Excited states and scattering phase shifts from lattice QCD

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Hadrons and Hadron Interactions in QCD

Kyoto, Japan

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Outline

- project 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
- preliminary results for 20 channels $I = 1, \ S = 0$
  - correlator matrices of size $100 \times 100$
  - large number of extended single-hadron operators
  - attempt to include all needed 2-hadron operators
- preliminary results for $I = \frac{1}{2}, \ S = 1, \ T_{1u}$
- $I = 1$ $P$-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

C. Morningstar

Excited States
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:
  \[
  q^A_{a\alpha j} = D^{(j)} \tilde{\psi}_{a\alpha}^{(A)}, \quad \bar{q}^A_{a\alpha j} = \bar{\tilde{\psi}}_{a\alpha}^{(A)} \gamma_4 D^{(j)}\dagger
  \]
- 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

\[ \Phi_{\alpha\beta}(p, t) = \sum_x e^{ip \cdot (x + \frac{1}{2} (d_\alpha + d_\beta))} \delta_{ab} q^B_{b\beta}(x, t) q^A_{a\alpha}(x, t) \]

\[ \Phi^{ABC}_{\alpha\beta\gamma}(p, t) = \sum_x e^{ip \cdot x} \varepsilon_{abc} q^C_{c\gamma}(x, t) q^B_{b\beta}(x, t) q^A_{a\alpha}(x, t) \]

Baryon configurations

- group-theory projections onto irreps of lattice symmetry group

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

- definite momentum \( p \), irreps of little group of \( p \)
Small $-a$ expansion of probes

- link variables in terms of continuum gluon field

$$U_\mu(x) = \mathcal{P} \exp \left\{ i g \int_x^{x+\hat{\mu}} d\eta \cdot A(\eta) \right\},$$

- classical small $-a$ expansion of displaced quark field:

$$U_j(x) U_k(x + \hat{j}) \psi_\alpha(x + \hat{j} + \hat{k}) = \exp(aD_j) \exp(aD_k) \psi_\alpha(x).$$

- where $D_j = \partial_j + igA_j$ is covariant derivative
- must take smearing of fields into account
- radiative corrections of expansion coefficients (hopefully small due to smearing)
isovector meson continuum probe operators

\[ M_{\mu j_1 j_2 \cdots} = \chi^d \Gamma_{\mu} D_{j_1} D_{j_2} \cdots \psi^u, \quad \chi = \overline{\psi} \gamma_4 \]

where $\Gamma_0 = 1$ and $\Gamma_k = \gamma_k$ (analogous table inserting $\gamma_4, \gamma_5, \gamma_4 \gamma_5$)

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<th>$J^{PG}$</th>
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isovector meson continuum probe operators

\[ M_{\mu j_1 j_2 \ldots} = \chi^d \Gamma_{\mu} D_{j_1} D_{j_2} \ldots \psi^u, \quad \chi = \overline{\psi} \gamma_4 \]

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<td>( M_{331} - M_{212} + M_{313} - M_{122} + M_{133} - M_{221} )</td>
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Two-hadron operators

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

$$c_{I_3aI_3b}^{I_3aI_3b} p_a \lambda_a; p_b \lambda_b \cdot B_{I_3aI_3b}^{I_3aI_3b} S_a \cdot B_{I_3bI_3b}^{I_3bI_3b} S_b$$

- 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 $R_{\text{ref}}^p$ that transforms $p_{\text{ref}}$ into $p$

- efficient creating large numbers of two-hadron operators

- generalizes to three, four, ... hadron operators
Testing our two-meson operators

- (left) $K\pi$ operator in $T_{1u} I = \frac{1}{2}$ channels
- (center and right) comparison with localized $\pi\pi$ operators

\[
(\pi\pi)^{A_1^+}(t) = \sum_x \pi^+(x, t) \pi^+(x, t),
\]
\[
(\pi\pi)^{T_{1u}^+}(t) = \sum_{x,k=1,2,3} \left\{ \pi^+(x, t) \Delta_k \pi^0(x, t) - \pi^0(x, t) \Delta_k \pi^+(x, t) \right\}
\]

- less contamination from higher states in our $\pi\pi$ 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

![Diagram showing slice-to-slice quark lines]

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

![Diagram showing 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 $K^{-1}$

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_{i}^{(r)} \eta_{j}^{(r)*}$$

- variance reduction using noise dilution
- dilution introduces projectors

$P^{(a)}P^{(b)} = \delta^{ab} P^{(a)}$, \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

$$K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_{a} X_{i}^{(r)[a]} \eta_{j}^{(r)[a]*}$$
Stochastic LapH method

