Excited states and scattering phase shifts from lattice QCD

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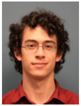
Overview

- goals:
  - comprehensive survey of QCD stationary states in finite volume
  - hadron scattering phase shifts, decay widths, matrix elements
  - focus: large 32^3 anisotropic lattices, $m_\pi \sim 240$ MeV

- extracting excited-state energies
- single-hadron and multi-hadron operators
- the stochastic LapH method
- level identification issues
- results for $I = 1,\ S = 0,\ T_{1u}^+$ channel
  - 100×100 correlator matrix, all needed 2-hadron operators
- other channels
- $I = 1$ P-wave $\pi\pi$ scattering phase shifts and width of ρ
- future work

Dramatis Personae

- current grad students:



Jake Fallica
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Andrew Hanlon
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former CMU postdocs:

Justin Foley
Software,
NVIDIA

Jimmy Juge
Faculty,
Stockton, CA

- past CMU grad students:

Brendan Fahy
2014
Postdoc KEK
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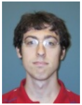
2013
Silicon Valley



David Lenkner
2013
Data Science
Auto., PGH

Ricky Wong
2011
Postdoc
Germany

John Bulava
2009
Faculty,
Dublin

Adam Lichtl
2006
SpaceX, LA

- thanks to NSF Teragrid/XSEDE:
  - Athena+Kraken at NICS
  - Ranger+Stampede at TACC

Temporal correlations from path integrals

- stationary-state energies from $N \times N$ Hermitian correlation matrix

$$C_{ij}(t) = \langle 0 | \, O_i(t+t_0) \, \overline{O}_j(t_0) \, | 0 \rangle$$

- judiciously designed operators $\overline{O}_j$ create states of interest

$$O_j(t) = O_j[\overline{\psi}(t), \psi(t), U(t)]$$

- correlators from path integrals over quark $\psi, \overline{\psi}$ and gluon U fields

$$C_{ij}(t) = \frac{\int \mathcal{D}(\overline{\psi}, \psi, U) \;\; O_i(t+t_0) \, \overline{O}_j(t_0) \;\; \exp\left(-S[\overline{\psi}, \psi, U]\right)}{\int \mathcal{D}(\overline{\psi}, \psi, U) \; \exp\left(-S[\overline{\psi}, \psi, U]\right)}$$

- involves the action

$$S[\overline{\psi}, \psi, U] = \overline{\psi} \; K[U] \; \psi + S_G[U]$$

- $K[U]$ is fermion Dirac matrix
- $S_G[U]$ is gluon action

Integrating the quark fields

- integrals over Grassmann-valued quark fields done exactly
- meson-to-meson example:

$$\begin{aligned}&\int \mathcal{D}(\overline{\psi},\psi)\ \psi_a\psi_b\ \overline{\psi}_c\overline{\psi}_d\ \exp\left(-\overline{\psi}K\psi\right)\\ =\ &\left(K^{-1}_{ad}K^{-1}_{bc}-K^{-1}_{ac}K^{-1}_{bd}\right)\det K.\end{aligned}$$

- baryon-to-baryon example:

$$\begin{aligned}&\int \mathcal{D}(\overline{\psi},\psi)\ \psi_{a_1}\psi_{a_2}\psi_{a_3}\ \overline{\psi}_{b_1}\overline{\psi}_{b_2}\overline{\psi}_{b_3}\ \exp\left(-\overline{\psi}K\psi\right)\\ =\ &\Big(-K^{-1}_{a_1b_1}K^{-1}_{a_2b_2}K^{-1}_{a_3b_3}+K^{-1}_{a_1b_1}K^{-1}_{a_2b_3}K^{-1}_{a_3b_2}+K^{-1}_{a_1b_2}K^{-1}_{a_2b_1}K^{-1}_{a_3b_3}\\ -\ &K^{-1}_{a_1b_2}K^{-1}_{a_2b_3}K^{-1}_{a_3b_1}-K^{-1}_{a_1b_3}K^{-1}_{a_2b_1}K^{-1}_{a_3b_2}+K^{-1}_{a_1b_3}K^{-1}_{a_2b_2}K^{-1}_{a_3b_1}\Big)\ \det K\end{aligned}$$

Monte Carlo integration

- correlators have form

$$C_{ij}(t) = \frac{\int \mathcal{D}U\ \det K[U]\ K^{-1}[U] \cdots K^{-1}[U]\ \ \exp\left(-S_G[U]\right)}{\int \mathcal{D}U\ \det K[U]\ \exp\left(-S_G[U]\right)}$$

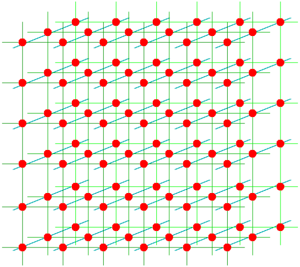
- resort to Monte Carlo method to integrate over gluon fields
- use Markov chain to generate sequence of gauge-field configurations

$$U_1, U_2, \ldots, U_N$$

- most computationally demanding parts:
  - including $\det K$ in updating
  - evaluating K^{-1} in numerator

Lattice QCD

- Monte Carlo method using computers requires hypercubic space-time lattice
- quarks reside on sites, gluons reside on links between sites
- for gluons, 8 dimensional integral on each link
- path integral dimension $32N_xN_yN_zN_t$
  - 268 million for $32^3\times 256$ lattice
- Metropolis method with global updating proposal
  - RHMC: solve Hamilton equations with Gaussian momenta
  - $\det K$ estimates with integral over pseudo-fermion fields
- systematic errors
  - discretization
  - finite volume



Excited states from correlation matrices

- in finite volume, energies are discrete (neglect wrap-around)

$$C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*}\ e^{-E_n t}, \qquad Z_j^{(n)} = \langle 0|\ O_j\ |n\rangle$$

- not practical to do fits using above form
- define new correlation matrix $\widetilde{C}(t)$ using a single rotation

$$\widetilde{C}(t) = U^\dagger\ C(\tau_0)^{-1/2}\ C(t)\ C(\tau_0)^{-1/2}\ U$$

- columns of U are eigenvectors of $C(\tau_0)^{-1/2}\, C(\tau_D)\, C(\tau_0)^{-1/2}$
- choose τ_0 and τ_D large enough so $\widetilde{C}(t)$ diagonal for $t > \tau_D$
- effective energies

$$\widetilde{m}_\alpha^{\rm eff}(t) = \frac{1}{\Delta t} \ln\left(\frac{\widetilde{C}_{\alpha\alpha}(t)}{\widetilde{C}_{\alpha\alpha}(t+\Delta t)}\right)$$

  tend to N lowest-lying stationary state energies in a channel
- 2-exponential fits to $\widetilde{C}_{\alpha\alpha}(t)$ yield energies E_α and overlaps $Z_j^{(n)}$

Building blocks for single-hadron operators

- building blocks: covariantly-displaced LapH-smeared quark fields
- stout links $\widetilde{U}_j(x)$
- Laplacian-Heaviside (LapH) smeared quark fields

$$\widetilde{\psi}_{a\alpha}(x) = \mathcal{S}_{ab}(x,y)\, \psi_{b\alpha}(y), \qquad \mathcal{S} = \Theta\left(\sigma_s^2 + \widetilde{\Delta}\right)$$

- 3d gauge-covariant Laplacian $\widetilde{\Delta}$ in terms of $\widetilde{U}$
- displaced quark fields:

$$q^A_{a\alpha j} = D^{(j)}\widetilde{\psi}^{(A)}_{a\alpha}, \qquad \overline{q}^A_{a\alpha j} = \widetilde{\overline{\psi}}^{(A)}_{a\alpha}\gamma_4\, D^{(j)\dagger}$$

- displacement $D^{(j)}$ is product of smeared links:

$$D^{(j)}(x,x') = \widetilde{U}_{j_1}(x)\, \widetilde{U}_{j_2}(x+d_2)\, \widetilde{U}_{j_3}(x+d_3) \ldots \widetilde{U}_{j_p}(x+d_p)\delta_{x',\, x+d_{p+1}}$$

