Lattice QCD Study of Excited Hadron Resonances

Colin Morningstar Carnegie Mellon University

Effective Field Theories and Lattice Gauge Theory TUM Insitute for Advanced Study, Garching, Germany

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Spectrum of QCD

- spectroscopy resurgence due to discovery of unexpected charmonium XYZ states
- GlueX and JLab Hall D search for hybrids, other exotics



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Key Points

- crucial role of interpolating operators for excited-state studies in lattice QCD
- lower-lying multi-hadron levels must be dealt with
- need to handle many quark lines: stochastic LapH method
- level identification using interpolating operators
- finite-volume energies ⇒ hadron resonance properties: masses, decay widths



- focus: large 32^3 anisotropic lattices, $m_{\pi} \sim 240$ MeV
- scattering phase shifts from finite-volume energies
- need for effective Hamiltonian approach
- tetraquark operators

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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

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

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 $Z_{i}^{(n)}$

Correlator matrix toy model

• **Theorem:** For every $t \ge 0$, let $\lambda_n(t)$ be the eigenvalues of an $N \times N$ Hermitian correlation matrix C(t) ordered such that $\lambda_0 \ge \lambda_1 \ge \cdots \ge \lambda_{N-1}$, then

$$\lim_{t \to \infty} \lambda_n(t) = b_n e^{-E_n t} \Big[1 + O(e^{-t\Delta_n}) \Big],$$

$$b_n > 0, \quad \Delta_n = \min_{m \neq n} |E_n - E_m|.$$

• Example: $N_e = 200$ eigenstates with energies

$$E_0 = 0.20,$$
 $E_n = E_{n-1} + \frac{0.08}{\sqrt{n}},$ $n = 1, 2, \dots, N_e - 1.$

for $N \times N$ correlator matrix, N = 12, overlaps

$$Z_j^{(n)} = \frac{(-1)^{j+n}}{1+0.05(j-n)^2}.$$

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Correlator matrix toy model (con't)

• toy model $N_e = 200$ with 12×12 correlator matrix C(t)



- left: effective energies of diagonal elements of correlator matrix
- middle: effective energies of eigenvalues of C(t)
- right: effective energies of eigenvalues of $C(\tau_0)^{-1/2} C(t) C(\tau_0)^{-1/2}$ for $\tau_0 = 1$

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:

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

• 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

 $S = V_s V_s^{\dagger}$

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

Extended operators for single hadrons

• quark displacements build up orbital, radial structure



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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



Two-hadron operators

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

 $c_{p_a\lambda_a; p_b\lambda_b}^{I_3I_{3a}S_a} B_{p_a\Lambda_a\lambda_ai_a}^{I_bI_{3b}S_b} B_{p_b\Lambda_b\lambda_bi_b}^{I_aI_{3a}S_a}$

- 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 p and isospin irreps
- crucial to know and fix all phases of single-hadron operators for all momenta
 - each class, choose reference direction $p_{\rm ref}$
 - each p, select one reference rotation R_{ref}^{p} that transforms p_{ref} into p
- efficient creating large numbers of two-hadron operators
- generalizes to three, four, ... hadron 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]
- introduce Z_4 noise vectors η in the LapH subspace

 $\eta_{\alpha k}(t), \quad t = time, \ \alpha = spin, \ k = eigenvector number$

• 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 $P^{(a)}$, then define

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

to obtain Monte Carlo estimate with drastically reduced variance

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

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The effectiveness of stochastic LapH

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



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



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More complicated correlators

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



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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

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

• on-axis momenta: little group $C_{4\nu}$

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

• planar-diagonal momenta: little group $C_{2\nu}$

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

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

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

• 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	0	G_2	Η		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

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Ensembles and run parameters

- focusing on two Monte Carlo ensembles
 - (32³|240): 412 configs 32³ × 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 to values on 24³
 - 8 t₀ values used on 32³ lattice

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

- effective energies $\widetilde{m}^{\text{eff}}(t)$ for levels 0 to 24 (32³|240)
- energies obtained from two-exponential fits (B. Fahy, PhD thesis)



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

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



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Level identification

overlaps for various operators



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
- left: experiment (masses and widths)



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Issues

- infinite-volume resonance parameters from finite-volume energies
 - · Luscher method too cumbersome, restrictive in applicability
 - use of hadron effective Hamiltonian techniques
- 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

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

A1um 1



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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

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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

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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

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- 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 (Y.C. Jhang, PhD thesis)



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



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



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Excited States

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- 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

kaon T1u 32



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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

