Excited States from the Stochastic LapH Method

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Outline

- goals
  - comprehensive survey of energy spectrum of QCD stationary states in a finite volume
  - hadron scattering phase shifts, decay widths, matrix elements
- extracting excited-state energies
- single-hadron operators
- multi-hadron operators
- the stochastic LapH method
- first results in ρ-channel: $I = 1, \; S = 0, \; T_{1u}^{+}$
  - used 56×56 matrix of correlators
  - 12 single-hadron operators
  - 17 "$\pi\pi$" operators
  - 14 "$\eta\pi$" operators, 3 "$\phi\pi$" operators
  - 10 "$K\overline{K}$" operators
- preliminary results using 59×59 matrix of correlators in the bosonic $I = \frac{1}{2}, \; S = 1, \; T_{1u}$

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  - Ranger+Stampede at TACC

Excited states from correlation matrices

- extract excited energies from matrices of temporal correlations
- $N \times N$ Hermitian correlation matrix $C_{ij}(t_F - t_0) = \langle 0 | \, O_i(t_F) \, \overline{O}_j(t_0) \, | 0 \rangle$
- N *principal correlators* $\lambda_\alpha(t, \tau_0)$ are eigenvalues of

$$C(\tau_0)^{-1/2} \, C(t) \, C(\tau_0)^{-1/2}$$

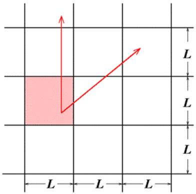
- large time separation: $\lim_{t\to\infty} \lambda_\alpha(t, \tau_0) = e^{-(t-\tau_0)E_\alpha}$
- N principal effective masses

$$m_\alpha^{\text{eff}}(t) = \ln\left(\frac{\lambda_\alpha(t, \tau_0)}{\lambda_\alpha(t+1, \tau_0)}\right)$$

  tend to N lowest-lying stationary state energies in a channel
- extracting energy of level α requires careful consideration of all lower-lying and nearby levels
  - multi-hadron states below most resonances

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

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

  - 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 $-$)

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:

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

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

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

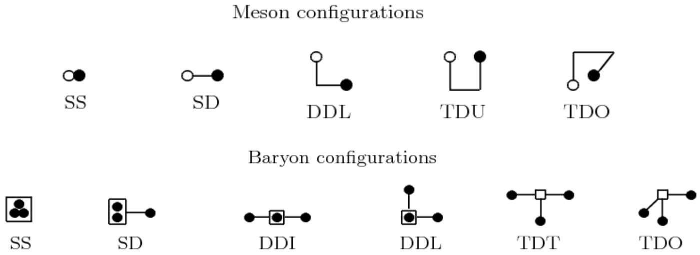
- to good approximation, LapH smearing operator is