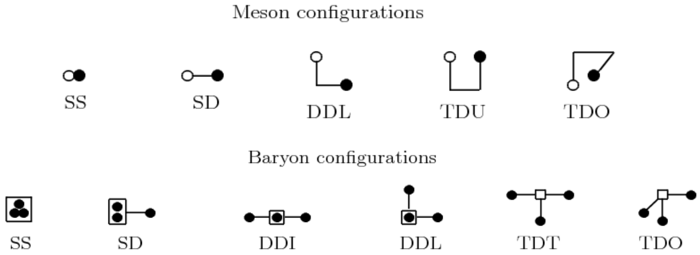
- to good approximation, LapH smearing operator is

$$\mathcal{S} = V_s V_s^\dagger$$

  - columns of matrix V_s are eigenvectors of $\widetilde{\Delta}$

Extended operators for single hadrons

- quark displacements build up orbital, radial structure



$$\overline{\Phi}^{AB}_{\alpha\beta}(\boldsymbol{p},t) \;=\; \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot(\mathbf{x}+\frac{1}{2}(\boldsymbol{d}_\alpha+\boldsymbol{d}_\beta))}\delta_{ab}\;\overline{q}^{B}_{b\beta}(\boldsymbol{x},t)\;q^{A}_{a\alpha}(\boldsymbol{x},t)$$

$$\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(\boldsymbol{p},t) \;=\; \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot\mathbf{x}}\varepsilon_{abc}\;\overline{q}^{C}_{c\gamma}(\boldsymbol{x},t)\;\overline{q}^{B}_{b\beta}(\boldsymbol{x},t)\;\overline{q}^{A}_{a\alpha}(\boldsymbol{x},t)$$

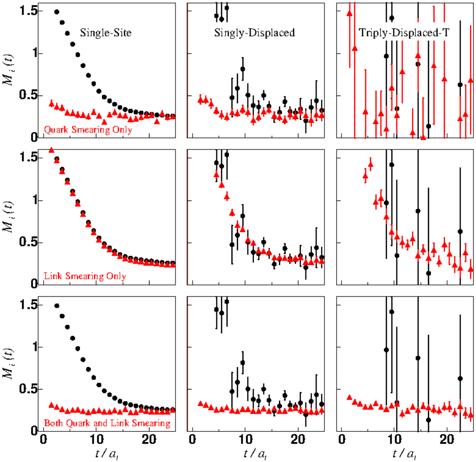
- group-theory projections onto irreps of lattice symmetry group

$$\overline{M}_l(t) = c^{(l)*}_{\alpha\beta}\;\overline{\Phi}^{AB}_{\alpha\beta}(t) \qquad\qquad \overline{B}_l(t) = c^{(l)*}_{\alpha\beta\gamma}\;\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(t)$$

- definite momentum $\boldsymbol{p}$, irreps of little group of $\boldsymbol{p}$

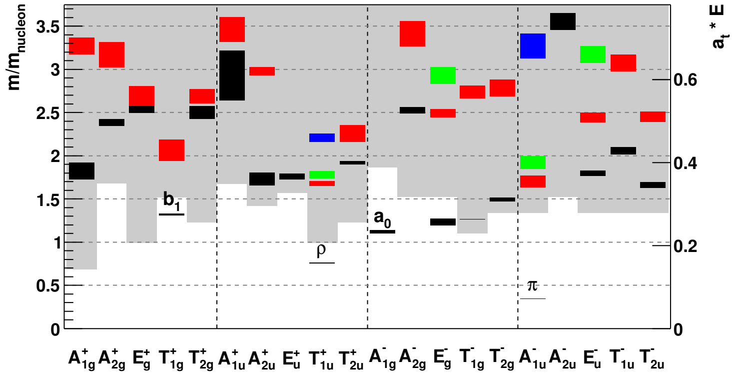
Importance of smeared fields

- effective masses of 3 selected nucleon operators shown
- noise reduction of displaced-operators from link smearing $n_\rho \rho = 2.5, n_\rho = 16$
- quark-field smearing $\sigma_s = 4.0, n_\sigma = 32$ reduces excited-state contamination



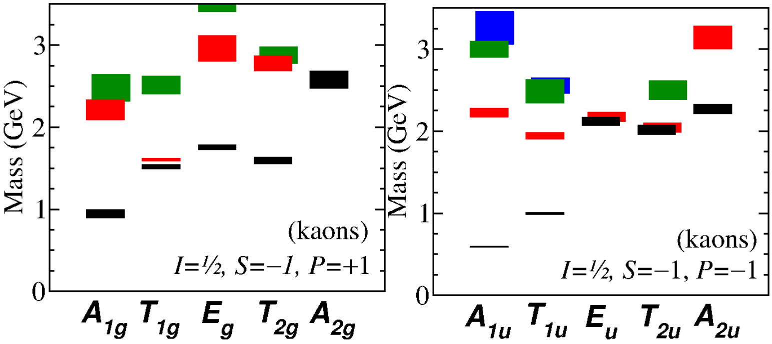
Early results on small 16^3 and 24^3 lattices

- Bob Sugar in 2005: “You’ll never see more than 2 levels”
- $I = 1,\ S = 0$ energies on 24^3 lattice, $m_\pi \sim 390$ MeV in 2010
- use of single-meson operators only
- shaded region shows where two-meson energies expected



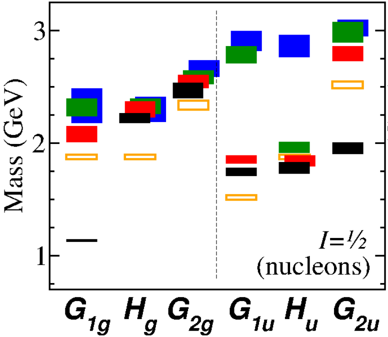
Early results on small lattices

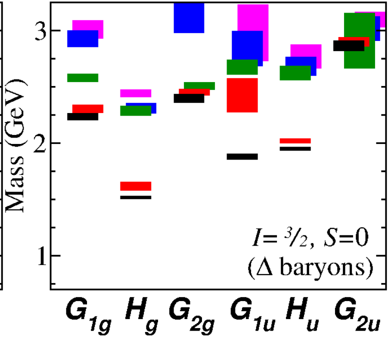
- kaons on 16^3 lattice, $m_\pi \sim 390$ MeV in 2008
- use of single-meson operators only



Early results on small lattices

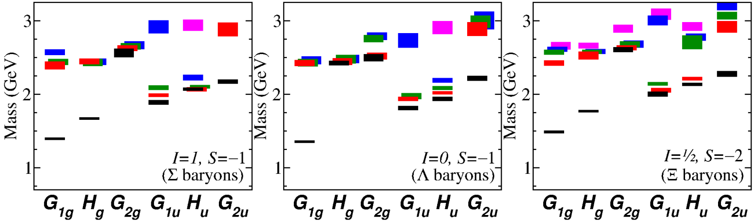
- $N, \ \Delta$ baryons on 16^3 lattice, $m_\pi \sim 390$ MeV in 2008
- use of single-baryon operators only





Early results on small lattices

- $\Sigma,\ \Lambda,\ \Xi$ baryons on 16^3 lattice, $m_\pi \sim 390$ MeV in 2008
- use of single-baryon operators only



Two-hadron operators

- our approach: superposition of products of single-hadron operators of definite momenta

$$c^{I_{3a} I_{3b}}_{\boldsymbol{p}_a \lambda_a;\ \boldsymbol{p}_b \lambda_b}\ B^{I_a I_{3a} S_a}_{\boldsymbol{p}_a \Lambda_a \lambda_a i_a}\ B^{I_b I_{3b} S_b}_{\boldsymbol{p}_b \Lambda_b \lambda_b i_b}$$

