

Ben Hörz

- '08 - '11 B.Sc. Physics, Humboldt-University Berlin
Thesis: Light Scattering by Large Particles in Geometrical Optics Approximation
(jointly with FU Berlin, polarization-resolved raytracing software suite)
- '11 - '13 M.Sc. Physics, Humboldt-University Berlin
Thesis: ChPT for 2+1+1 Flavor of Wilson Fermions with Twisted Masses (O. Bär)
- '13 - '16 (exp.) Ph.D. in Mathematics, Trinity College Dublin
Resonances from Lattice QCD (J. Bulava)
- 15/08 - 15/12 Fulbright visiting researcher at Carnegie Mellon University (C. Morningstar)

Excited states from Lattice QCD

Ben Hörz
Trinity College Dublin

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- Quantum chromodynamics describes the strong interaction in the Standard Model
- Euclidean path integral $(a, L, T) \leftrightarrow$ statistical ensemble

$$\langle 0 | \bar{\psi} \Gamma \psi(x) \bar{\psi} \Gamma' \psi(y) | 0 \rangle_c =$$

$$\int D\mathcal{U} \operatorname{tr} \left[M^{-1}(x, y) \Gamma M^{-1}(y, x) \Gamma' \right] \frac{\det M e^{-S_g}}{Z}$$

- Monte Carlo with importance sampling of the path integral gives Euclidean correlation functions
- Dirac matrix M is large, sparse, ill-conditioned
- Its inverse is required for calculating correlation functions

Spectroscopy

- decomposition of correlation matrix in terms of Hamiltonian eigenstates

$$C_{ij}(t) = \sum_n \langle 0 | O_i | n \rangle \langle n | \bar{O}_j | 0 \rangle e^{-E_n t}$$

- symmetries of the system \Leftrightarrow block-diagonalization of Hamiltonian (*quantum numbers*)
- matrix of temporal correlators facilitates extraction of $E_n, n = 1, 2, \dots$
- energy eigenvalues of multi-particle states in a box with periodic boundary conditions are shifted by their interactions

[Lüscher '86, '90, '91; Rummukainen, Gottlieb '95]

- renewed theoretical interest

e.g. [Kim, Sachrajda, Sharpe '05; Briceño, Hansen, Walker-Loud '14]

and applications

e.g. [Wilson et al '15; Briceño et al '15]

Timelike pion form factor from Lattice QCD

- behavior of Lüscher quantization condition under small perturbations encodes even more information [Meyer '12]
- derivation by Meyer closely related to Lellouch-Lüscher formalism [Lellouch, Lüscher '01]
- Key formula

$$|F_\pi(s)|^2 = \frac{3\pi s}{2L^3 p^5} g(\gamma) \left(q\phi'(q) + p \frac{\partial \delta_1(p)}{\partial p} \right) \left| \langle 0 | V^{(\mathbf{P},\Lambda)} | \mathbf{P}, \Lambda, \mathbf{n} \rangle \right|^2$$

- special case of $0 \rightarrow 2$ transition amplitude

[Briceño, Hansen '15]

The stochastic LapH method

All-to-all propagators

- all-to-all propagators required for two-particle states, each with definite momentum
- Dirac matrix M is ill-conditioned and intractable
- two key insights:
 - 1 important physics is captured by a low-dimensional subspace
→ *distillation*
 - 2 achievable overall accuracy is limited by incomplete sampling of the path integral
→ stochastic

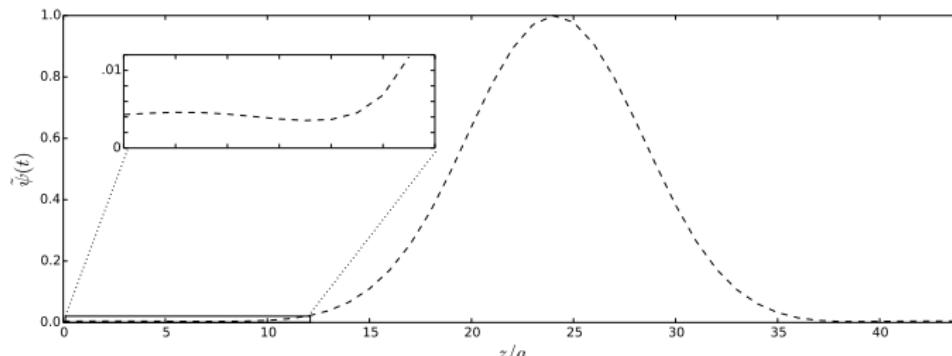
The stochastic LapH method

Distillation

- important contributions to the quark propagator are encoded in subspace

$$-\Delta v_n = \lambda_n v_n$$

- spanned by $N_{\text{ev}} \ll 12 \times L^3$ eigenvectors of covariant 3D Laplace operator [Peardon et al '08]
- projector into subspace acts like smearing operator



The stochastic LapH method

- distillation has proven successful in baryon, two-meson, charmonium, ... spectroscopy

[HadSpec Collaboration '12 ff.]