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

  \[
  \begin{align*}
  P_{ij}^{(a)} &= \delta_{ij} \quad a = 0 \quad \text{(none)} \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{ai} \quad a = 0, 1, \ldots, N-1 \quad \text{(full)} \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{a,i/K} \quad a = 0, 1, \ldots, K-1 \quad \text{(interlace-$K$)} \\
  P_{ij}^{(a)} &= \delta_{ij}\delta_{a,i \mod k} \quad a = 0, 1, \ldots, K-1 \quad \text{(block-$K$)}
  \end{align*}
  \]
- 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
  \[ Q = D^{(j)} SK^{-1} \gamma_4 SD^{(k)} \]

- 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, \(u, v\) compound: space, time, color, spin, displacement type)
  \[ Q_{uv}^{(AB)} \approx \frac{1}{N_R} \delta_{AB} \sum_{r=1}^{N_R} \sum_{b} \varphi_u^{[b]}(\rho^r) \bar{Q}_v^{[b]}(\rho^r)^* \]

- occasionally use \(\gamma_5\)-Hermiticity to switch source and sink
  \[ Q_{uv}^{(AB)} \approx \frac{1}{N_R} \delta_{AB} \sum_{r=1}^{N_R} \sum_{b} \bar{Q}_u^{[b]}(\rho^r) \bar{\varphi}_v^{[b]}(\rho^r)^* \]

  defining \(\bar{Q}(\rho) = -\gamma_5 \gamma_4 Q(\rho)\) and \(\bar{\varphi}(\rho) = \gamma_5 \gamma_4 \varphi(\rho)\)
Source-sink factorization in stochastic LapH

- baryon correlator has form
  \[ C_{\bar{l}l} = c_{ijkl}^{(l)} c_{\bar{j}k}^{(l)*} Q_i^A Q_j^B Q_k^C \]

- stochastic estimate with dilution
  \[ C_{\bar{l}l} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} c_{ijkl}^{(l)} c_{\bar{j}k}^{(l)*} \left( \varphi_i^{(Ar)} [d_A] \varphi_j^{(Br)} [d_B] \varphi_k^{(Cr)} [d_C] \right) \]
  \[ \times \left( \varphi_j^{(Br)} [d_B] \varphi_j^{(Br)*} \right) \left( \varphi_k^{(Cr)} [d_C] \varphi_k^{(Cr)*} \right) \]

- define baryon source and sink
  \[ B_l^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) = c_{ijkl}^{(l)} \varphi_i^{(Ar)} [d_A] \varphi_j^{(Br)} [d_B] \varphi_k^{(Cr)} [d_C] \]
  \[ B_{\bar{l}}^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) = c_{ijkl}^{(l)} \varphi_i^{(Ar)} [d_A] \varphi_j^{(Br)} [d_B] \varphi_k^{(Cr)} [d_C] \]

- correlator is dot product of source vector with sink vector
  \[ C_{\bar{l}l} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} B_l^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C) \overline{B_{\bar{l}}^{(r)[d_A d_B d_C]} (\varphi^A, \varphi^B, \varphi^C)} \]
Correlators and quark line diagrams

- baryon correlator

\[ C_{\vec{\nu}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} B_l^{(r)[d_A d_B d_C]} (\phi^A, \phi^B, \phi^C) B_{\bar{\nu}}^{(r)[d_A d_B d_C]} (\bar{\phi}^A, \bar{\phi}^B, \bar{\phi}^C)^* \]

- 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 ⇒ 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 $O_h$
    \[ A_{1a}, A_{2g\alpha}, E_a, T_{1a}, T_{2a}, G_{1a}, G_{2a}, H_a, \quad a = g, u \]
  - 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

- irreps of commonly-known hadrons at rest

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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 $\sigma^2_s = 0.33$ 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
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      |
| \(\pi\pi\) | 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      |
| \(K\bar{K}\) | 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      |
| \(K\bar{K}\) | 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

| (24²|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        |

| (24²|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        |

G. Morningstar

Excited States 26
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 \( Z_j^{(n)} \)
$I = 1$, $S = 0$, $T_{1u}^{+}$ 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 $\tilde{m}^{\text{eff}}(t)$ 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 $\bar{O}_j$ act on vacuum, create a “probe state” $|\Phi_j\rangle$,
    $Z$’s are overlaps of probe state with each eigenstate
    $$|\Phi_j\rangle \equiv \bar{O}_i|0\rangle, \quad Z_j^{(n)} = \langle \Phi_j | n \rangle$$
  - 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
Identifying quark-antiquark resonances

