Dealing with multi-quark operators in lattice QCD

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XSEDE

Extreme Science and Engineering Discovery Environment

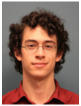
Overview

- 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
CMU

Andrew Hanlon
Pitt

Bijit Singha
CMU

- former CMU postdocs:

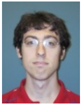
Justin Foley
Software,
NVIDIA

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
  - Comet at SDSC

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

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

Integrating the quark fields

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

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

- baryon-to-baryon example:

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

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

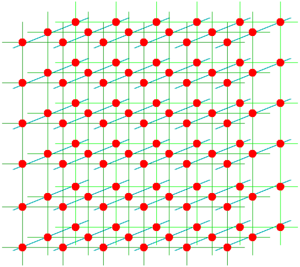
$$U_1, U_2, \ldots, U_N$$

- 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 $Z_j^{(n)}$

Excited states in lattice QCD timeline

- LHPC spectroscopy effort: Isgur and Negele 2001
- initial excited-state skepticism: Bob Sugar
- operator construction PRD **72**, 094506 (2005)
- Lichtl at Lattice 2005 in Dublin: "we'll get twelve levels or more"
- first quenched results: PRD **76** 074504 (2007)
  - point-to-all propagators
- need to incorporate multi-hadron operators begins 2007
- distillation for small lattices: PRD **80**, 054506 (2009)
- stochastic LapH for large lattices: PRD **83**, 114505 (2011)

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:

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

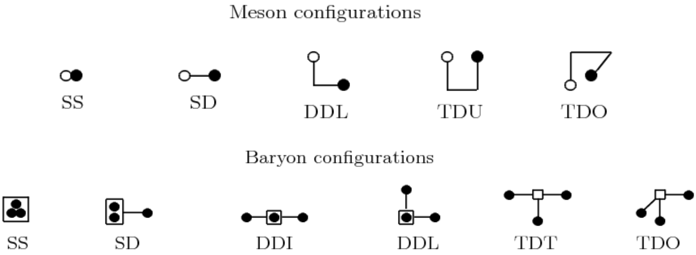
- to good approximation, LapH smearing operator is

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

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

Extended operators for single hadrons

- quark displacements build up orbital, radial structure



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

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

- group-theory projections onto irreps of lattice symmetry group

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

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

Two-hadron operators

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

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

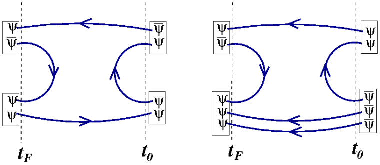
- fixed total momentum $\boldsymbol{p} = \boldsymbol{p}_a + \boldsymbol{p}_b$, fixed $\Lambda_a, i_a, \Lambda_b, i_b$
- group-theory projections onto little group of $\boldsymbol{p}$ and isospin irreps
- restrict attention to certain classes of momentum directions
  - on axis $\pm\hat{\boldsymbol{x}},\ \pm\hat{\boldsymbol{y}},\ \pm\hat{\boldsymbol{z}}$
  - planar diagonal $\pm\hat{\boldsymbol{x}}\pm\hat{\boldsymbol{y}},\ \pm\hat{\boldsymbol{x}}\pm\hat{\boldsymbol{z}},\ \pm\hat{\boldsymbol{y}}\pm\hat{\boldsymbol{z}}$
  - cubic diagonal $\pm\hat{\boldsymbol{x}}\pm\hat{\boldsymbol{y}}\pm\hat{\boldsymbol{z}}$
- 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

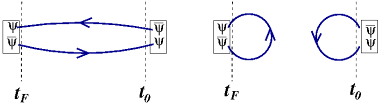
- quark propagator is inverse K^{-1} of Dirac matrix
  - rows/columns involve lattice site, spin, color
  - very large $N_{\rm tot} \times N_{\rm tot}$ matrix for each flavor
$$N_{\rm tot} = N_{\rm site} N_{\rm spin} N_{\rm color}$$
  - for $32^3 \times 256$ lattice, $N_{\rm tot} \sim 101$ million
- 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:

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

- 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

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

- define baryon source and sink

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

- correlator is dot product of source vector with sink vector

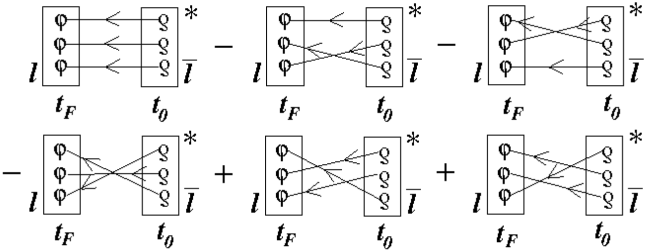
$$C_{l\bar{l}} \approx \frac{1}{N_R}\sum_{r}\sum_{d_A d_B d_C} \mathcal{B}^{(r)[d_A d_B d_C]}_{l}(\varphi^{A},\varphi^{B},\varphi^{C})\,\mathcal{B}^{(r)[d_A d_B d_C]}_{\bar{l}}(\varrho^{A},\varrho^{B},\varrho^{C})^{*}$$