- but, for constant physical smearing: $N_{\text{ev}} \propto V = L^3$
- use stochastic estimation in the low-dimensional subspace

[Morningstar et al '11]

- for random noise vectors $\eta_i^{(r)} \in Z_4, i = 1, \dots, N_{\text{ev}}$

$$M'_{ij}^{-1} = \lim_{N_\eta \rightarrow \infty} \frac{1}{N_\eta} \sum_{r=1}^{N_\eta} X_i^{(r)} \eta_j^{(r)*}, \quad \text{where } M' X^{(r)} = \eta^{(r)}$$

- practical stochastic estimates using dilution [Foley et al '05]

The stochastic LapH method

- #inversions $\propto N_\eta \times N_{\text{dil}}$ instead of N_{ev}
- one noise per quark line for unbiased estimate of a diagram
- required N_{dil} is independent of V
- local coherence of low-quark modes - the phenomenon that powers deflation

[Lüscher '07]

Other nice features of *stochastic LapH*:

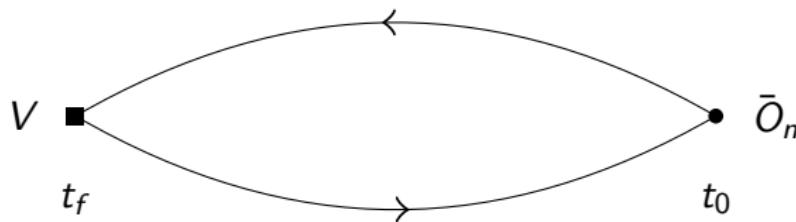
- each quark line outer product of a “source” η and a “sink” X
- minimal storage required to save propagator (a few complex numbers)
- factorization of objects required for correlator construction
- universally applicable method

e.g. string breaking [Koch, .., BH et al '15]

The stochastic LapH method

$$|F_\pi(s)|^2 = \frac{3\pi s}{2L^3 p^5} g(\gamma) \left(q\phi'(q) + p \frac{\partial \delta_1(p)}{\partial p} \right) \left| \langle 0 | V^{(\mathbf{d}, \Lambda)} | \mathbf{d}, \Lambda, \mathbf{n} \rangle \right|^2$$

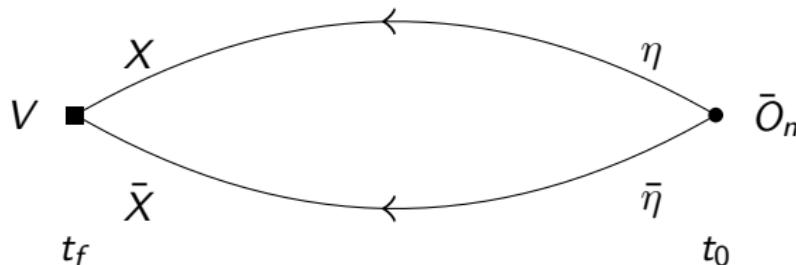
$$V_\mu^{(\text{imp, ren})} = Z_V (1 + b_V am) \left(\bar{\psi} \gamma_\mu \psi + i a c_V \partial_\nu \left\{ \bar{\psi} \sigma_{\mu\nu} \psi \right\} \right)$$



- could enforce π form factor = 1 at $Q^2 = 0$
c.f. [Shultz, Dudek, Edwards '15]
- want to use non-perturbative $Z_V \rightarrow$ 'unsmeared' V

The stochastic LapH method

- quark propagator has outer-product form $M^{-1} = X\eta^\dagger$



- use γ_5 -hermiticity to switch source and sink $\rightarrow \bar{\eta}, \bar{X}$
- compute *current sink functions* right after inversions, before smearing and writing to disk