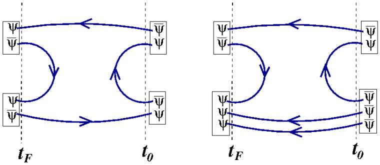
- fixed total momentum $\boldsymbol{p} = \boldsymbol{p}_a + \boldsymbol{p}_b$, fixed $\Lambda_a, i_a, \Lambda_b, i_b$
- group-theory projections onto little group of $\boldsymbol{p}$ and isospin irreps
- restrict attention to certain classes of momentum directions
  - on axis $\pm\widehat{\boldsymbol{x}},\ \pm\widehat{\boldsymbol{y}},\ \pm\widehat{\boldsymbol{z}}$
  - planar diagonal $\pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{y}},\ \pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{z}},\ \pm\widehat{\boldsymbol{y}} \pm \widehat{\boldsymbol{z}}$
  - cubic diagonal $\pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{y}} \pm \widehat{\boldsymbol{z}}$
- crucial to know and fix all phases of single-hadron operators for all momenta
  - each class, choose reference direction $\boldsymbol{p}_{\rm ref}$
  - each $\boldsymbol{p}$, select one reference rotation $R^{\boldsymbol{p}}_{\rm ref}$ that transforms $\boldsymbol{p}_{\rm ref}$ into $\boldsymbol{p}$
- efficient creating large numbers of two-hadron operators
- generalizes to three, four, ... hadron operators

Quark propagation

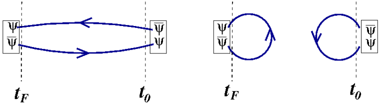
- quark propagator is inverse K^{-1} of Dirac matrix
  - rows/columns involve lattice site, spin, color
  - very large $N_{\rm tot} \times N_{\rm tot}$ matrix for each flavor
$$N_{\rm tot} = N_{\rm site} N_{\rm spin} N_{\rm color}$$
  - for $32^3 \times 256$ lattice, $N_{\rm tot} \sim 101$ million
- not feasible to compute (or store) all elements of K^{-1}
- solve linear systems $Kx = y$ for source vectors y
- translation invariance can drastically reduce number of source vectors y needed
- multi-hadron operators and isoscalar mesons require large number of source vectors y

Quark line diagrams

- temporal correlations involving our two-hadron operators need
  - slice-to-slice quark lines (from all spatial sites on a time slice to all spatial sites on another time slice)
  - sink-to-sink quark lines



- isoscalar mesons also require sink-to-sink quark lines



- solution: the stochastic LapH method!

Stochastic estimation of quark propagators

- do not need exact inverse of Dirac matrix $K[U]$
- use noise vectors η satisfying $E(\eta_i) = 0$ and $E(\eta_i \eta_j^*) = \delta_{ij}$
- Z_4 noise is used $\{1, i, -1, -i\}$
- solve $K[U]X^{(r)} = \eta^{(r)}$ for each of N_R noise vectors $\eta^{(r)}$, then obtain a Monte Carlo estimate of all elements of K^{-1}

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_i^{(r)} \eta_j^{(r)*}$$

- variance reduction using noise dilution
- dilution introduces projectors

$$P^{(a)} P^{(b)} = \delta^{ab} P^{(a)}, \qquad \sum_a P^{(a)} = 1, \qquad P^{(a)\dagger} = P^{(a)}$$

- define

$$\eta^{[a]} = P^{(a)} \eta, \qquad X^{[a]} = K^{-1} \eta^{[a]}$$

to obtain Monte Carlo estimate with drastically reduced variance

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a X_i^{(r)[a]} \eta_j^{(r)[a]*}$$

Stochastic LapH method

- introduce Z_N noise in the LapH subspace

$$\rho_{\alpha k}(t), \qquad t = \text{time},\ \alpha = \text{spin},\ k = \text{eigenvector number}$$

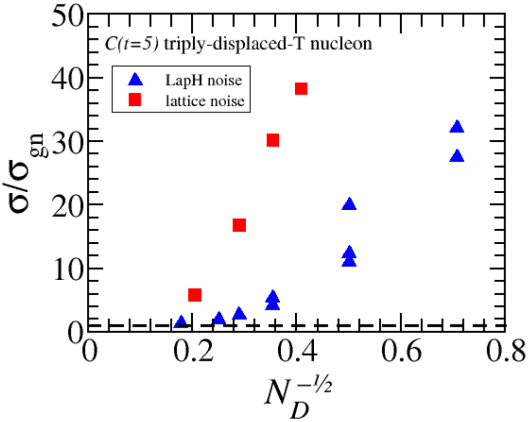
- four dilution schemes:

$$
\begin{array}{lll}
P^{(a)}_{ij} = \delta_{ij} & a = 0 & \text{(none)} \\
P^{(a)}_{ij} = \delta_{ij}\delta_{ai} & a = 0,1,\ldots,N-1 & \text{(full)} \\
P^{(a)}_{ij} = \delta_{ij}\delta_{a,Ki/N} & a = 0,1,\ldots,K-1 & \text{(interlace-}K\text{)} \\
P^{(a)}_{ij} = \delta_{ij}\delta_{a,i \bmod k} & a = 0,1,\ldots,K-1 & \text{(block-}K\text{)}
\end{array}
$$

- apply dilutions to
  - time indices (full for fixed src, interlace-16 for relative src)
  - spin indices (full)
  - LapH eigenvector indices (interlace-8 mesons, interlace-4 baryons)

The effectiveness of stochastic LapH

- comparing use of lattice noise vs noise in LapH subspace
- N_D is number of solutions to $Kx = y$



Quark line estimates in stochastic LapH

- each of our quark lines is the product of matrices

$$\mathcal{Q} = D^{(j)}\mathcal{S}K^{-1}\gamma_4\mathcal{S}D^{(k)\dagger}$$

- displaced-smeared-diluted quark source and quark sink vectors:

$$\begin{aligned}\varrho^{[b]}(\rho) &= D^{(j)}V_sP^{(b)}\rho\\ \varphi^{[b]}(\rho) &= D^{(j)}\mathcal{S}K^{-1}\gamma_4\, V_sP^{(b)}\rho\end{aligned}$$

- estimate in stochastic LapH by (A, B flavor, u, v compound: space, time, color, spin, displacement type)

$$\mathcal{Q}_{uv}^{(AB)} \approx \frac{1}{N_R}\delta_{AB}\sum_{r=1}^{N_R}\sum_b \varphi_u^{[b]}(\rho^r)\ \varrho_v^{[b]}(\rho^r)^*$$

- occasionally use γ_5-Hermiticity to switch source and sink

$$\mathcal{Q}_{uv}^{(AB)} \approx \frac{1}{N_R}\delta_{AB}\sum_{r=1}^{N_R}\sum_b \overline{\varrho}_u^{[b]}(\rho^r)\ \overline{\varphi}_v^{[b]}(\rho^r)^*$$

defining $\overline{\varrho}(\rho) = -\gamma_5\gamma_4\varrho(\rho)$ and $\overline{\varphi}(\rho) = \gamma_5\gamma_4\varphi(\rho)$

Source-sink factorization in stochastic LapH

- baryon correlator has form

$$C_{l\bar{l}} = c^{(l)}_{ijk}\, c^{(\bar{l})*}_{\bar{i}\bar{j}\bar{k}}\, \mathcal{Q}^{A}_{i\bar{i}}\, \mathcal{Q}^{B}_{j\bar{j}}\, \mathcal{Q}^{C}_{k\bar{k}}$$

- stochastic estimate with dilution

$$\begin{aligned} C_{l\bar{l}} \quad &\approx \quad \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} c^{(l)}_{ijk}\, c^{(\bar{l})*}_{\bar{i}\bar{j}\bar{k}} \left(\varphi^{(Ar)[d_A]}_{i}\, \varrho^{(Ar)[d_A]*}_{\bar{i}} \right) \\ &\times \quad \left(\varphi^{(Br)[d_B]}_{j}\, \varrho^{(Br)[d_B]*}_{\bar{j}} \right) \left(\varphi^{(Cr)[d_C]}_{k}\, \varrho^{(Cr)[d_C]*}_{\bar{k}} \right) \end{aligned}$$

- define baryon source and sink

$$\begin{aligned} \mathcal{B}^{(r)[d_A d_B d_C]}_{l}(\varphi^A, \varphi^B, \varphi^C) \quad &= \quad c^{(l)}_{ijk}\ \varphi^{(Ar)[d_A]}_{i}\, \varphi^{(Br)[d_B]}_{j}\, \varphi^{(Cr)[d_C]}_{k} \\ \mathcal{B}^{(r)[d_A d_B d_C]}_{l}(\varrho^A, \varrho^B, \varrho^C) \quad &= \quad c^{(l)}_{ijk}\ \varrho^{(Ar)[d_A]}_{i}\, \varrho^{(Br)[d_B]}_{j}\, \varrho^{(Cr)[d_C]}_{k} \end{aligned}$$