Correlators and quark line diagrams

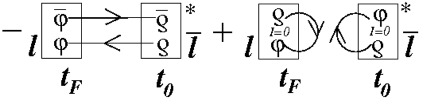
- baryon correlator

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

- express diagrammatically

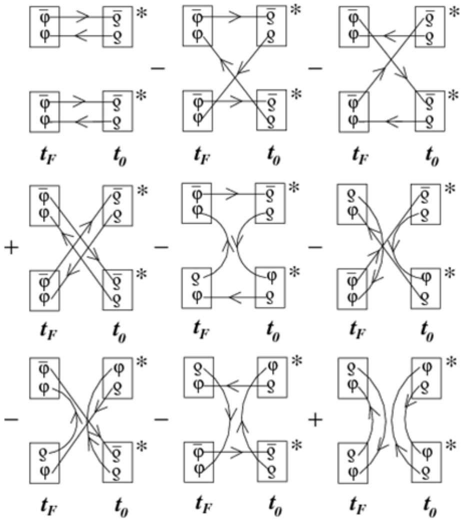


- meson correlator



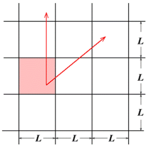
More complicated correlators

- 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

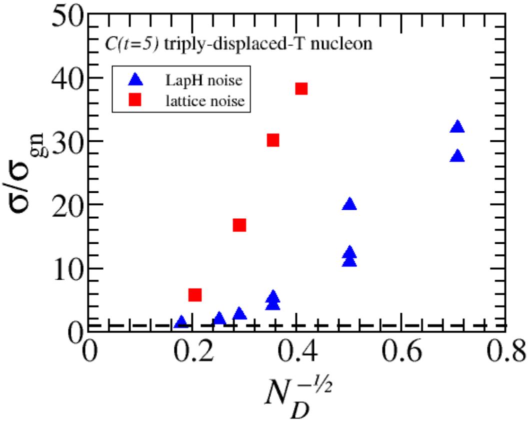
- numbers of occurrences of Λ irreps in J subduced

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

The effectiveness of stochastic LapH

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



Ensembles and run parameters

- focusing on two Monte Carlo ensembles
  - $(32^3|240)$: 412 configs $32^3 \times 256$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 4.4$
  - $(24^3|390)$: 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

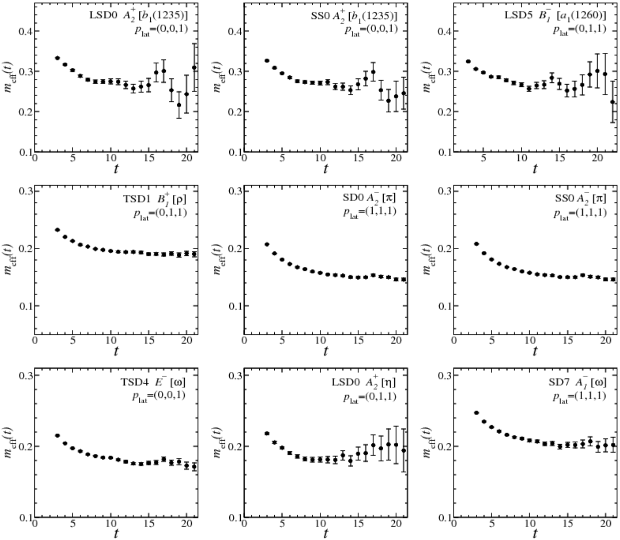
Kraken at NICS

Stampede at TACC

Comet at SDSC

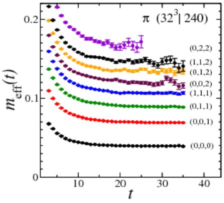
Testing single-hadron operators

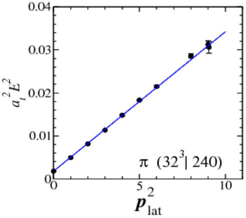
- meson effective masses on $(24^3|390)$ ensemble

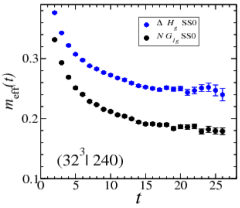


Testing single-hadron operators (con't)

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





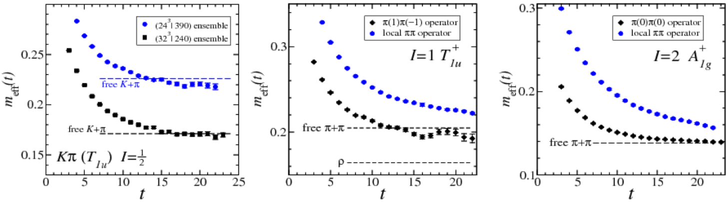


Testing our two-meson operators

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

$$(\pi\pi)^{A_{1g}^{+}}(t) \quad = \quad \sum_{\boldsymbol{x}} \pi^{+}(\boldsymbol{x},t)\ \pi^{+}(\boldsymbol{x},t),$$