Anisotropic Wilson Fermions

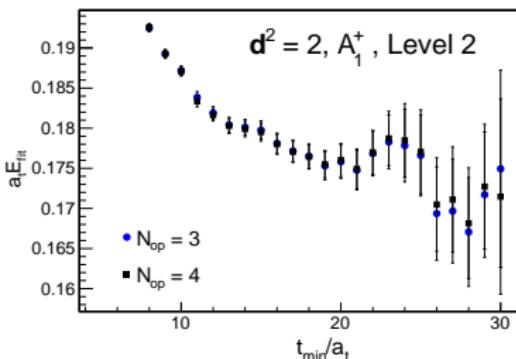
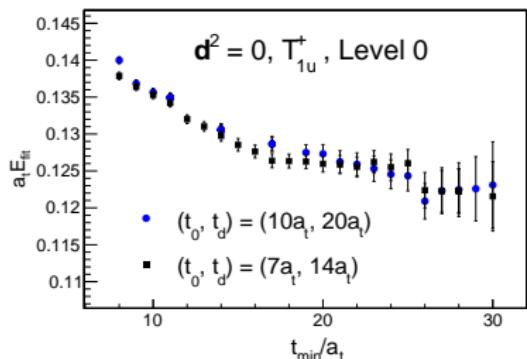
Exploratory study on $\pi - \pi$ scattering (here $I = 1$ - ρ -channel):

- $N_f = 2 + 1$ anisotropic Wilson clover

[HadSpec Collaboration '09]

- $a_s/a_t \approx 3.44$
→ large volume, but good temporal resolution
- $32^3 \times 256, m_\pi \approx 240 \text{ MeV}, a_s \approx 0.12 \text{ fm}, L \approx 4 \text{ fm}$
- $m_\pi T \approx 10$
→ safe from thermal effects

Anisotropic Wilson Fermions

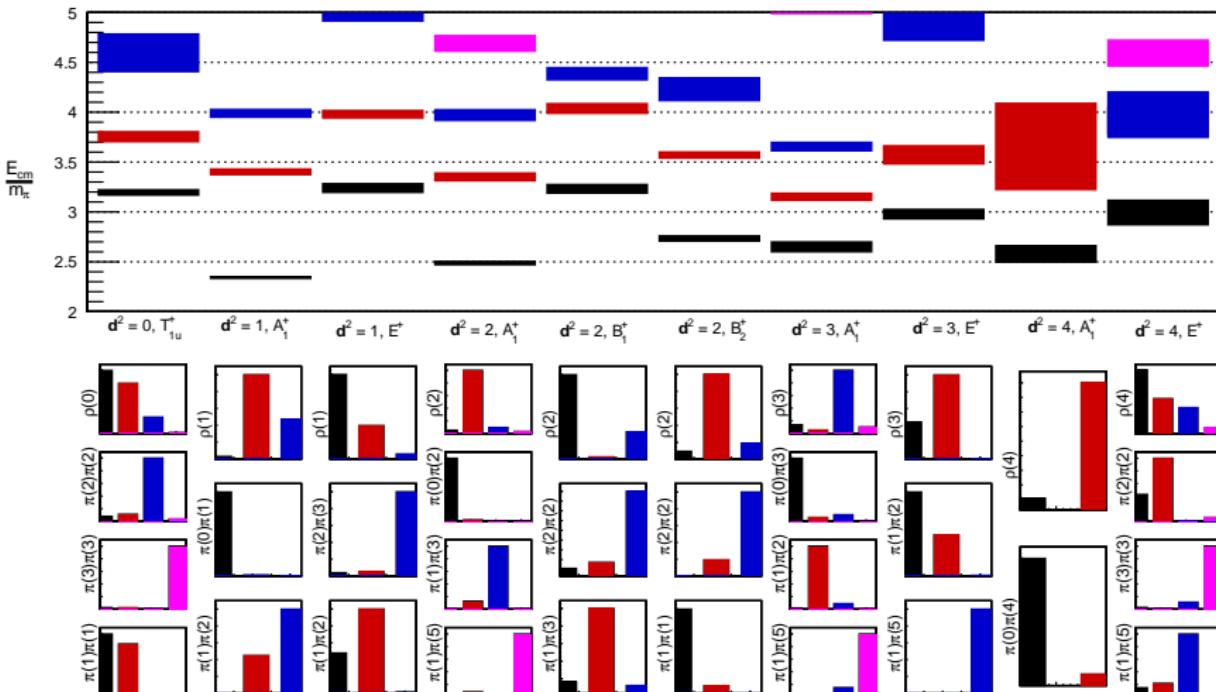


- GEVP on the mean at fixed (t_0, t_d) to form

$$\hat{C}_{mn}(t) = (\nu_n, C(t)\nu_m)$$

- Fit diagonal elements to single exponential
- Monitor consistency across GEVP parameters and fit models

