Morningstar, Bulava, Singha, Brett, Fallica, Hanlon, BH 1707.05817]

A simple (yet relevant) resonance: $\rho(770)$

[plot adapted from Bulava, Fahy, BH, Juge, Morningstar, Wong 1604.05593]





- elastic $\pi\pi$ scattering neglecting $\ell \geq 3$ partial wave
  spectrum $\Leftrightarrow$ scattering amplitude
- benchmark system for the lattice

e.g. Lang et al. 1105.5636, Aoki et al. 1106.5365, ..., Dudek et al. 1212.0830, ...

- recent interest due to its contribution to $(g-2)_\mu$ HVP

[Meyer, Wittig 1807.09370]

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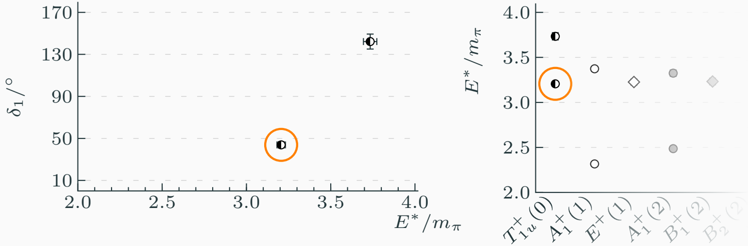

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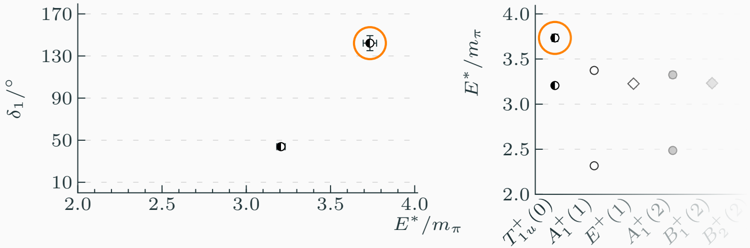

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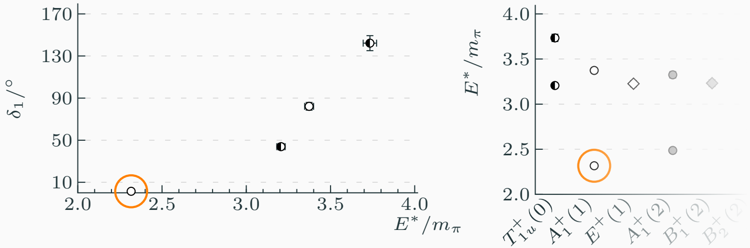

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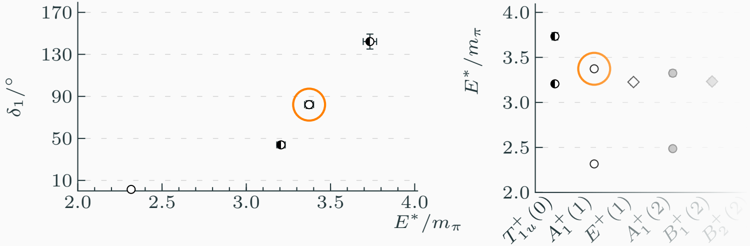

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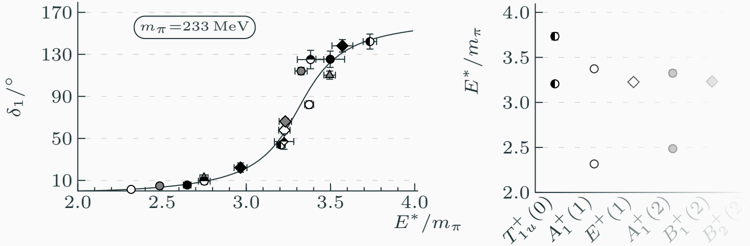

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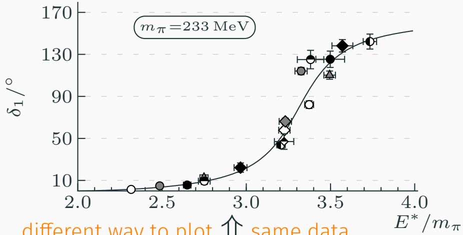
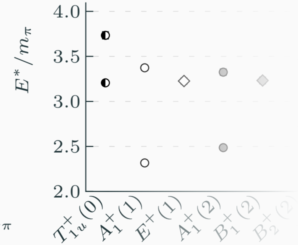
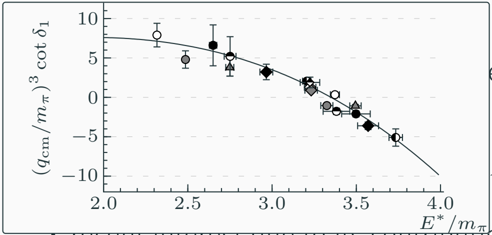




different way to plot ⇕ same data



3 partial wave

e

1105.5636, Aoki et al. 1106.5365, ..., Dudek et al. 1212.0830, ...

