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
  - $100 \times 100$ correlator matrix, all needed 2-hadron operators
- other channels
- $I = 1$ $P$-wave $\pi \pi$ scattering phase shifts and width of $\rho$
- future work
Dramatis Personae

- current grad students:
  - Jake Fallica
    - CMU
  - Andrew Hanlon
    - Pitt

- former CMU postdocs:
  - Justin Foley
    - Software, NVIDIA
  - Jimmy Juge
    - Faculty, Stockton, CA

- past CMU grad students:
  - Brendan Fahy
    - 2014 Postdoc KEK
      - Japan
  - You-Cyuan Jhang
    - 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
  
  \[ C_{ij}(t) = \langle 0 | O_i(t + t_0) \bar{O}_j(t_0) | 0 \rangle \]

- Judiciously designed operators $\bar{O}_j$ create states of interest
  
  \[ O_j(t) = O_j[\bar{\psi}(t), \psi(t), U(t)] \]

- Correlators from path integrals over quark $\psi, \bar{\psi}$ and gluon $U$ fields
  
  \[ C_{ij}(t) = \frac{\int D(\bar{\psi}, \psi, U) \; O_i(t + t_0) \bar{O}_j(t_0) \exp \left( -S[\bar{\psi}, \psi, U] \right)}{\int D(\bar{\psi}, \psi, U) \exp \left( -S[\bar{\psi}, \psi, U] \right)} \]

- Involves the action
  
  \[ S[\bar{\psi}, \psi, U] = \bar{\psi} \; K[U] \; \psi + S_G[U] \]

- $K[U]$ 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:
  \[
  \int \mathcal{D}(\bar{\psi}, \psi) \, \psi_a \psi_b \, \bar{\psi}_c \bar{\psi}_d \, \exp(-\bar{\psi}K\psi) = \left( K_{ad}^{-1} K_{bc}^{-1} - K_{ac}^{-1} K_{bd}^{-1} \right) \det K.
  \]

- Baryon-to-baryon example:
  \[
  \int \mathcal{D}(\bar{\psi}, \psi) \, \psi_{a_1} \psi_{a_2} \psi_{a_3} \, \bar{\psi}_{b_1} \bar{\psi}_{b_2} \bar{\psi}_{b_3} \, \exp(-\bar{\psi}K\psi) = \left(-K_{a_1 b_1}^{-1} K_{a_2 b_2}^{-1} K_{a_3 b_3}^{-1} + K_{a_1 b_1}^{-1} K_{a_2 b_2}^{-1} K_{a_3 b_2}^{-1} + K_{a_1 b_2}^{-1} K_{a_2 b_1}^{-1} K_{a_3 b_3}^{-1} \right. \\
  \left. - K_{a_1 b_2}^{-1} K_{a_2 b_3}^{-1} K_{a_3 b_1}^{-1} - K_{a_1 b_3}^{-1} K_{a_2 b_1}^{-1} K_{a_3 b_2}^{-1} + K_{a_1 b_3}^{-1} K_{a_2 b_2}^{-1} K_{a_3 b_1}^{-1} \right) \det K.
  \]
Monte Carlo integration

- Correlators have form

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

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

• not practical to do fits using above form
• define new correlation matrix \( \tilde{C}(t) \) using a single rotation
  \[ \tilde{C}(t) = U^\dagger C(\tau_0)^{-1/2} C(t) C(\tau_0)^{-1/2} U \]
  columns of \( U \) are eigenvectors of \( C(\tau_0)^{-1/2} C(\tau_D) C(\tau_0)^{-1/2} \)
• choose \( \tau_0 \) and \( \tau_D \) large enough so \( \tilde{C}(t) \) diagonal for \( t > \tau_D \)
• effective energies
  \[ \tilde{m}_\alpha^{\text{eff}}(t) = \frac{1}{\Delta t} \ln \left( \frac{\tilde{C}_{\alpha\alpha}(t)}{\tilde{C}_{\alpha\alpha}(t + \Delta t)} \right) \]
  tend to \( N \) lowest-lying stationary state energies in a channel
• 2-exponential fits to \( \tilde{C}_{\alpha\alpha}(t) \) yield energies \( E_\alpha \) and overlaps \( Z_j^{(n)} \)
Building blocks for single-hadron operators