Anisotropic Wilson Fermions

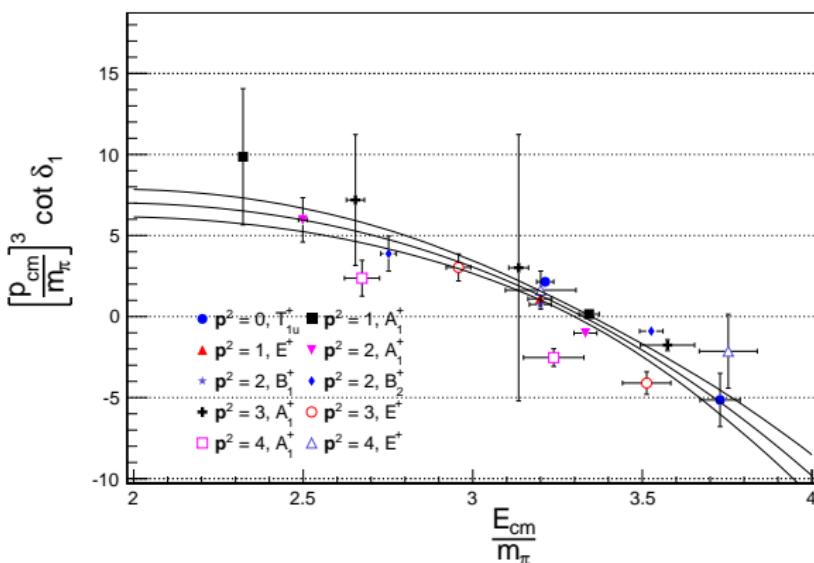


Lüscher quantization condition in moving frames

$$\mathbf{P} = \frac{2\pi}{L}\mathbf{d}, \quad \mathbf{p} = \frac{2\pi}{L}\mathbf{q}, \quad \gamma = \frac{E}{\sqrt{s}}, \quad w_{lm} = \frac{8Z_{lm}(\mathbf{d}, \gamma, \mathbf{q}^2)}{\gamma\pi^{-3/2}L^3q^{l-2}}$$

\mathbf{d}	Λ	$p^3 \cot \delta_1$	#operators
(0,0,0)	T_{1u}^+	w_{00}	4
(0,0,n)	A_1^+	$w_{00} + \frac{2}{\sqrt{5}}w_{20}$	3 / 2
	E^+	$w_{00} - \frac{1}{\sqrt{5}}w_{20}$	3 / 4
(0,1,1)	A_1^+	$w_{00} + \frac{1}{2\sqrt{5}}w_{20} + \sqrt{\frac{6}{5}}iw_{21} - \sqrt{\frac{3}{10}}w_{22}$	4
	B_1^+	$w_{00} - \frac{1}{\sqrt{5}}w_{20} + \sqrt{\frac{6}{5}}w_{22}$	3
	B_2^+	$w_{00} + \frac{1}{2\sqrt{5}}w_{20} - \sqrt{\frac{6}{5}}iw_{21} - \sqrt{\frac{3}{10}}w_{22}$	3
(1,1,1)	A_1^+	$w_{00} - 2\sqrt{\frac{6}{5}}iw_{22}$	4
	E^+	$w_{00} + \sqrt{\frac{6}{5}}iw_{22}$	3

Anisotropic Wilson Fermions



$$p^3 \cot \delta_1 = (m_r^2 - s) \frac{6\pi}{g_{\rho\pi\pi}^2} \sqrt{s} \quad \text{Breit-Wigner fit}$$

$$g_{\rho\pi\pi} = 6.16(36), \quad \frac{m_r}{m_\pi} = 3.324(24), \quad \frac{\chi^2}{d.o.f.} = 1.43$$

Anisotropic Wilson Fermions

Recent results from the JLab group on the same ensemble:

[Wilson et al '15]

$$g_{\rho\pi\pi}^{\text{JLab}} = 5.688(75)$$

$$g_{\rho\pi\pi} = 6.16(36)$$

- exact distillation requires 170 times as many inversions
- discrepancy in $g_{\rho\pi\pi}$ illustrates need for careful checks of systematic effects in these calculations
- how to approach the chiral limit?
 - direct calculations - $4m_\pi < m_\rho$ at m_π^{phys}
 - EFT approach: Unitarized ChPT [Bolton, Briceño, Wilson '15]