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

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

Extended operators for single hadrons

- quark displacements build up orbital, radial structure



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

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

- group-theory projections onto irreps of lattice symmetry group

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

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

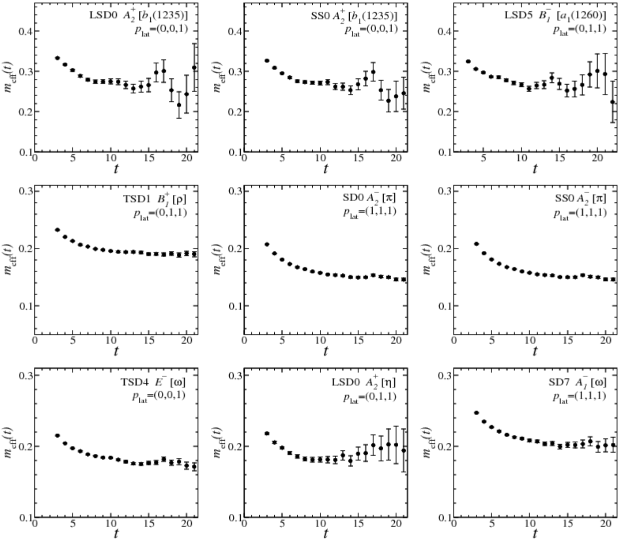
Ensembles and run parameters

- 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

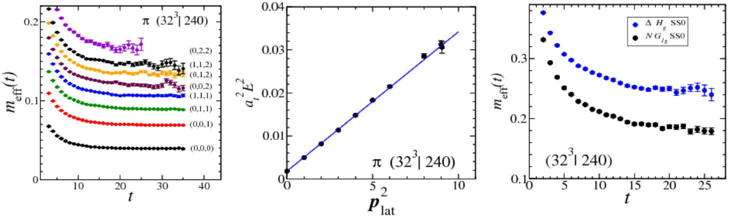
Testing single-hadron operators

- meson effective masses on $(24^3|390)$ ensemble



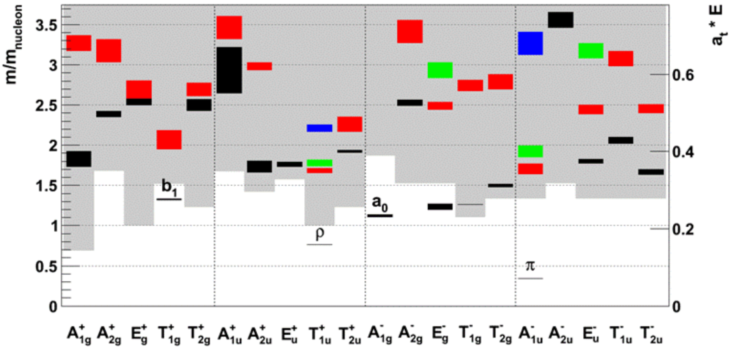
Testing single-hadron operators (con't)

- (left and center) pion energies on $(32^3|240)$ ensemble
- (right) nucleon and Δ baryons



Isovector meson spectrum: a first glance

- first glance at isovector meson spectrum
- single-hadron operators only, 170 configs of $(24^3|390)$ ensemble
- shaded region shows where multi-hadron states possible



- multi-hadron operators could be crucial!!

Two-hadron operators

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

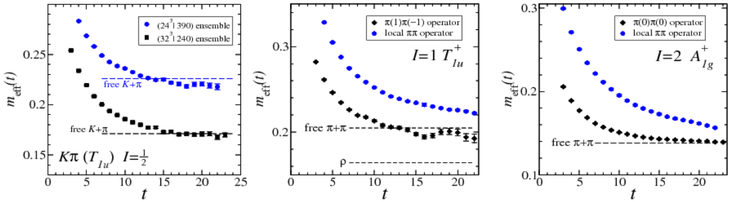
$$c^{I_{3a} I_{3b}}_{\boldsymbol{p}_a \lambda_a;\ \boldsymbol{p}_b \lambda_b}\ B^{I_a I_{3a} S_a}_{\boldsymbol{p}_a \Lambda_a \lambda_a i_a}\ B^{I_b I_{3b} S_b}_{\boldsymbol{p}_b \Lambda_b \lambda_b i_b}$$

- 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

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

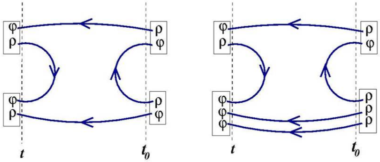
$$(\pi\pi)^{A_{1g}^+}(t) = \sum_{\boldsymbol{x}} \pi^+(\boldsymbol{x},t)\ \pi^+(\boldsymbol{x},t),$$
$$(\pi\pi)^{T_{1u}^+}(t) = \sum_{\boldsymbol{x},k=1,2,3} \left\{ \pi^+(\boldsymbol{x},t)\ \Delta_k \pi^0(\boldsymbol{x},t) - \pi^0(\boldsymbol{x},t)\ \Delta_k \pi^+(\boldsymbol{x},t) \right\}$$



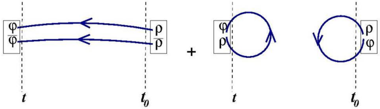
- less contamination from higher states in our $\pi\pi$ operators

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:

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

- 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)

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:

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

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

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

- occasionally use γ_5-Hermiticity to switch source and sink

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

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

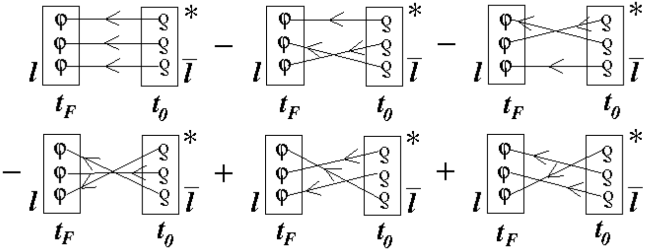
$$C_{l\bar{l}} \approx \frac{1}{N_R}\sum_{r}\sum_{d_A d_B d_C} \mathcal{B}^{(r)[d_A d_B d_C]}_{l}(\varphi^{A},\varphi^{B},\varphi^{C})\, \mathcal{B}^{(r)[d_A d_B d_C]}_{\bar{l}}(\varrho^{A},\varrho^{B},\varrho^{C})^{*}$$