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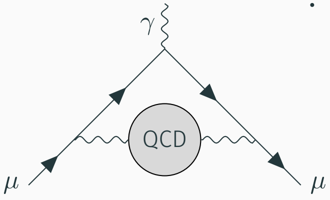
[Meyer, Wittig 1807.09370]

Matrix elements: Timelike pion form factor



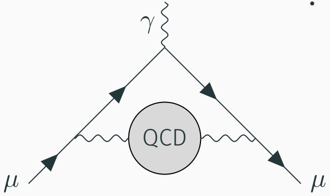
- muon anomalous magnetic moment $(g-2)_\mu$
  - HVP governed by

    $R_{\text{had}} = \sigma(e^+e^- \to \text{hadrons}) / \frac{4\pi\alpha_{\text{em}}(s)^2}{3s}$

  - two-pion state dominates at low energies

    $R_{\text{had}}(s) = \frac{1}{4}\left(1 - \frac{4m_\pi^2}{s}\right)^{\frac{3}{2}} |F_\pi(s)|^2$

    $F_\pi(s)$: $\gamma^* \to \pi\pi$



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    $\gamma^* \to \pi\pi$

infinite volume

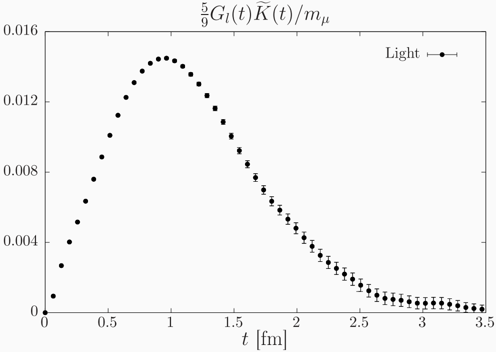
finite volume

$$|F_\pi(E^*)|^2 = g_\Lambda(\gamma)\, q \frac{\partial(\delta_1 + F)}{\partial q} \frac{3\pi E^{*2}}{2q^5L^3} \left|\langle 0|V^{(\mathbf{d},\Lambda)}|\mathbf{d}\Lambda E^*\rangle\right|^2$$

Lellouch, Lüscher hep-lat/0003023
Meyer 1105.1892
Feng et al. 1412.6319

requires
scattering amplitude

Vector-correlator reconstruction

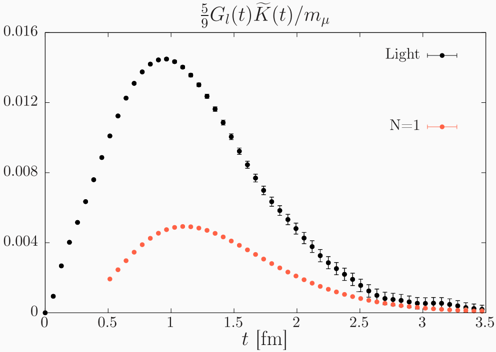


$m_\pi = 200\,\mathrm{MeV}, L = 4.1\,\mathrm{fm}$

[Gérardin, Cè, von Hippel, BH, Meyer, Mohler, Ottnad, Wilhelm, Wittig 1904.03120]

- time-momentum representation
  [Bernecker, Meyer 1107.4388]
- clear spectral decomposition

$$G_l(t) \sim \sum_{\mathbf{x}} \langle 0|V(\mathbf{x},t)V^\dagger(0)|0\rangle$$
$$\approx \sum_{n}^{N} |\langle 0|V|T_{1u},n\rangle|^2\, \mathrm{e}^{-E_n t}$$



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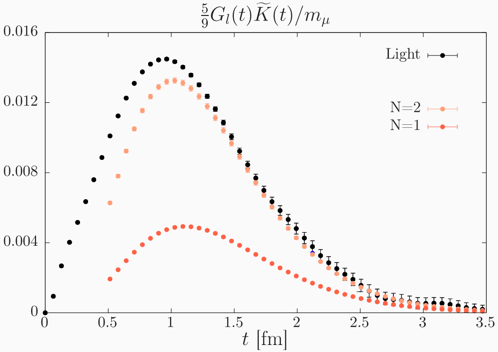