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

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

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

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

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

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

- to good approximation, LapH smearing operator is

$$S = V_s V_s^\dagger$$

- columns of matrix $V_s$ are eigenvectors of $\tilde{\Delta}$
Extended operators for single hadrons

- quark displacements build up orbital, radial structure

**Meson configurations**

**Baryon configurations**

\[
\Phi_{AB}^{\alpha\beta}(p, t) = \sum_x e^{i p \cdot (x + \frac{1}{2} (d_\alpha + d_\beta))} \delta_{ab} \overline{q}_b^B(x, t) q_a^A(x, t)
\]

\[
\Phi_{ABC}^{\alpha\beta\gamma}(p, t) = \sum_x e^{i p \cdot x} \varepsilon_{abc} \overline{q}_c^C(x, t) \overline{q}_b^B(x, t) \overline{q}_a^A(x, t)
\]

- group-theory projections onto irreps of lattice symmetry group

\[
\overline{M}_l(t) = c^{(l)*}_{\alpha\beta} \Phi_{AB}^{\alpha\beta}(t) \quad \overline{B}_l(t) = c^{(l)*}_{\alpha\beta\gamma} \Phi_{ABC}^{\alpha\beta\gamma}(t)
\]

- definite momentum \( p \), irreps of little group of \( p \)
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

Graphs showing mass distribution for different states.

- $I=\frac{1}{2}, S=-1, P=+1$
  - $A_{1g}$, $T_{1g}$, $E_g$, $T_{2g}$, $A_{2g}$

- $I=\frac{1}{2}, S=-1, P=-1$
  - $A_{1u}$, $T_{1u}$, $E_u$, $T_{2u}$, $A_{2u}$
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

\[ c_{p_a \lambda_a}^{I_3 a} p_{b \lambda_b} B_{p_a \Lambda_a \lambda_a i_a} B_{p_b \Lambda_b \lambda_b i_b} \]

- fixed total momentum \( p = p_a + p_b \), fixed \( \Lambda_a, i_a, \Lambda_b, i_b \)

- group-theory projections onto little group of \( p \) and isospin irreps

- restrict attention to certain classes of momentum directions
  - on axis \( \pm \hat{x}, \pm \hat{y}, \pm \hat{z} \)
  - planar diagonal \( \pm \hat{x} \pm \hat{y}, \pm \hat{x} \pm \hat{z}, \pm \hat{y} \pm \hat{z} \)
  - cubic diagonal \( \pm \hat{x} \pm \hat{y} \pm \hat{z} \)

- crucial to know and fix all phases of single-hadron operators for all momenta
  - each class, choose reference direction \( p_{\text{ref}} \)
  - each \( p \), select one reference rotation \( R^p_{\text{ref}} \) that transforms \( p_{\text{ref}} \) into \( p \)

- efficient creating large numbers of two-hadron operators

- generalizes to three, four, \ldots two-hadron operators
Quark propagation

- Quark propagator is inverse $K^{-1}$ of Dirac matrix
  - Rows/columns involve lattice site, spin, color
  - Very large $N_{\text{tot}} \times N_{\text{tot}}$ matrix for each flavor
    
    
    \[ N_{\text{tot}} = N_{\text{site}}N_{\text{spin}}N_{\text{color}} \]

- For $32^3 \times 256$ lattice, $N_{\text{tot}} \sim 101$ 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 $\eta$ 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 $K^{-1}$

$$K^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X^{(r)}_i \eta^{(r)*}_j$$

- variance reduction using noise dilution
- dilution introduces projectors

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

- define

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

to obtain Monte Carlo estimate with drastically reduced variance

$$K^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a X^{(r)[a]}_i \eta^{(r)[a]*}_j$$
Stochastic LapH method

- introduce $Z_N$ noise in the LapH subspace
  \[ \rho_{\alpha k}(t), \quad t = \text{time}, \alpha = \text{spin}, \, k = \text{eigenvector number} \]

- four dilution schemes:
  \[
  \begin{align*}
  P_{ij}^{(a)} &= \delta_{ij} \quad &a = 0 &\quad \text{(none)} \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{ai} \quad &a = 0, 1, \ldots, N - 1 &\quad \text{(full)} \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{a,Ki/N} \quad &a = 0, 1, \ldots, K - 1 &\quad \text{(interlace-}K) \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{a, i \mod k} \quad &a = 0, 1, \ldots, K - 1 &\quad \text{(block-}K) \\
  \end{align*}
  \]