Correlators and quark line diagrams

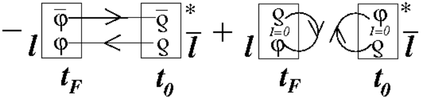
- baryon correlator

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

- express diagrammatically

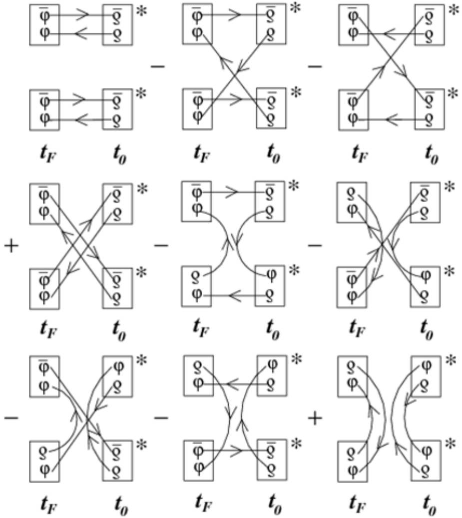


- meson correlator



More complicated correlators

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

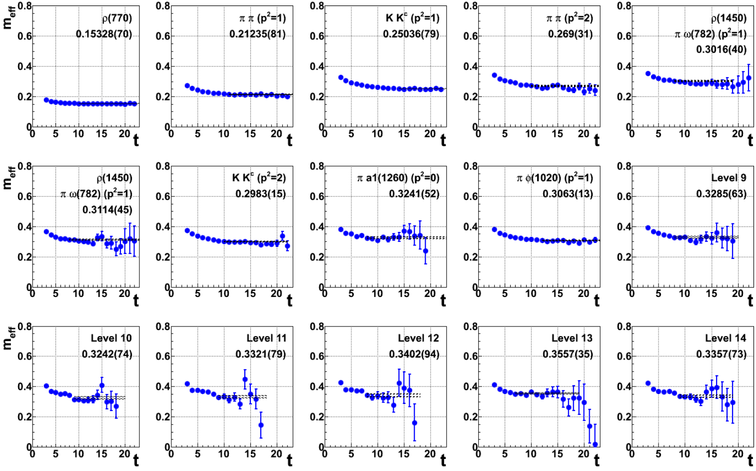


First results

- first part of summer spent testing last_laph software
  - testing of all flavor channels for single and two-mesons completed
  - comparison of results from last_laph with independent code
  - myriad of orthgonality tests
- first focus on the resonance-rich ρ-channel: $I = 1,\ S = 0,\ T_{1u}^{+}$
- experiment: $\rho(770)$, $\rho(1450)$, $\rho(1570)$, $\rho_3(1690)$, $\rho(1700)$
  - interpretation of these states still controversial
- first results: 56×56 matrix of correlators $(24^3|390)$ ensemble
  - 12 single-hadron (quark-antiquark) operators
  - 17 "$\pi\pi$" operators
  - 14 "$\eta\pi$" operators, 3 "$\phi\pi$" operators
  - 10 "$K\overline{K}$" operators
- our results are only weeks old!
- good condition number, diagonalization using $\tau_0 = 4$
- still finalizing analysis code

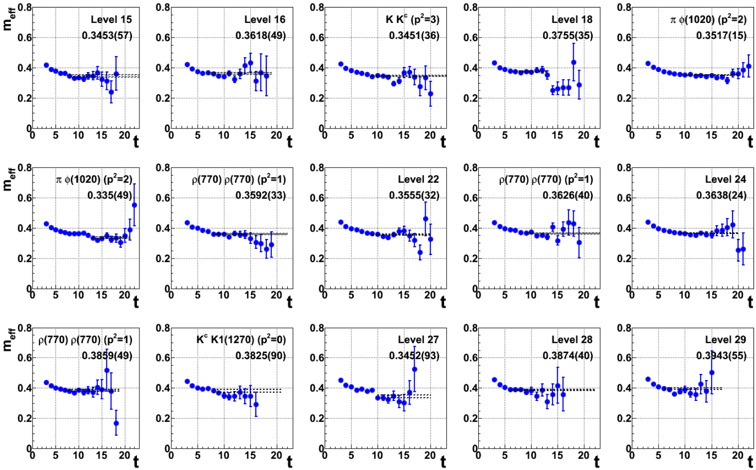
Bosonic $I = 1,\ S = 0,\ T_{1u}^{+}$ channel