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

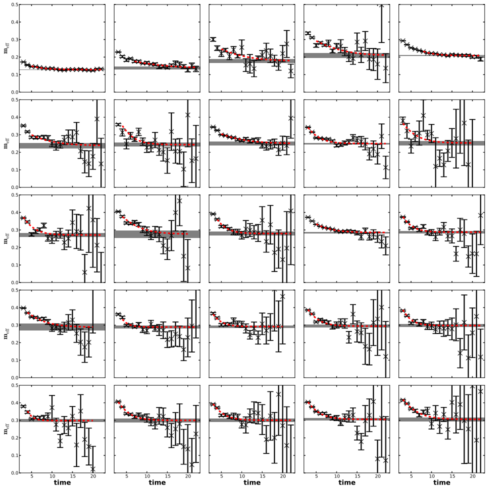


- less contamination from higher states in our $\pi\pi$ operators

Status report

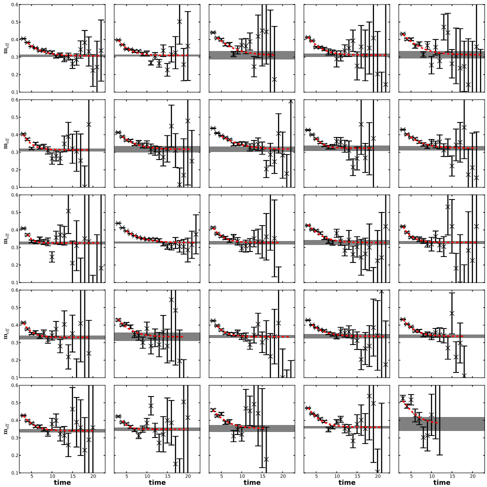
- correlator software last_laph completed summer 2013
  - testing of all flavor channels for single and two-mesons completed fall 2013
  - testing of all flavor channels for single baryon and meson-baryons completed summer 2014
- small-a expansions of all operators completed
- first focus on the resonance-rich 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 $I = 1,\ S = 0$

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ for levels 0 to 24 (B. Fahy, PhD thesis)
- energies obtained from two-exponential fits



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

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

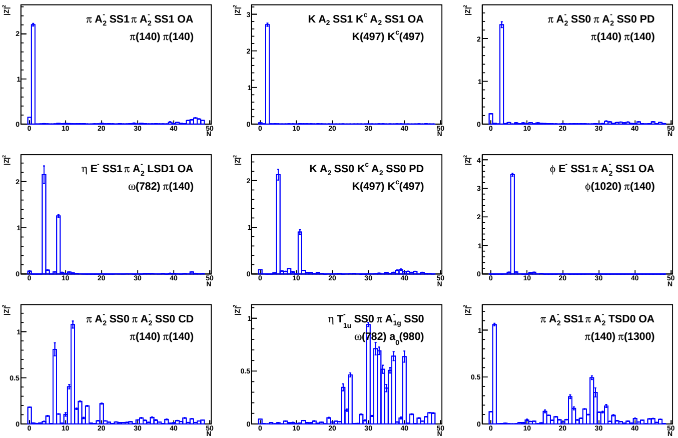


Level identification

- 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

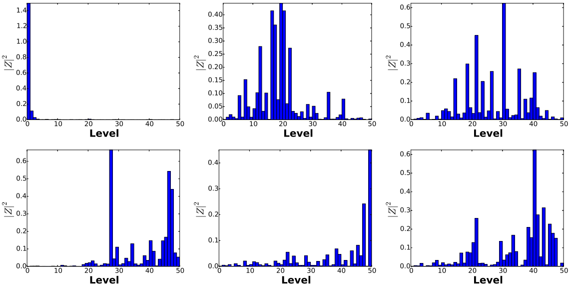
- overlaps for various operators



Identifying quark-antiquark resonances

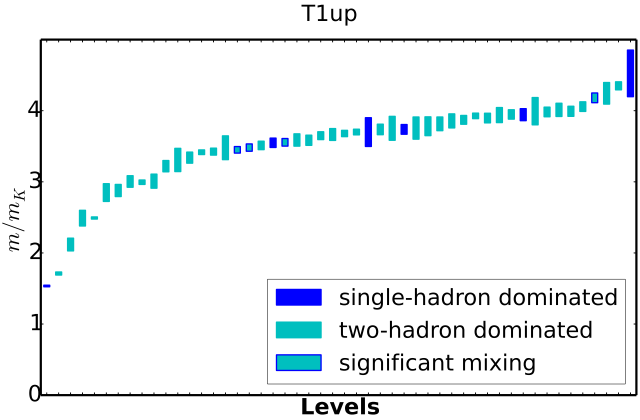
- resonances: finite-volume "precursor states"
- probes: *optimized* single-hadron operators
  - analyze matrix of just single-hadron operators $O_i^{[SH]}$ (12×12)
  - perform single-rotation as before to build probe operators $O_m'^{[SH]} = \sum_i v_i'^{(m)*} O_i^{[SH]}$
- obtain Z' factors of these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