- correlator is dot product of source vector with sink vector

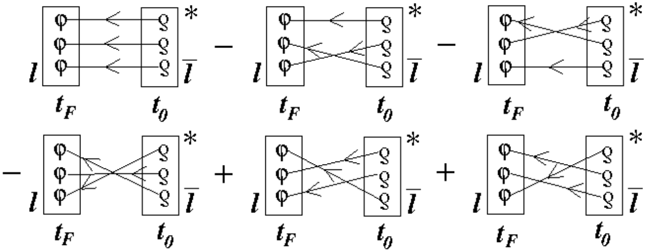
$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} \mathcal{B}^{(r)[d_A d_B d_C]}_{l}(\varphi^A, \varphi^B, \varphi^C)\, \mathcal{B}^{(r)[d_A d_B d_C]}_{\bar{l}}(\varrho^A, \varrho^B, \varrho^C)^*$$

Correlators and quark line diagrams

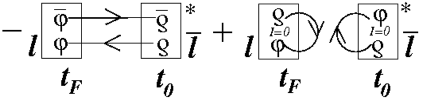
- baryon correlator

$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} \mathcal{B}_l^{(r)[d_A d_B d_C]}(\varphi^A, \varphi^B, \varphi^C)\, \mathcal{B}_{\bar{l}}^{(r)[d_A d_B d_C]}(\varrho^A, \varrho^B, \varrho^C)^*$$

- express diagrammatically

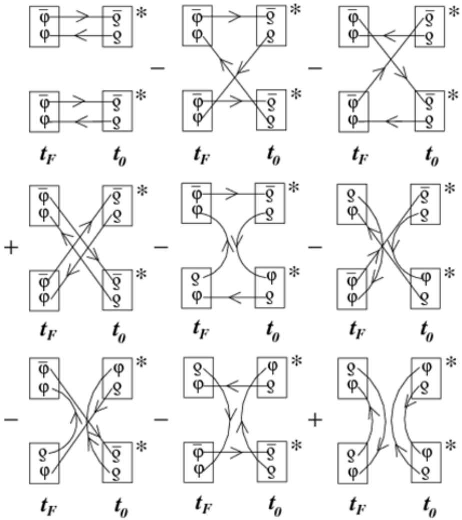


- meson correlator



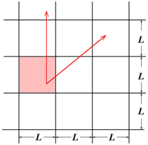
More complicated correlators

- two-meson to two-meson correlators (non isoscalar mesons)



Quantum numbers in toroidal box

- periodic boundary conditions in cubic box
  - not all directions equivalent $\Rightarrow$ using J^{PC} is wrong!!



- label stationary states of QCD in a periodic box using irreps of cubic space group even in continuum limit
  - zero momentum states: little group O_h

$$A_{1a}, A_{2ga}, E_a, T_{1a}, T_{2a}, \quad G_{1a}, G_{2a}, H_a, \qquad a = g, u$$

  - on-axis momenta: little group C_{4v}

$$A_1, A_2, B_1, B_2, E, \quad G_1, G_2$$

  - planar-diagonal momenta: little group C_{2v}

$$A_1, A_2, B_1, B_2, \quad G_1, G_2$$

  - cubic-diagonal momenta: little group C_{3v}

$$A_1, A_2, E, \quad F_1, F_2, G$$

- include G parity in some meson sectors (superscript $+$ or $-$)

Spin content of cubic box irreps

- numbers of occurrences of Λ irreps in J subduced

J	A_1	A_2	E	T_1	T_2
0	1	0	0	0	0
1	0	0	0	1	0
2	0	0	1	0	1
3	0	1	0	1	1
4	1	0	1	1	1
5	0	0	1	2	1
6	1	1	1	1	2
7	0	1	1	2	2

J	G_1	G_2	H	J	G_1	G_2	H
$\frac{1}{2}$	1	0	0	$\frac{9}{2}$	1	0	2
$\frac{3}{2}$	0	0	1	$\frac{11}{2}$	1	1	2
$\frac{5}{2}$	0	1	1	$\frac{13}{2}$	1	2	2
$\frac{7}{2}$	1	1	1	$\frac{15}{2}$	1	1	3

Common hadrons

- irreps of commonly-known hadrons at rest

Hadron	Irrep	Hadron	Irrep	Hadron	Irrep
π	A_{1u}^-	K	A_{1u}	η, η'	A_{1u}^+
ρ	T_{1u}^+	ω, ϕ	T_{1u}^-	K^*	T_{1u}
a_0	A_{1g}^+	f_0	A_{1g}^+	h_1	T_{1g}^-
b_1	T_{1g}^+	K_1	T_{1g}	π_1	T_{1u}^-
N, Σ	G_{1g}	Λ, Ξ	G_{1g}	Δ, Ω	H_g

Ensembles and run parameters

- plan to use three Monte Carlo ensembles
  - $(32^3|240)$: 412 configs $32^3 \times 256$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 4.4$
  - $(24^3|240)$: 584 configs $24^3 \times 128$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 3.3$
  - $(24^3|390)$: 551 configs $24^3 \times 128$, $m_\pi \approx 390$ MeV, $m_\pi L \sim 5.7$
- anisotropic improved gluon action, clover quarks (stout links)
- QCD coupling $\beta = 1.5$ such that $a_s \sim 0.12$ fm, $a_t \sim 0.035$ fm
- strange quark mass $m_s = -0.0743$ nearly physical (using kaon)
- work in $m_u = m_d$ limit so $SU(2)$ isospin exact
- generated using RHMC, configs separated by 20 trajectories

- stout-link smearing in operators $\xi = 0.10$ and $n_\xi = 10$
- LapH smearing cutoff $\sigma_s^2 = 0.33$ such that
  - $N_v = 112$ for 24^3 lattices
  - $N_v = 264$ for 32^3 lattices
- source times:
  - 4 widely-separated t_0 values on 24^3
  - 8 t_0 values used on 32^3 lattice

Use of XSEDE resources

- use of XSEDE resources crucial
- Monte Carlo generation of gauge-field configurations: $\sim$ 200 million core hours
- quark propagators: $\sim$ 100 million core hours
- hadrons + correlators: $\sim$ 40 million core hours
- storage: $\sim$ 300 TB

Kraken at NICS

Stampede at TACC

Status report

- correlator software last_laph completed summer 2013
  - testing of all flavor channels for single and two-mesons completed fall 2013
  - testing of all flavor channels for single baryon and meson-baryons completed summer 2014
- small-a expansions of all operators completed
- first focus on the resonance-rich ρ-channel: $I=1,\ S=0,\ T_{1u}^{+}$
- results from 63×63 matrix of correlators $(32^3|240)$ ensemble
  - 10 single-hadron (quark-antiquark) operators
  - "$\pi\pi$" operators
  - "$\eta\pi$" operators, "$\phi\pi$" operators
  - "$K\overline{K}$" operators
- inclusion of all possible 2-meson operators
- 3-meson operators currently neglected
- still finalizing analysis code sigmond
- next focus: the 20 bosonic channels with $I=1,\ S=0$

Operator accounting

- numbers of operators for $I=1,\ S=0,\ P=(0,0,0)$ on 32^3 lattice

$(32^2\|240)$	A_{1g}^+	A_{1u}^+	A_{2g}^+	A_{2u}^+	E_g^+	E_u^+	T_{1g}^+	T_{1u}^+	T_{2g}^+	T_{2u}^+
SH	9	7	13	13	9	9	14	23	15	16
"$\pi\pi$"	10	17	8	11	8	17	23	30	17	27
"$\eta\pi$"	6	15	10	7	11	18	31	20	21	23
"$\phi\pi$"	6	15	9	7	12	19	37	11	23	23
"$K\overline{K}$"	0	5	3	5	3	6	9	12	5	10
Total	31	59	43	43	43	69	114	96	81	99