- resonances: finite-volume “precursor states”
- probes: optimized single-hadron operators
  - analyze matrix of just single-hadron operators $O_{i}^{[SH]} \ (12 \times 12)$
  - 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 $\bar{q}q$-dominant states as ratios over $m_K$ for $(32^3|240)$ ensemble (resonance precursor states)
- left: experiment

![Graph showing comparison between experiment and lattice calculations](image-url)
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
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

C. Morningstar Excited States
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

\[ C^L(P) = \sigma \sigma^+ + \sigma iK \sigma^+ + \cdots \]

- Bethe-Salpeter kernel

\[ iK = \times + \bullet + \circ + \cdots \]

- $C^\infty(P)$ 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
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 $i\mathcal{M}$

\[ A = \sigma + \sigma iK + \sigma iK + \ldots \]

\[ A' = \sigma^\dagger + iK \sigma^\dagger + \ldots \]

\[ i\mathcal{M} = iK + iK + iK + \ldots \]
subtracted correlator $C_{\text{sub}}(P) = C^L(P) - C^\infty(P)$ given by

$$C_{\text{sub}}(P) = \begin{array}{c}
A \quad A' \\
\mathcal{F} \quad \mathcal{F}
\end{array} + \begin{array}{c}
A \quad iM \\
\mathcal{F} \quad \mathcal{F}
\end{array} + \begin{array}{c}
A \quad iM \\
\mathcal{F} \quad \mathcal{F}
\end{array} + \begin{array}{c}
iM \quad A' \\
\mathcal{F} \quad \mathcal{F}
\end{array} + \ldots$$

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 $\mathbf{P} = (2\pi/L)d$, 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:

\[
E_{cm} = \sqrt{E^2 - \mathbf{P}^2}, \quad \gamma = \frac{E}{E_{cm}},
\]

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

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

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

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

where $F$ matrix defined next slide

C. Morningstar

Excited States
Phase shifts from finite-volume energies (con’t)

- $F$ matrix in $JLS$ basis states given by
  \[
  F_{J'm_j'L'S'a'}^{(s,\gamma,u)}; Jm_jLSa = \frac{\rho_a}{2} \delta_{a'a} \delta_{S'S} \left\{ \delta_{J'J} \delta_{m_j'm_j} \delta_{L'L} \\
  + W_{L'm_{L'}; Lm_L}^{(s,\gamma,u)} \langle J'm_j' | L'm_{L'}, Ss_S \rangle \langle Lm_L, Ss_S | Jm_J \rangle \right\},
  \]
- 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
  \[
  W_{L'm_{L'}; Lm_L}^{(s,\gamma,u)} = \frac{2i}{\pi \gamma u^{l+1}} \mathcal{Z}_{lm}(s, \gamma, u^2) \int d^2\Omega \ Y_{L'm_{L'}}^*(\Omega) Y_{lm}(\Omega) Y_{Lm_L}(\Omega)
  \]
- Rummukainen-Gottlieb-Lüscher (RGL) shifted zeta functions $\mathcal{Z}_{lm}$ 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

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

$$+ \delta_l 0 \gamma \pi e^{\Lambda u^2} \left( 2u D(u \sqrt{\Lambda}) - \Lambda^{-1/2} \right)$$

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

where

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

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

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

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

choose $\Lambda \approx 1$ for convergence of the summation

integral done Gauss-Legendre quadrature, Dawson with Rybicki
for \( P \)-wave phase shift \( \delta_1(E_{\text{cm}}) \) for \( \pi\pi \) \( I = 1 \) scattering

\[
\cot \delta_1 = \frac{\mathcal{Z}_{lm}(s, \gamma, u^2)}{\gamma \pi^{3/2} u^{l+1}}
\]

<table>
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<th>( d )</th>
<th>( \Lambda )</th>
<th>( \cot \delta_1 )</th>
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<td>( T^{+}_{1\mu} )</td>
<td>( \text{Re } w_{0,0} )</td>
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<tr>
<td>(1,1,1)</td>
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</tbody>
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\[ C. \text{ Morningstar} \]
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 $\left(\pi/(16\xi)\right)^2$, 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)

\[
\tan(\delta_1) = \frac{\Gamma/2}{m_r - E} + A \quad \text{and} \quad \Gamma = \frac{g^2}{48\pi m_r^2} \left(m_r^2 - 4m_\pi^2\right)^{3/2}
\]
References


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 $\rightarrow$ need new effective field theory techniques