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



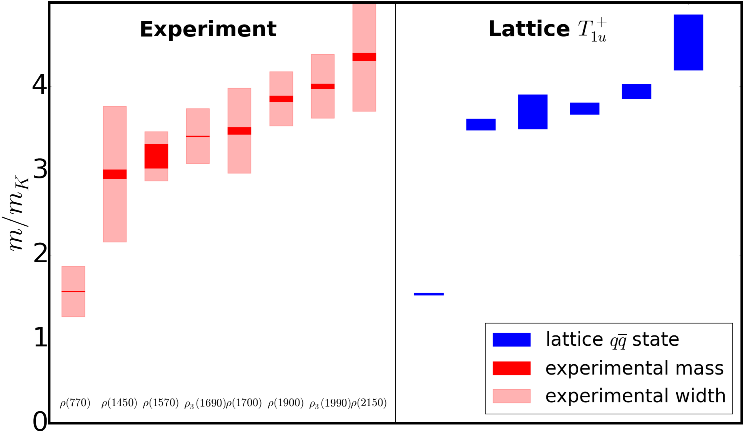
Staircase of energy levels

- 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

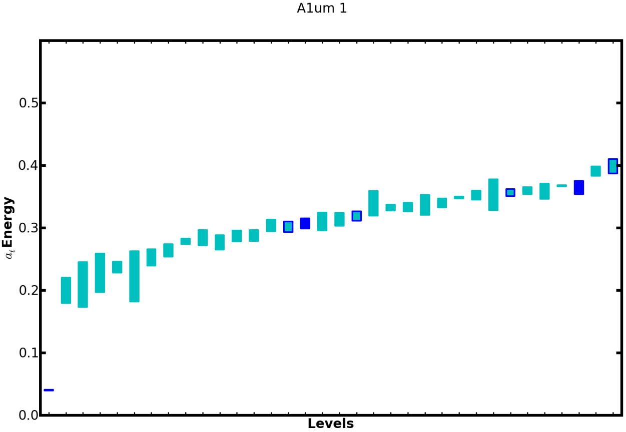


Issues

- 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

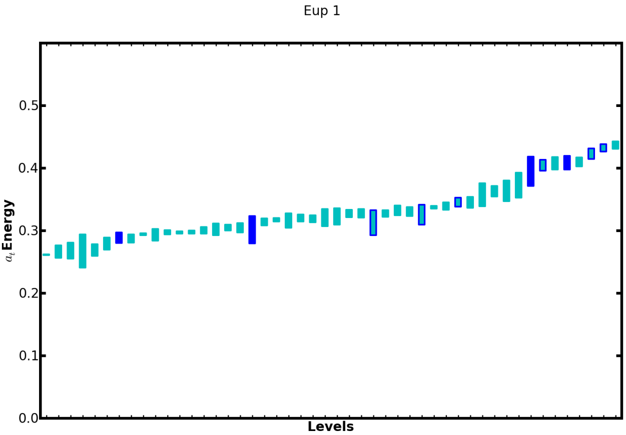
Bosonic $I = 1,\ S = 0,\ A_{1u}^{-}$ channel

- 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



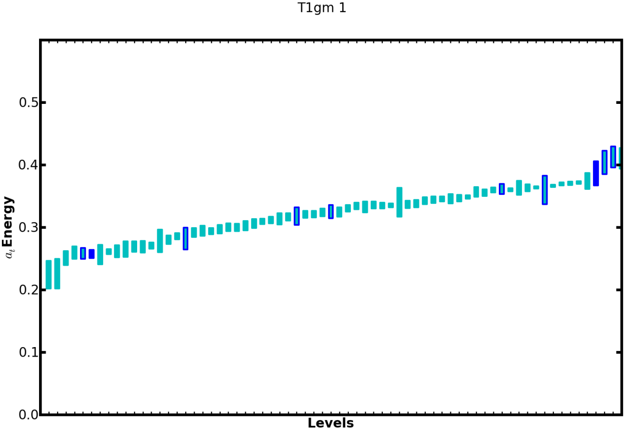
Bosonic $I=1,\ S=0,\ E_u^+$ channel

- 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



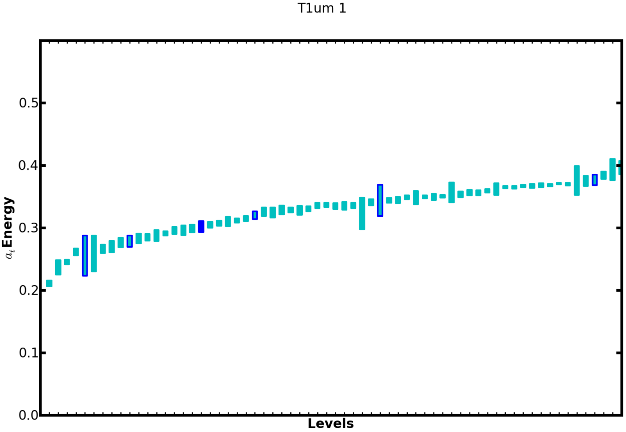
Bosonic $I = 1,\ S = 0,\ T_{1g}^{-}$ channel

- 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



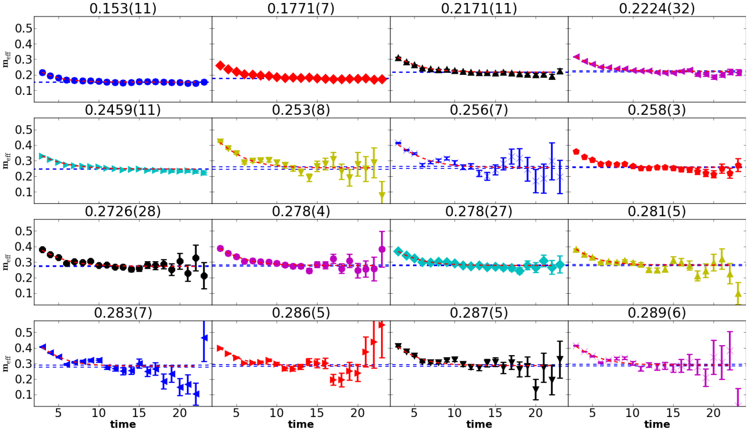
Bosonic $I = 1,\ S = 0,\ T_{1u}^{-}$ channel

- 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



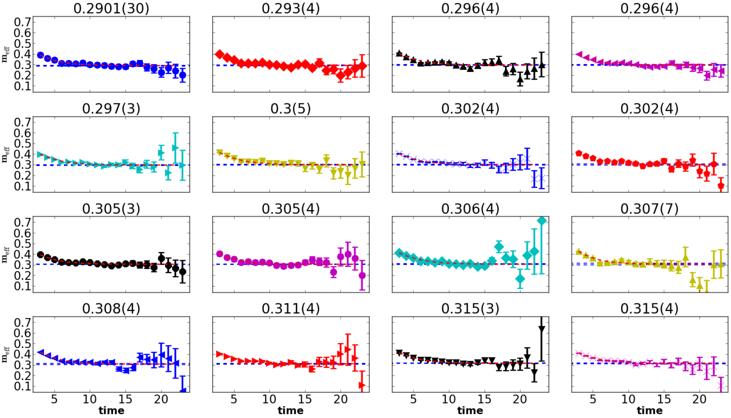
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