CLS effort with open boundary conditions

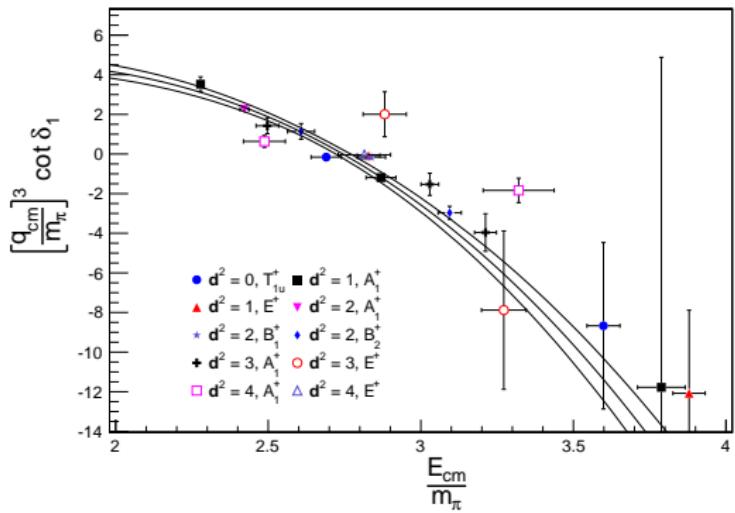
- we have initiated a spectroscopy project using the recent $N_f = 2 + 1$ ensembles generated through the CLS effort

[Bruno et al '14]

- Lattice setup (N200)

- $L^3 \times T = 48^3 \times 128$
- $\mathcal{O}(a)$ -improved Wilson fermions, Lüscher-Weisz gauge action, open temporal BC
- $m_\pi \approx 280$ MeV, $m_K \approx 460$ MeV, $a \approx 0.064$ fm
- $m_\pi L \approx 4.4$, $2m_K/m_\pi \approx 3.3$

CLS effort with open boundary conditions



$$p^3 \cot \delta_1 = (m_r^2 - s) \frac{6\pi}{g_{\rho\pi\pi}^2} \sqrt{s} \quad \text{Breit-Wigner fit}$$

$$g_{\rho\pi\pi} = 5.68(24), \quad \frac{m_r}{m_\pi} = 2.745(24), \quad \frac{\chi^2}{d.o.f.} = 1.2$$

PRELIMINARY

CLS effort with open boundary conditions

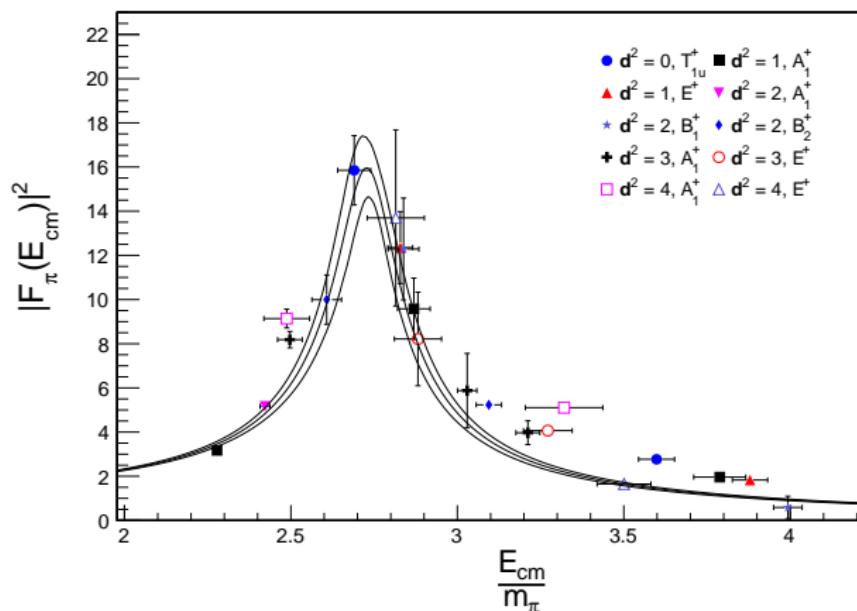
Timelike pion form factor

$$|F_\pi(s)|^2 = \frac{3\pi s}{2L^3 p^5} g(\gamma) \left(q\phi'(q) + p \frac{\partial \delta_1(p)}{\partial p} \right) \left| \langle 0 | V^{(\mathbf{d}, \Lambda)} | \mathbf{d}, \Lambda, \mathbf{n} \rangle \right|^2$$

- extract energy levels for given momentum \mathbf{d} and irrep Λ ✓
- use all levels across all irreps to map out the phase shift $\delta_1(p)$ and parametrize it ✓
- compute $\phi'(q)$ for each energy level numerically ✓
- extract the finite volume current matrix element

[Bulava, BH et al '15]