$(32^2\|240)$	A_{1g}^-	A_{1u}^-	A_{2g}^-	A_{2u}^-	E_g^-	E_u^-	T_{1g}^-	T_{1u}^-	T_{2g}^-	T_{2u}^-
SH	10	8	11	10	12	9	21	15	19	16
"$\pi\pi$"	3	7	7	3	8	11	22	12	12	15
"$\eta\pi$"	26	15	10	12	24	21	25	33	28	30
"$\phi\pi$"	26	15	10	12	27	22	26	38	30	32
"$K\overline{K}$"	11	3	4	2	11	5	12	5	12	6
Total	76	48	42	39	82	68	106	103	101	99

Operator accounting

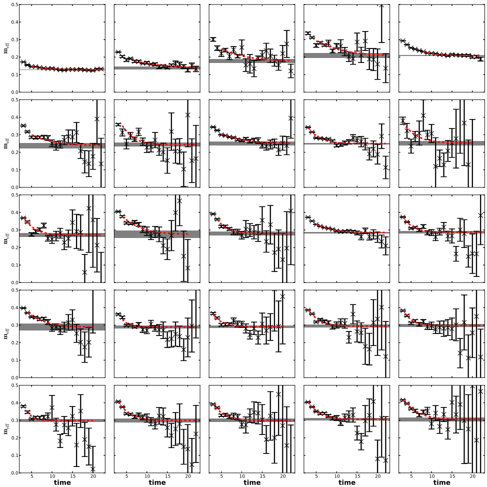
- numbers of operators for $I = 1,\ S = 0,\ P = (0,0,0)$ on 24^3 lattice

$(24^2\|390)$	A^+_{1g}	A^+_{1u}	A^+_{2g}	A^+_{2u}	E^+_g	E^+_u	T^+_{1g}	T^+_{1u}	T^+_{2g}	T^+_{2u}
SH	9	7	13	13	9	9	14	23	15	16
"$\pi\pi$"	6	12	2	6	8	9	15	17	10	12
"$\eta\pi$"	2	10	8	4	8	11	21	14	14	13
"$\phi\pi$"	2	10	8	4	8	11	23	3	14	13
"$K\overline{K}$"	0	4	1	4	1	4	8	10	4	6
Total	19	43	32	31	34	44	81	67	57	60

$(24^2\|390)$	A^-_{1g}	A^-_{1u}	A^-_{2g}	A^-_{2u}	E^-_g	E^-_u	T^-_{1g}	T^-_{1u}	T^-_{2g}	T^-_{2u}
SH	10	8	11	10	12	9	20	15	19	16
"$\pi\pi$"	1	5	6	2	3	7	18	8	10	9
"$\eta\pi$"	19	9	4	6	13	12	11	18	15	14
"$\phi\pi$"	18	9	4	6	14	12	11	19	15	15
"$K\overline{K}$"	7	2	2	2	6	4	9	4	8	4
Total	55	33	27	26	48	44	69	64	67	58

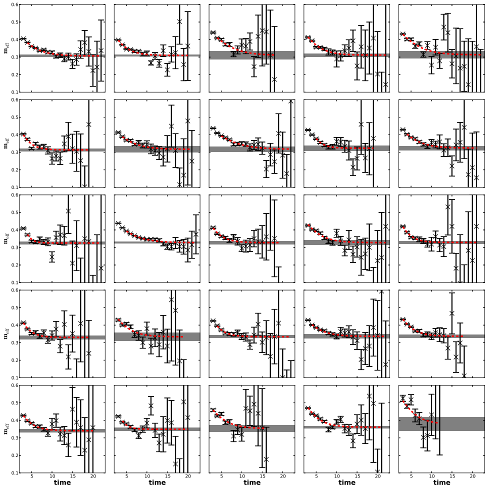
$I = 1,\ S = 0,\ T_{1u}^{+}$ channel

- effective energies $\widetilde{m}^{\rm eff}(t)$ for levels 0 to 24
- energies obtained from two-exponential fits



$I = 1,\ S = 0,\ T_{1u}^{+}$ energy extraction, continued

- effective energies $\widetilde{m}^{\text{eff}}(t)$ for levels 25 to 49
- energies obtained from two-exponential fits



Level identification

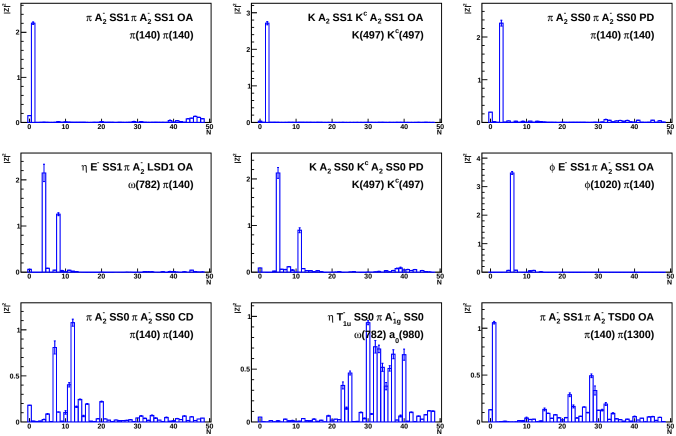
- level identification inferred from Z overlaps with probe operators
- analogous to experiment: infer resonances from scattering cross sections
- keep in mind:
  - probe operators $\overline{O}_j$ act on vacuum, create a “probe state” $|\Phi_j\rangle$, Z's are overlaps of probe state with each eigenstate

$$|\Phi_j\rangle \equiv \overline{O}_i|0\rangle, \qquad Z_j^{(n)} = \langle\Phi_j|n\rangle$$

  - have limited control of “probe states” produced by probe operators
    - ideal to be ρ, single $\pi\pi$, and so on
    - use of small$-a$ expansions to characterize probe operators
    - use of smeared quark, gluon fields
    - field renormalizations
  - mixing is prevalent
  - identify by dominant probe state(s) whenever possible

Level identification

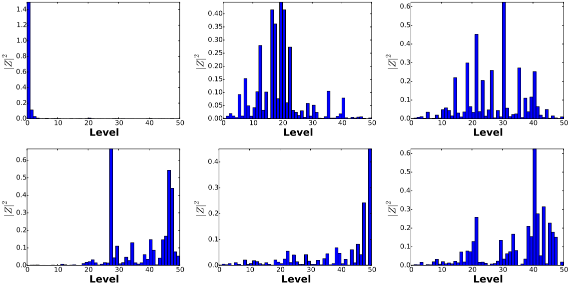
- overlaps for various operators



Identifying quark-antiquark resonances

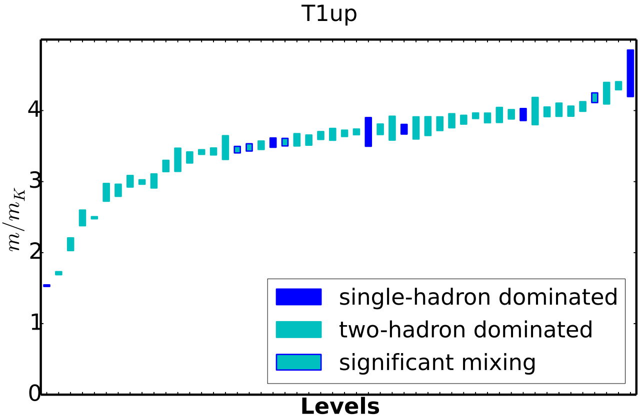
- resonances: finite-volume “precursor states”
- probes: *optimized* single-hadron operators
  - analyze matrix of just single-hadron operators $O_i^{[SH]}$ (12×12)
  - perform single-rotation as before to build probe operators $O_m'^{[SH]} = \sum_i v_i'^{(m)*} O_i^{[SH]}$
- obtain Z' factors of these probe operators

$$Z_m'^{(n)} = \langle 0|\ O_m'^{[SH]}\ |n\rangle$$



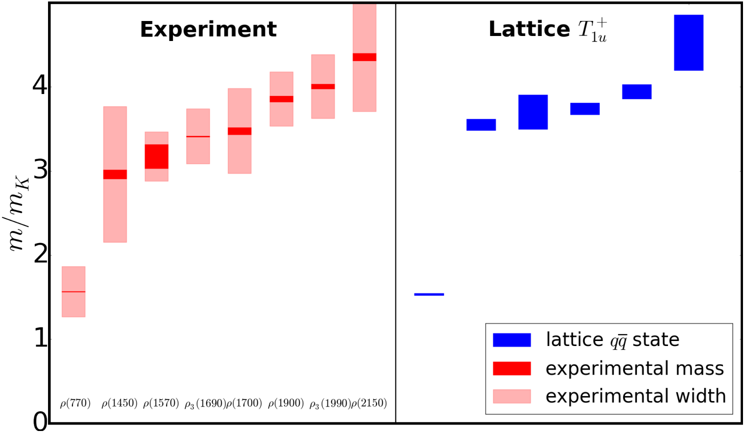
Staircase of energy levels

- stationary state energies $I = 1,\ S = 0,\ T_{1u}^{+}$ channel on $(32^3 \times 256)$ anisotropic lattice