- 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
  \[ Q = D^{(j)} SK^{-1} \gamma_4 SD^{(k)\dagger} \]
- displaced-smeared-diluted quark source and quark sink vectors:
  \[ Q^{[b]}(\rho) = D^{(j)} V_s P^{(b)} \rho \]
  \[ \varphi^{[b]}(\rho) = D^{(j)} SK^{-1} \gamma_4 V_s P^{(b)} \rho \]
- estimate in stochastic LapH by \((A, B\) flavor, \(u, \nu\) compound: space, time, color, spin, displacement type)
  \[ Q_{uv}^{(AB)} \approx \frac{1}{N_R} \delta_{AB} \sum_{r=1}^{N_R} \sum_{b} \varphi^{[b]}(\rho^r) Q^{[b]}(\rho^r)^* \]
- occasionally use \(\gamma_5\)-Hermiticity to switch source and sink
  \[ Q_{uv}^{(AB)} \approx \frac{1}{N_R} \delta_{AB} \sum_{r=1}^{N_R} \sum_{b} \overline{Q}^{[b]}(\rho^r) \overline{\varphi}^{[b]}(\rho^r)^* \]
  defining \(\overline{\varphi}(\rho) = -\gamma_5 \gamma_4 \varphi(\rho)\) and \(\overline{\varphi}(\rho) = \gamma_5 \gamma_4 \varphi(\rho)\)
Source-sink factorization in stochastic LapH

- baryon correlator has form

\[ C_{\vec{l}\vec{l}} = c_{ijk}^l c_{ijk}^{\vec{l}} \ast Q_i^A Q_j^B Q_k^C \]

- stochastic estimate with dilution

\[ C_{\vec{l}\vec{l}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} c_{ijk}^l c_{ijk}^{\vec{l}} \ast \left( \varphi_i^{(Ar)}[d_A] \varphi_i^{(Ar)}[d_A]^* \right) \times \left( \varphi_j^{(Br)}[d_B] \varphi_j^{(Br)}[d_B]^* \right) \times \left( \varphi_k^{(Cr)}[d_C] \varphi_k^{(Cr)}[d_C]^* \right) \]

- define baryon source and sink

\[
\begin{align*}
B_l^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) &= c_{ijk}^l \varphi_i^{(Ar)}[d_A] \varphi_j^{(Br)}[d_B] \varphi_k^{(Cr)}[d_C] \\
B_{\vec{l}}^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) &= c_{ijk}^{\vec{l}} Q_i^{(Ar)}[d_A] Q_j^{(Br)}[d_B] Q_k^{(Cr)}[d_C]
\end{align*}
\]

- correlator is dot product of source vector with sink vector

\[ C_{\vec{l}\vec{l}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} B_l^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) B_{\vec{l}}^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C)^* \]
Correlators and quark line diagrams

- **baryon correlator**

\[
\mathcal{C}_{\bar{l}l} \approx \frac{1}{N_R} \sum_r \sum_{d_Ad_Bd_C} \mathcal{B}_l^{(r)[d_Ad_Bd_C]} (\phi^A, \phi^B, \phi^C) \mathcal{B}_{\bar{l}}^{(r)[d_Ad_Bd_C]} (\bar{\phi}^A, \bar{\phi}^B, \bar{\phi}^C) *
\]

- **express diagrammatically**

- **meson correlator**

\[
- \mathcal{C} \mathcal{G} \left[ \begin{array}{c} \phi \\ \phi \\ \phi \\ \phi \\ \phi \\ \phi \end{array} \right] \left[ \begin{array}{c} \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \end{array} \right] + \mathcal{C} \mathcal{G} \left[ \begin{array}{c} \phi \\ \phi \\ \phi \\ \phi \\ \phi \\ \phi \end{array} \right] \left[ \begin{array}{c} \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \\ \bar{\phi} \end{array} \right]
\]
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 ⇒ 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 $O_h$
    $$A_{1a}, A_{2g}, E_g, T_{1a}, T_{2a}, \quad G_{1a}, G_{2a}, H_a, \quad a = g, u$$
  - 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 $\Lambda$ irreps in $J$ subduced

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### Common hadrons

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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: \( \sim 200 \text{ million core hours} \)
- quark propagators: \( \sim 100 \text{ million core hours} \)
- hadrons + correlators: \( \sim 40 \text{ million core hours} \)
- storage: \( \sim 300 \text{ TB} \)