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



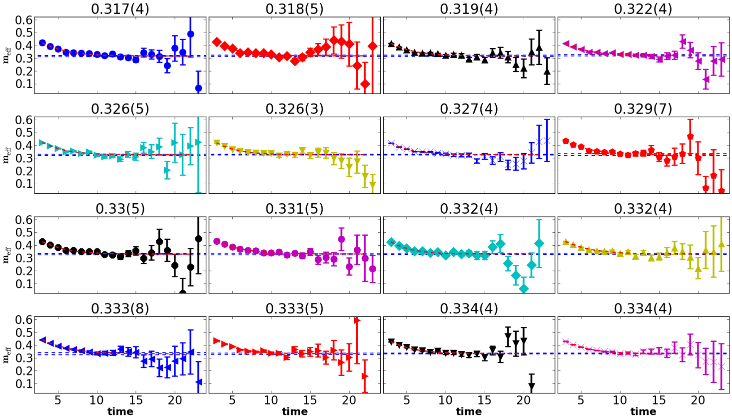
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- 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



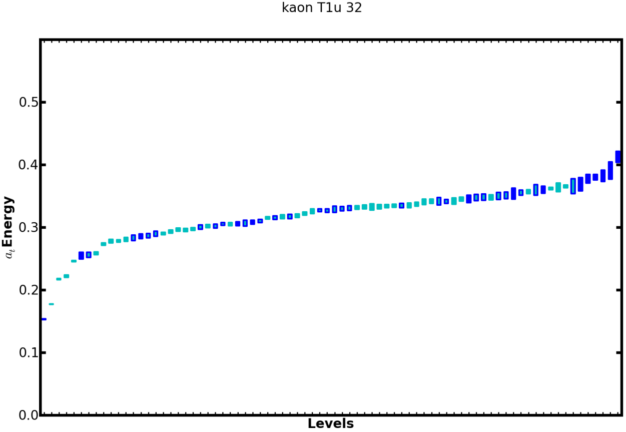
Bosonic $I = \frac{1}{2},\ S = 1,\ T_{1u}$ channel

- effective energies $\widetilde{m}^{\mathrm{eff}}(t)$ 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



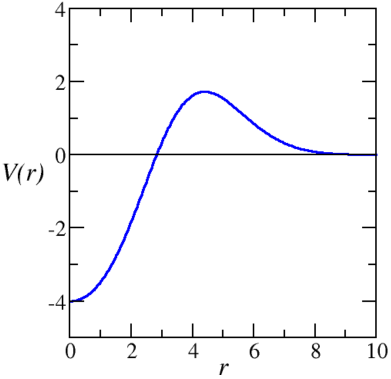
Scattering phase shifts in lattice QCD timeline

- DeWitt 1956: finite-volume energies related to scattering phase shifts
- Lüscher 1984: quantum mechanics in a box
- Rummukainen and Gottlieb 1995: nonzero total momenta
- Kim, Sachrajda, and Sharpe 2005: field theoretic derivation
- explosion of papers since then
- generalized to arbitrary spin, multiple channels

Resonances in a box: an example

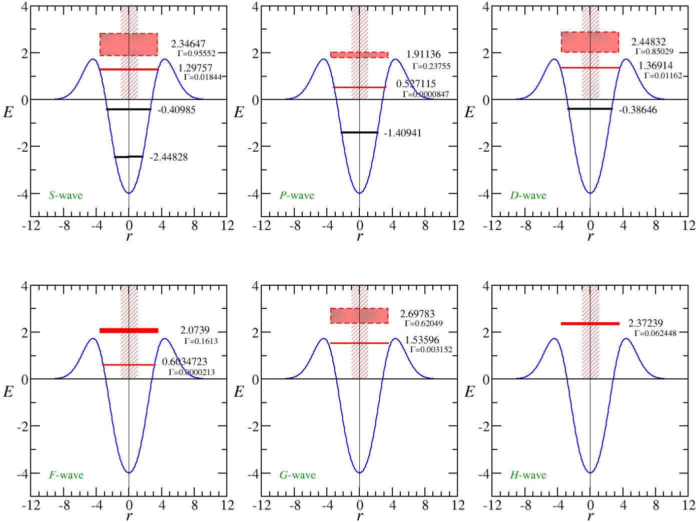
- consider a simple quantum mechanical example
- Hamiltonian

$$H = \frac{1}{2}\boldsymbol{p}^2 + V(r), \qquad V(r) = \left(-4 + \frac{1}{16}r^4\right) e^{-r^2/8}$$