Summary and comparison with experiment

- right: energies of $\overline{q}q$-dominant states as ratios over m_K for $(32^3|240)$ ensemble (resonance precursor states)
- left: experiment

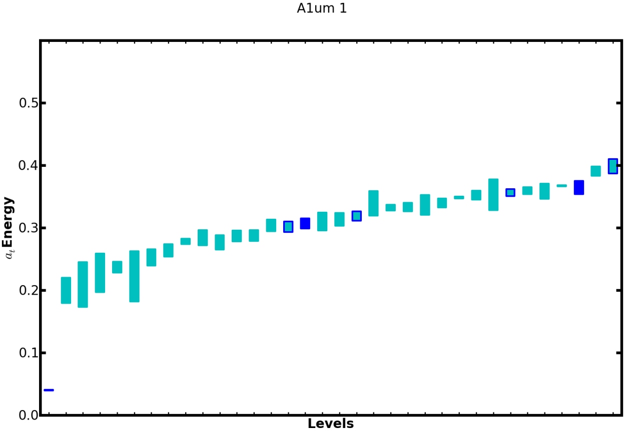


Issues

- address presence of 3 and 4 meson states
- in other channels, address scalar particles in spectrum
  - scalar probe states need vacuum subtractions
  - hopefully can neglect due to OZI suppression
- infinite-volume resonance parameters from finite-volume energies
  - Luscher method too cumbersome, restrictive in applicability
  - need for new hadron effective field theory techniques

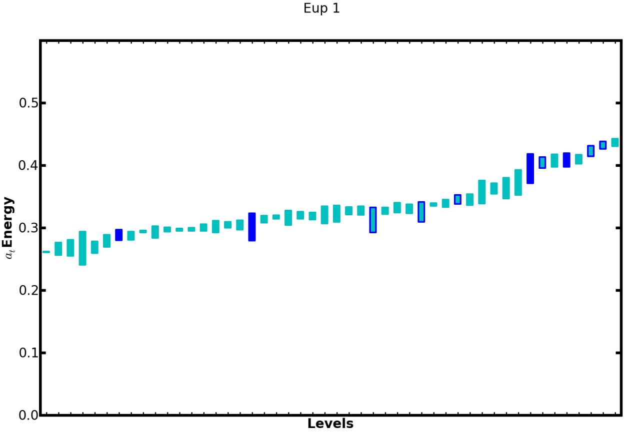
Bosonic $I = 1,\ S = 0,\ A_{1u}^-$ channel

- finite-volume stationary-state energies: "staircase" plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators



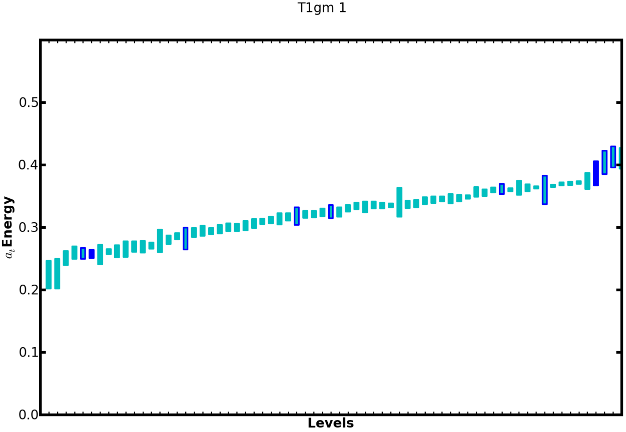
Bosonic $I = 1,\ S = 0,\ E_u^+$ channel

- finite-volume stationary-state energies: “staircase” plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators



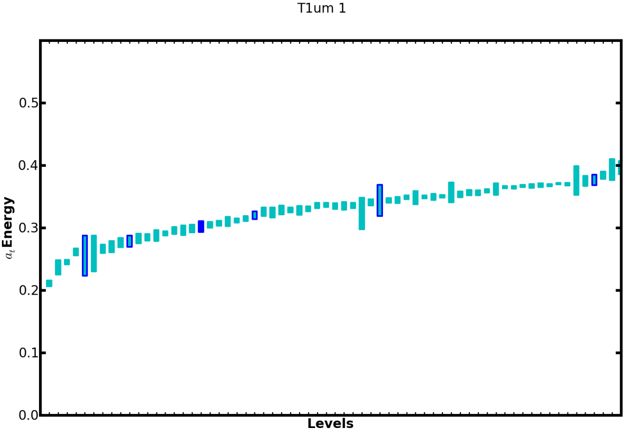
Bosonic $I = 1,\ S = 0,\ T_{1g}^-$ channel

- finite-volume stationary-state energies: “staircase” plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators



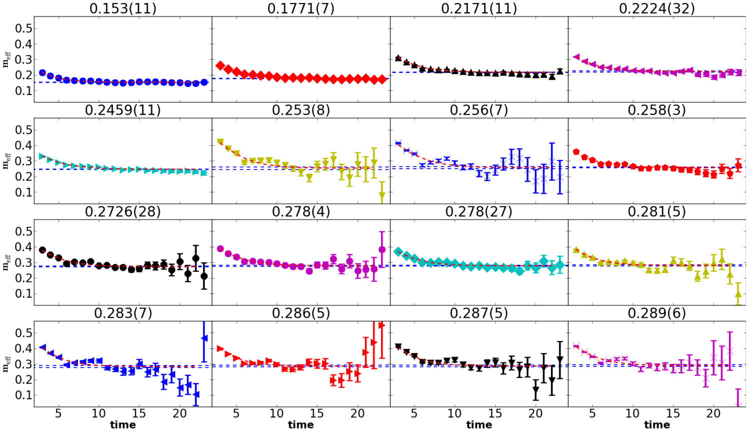
Bosonic $I = 1,\ S = 0,\ T_{1u}^{-}$ channel

- finite-volume stationary-state energies: “staircase” plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators



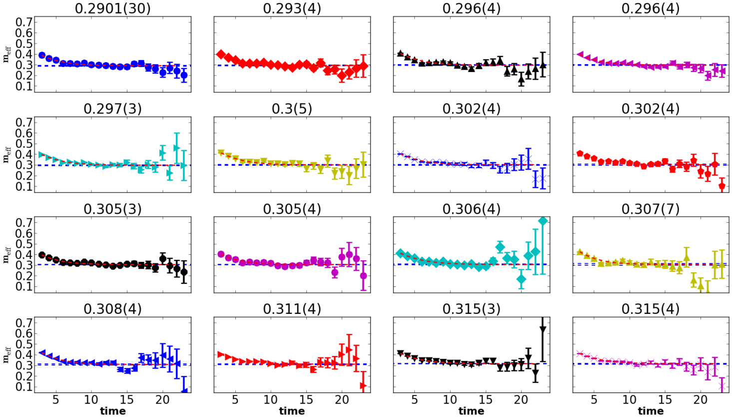
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- kaon channel: effective energies $\widetilde{m}^{\text{eff}}(t)$ for levels 0 to 8
- results for $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- two-exponential fits