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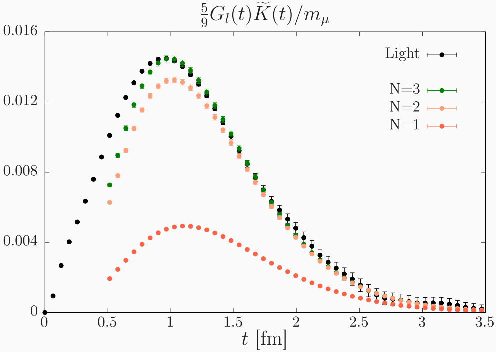

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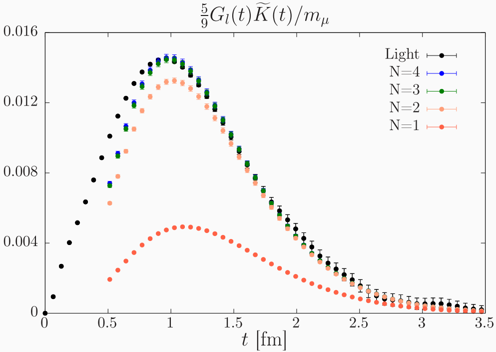

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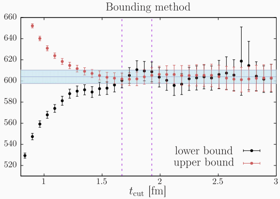
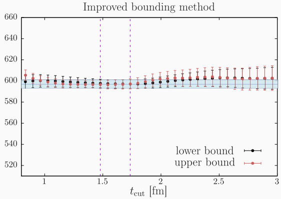
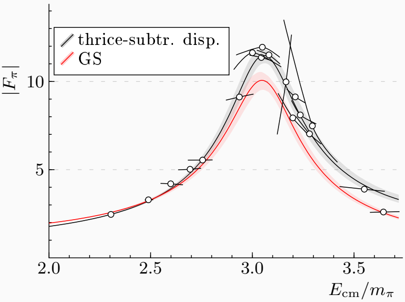
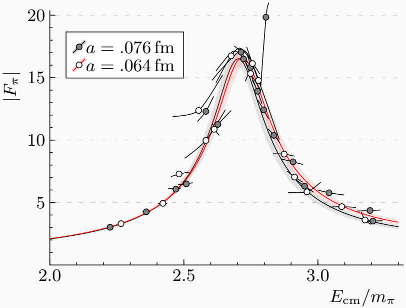




[Andersen, Bulava, BH, Morningstar 1808.05007]



$m_\pi = 260\,\text{MeV}$



$m_\pi = 280\,\text{MeV}$

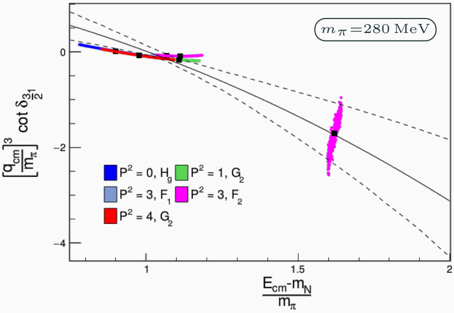
allows for a check of HVP FV effects

$\rightsquigarrow$ formalism and technology under control for two-meson systems

Δ resonance $(I = 3/2\ N\pi$ scattering$)$

- combinatorically harder than meson-meson
- typically worse signal-to-noise
- scattering of particles with spin
  rotational-symmetry breaking more restricting

[Andersen, Bulava, BH, Morningstar 1710.01557]



- Breit-Wigner shape
- $\Delta(1232)$ found on threshold
- more precision required for matrix elements
  (limited by correlator construction)

NN scattering

[Briceño, Davoudi, Luu 1305.4903]

	0^+	0^-	1^+	1^-	2^+	2^-	3^+
$I=0$	–	–	$\{(0,1),(2,1)\}$	$(1,0)$	$(2,1)$	–	$(2,1)$
$I=1$	(0,0)	$(1,1)$	–	$(1,1)$	$(2,0)$	$(1,1)$	–

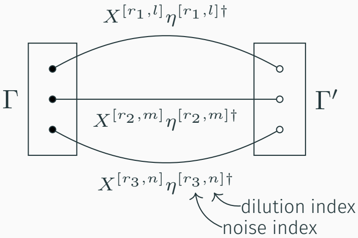
(L,S)