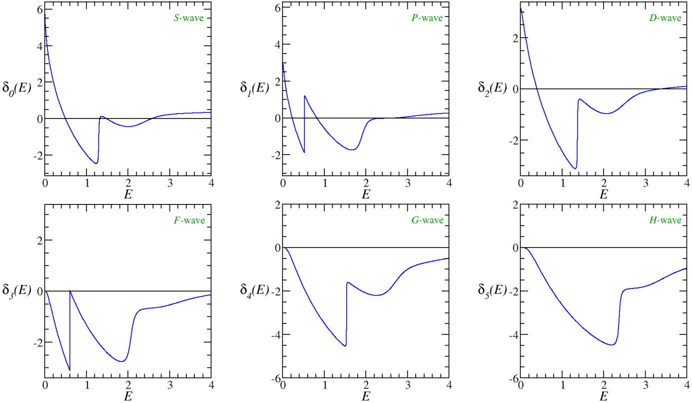
Spectrum of example Hamiltonian

- spectrum for $E < 4$ and $l = 0, 1, 2, 3, 4, 5$ of example system



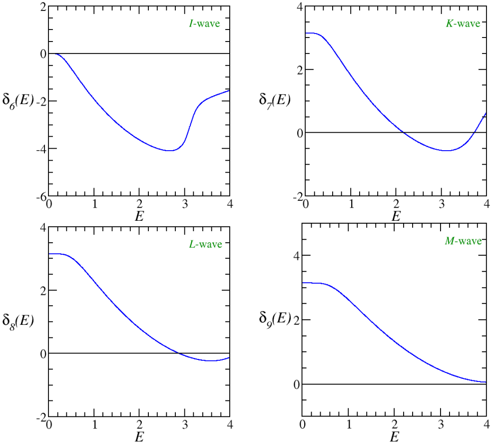
Scattering phase shifts

- scattering phase shifts for various partial waves



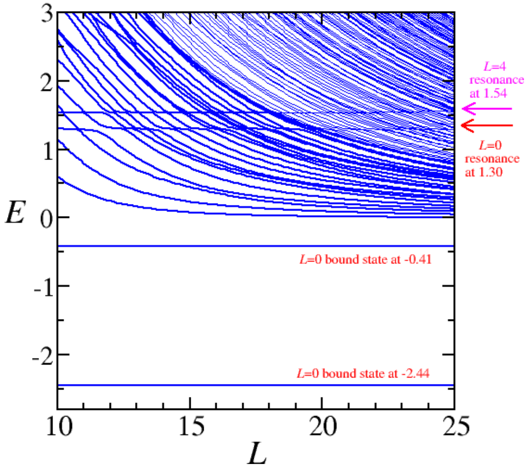
More scattering phase shifts

- scattering phase shifts for higher partial waves



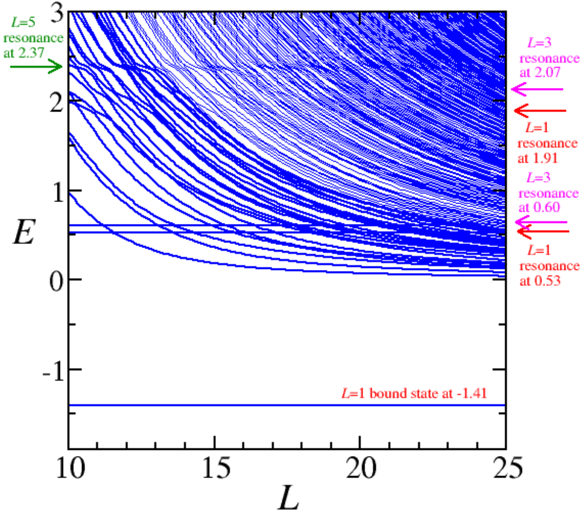
Spectrum in box: A_{1g} channel

- spectrum discrete in box, periodic b.c., momenta quantized
- stationary-state energies in A_{1g} channel shown below
- narrow resonance is avoided level crossing, broad resonances?



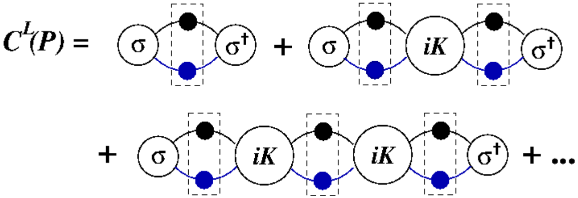
Spectrum in box: T_{1u} channel

- stationary-state energies in T_{1u} channel shown below

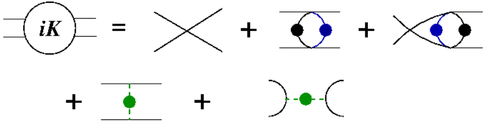


Scattering phase shifts from finite-volume energies

- correlator of two-particle operator σ in finite volume



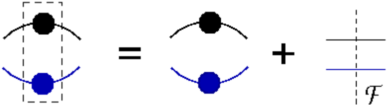
- Bethe-Salpeter kernel



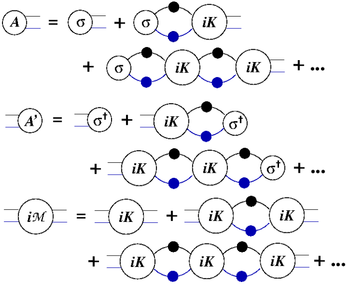
- $C^\infty(P)$ has branch cuts where two-particle thresholds begin
- momentum quantization in finite volume: cuts $\rightarrow$ series of poles
- C^L poles: two-particle energy spectrum of finite volume theory

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

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

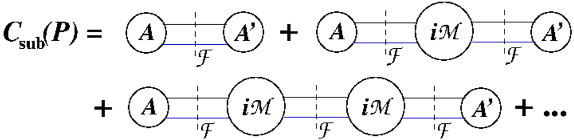


- define the following quantities: A, A', invariant scattering amplitude $i\mathcal{M}$