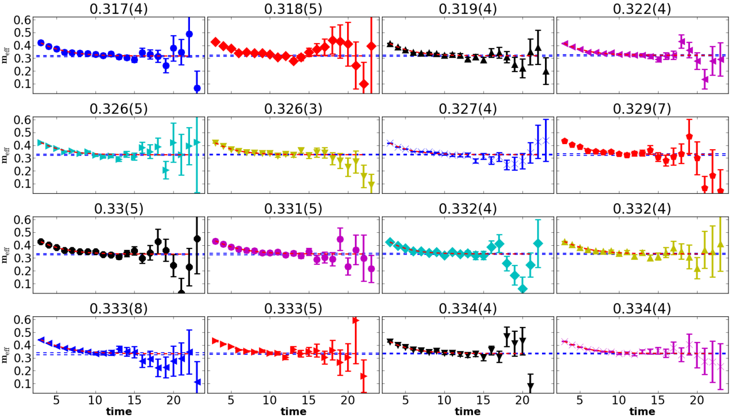
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- effective energies $\widetilde{m}^{\rm eff}(t)$ for levels 9 to 17
- results for $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- two-exponential fits



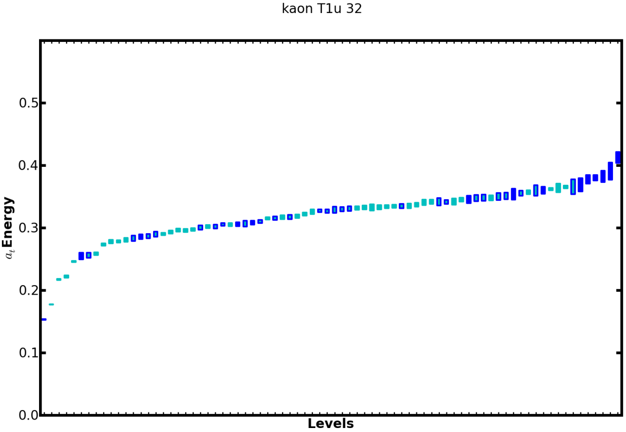
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- effective energies $\widetilde{m}^{\rm eff}(t)$ for levels 18 to 23
- dashed lines show energies from single exponential fits



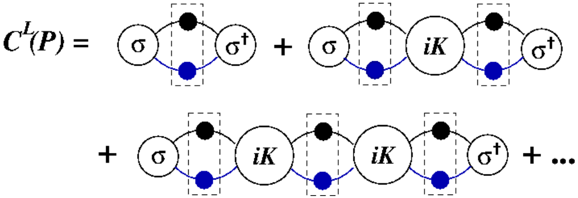
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- finite-volume stationary-state energies: “staircase” plot
- $32^3 \times 256$ lattice for $m_\pi \sim 240$ MeV
- use of single- and two-meson operators only
- blue: levels of max ovelaps with SH optimized operators

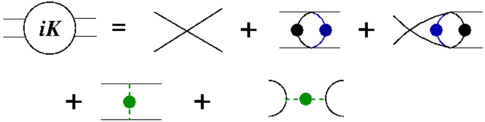


Scattering phase shifts from finite-volume energies

- correlator of two-particle operator σ in finite volume



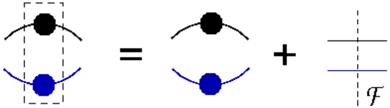
- Bethe-Salpeter kernel



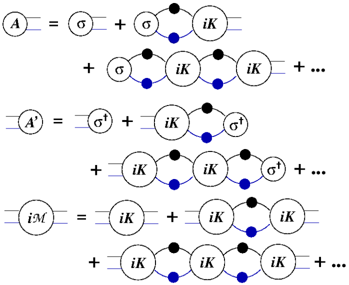
- $C^{\infty}(P)$ has branch cuts where two-particle thresholds begin
- momentum quantization in finite volume: cuts $\rightarrow$ series of poles
- C^{L} poles: two-particle energy spectrum of finite volume theory

Phase shift from finite-volume energies (con't)

- finite-volume momentum sum is infinite-volume integral plus correction $\mathcal{F}$

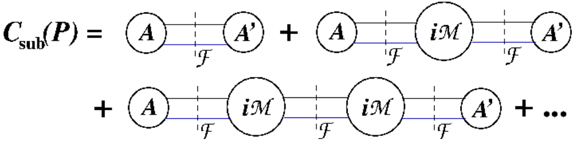


- define the following quantities: A, A', invariant scattering amplitude $i\mathcal{M}$



Phase shifts from finite-volume energies (con't)

- subtracted correlator $C_{\mathrm{sub}}(P) = C^L(P) - C^\infty(P)$ given by



- sum geometric series

$$C_{\mathrm{sub}}(P) = A\,\mathcal{F}(1 - i\mathcal{M}\mathcal{F})^{-1}\,A'.$$

- poles of $C_{\mathrm{sub}}(P)$ are poles of $C^L(P)$ from $\det(1 - i\mathcal{M}\mathcal{F}) = 0$

Phase shifts from finite-volume energies (con't)

- work in spatial L^3 volume with periodic b.c.
- total momentum $\boldsymbol{P} = (2\pi/L)\boldsymbol{d}$, where $\boldsymbol{d}$ vector of integers
- masses m_1 and m_2 of particle 1 and 2
- calculate lab-frame energy E of two-particle interacting state in lattice QCD
- boost to center-of-mass frame by defining:

$$\begin{aligned} E_{\rm cm} &= \sqrt{E^2 - \boldsymbol{P}^2}, \qquad \gamma = \frac{E}{E_{\rm cm}}, \\ \boldsymbol{q}_{\rm cm}^2 &= \frac{1}{4}E_{\rm cm}^2 - \frac{1}{2}(m_1^2 + m_2^2) + \frac{(m_1^2 - m_2^2)^2}{4E_{\rm cm}^2}, \\ u^2 &= \frac{L^2 \boldsymbol{q}_{\rm cm}^2}{(2\pi)^2}, \qquad \boldsymbol{s} = \left(1 + \frac{(m_1^2 - m_2^2)}{E_{\rm cm}^2}\right)\boldsymbol{d} \end{aligned}$$

- E related to S matrix (and phase shifts) by

$$\det[1 + F^{(\boldsymbol{s},\gamma,u)}(S - 1)] = 0,$$

where F matrix defined next slide

Phase shifts from finite-volume energies (con't)

- F matrix in JLS basis states given by

$$F^{(\boldsymbol{s},\gamma,u)}_{J'm_{J'}L'S'a';\; Jm_JLSa} = \frac{\rho_a}{2}\delta_{a'a}\delta_{S'S}\Big\{\delta_{J'J}\delta_{m_{J'}m_J}\delta_{L'L}$$
$$+W^{(\boldsymbol{s},\gamma,u)}_{L'm_{L'};\; Lm_L}\langle J'm_{J'}|L'm_{L'},Sm_S\rangle\langle Lm_L,Sm_S|Jm_J\rangle\Big\},$$

- total angular mom J, J', orbital mom L, L', intrinsic spin S, S'
- a, a' channel labels
- $\rho_a = 1$ distinguishable particles, $\rho_a = \frac{1}{2}$ identical

$$W^{(\boldsymbol{s},\gamma,u)}_{L'm_{L'};\; Lm_L} = \frac{2i}{\pi\gamma u^{l+1}}\mathcal{Z}_{lm}(\boldsymbol{s},\gamma,u^2)\int d^2\Omega\; Y^*_{L'm_{L'}}(\Omega)Y^*_{lm}(\Omega)Y_{Lm_L}(\Omega)$$

- Rummukainen-Gottlieb-Lüscher (RGL) shifted zeta functions $\mathcal{Z}_{lm}$ defined next slide
- $F^{(\boldsymbol{s},\gamma,u)}$ diagonal in channel space, mixes different J, J'
- recall S diagonal in angular momentum, but off-diagonal in channel space

RGL shifted zeta functions

- compute $\mathcal{Z}_{lm}$ using

$$\mathcal{Z}_{lm}(\boldsymbol{s},\gamma,u^2) = \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \frac{\mathcal{Y}_{lm}(\boldsymbol{z})}{(\boldsymbol{z}^2-u^2)} e^{-\Lambda(\boldsymbol{z}^2-u^2)}$$

$$+\delta_{l0}\gamma\pi e^{\Lambda u^2}\left(2uD(u\sqrt{\Lambda})-\Lambda^{-1/2}\right)$$

$$+\frac{i^l\gamma}{\Lambda^{l+1/2}}\int_0^1 dt\left(\frac{\pi}{t}\right)^{l+3/2} e^{\Lambda t u^2} \sum_{\substack{\boldsymbol{n}\in\mathbb{Z}^3\\ \boldsymbol{n}\neq 0}} e^{\pi i\boldsymbol{n}\cdot\boldsymbol{s}}\mathcal{Y}_{lm}(\mathbf{w})\; e^{-\pi^2\mathbf{w}^2/(t\Lambda)}$$