![Kraken at NICS](image1.png)  ![Stampede at TACC](image2.png)

C. Morningstar  Excited States
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 \(\rho\)-channel: \(I = 1, S = 0, T_{1u}^+\)

results from \(63 \times 63\) matrix of correlators \((32^3|240)\) ensemble
  • 10 single-hadron (quark-antiquark) operators
  • “\(\pi\pi\)” operators
  • “\(\eta\pi\)” operators, “\(\phi\pi\)” operators
  • “\(K\bar{K}\)” 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          |
| "ππ"     | 10          | 17          | 8           | 11          | 8       | 17      | 23          | 30          | 17          | 27          |
| "ηπ"     | 6           | 15          | 10          | 7           | 11      | 18      | 31          | 20          | 21          | 23          |
| "φπ"     | 6           | 15          | 9           | 7           | 12      | 19      | 37          | 11          | 23          | 23          |
| "K̄K̄"   | 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          |
| "ππ"     | 3           | 7           | 7           | 3           | 8       | 11      | 22          | 12          | 12          | 15          |
| "ηπ"     | 26          | 15          | 10          | 12          | 24      | 21      | 25          | 33          | 28          | 30          |
| "φπ"     | 26          | 15          | 10          | 12          | 27      | 22      | 26          | 38          | 30          | 32          |
| "K̄K̄"   | 11          | 3           | 4           | 2           | 11      | 5       | 12          | 5           | 12          | 6           |
| Total    | 76          | 48          | 42          | 39          | 82      | 68      | 106         | 103         | 101         | 99          |

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Excited States 31
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         |
| “$K\bar{K}$” | 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         |
| “$K\bar{K}$” | 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 \( \tilde{m}^{\text{eff}}(t) \) for levels 0 to 24
- energies obtained from two-exponential fits
$I = 1, \ S = 0, \ T_{1u}^+ \ energy\ extraction, \ continued$

- effective energies $\tilde{m}_{eff}(t)$ 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:
    $$|\Phi_j\rangle \equiv \overline{O}_i|0\rangle, \quad Z_j^{(n)} = \langle \Phi_j | n \rangle$$
  - Have limited control of “probe states” produced by probe operators:
    - Ideal to be $\rho$, 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

\[
\begin{align*}
\pi A_2^+ S S1 \pi A_2^+ S S1 OA \\
\pi(140) \pi(140)
\end{align*}
\]

\[
\begin{align*}
K A_2 S S1 K^+ A_2 S S1 OA \\
K(497) K^+(497)
\end{align*}
\]

\[
\begin{align*}
\pi A_2^+ S S0 \pi A_2^+ S S0 PD \\
\pi(140) \pi(140)
\end{align*}
\]

\[
\begin{align*}
\eta E S S1 \pi A_2^- L S D1 OA \\
\omega(782) \pi(140)
\end{align*}
\]

\[
\begin{align*}
K A_2 S S0 K^+ A_2 S S0 PD \\
K(497) K^+(497)
\end{align*}
\]

\[
\begin{align*}
\phi E S S1 \pi A_2^- S S1 OA \\
\phi(1020) \pi(140)
\end{align*}
\]

\[
\begin{align*}
\pi A_2^+ S S0 \pi A_2^- S S0 C D \\
\pi(140) \pi(140)
\end{align*}
\]

\[
\begin{align*}
\eta T_{1u} S S0 \pi A_1^+ S S0 \\
\omega(782) a_0(980)
\end{align*}
\]

\[
\begin{align*}
\pi A_2^+ S S1 \pi A_2^- T S D0 OA \\
\pi(140) \pi(1300)
\end{align*}
\]
Identifying quark-antiquark resonances

- resonances: finite-volume “precursor states”
- probes: *optimized* single-hadron operators
  - analyze matrix of just single-hadron operators $O^{[SH]}_i$ ($12 \times 12$)
  - perform single-rotation as before to build probe operators
    $$O^{[SH]}_m = \sum_i v_i^{(m)*} O^{[SH]}_i$$
- obtain $Z'$ factors of these probe operators
  $$Z'_m(n) = \langle 0 | O^{[SH]}_m | n \rangle$$
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 $\bar{q}q$-dominant states as ratios over $m_K$ for $(32^3|240)$ ensemble (resonance precursor states)
- left: experiment