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

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



- sum geometric series

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

- poles of $C_{\rm sub}(P)$ are poles of $C^L(P)$ from $\det(1 - i\mathcal{M}\mathcal{F}) = 0$
- key tool: for $g_c(\boldsymbol{p})$ spatially contained and regular

$$\frac{1}{L^3}\sum_{\boldsymbol{p}} g_c(\boldsymbol{p}) = \int \frac{d^3k}{(2\pi)^3}\ g_c(\mathbf{k}) + O(e^{-mL})$$

$$\frac{1}{L^3}\sum_{\boldsymbol{p}} \frac{g_c(\boldsymbol{p}^2)}{(\boldsymbol{p}^2 - a^2)} = \frac{1}{L^3}\sum_{\boldsymbol{p}} \frac{g_c(a^2)}{(\boldsymbol{p}^2 - a^2)} + \int \frac{d^3k}{(2\pi)^3} \frac{g_c(\boldsymbol{p}^2) - g(a^2)}{(\boldsymbol{p}^2 - a^2)} + O(e^{-mL})$$

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:

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

- 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

$$\mathcal{Z}_{lm}(\boldsymbol{s},\gamma,u^2) = \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \frac{\mathcal{Y}_{lm}(\boldsymbol{z})}{(\boldsymbol{z}^2-u^2)} e^{-\Lambda(\boldsymbol{z}^2-u^2)} + \delta_{l0}\frac{\gamma\pi}{\sqrt{\Lambda}} F_0(\Lambda u^2)$$

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

- where

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

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

$$F_0(x) = -1 + \frac{1}{2}\int_0^1 dt\ \frac{e^{tx}-1}{t^{3/2}}$$

- choose $\Lambda \approx 1$ for convergence of the summation
- integral done Gauss-Legendre quadrature
- $F_0(x)$ given in terms of Dawson or erf function

Block diagonalization of F matrix

- quantization condition is large determinant relation:

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

- define the matrix

$$B^{(R)}_{J'm_{J'}L'S'a';\ Jm_JLSa} = \delta_{J'J}\delta_{L'L}\delta_{S'S}\delta_{a'a}D^{(J)*}_{m_{J'}m_J}(R)$$

- can show that under lattice symmetry operator R,

$$F^{(R\boldsymbol{s},\gamma,u)} = B^{(R)}\ F^{(\boldsymbol{s},\gamma,u)}\ B^{(R)\dagger}$$

- can block diagonalize F by diagonalizing $D^{(J)}_{m'm}(R)$ for each J
- change of basis: little group irrep Λ, row λ, n occurrence of Λ in $D^{(J)}_{m'm}(R)$

$$|\Lambda\lambda nJLSa\rangle = \sum_{m_J} c^{\Lambda\lambda n}_{Jm_J}|Jm_JLSa\rangle$$

- F diagonal in Λ, λ, but not in n_Λ
- can now focus on the matrix elements:

$$F^{(\boldsymbol{s},\gamma,u)(\Lambda,\lambda)}_{J'n'L'S'a';\ JnLSa}$$

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

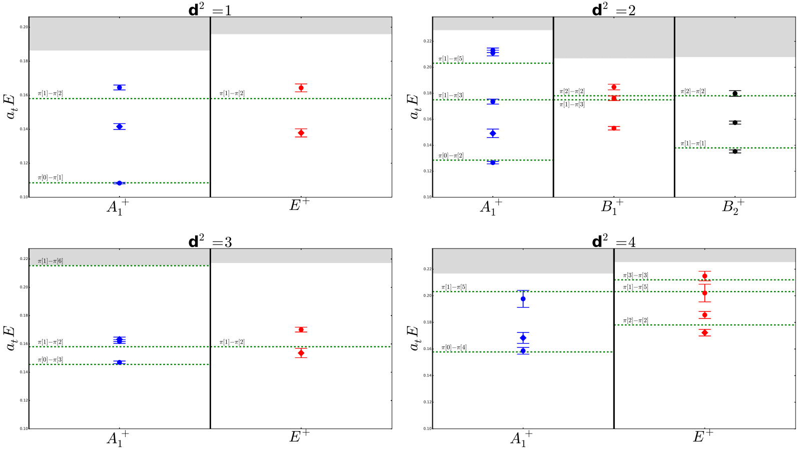
- for P-wave phase shift $\delta_1(E_{\rm cm})$ for $\pi\pi$ $I = 1$ scattering
- define

$$w_{lm} = \frac{\mathcal{Z}_{lm}(\boldsymbol{s}, \gamma, u^2)}{\gamma \pi^{3/2} u^{l+1}}$$

$\boldsymbol{d}$	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

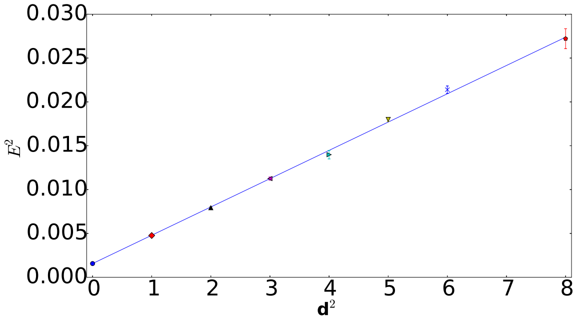


Pion dispersion relation

- 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 $\xi = a_s/a_t$

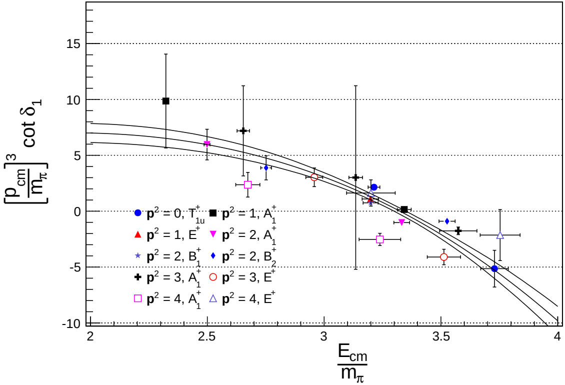


$I = 1$ $\pi\pi$ scattering phase shift and width of the ρ

- results $32^3 \times 256$, $m_\pi \approx 240$ MeV:

$$g_{\rho\pi\pi} = 6.16(36),\ m_\rho/m_\pi = 3.324(24),\ \chi^2/\text{dof} = 1.43$$