- where

$$\boldsymbol{z} = \boldsymbol{n} - \gamma^{-1}\left[\tfrac{1}{2}+(\gamma-1)s^{-2}\boldsymbol{n}\cdot\boldsymbol{s}\right]\boldsymbol{s},$$

$$\mathbf{w} = \boldsymbol{n} - (1-\gamma)s^{-2}\boldsymbol{s}\cdot\boldsymbol{n}\boldsymbol{s}, \qquad \mathcal{Y}_{lm}(\mathbf{x}) = |\mathbf{x}|^l\; Y_{lm}(\widehat{\mathbf{x}})$$

$$D(x) = e^{-x^2}\int_0^x dt\; e^{t^2} \qquad \text{(Dawson function)}$$

- choose $\Lambda \approx 1$ for convergence of the summation
- integral done Gauss-Legendre quadrature, Dawson with Rybicki

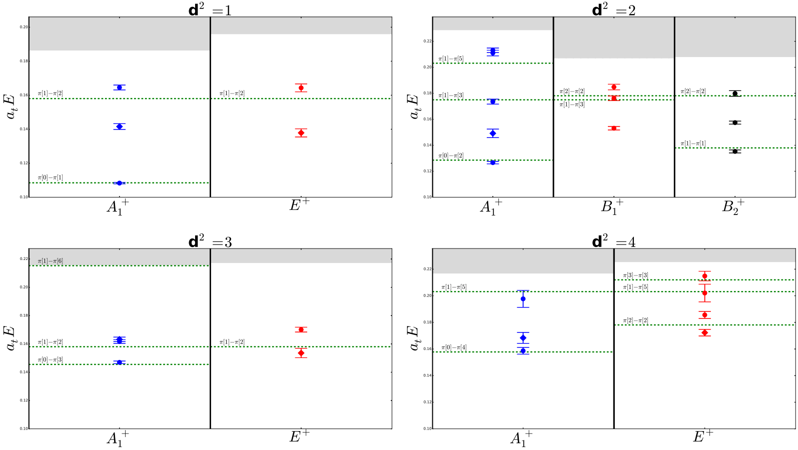
P-wave $I = 1$ $\pi\pi$ scattering

- for P-wave phase shift $\delta_1(E_{\rm cm})$ for $\pi\pi$ $I = 1$ scattering
- define
$$w_{lm} = \frac{\mathcal{Z}_{lm}(\boldsymbol{s}, \gamma, u^2)}{\gamma \pi^{3/2} u^{l+1}}$$

$\boldsymbol{d}$	Λ	$\cot \delta_1$
(0,0,0)	T_{1u}^{+}	$\mathrm{Re}\ w_{0,0}$
(0,0,1)	A_1^{+}	$\mathrm{Re}\ w_{0,0} + \frac{2}{\sqrt{5}}\mathrm{Re}\ w_{2,0}$
	E^{+}	$\mathrm{Re}\ w_{0,0} - \frac{1}{\sqrt{5}}\mathrm{Re}\ w_{2,0}$
(0,1,1)	A_1^{+}	$\mathrm{Re}\ w_{0,0} + \frac{1}{2\sqrt{5}}\mathrm{Re}\ w_{2,0} - \sqrt{\frac{6}{5}}\mathrm{Im}\ w_{2,1} - \sqrt{\frac{3}{10}}\mathrm{Re}\ w_{2,2},$
	B_1^{+}	$\mathrm{Re}\ w_{0,0} - \frac{1}{\sqrt{5}}\mathrm{Re}\ w_{2,0} + \sqrt{\frac{6}{5}}\mathrm{Re}\ w_{2,2},$
	B_2^{+}	$\mathrm{Re}\ w_{0,0} + \frac{1}{2\sqrt{5}}\mathrm{Re}\ w_{2,0} + \sqrt{\frac{6}{5}}\mathrm{Im} w_{2,1} - \sqrt{\frac{3}{10}}\mathrm{Re}\ w_{2,2}$
(1,1,1)	A_1^{+}	$\mathrm{Re}\ w_{0,0} + 2\sqrt{\frac{6}{5}}\mathrm{Im}\ w_{2,2}$
	E^{+}	$\mathrm{Re}\ w_{0,0} - \sqrt{\frac{6}{5}}\mathrm{Im}\ w_{2,2}$

Finite-volume $\pi\pi$ $I = 1$ energies

- $\pi\pi$-state energies for various $\boldsymbol{d}^2$
- dashed lines are non-interacting energies, shaded region above inelastic thresholds

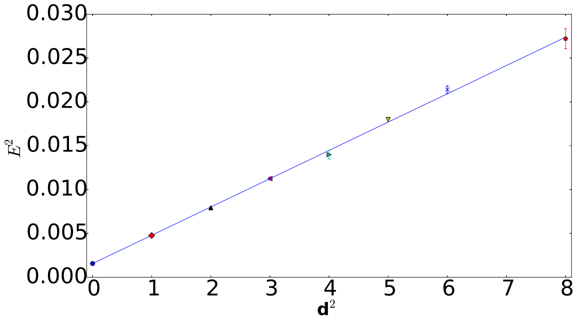


Pion dispersion relation

- boost to cm frame requires aspect ratio on anisotropic lattice
- aspect ratio ξ from pion dispersion

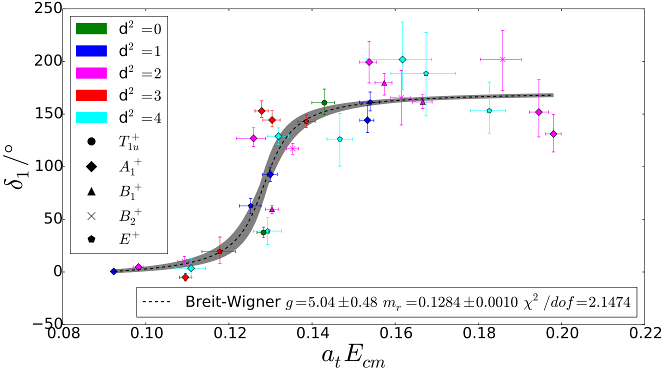
$$(a_t E)^2 = (a_t m)^2 + \frac{1}{\xi^2}\left(\frac{2\pi a_s}{L}\right)^2 \boldsymbol{d}^2$$

- slope below equals $(\pi/(16\xi))^2$, where $\xi = a_s/a_t$



$I = 1$ $\pi\pi$ scattering phase shift and width of the ρ

- preliminary results $32^3 \times 256$, $m_\pi \approx 240$ MeV
- additional collaborator: Ben Hoerz (Dublin)



- fit $\tan(\delta_1) = \dfrac{\Gamma/2}{m_r - E} + A$ and $\Gamma = \dfrac{g^2}{48\pi m_r^2}(m_r^2 - 4m_\pi^2)^{3/2}$

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- S. Basak et al., *Lattice QCD determination of patterns of excited baryon states*, Phys. Rev. D **76**, 074504 (2007).
- C. Morningstar et al., *Improved stochastic estimation of quark propagation with Laplacian Heaviside smearing in lattice QCD*, Phys. Rev. D **83**, 114505 (2011).
- C. Morningstar et al., *Extended hadron and two-hadron operators of definite momentum for spectrum calculations in lattice QCD*, Phys. Rev. D **88**, 014511 (2013).

Conclusion

- goal: comprehensive survey of energy spectrum of QCD stationary states in a finite volume
- stochastic LapH method works very well
  - allows evaluation of all needed quark-line diagrams
  - source-sink factorization facilitates large number of operators
  - last_laph software completed for evaluating correlators
- analysis software sigmond urgently being developed
- analysis of 20 channels $I = 1,\ S = 0$ for $(24^3|390)$ and $(32^3|240)$ ensembles nearing completion
- can evaluate and analyze correlator matrices of unprecedented size 100×100 due to XSEDE resources
- study various scattering phase shifts also planned
- infinite-volume resonance parameters from finite-volume energies $\longrightarrow$ need new effective field theory techniques