---

**Experiment**

<table>
<thead>
<tr>
<th>Energy (GeV)</th>
<th>Experimental mass</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.77</td>
<td>$\rho(770)$</td>
</tr>
<tr>
<td>1.45</td>
<td>$\rho(1450)$</td>
</tr>
<tr>
<td>1.57</td>
<td>$\rho(1570)$</td>
</tr>
<tr>
<td>1.69</td>
<td>$\rho_2(1690)$</td>
</tr>
<tr>
<td>1.70</td>
<td>$\rho(1700)$</td>
</tr>
<tr>
<td>1.90</td>
<td>$\rho(1900)$</td>
</tr>
<tr>
<td>1.99</td>
<td>$\rho_3(1990)$</td>
</tr>
<tr>
<td>2.15</td>
<td>$\rho(2150)$</td>
</tr>
</tbody>
</table>

**Lattice $T_{1u}^+$**

- lattice $q\bar{q}$ state
- experimental mass
- experimental width
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 overlaps 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 overlaps with SH optimized operators

![Energy vs Levels Plot]

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Excited States
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 overlaps 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 overlaps with SH optimized operators
Bosonic $I = \frac{1}{2}$, $S = 1$, $T_{1u}$ channel

- kaon channel: effective energies $\tilde{m}_{\text{eff}}(t)$ 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 $\tilde{m}_{\text{eff}}(t)$ 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 $\tilde{m}^{\text{eff}}(t)$ 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 overlaps with SH optimized operators
Scattering phase shifts from finite-volume energies

- correlator of two-particle operator $\sigma$ in finite volume

$$C^L(P) = \sigma \sigma^\dagger + \sigma iK \sigma^\dagger + \cdots$$

- Bethe-Salpeter kernel

$$iK = \times + \cdots$$

- $C^\infty(P)$ 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
finite-volume momentum sum is infinite-volume integral plus correction $\mathcal{F}$

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

$$A = \sigma + \sigma iK + \sigma iK + \sigma iK + \ldots$$

$$A' = \sigma^\dagger + iK \sigma^\dagger + iK \sigma^\dagger + iK \sigma^\dagger + \ldots$$

$$i\mathcal{M} = iK + iK iK + iK iK + iK iK + \ldots$$
Phase shifts from finite-volume energies (con’t)

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

\[
C_{\text{sub}}(P) = A \frac{1}{\mathcal{F}} + A \frac{iM}{\mathcal{F}} A' + A \frac{iM}{\mathcal{F}} iM \frac{iM}{\mathcal{F}} A' + \ldots
\]

- sum geometric series

\[
C_{\text{sub}}(P) = A \mathcal{F}(1 - iM\mathcal{F})^{-1} A'.
\]

- poles of \( C_{\text{sub}}(P) \) are poles of \( C^L(P) \) from \( \det(1 - iM\mathcal{F}) = 0 \)
Phase shifts from finite-volume energies (con’t)

- work in spatial $L^3$ volume with periodic b.c.
- total momentum $P = (2\pi/L)d$, where $d$ 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:

$$E_{\text{cm}} = \sqrt{E^2 - P^2}, \quad \gamma = \frac{E}{E_{\text{cm}}},$$

$$q_{\text{cm}}^2 = \frac{1}{4} E_{\text{cm}}^2 - \frac{1}{2} (m_1^2 + m_2^2) + \frac{(m_1^2 - m_2^2)^2}{4 E_{\text{cm}}^2},$$

$$u^2 = \frac{L^2 q_{\text{cm}}^2}{(2\pi)^2}, \quad s = \left(1 + \frac{(m_1^2 - m_2^2)}{E_{\text{cm}}^2}\right) d$$

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

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

where $F$ matrix defined next slide
Phase shifts from finite-volume energies (con’t)