FV

	[000]	$[00n]$	$[0nn]$
0^+	A_{1g}	A_1	A_1
0^-	A_{1u}	A_2	A_2
1^+	T_{1g}	$(A_2 \oplus E)$	$(A_2 \oplus B_1$
1^-	T_{1u}	$(A_1 \oplus E)$	$(A_1 \oplus B_1$
2^+	$E_g \oplus T_{2g}$	$(A_1 \oplus B_1) \oplus (B_2 \oplus E)$	$(A_1 \oplus B_2) \oplus (A_1$
2^-	$E_u \oplus T_{2u}$	$(A_2 \oplus B_2) \oplus (B_1 \oplus E)$	$(A_2 \oplus B_1) \oplus (A_1$
3^+	$A_{2g} \oplus T_{1g} \oplus T_{2g}$	$B_1 \oplus (A_2 \oplus E) \oplus (B_2 \oplus E)$	$B_2 \oplus (A_2 \oplus B_1 \oplus B_2)$

$\rightsquigarrow$ large degeneracy – many operators – even more correlation functions

[Morningstar et al. 1104.3870]



- quark propagators outer products

$$DX^{[r,l]} = \eta^{[r,l]}$$

- define baryon-sink function
  (analogously for source)

$$\mathcal{B}^{[z]}(l,m,n) = \sum_{\mathbf{x}} \mathrm{e}^{-i\mathbf{p}\mathbf{x}} \epsilon_{abc} \Gamma_{\alpha\beta\gamma} X^{[r_1,l]}_{\alpha a} X^{[r_2,m]}_{\beta b} X^{[r_3,n]}_{\gamma c}$$

combined noise, momentum, Γ index

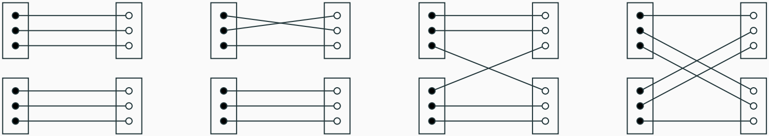
computing correlation functions $\equiv$ tensor contractions

rank-3 tensors $\mathcal{B}^{[z]}(l,m,n)$ – dilution index range $N_{\mathrm{dil}} = O(64)$

- factorizes computation of observable
  (baryon functions computed timeslice by timeslice)

- reusable for multi-hadron correlators

Two-nucleon correlation function



48 diagrams ($I = 1$ NN), 36 diagrams ($I = 0$ NN)

- ‘unroll’ group-theoretic linear combinations

  (*many* elemental diagrams to compute – a lot of redundancy)

- quark-level optimization investigated before

  Doi, Endres 1205.0585
  Detmold, Orginos 1207.1452
  Wynen et al. 1810.12747

- contraction order matters at tensor level

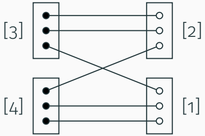
  well-known in quantum chemistry

  Hartono et al. *Automated Operation Minimization of Tensor Contraction Expressions in Electronic Structure Calculations*, 2005
  Hartono et al. *Identifying Cost-Effective Common Subexpressions to Reduce Operation Count in Tensor Contraction Evaluations*, 2006

  more recently in the context of tensor networks

  Pfeifer et al. *Faster identification of optimal contraction sequences for tensor networks*, 1304.6112

Two-nucleon correlation function (II)



- single-term optimization
  (find the best contraction(s) in a diagram)

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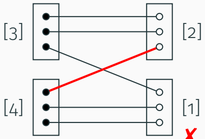

✗ $N_{\rm dil}^5$

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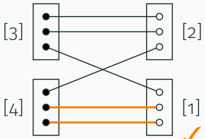

✓ N_{dil}^4

- single-term optimization

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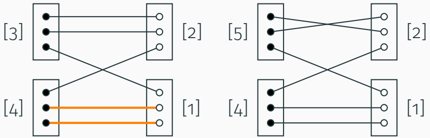
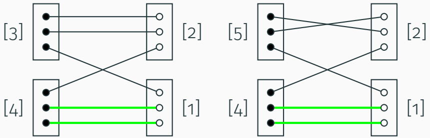


- single-term optimization
  (find the best contraction(s) in a diagram)

- global optimization
  (compare utility across all diagrams)

Two-nucleon correlation function (II)