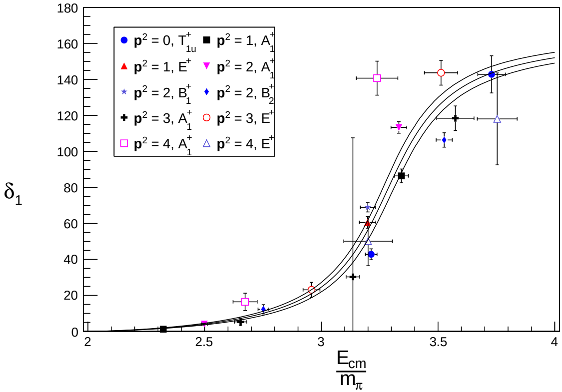
- additional collaborator: Ben Hoerz (Dublin)



- fit $\quad g_{\rho\pi\pi}^2 q_{\text{cm}}^3 \cot(\delta_1) = 6\pi E_{\text{cm}}(m_\rho^2 - E_{\text{cm}}^2)$

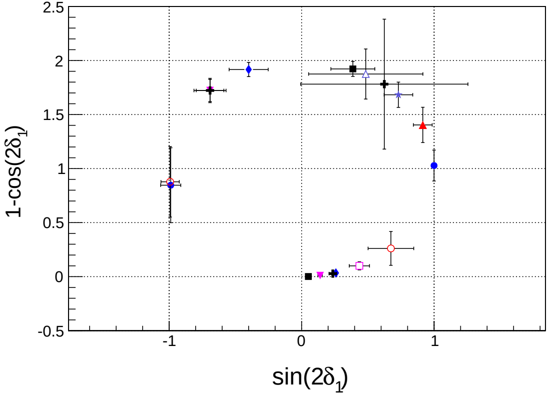
$I = 1$ $\pi\pi$ scattering phase shift and width of the ρ

- results $32^3 \times 256$, $m_\pi \approx 240$ MeV:
  $g_{\rho\pi\pi} = 6.16(36),\ m_\rho/m_\pi = 3.324(24),\ \chi^2/\text{dof} = 1.43$



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

- Argand plot of P-wave scattering phase shift

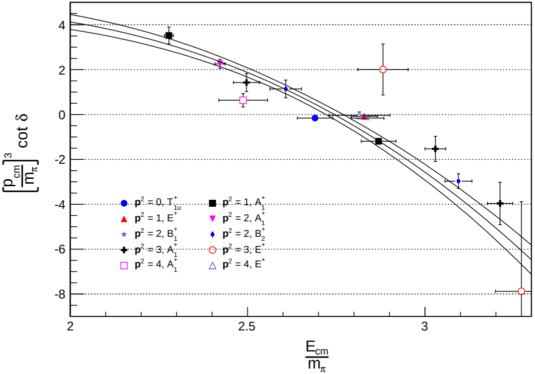


$I = 1$ $\pi\pi$ scattering phase shift and width of the ρ

- results $48^3 \times 128$, $m_\pi \approx 280$ MeV isotropic improved Wilson:

$$g_{\rho\pi\pi} = 5.68(24),\; m_\rho/m_\pi = 2.745(24),\; \chi^2/\text{dof} = 1.20$$

- plot from Ben Hoerz (Dublin)

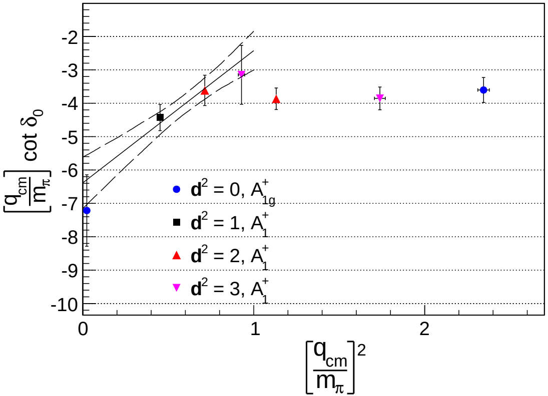


- fit $\quad g^2_{\rho\pi\pi} q^3_{\rm cm} \cot(\delta_1) = 6\pi E_{\rm cm}(m_\rho^2 - E_{\rm cm}^2)$

$I = 2\ \pi\pi$ scattering phase shift

- results $32^3 \times 256$, $m_\pi \approx 240$ MeV
- very small phase shifts

$$m_\pi a_0 = -0.157(19),\ \ m_\pi r_{\rm eff} = 7.9(2.4),\ \ \chi^2/{\rm dof} = 0.61$$



- fit $\quad q_{\rm cm}\cot(\delta_1) = \dfrac{1}{a_0} + \dfrac{1}{2} q_{\rm cm}^2 r_{\rm eff}$

References

- S. Basak et al., *Group-theoretical construction of extended baryon operators in lattice QCD*, Phys. Rev. D **72**, 094506 (2005).
- 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