- $F$ matrix in $JLS$ basis states given by
  \[
  F_{J'm_j',L'S'\alpha'}^{(s,\gamma,u)}; JmJLSa = \frac{\rho_a}{2} \delta_{\alpha'\alpha} \delta_{S'S} \left\{ \delta_{J'J} \delta_{m_j'm_j} \delta_{L'L} + W_{L'm_{L'}; Lm_L}^{(s,\gamma,u)} \langle J'm_j' | L'm_{L'}, S_{m} \rangle \langle Lm_L, S_{m} | Jm_J \rangle \right\},
  \]
- total angular mom $J, J'$, orbital mom $L, L'$, intrinsic spin $S, S'$
- $\alpha, \alpha'$ channel labels
- $\rho_a = 1$ distinguishable particles, $\rho_a = \frac{1}{2}$ identical
- $W_{L'm_{L'}; Lm_L}^{(s,\gamma,u)} = \frac{2i}{\pi \gamma u^{l+1}} Z_{lm}(s, \gamma, u^2) \int d^2\Omega \ Y_{L'm_{L'}}^*(\Omega) Y_{lm}^*(\Omega) Y_{Lm_L}(\Omega)$
- Rummukainen-Gottlieb-Lüscher (RGL) shifted zeta functions $Z_{lm}$ defined next slide
- $F^{(s,\gamma,u)}$ diagonal in channel space, mixes different $J, J'$
- recall $S$ diagonal in angular momentum, but off-diagonal in channel space
compute $Z_{lm}$ using

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

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

$$+ \frac{i^l \gamma}{\Lambda^{l+1/2}} \int_0^1 dt \left(\frac{\pi}{t}\right)^{l+3/2} e^{\Lambda tu^2} \sum_{n \in \mathbb{Z}^3} e^{\pi in \cdot s} Y_{lm}(w) e^{-\pi^2 w^2/(t\Lambda)}$$

where

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

$$w = n - (1 - \gamma)s^{-2} s \cdot ns,$$  

$$Y_{lm}(x) = |x|^l Y_{lm}(\hat{x})$$

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

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 $\delta_1(E_{\text{cm}})$ for $\pi\pi$ $I = 1$ scattering
- Define

\[
w_{lm} = \frac{Z_{lm}(s, \gamma, u^2)}{\gamma \pi^{3/2} u^{l+1}}\]

<table>
<thead>
<tr>
<th>$d$</th>
<th>$\Lambda$</th>
<th>$\cot \delta_1$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$(0,0,0)$</td>
<td>$T_{1u}^+$</td>
<td>$\text{Re } w_{0,0}$</td>
</tr>
<tr>
<td>$(0,0,1)$</td>
<td>$A_1^+$</td>
<td>$\text{Re } w_{0,0} + \frac{2}{\sqrt{5}} \text{Re } w_{2,0}$</td>
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<td></td>
<td>$E^+$</td>
<td>$\text{Re } w_{0,0} - \frac{1}{\sqrt{5}} \text{Re } w_{2,0}$</td>
</tr>
<tr>
<td>$(0,1,1)$</td>
<td>$A_1^+$</td>
<td>$\text{Re } w_{0,0} + \frac{1}{2\sqrt{5}} \text{Re } w_{2,0} - \sqrt{\frac{6}{5}} \text{Im } w_{2,1} - \sqrt{\frac{3}{10}} \text{Re } w_{2,2}$</td>
</tr>
<tr>
<td></td>
<td>$B_{1}^+$</td>
<td>$\text{Re } w_{0,0} - \frac{1}{\sqrt{5}} \text{Re } w_{2,0} + \sqrt{\frac{6}{5}} \text{Re } w_{2,2}$</td>
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<td>$B_{2}^+$</td>
<td>$\text{Re } w_{0,0} + \frac{1}{2\sqrt{5}} \text{Re } w_{2,0} + \sqrt{\frac{6}{5}} \text{Im } w_{2,1} - \sqrt{\frac{3}{10}} \text{Re } w_{2,2}$</td>
</tr>
<tr>
<td>$(1,1,1)$</td>
<td>$A_1^+$</td>
<td>$\text{Re } w_{0,0} + 2 \sqrt{\frac{6}{5}} \text{Im } w_{2,2}$</td>
</tr>
<tr>
<td></td>
<td>$E^+$</td>
<td>$\text{Re } w_{0,0} - \sqrt{\frac{6}{5}} \text{Im } w_{2,2}$</td>
</tr>
</tbody>
</table>
Finite-volume $\pi\pi I = 1$ energies

- $\pi\pi$-state energies for various $d^2$
- 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 $\xi$ from pion dispersion

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

- Slope below equals \((\pi/(16\xi))^2\), where $\xi = a_s/a_t$
$I = 1 \pi \pi$ scattering phase shift and width of the $\rho$

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

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


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 $100 \times 100$ due to XSEDE resources
- study various scattering phase shifts also planned
- infinite-volume resonance parameters from finite-volume energies need new effective field theory techniques