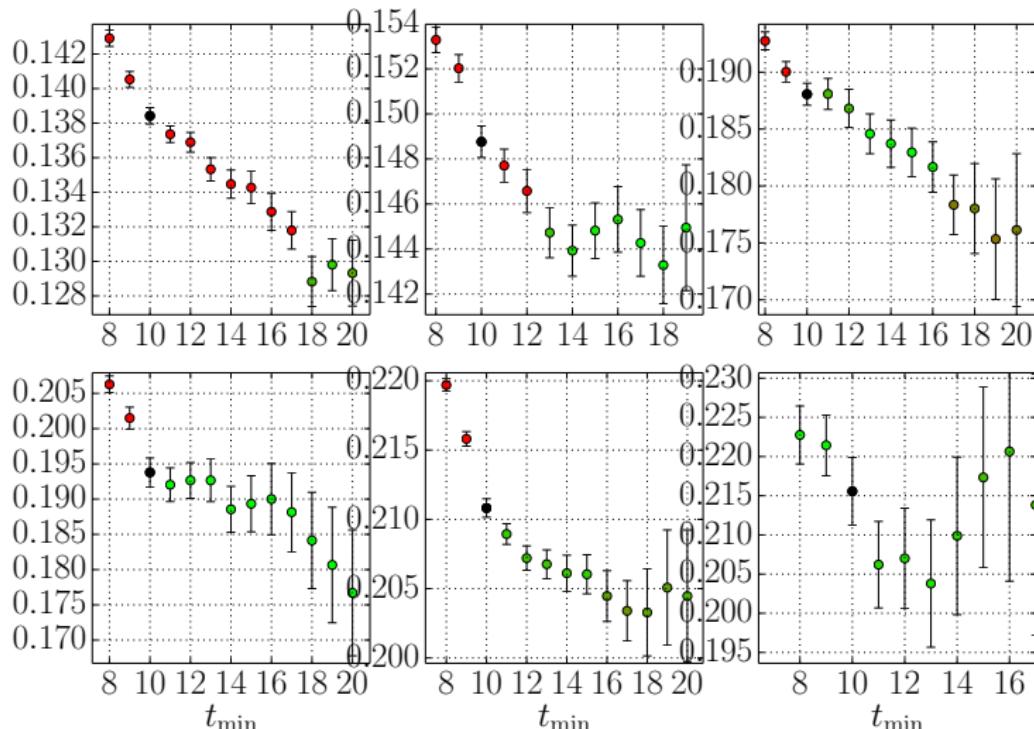
CLS effort with open boundary conditions



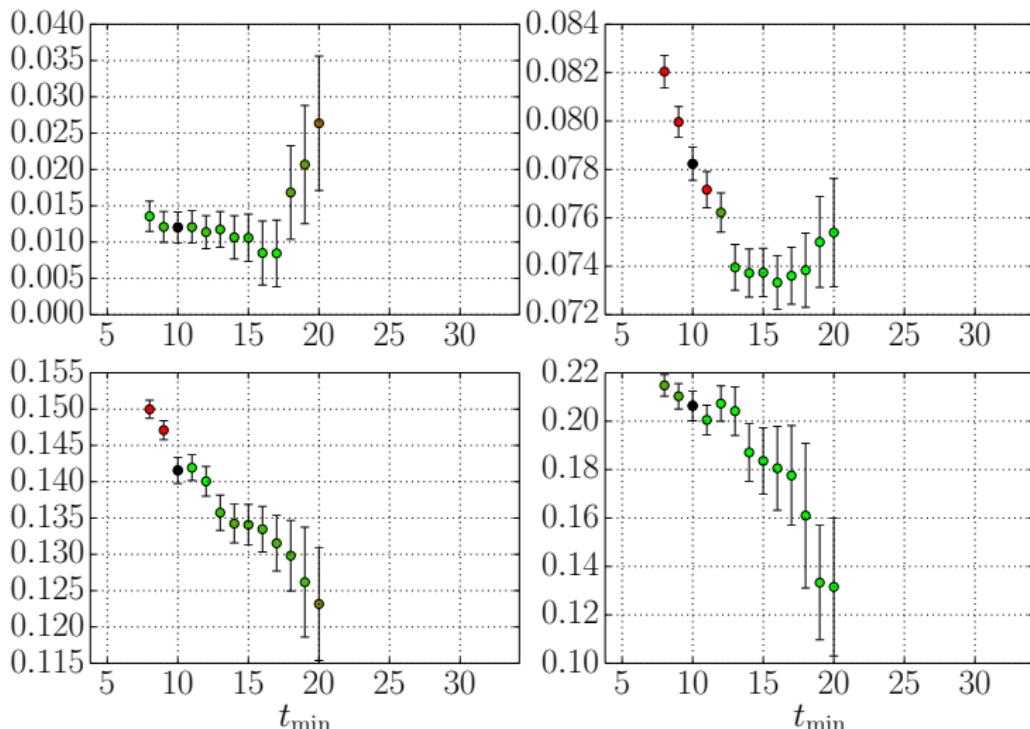
PRELIMINARY

- curve is the Gounaris-Sakurai parametrization of $|F_\pi(E_{cm})|^2$
- no fit - prediction using the values of m_r and $g_{\rho\pi\pi}$ from the phase shift analysis

- advances in spectroscopy methods
- Lüscher-type methods can be put to practical use
- but: keep systematics in mind
 - analysis techniques
 - cutoff effects
 - exponential finite volume effects
 - chiral limit
- interplay between theory and practitioners
- exciting prospects
 - three-particle states, four-particle states
 - baryon resonances, scalar resonances
 - ...