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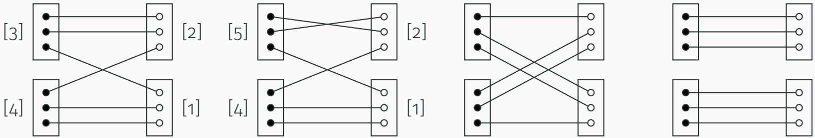
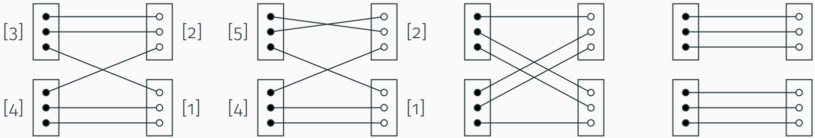
- global optimization
  (compare utility across all diagrams)

Two-nucleon correlation function (II)



- single-term optimization
  (find the best contraction(s) in a diagram)
- global optimization
  (compare utility across all diagrams)
- NN diagrams can be evaluated at $2N_{\mathrm{dil}}^4 + N_{\mathrm{dil}}^2$ or $2N_{\mathrm{dil}}^3$
  (need to keep track of noise indices etc.)

Two-nucleon correlation function (II)



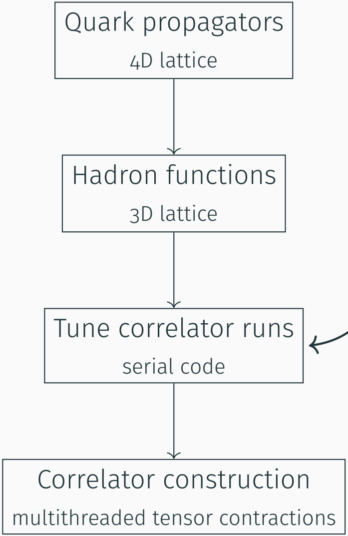
- single-term optimization
  (find the best contraction(s) in a diagram)

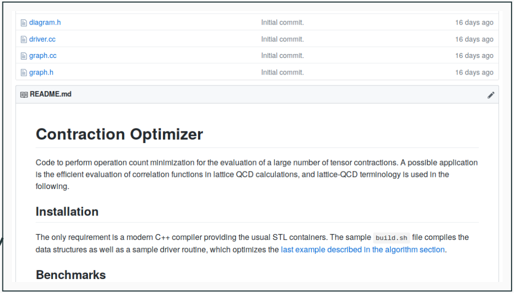
- global optimization
  (compare utility across all diagrams)

- NN diagrams can be evaluated at $2N_{\mathrm{dil}}^4 + N_{\mathrm{dil}}^2$ or $2N_{\mathrm{dil}}^3$
  (need to keep track of noise indices etc.)

- a single NN correlator:

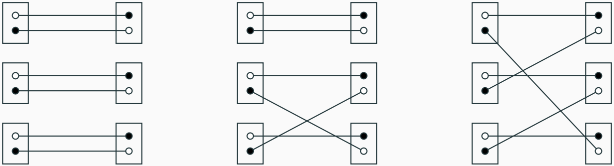
	N_{dil}^2	N_{dil}^3	N_{dil}^4
w/o CSE	12,992	3,584	25,984
w/ CSE	2,352	64	1,080



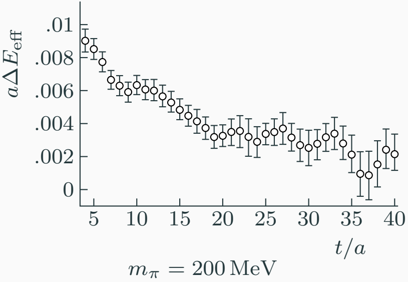


- backend-agnostic implementation in C++ with Python interface
- will be publicly available after licensing

Another example: $I = 3\ \pi\pi\pi$



- whole machinery readily applicable



- at-rest ground state $\pi(0)\pi(0)\pi(0)$

	N_{dil}^2	N_{dil}^3
w/o CSE	47,520	60,480
w/ CSE	450	360

- $\Delta E = E_{3\pi} - 3m_\pi$

Summary & Next Steps

- two-hadron interactions from lattice QCD …

  (calculations maturing, starting to assess standard lattice systematics)

- …and with practical relevance

  (helping to improve $(g-2)_\mu$/HVP from lattice QCD)

- addressing (gross) inefficiencies as we go

  (contractions hopefully won't be a problem again any time soon)

- stay tuned for
  - NN scattering
  - $N\Sigma$, $N\Lambda$ scattering
  - …