- “principal” effective masses



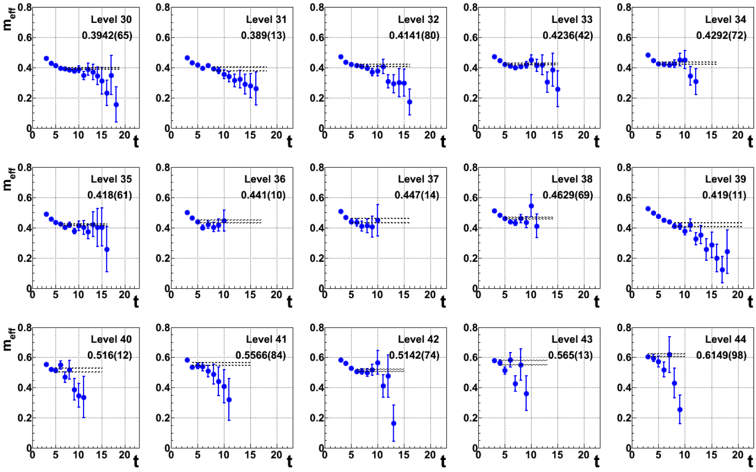
Bosonic $I = 1,\ S = 0,\ T_{1u}^{+}$ channel

- more “principal” effective masses



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

- even more “principal” effective masses



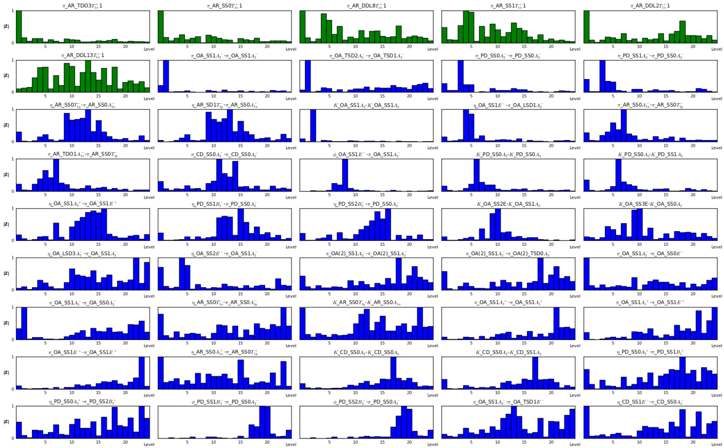
Bosonic $I = 1,\ S = 0,\ T_{1u}^{+}$ channel

- spectrum discrete so two-point functions have form

$$C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*}\ e^{-E_n t}$$

$$Z_j^{(n)*} = \langle n|\ \overline{O}_j\ |0\rangle, \qquad Z_j^{(n)} = \langle 0|\ O_j\ |n\rangle$$

- *preliminary* estimates of Z overlaps for various operators:



Issues

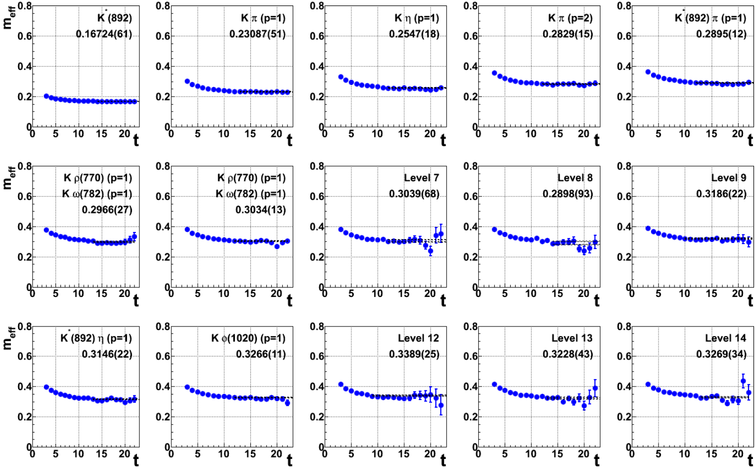
- next challenge: identifying the levels
- must address presence of 3 and 4 meson states
- must address scalar particles in spectrum
  - vacuum subtractions
  - neglect due to OZI suppression?