Iisoscalar pion-pion and kaon-kaon scattering, $\mathbf{d} = [0, 1, 1]$



Iisoscalar pion-pion and kaon-kaon scattering, $\mathbf{d} = [0, 0, 0]$

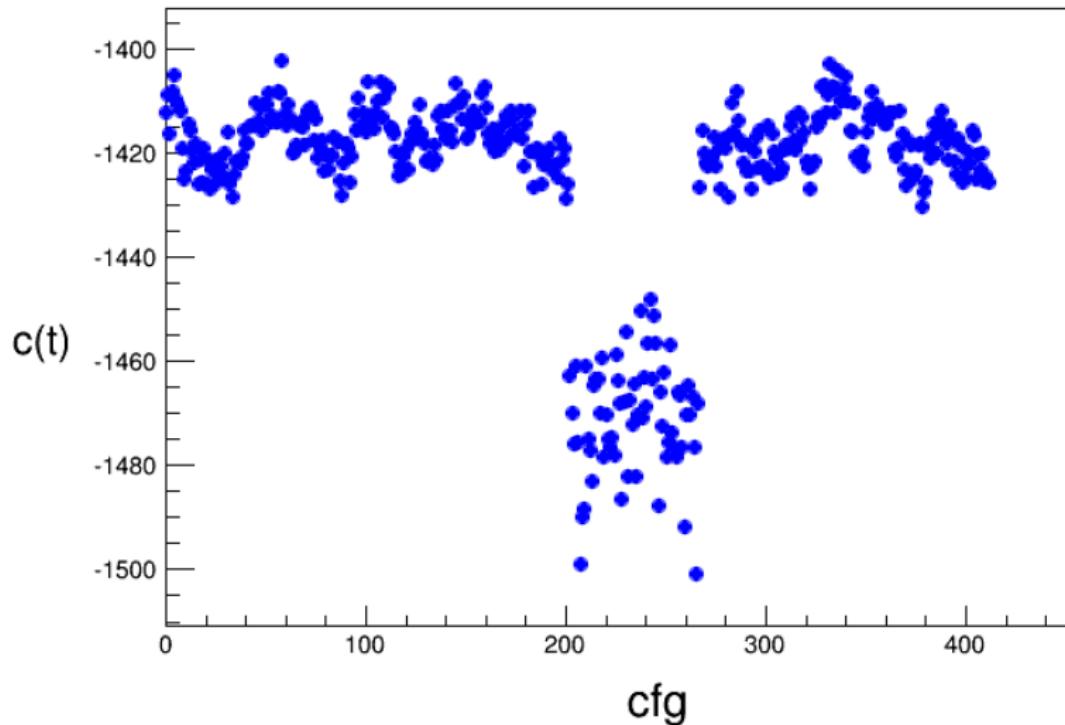


Figure: History of vacuum expectation value of SS η [0,0,0] A_{1g}^+

Temporal boundary effects

- boundary effects expected to decay as $e^{-2m_\pi t}$ near the chiral limit [Bruno et al. 2015]
- we do see large boundary effects in the spectrum of the lattice Laplacian

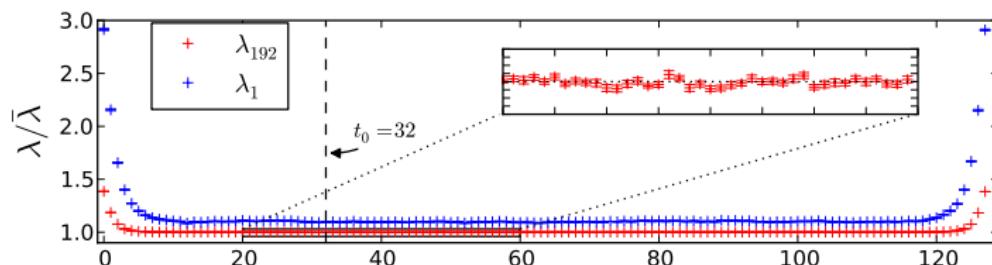


Figure: Smallest and largest retained EV of the lattice Laplacian normalized by their plateau average ($N_{\text{cfg}} = 26$). Lowest EV offset for legibility.