Scattering phase shifts from finite-volume energies

• correlator of two-particle operator σ in finite volume



• $C^{\infty}(P)$ 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 *F*



 define the following quantities: A, A', invariant scattering amplitude iM



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

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



sum geometric series

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

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

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

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

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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:

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

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

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

where F matrix defined next slide

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

F matrix in JLS basis states given by

$$F_{J'm_{J'}L'S'a'; Jm_{J}LSa}^{(s,\gamma,u)} = \frac{\rho_a}{2} \delta_{a'a} \delta_{S'S} \bigg\{ \delta_{J'J} \delta_{m_{J'}m_{J}} \delta_{L'L}$$

 $+ W_{L'm_{L'}; Lm_{L}}^{(s,\gamma,u)} \langle J'm_{J'} | L'm_{L'}, Sm_{S} \rangle \langle Lm_{L}, Sm_{S} | Jm_{J} \rangle \bigg\},$ • 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 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

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RGL shifted zeta functions

• compute Z_{lm} using

$$\begin{aligned} \mathcal{Z}_{lm}(\boldsymbol{s},\gamma,\boldsymbol{u}^2) &= \sum_{\boldsymbol{n}\in\mathbb{Z}^3} \frac{\mathcal{Y}_{lm}(\boldsymbol{z})}{(\boldsymbol{z}^2-\boldsymbol{u}^2)} e^{-\Lambda(\boldsymbol{z}^2-\boldsymbol{u}^2)} + \delta_{l0} \frac{\gamma\pi}{\sqrt{\Lambda}} F_0(\Lambda\boldsymbol{u}^2) \\ &+ \frac{i^l\gamma}{\Lambda^{l+1/2}} \int_0^1 dt \left(\frac{\pi}{t}\right)^{l+3/2} e^{\Lambda t\boldsymbol{u}^2} \sum_{\boldsymbol{n}\in\mathbb{Z}^3\atop\boldsymbol{n}\neq0} e^{\pi\boldsymbol{i}\boldsymbol{n}\cdot\boldsymbol{s}} \mathcal{Y}_{lm}(\boldsymbol{w}) \ e^{-\pi^2 \boldsymbol{w}^2/(t\Lambda)} \end{aligned}$$

where

$$z = \mathbf{n} - \gamma^{-1} \begin{bmatrix} \frac{1}{2} + (\gamma - 1)s^{-2}\mathbf{n} \cdot \mathbf{s} \end{bmatrix} \mathbf{s},$$

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

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

- 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:

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

define the matrix

 $B_{J'm_{J'}L'S'a'; Jm_JLSa}^{(R)} = \delta_{J'J}\delta_{L'L}\delta_{S'S}\delta_{a'a}D_{m_{J'}m_{J}}^{(J)*}(R)$

can show that under lattice symmetry operator R,

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

- can block diagonalize F by diagonalizing $D_{m'm}^{(J)}(R)$ for each J
- change of basis: little group irrep Λ , row λ , *n* occurrence of Λ in $D_{m'm}^{(J)}(R)$ $|\Lambda\lambda nJLSa\rangle = \sum c_{Jm_J}^{\Lambda\lambda n} |Jm_JLSa\rangle$
- *F* diagonal in Λ , λ , but not in $n_{\Lambda}^{m_{J}}$
- can now focus on the matrix elements:

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

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

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



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

• $\pi\pi$ -state energies for various d^2



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

• results $32^3 \times 256$, $m_\pi \approx 240$ MeV: $g_{\rho\pi\pi} = 5.99(26), \ m_\rho/m_\pi = 3.350(24), \ \chi^2/dof = 1.04$



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

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



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

• compendium of results for $g_{\rho\pi\pi}$



Effective Hamiltonian method

- relating finite-volume energies to resonance parameters via "Lüscher method" very complicated
- alternative: use an effective hadron Hamiltonian matrix
 - Wu et al, PRC 90, 055206 (2014)
- use single and two-particle states as basis states
- interaction terms from symmetry + assumed form wrt momenta
- parameters of Hamiltonian determined from fits to finite-volume spectra
- Lippmann-Schwinger (or other methods) to extract infinite-volume resonances

Tetraquark operators

- determine impact on spectrum when tetraquark operators included
- single-site and displaced quarks



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Conclusion

- excited states are difficult!
- crucial role of interpolating operators for excited-state studies in lattice QCD
- large number of finite-volume energies in large number of channels now possible
- stochastic LapH method works very well
 - allows evaluation of all needed quark-line diagrams
- scattering phase shifts can be computed
- infinite-volume resonance parameters from finite-volume energies → need for simpler effective Hamiltonian/field theory techniques
- role of tetraquark operators to be studied