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

- also have results for the kaon channel: $I = \frac{1}{2},\ S = 1,\ T_{1u}$
- experiment: $K^*(892)$, $K^*(1410)$, $K^*(1680)$, $K_3^*(1780)$
- first results: 59×59 matrix of correlators $(24^3|390)$ ensemble
  - 10 single-hadron (quark-antiquark) operators
  - 25 "$K\pi$" operators
  - 12 "$K\eta$" operators, 12 "$K\phi$" operators

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

- “principal” effective masses



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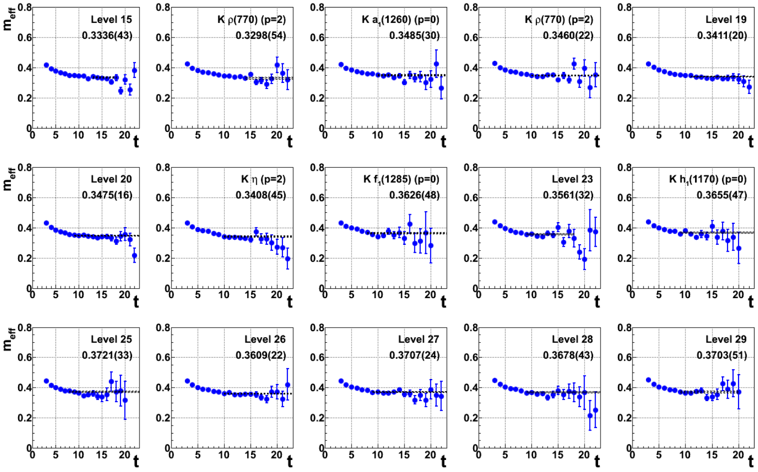

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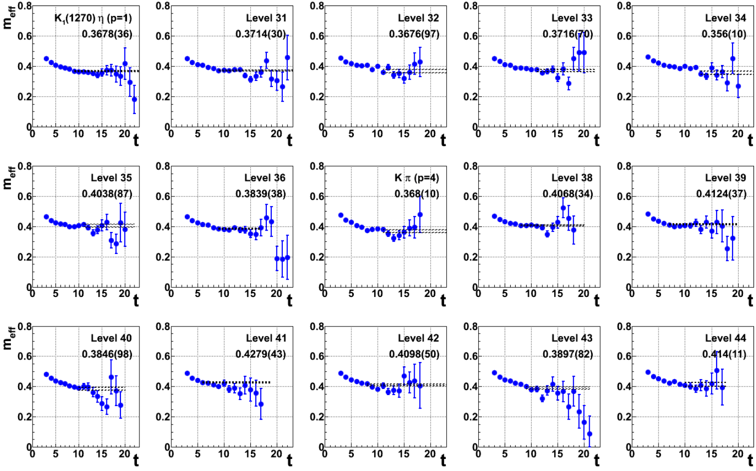
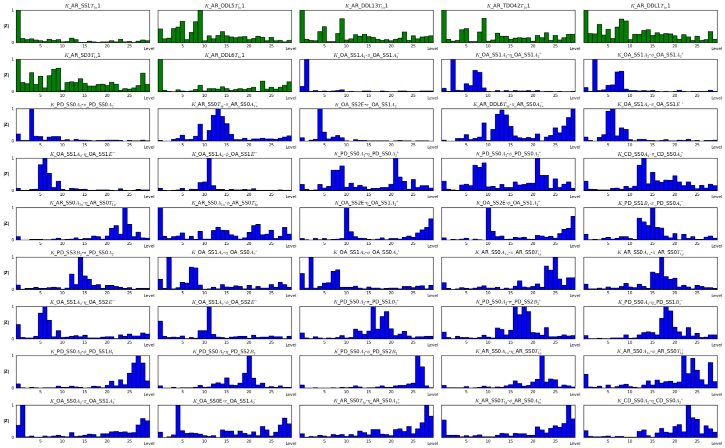
- even more "principal" effective masses



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

- *preliminary* estimates of Z overlaps for various operators:



Conclusion and future work

- 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
- showed first results in ρ-channel: $I = 1,\ S = 0,\ T_{1u}^{+}$ using 56×56 matrix of correlators
- preliminary results using 59×59 matrix of correlators in the bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$
- large number of channels to study over the next year!
- first peek: results on $(32^3|240)$ ensemble look even better so far!!
- investigations of various scattering phase shifts also planned for near future

References

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