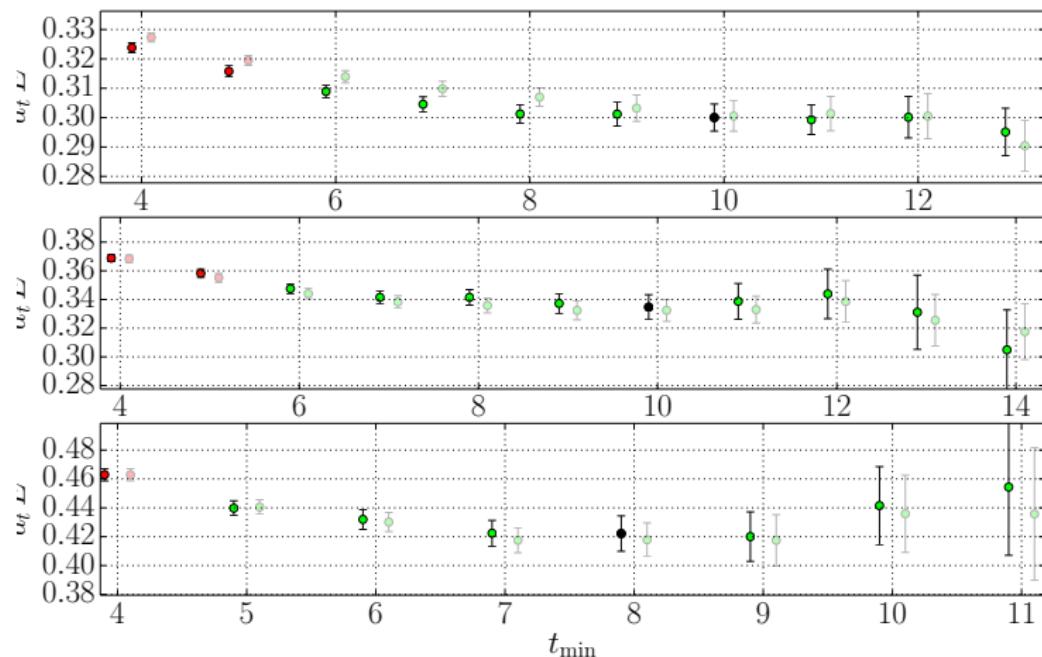


Figure: Correlated single-exponential fits to the rotated correlators in $[0,1,1] A_1^+$.

- evaluate correlation functions

$$D_i(t) = \langle V^{(\mathbf{d},\Lambda)}(t_0 + t) \bar{O}_i^{(\mathbf{d},\Lambda)}(t_0) \rangle$$

- $V^{(\mathbf{d},\Lambda)}$ are linear combinations of

$$(V_R)_\mu^a = Z_V(1 + b_V a m_q) \left\{ V_\mu^a + a c_V \tilde{\partial}_\nu T_{\mu\nu}^a \right\}$$

that transform irreducibly under the lattice symmetries

- nonperturbative Z_V [Dalla Brida '15]
one-loop b_V, c_V [Aoki, Frezzotti, Weisz '99]
- GEVP eigenvectors from “ordinary” correlation matrix gives *optimized* current correlation functions

$$\hat{D}_i(t) = (D(t), v_i) \stackrel{t \rightarrow \infty}{=} \langle 0 | V^{(\mathbf{d},\Lambda)} | \mathbf{d} \wedge i \rangle \langle \mathbf{d} \wedge i | \bar{O}_i^{(\mathbf{d},\Lambda)} | 0 \rangle \times e^{-E_i^{(\mathbf{d},\Lambda)} t}$$

$$\hat{D}_i(t) = \langle 0 | V^{(\mathbf{d}, \Lambda)} | \mathbf{d} \wedge i \rangle \langle \mathbf{d} \wedge i | \bar{O}_i^{(\mathbf{d}, \Lambda)} | 0 \rangle \times e^{-E_i^{(\mathbf{d}, \Lambda)} t}$$

- the three ratios all tend to the desired matrix element

$$R_1^{(i)}(t) = \frac{\hat{D}_i(t)}{\hat{C}_{ii}^{\frac{1}{2}}(t) e^{-\frac{1}{2} E_i t}},$$

$$R_2^{(i)}(t) = \frac{\hat{D}_i(t) \langle \mathbf{d} \wedge i | \bar{O}_i^{(\mathbf{d}, \Lambda)} | 0 \rangle}{\hat{C}_{ii}(t)},$$

$$R_3^{(i)}(t) = \frac{\hat{D}_i(t)}{\langle \mathbf{d} \wedge i | \bar{O}_i^{(\mathbf{d}, \Lambda)} | 0 \rangle e^{-E_i t}},$$