Exploring Excited Hadrons in Lattice QCD

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Excited QCD: Zakopane, Poland
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The frontier awaits

- experiments show many excited-state hadrons exist
- significant experimental efforts to map out QCD resonance spectrum → JLab Hall B, Hall D, ELSA, etc.
- great need for *ab initio* calculations → lattice QCD
The challenge of exploration!

- most excited hadrons are unstable (resonances)
- excited states more difficult to extract in Monte Carlo calculations
  - correlation matrices needed
  - operators with very good overlaps onto states of interest
- must extract all states lying below a state of interest
  - as pion get lighter, more and more multi-hadron states
- best multi-hadron operators made from constituent hadron operators with well-defined relative momenta
  - need for all-to-all quark propagators
- disconnected diagrams
Hadron Spectrum Collaboration (HSC)

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- R. Edwards, B. Joo, H.W. Lin, D. Richards (Jefferson Lab.)
- E. Engelson, S. Wallace (U. Maryland)
- J. Dudek (Old Dominion)
- K.J. Juge (U. of Pacific)
- N. Mathur (Tata Institute)
- M. Peardon, S. Ryan (Trinity Coll. Dublin)
Overview of our spectrum project

- obtain stationary state energies of QCD in various boxes
  - 1st milestone: quenched excited states with heavy pion \( \rightarrow \) done
  - 2nd milestone: \( N_f=2 \) excited states with heavy pion \( \rightarrow \) done
  - 3rd milestone: \( N_f=2+1 \) excited states with light pion
    - unexplored territory in lattice QCD
    - multi-hadron operators needed \( \rightarrow \) many-to-many quark propagators
    - recent technology breakthrough \( \rightarrow \) new quark smearing
    - results during next year will tell the tale
- interpretation of finite-volume energies
  - spectrum matching to construct effective hadron theory?
  - Monte Carlo simulations using effective theory
  - infinite-volume, realistic pions in effective theory
Monte Carlo method

- hadron operators  \( \phi = \phi[\bar{\psi}, \psi, U] \)  \( \psi = \) quark  \( U = \) gluon field
- temporal correlations from path integrals
  \[
  \langle \phi(t)\phi(0) \rangle = \frac{\int D[\bar{\psi}, \psi, U] \phi(t)\phi(0) e^{-\bar{\psi}M[U]\psi - S[U]}}{\int D[\bar{\psi}, \psi, U] e^{-\bar{\psi}M[U]\psi - S[U]}}
  \]
- integrate exactly over quark Grassmann fields
  \[
  \langle \phi(t)\phi(0) \rangle = \frac{\int DU \det M[U]\left(M^{-1}[U]\cdots\right) e^{-S[U]}}{\int DU \det M[U] e^{-S[U]}}
  \]
- resort to Monte Carlo method to integrate over gluon fields
- generate sequence of field configurations  \( U_1, U_2, U_3, \ldots, U_N \) using Markov chain procedure
  - use of parallel computations on supercomputers
  - especially intensive as quark mass (pion mass) gets small
Lattice regularization

- hypercubic space-time lattice regulator needed for Monte Carlo
- quarks reside on sites, gluons reside on links between sites
- lattice excludes short wavelengths from theory (regulator)
- regulator removed using standard renormalization procedures (continuum limit)
- systematic errors
  - discretization
  - finite volume
Excited-state energies from Monte Carlo

- Extracting excited-state energies requires matrix of correlators.
- For a given $N \times N$ correlator matrix $C_{\alpha\beta}(t) = \langle 0 | O_\alpha(t) O_\beta^+(0) | 0 \rangle$, one defines the $N$ principal correlators $\lambda_\alpha(t, t_0)$ as the eigenvalues of
  \[ C(t_0)^{-1/2} C(t) C(t_0)^{-1/2} \]
  where $t_0$ (the time defining the “metric”) is small.
- Can show that $\lim_{t \to \infty} \lambda_\alpha(t, t_0) = e^{-(t-t_0)E_\alpha}(1 + e^{-t\Delta E_\alpha})$.
- $N$ principal effective masses defined by $m_\alpha^{\text{eff}}(t) = \ln \left( \frac{\lambda_\alpha(t, t_0)}{\lambda_\alpha(t+1, t_0)} \right)$ now tend (plateau) to the $N$ lowest-lying stationary-state energies.
- Analysis:
  - Fit each principal correlator to single exponential.
  - Optimize on earlier time slice, matrix fit to optimized matrix.
  - Both methods as consistency check.

February 11, 2009  C. Morningstar
Operator design issues

- statistical noise increases with temporal separation $t$
- use of very good operators is crucial or noise swamps signal
- recipe for making better operators
  - crucial to construct operators using *smeared* fields
    - link variable smearing
    - quark field smearing
  - spatially extended operators
  - use large set of operators (variational coefficients)
Three stage approach (PRD72:094506, 2005)

- concentrate on baryons at rest (zero momentum)
- operators classified according to the irreps of $O_h$
  
  $$G_{1g}, G_{1u}, G_{2g}, G_{2u}, H_g, H_u$$
- (1) basic building blocks: smeared, covariant-displaced quark fields
  
  $$(\tilde{D}_j^{(p)}\tilde{\psi}(x))_{A\alpha} \quad p \text{- link displacement (} j = 0, \pm 1, \pm 2, \pm 3)$$
- (2) construct elemental operators (translationally invariant)
  
  $$B^F(x) = \phi_{ABC}^F \epsilon_{abc} (\tilde{D}_i^{(p)}\tilde{\psi}(x))_{A\alpha} (\tilde{D}_j^{(p)}\tilde{\psi}(x))_{B\beta} (\tilde{D}_k^{(p)}\tilde{\psi}(x))_{C\gamma}$$

  - flavor structure from isospin
  - color structure from gauge invariance

- (3) group-theoretical projections onto irreps of $O_h$
  
  $$B_i^{A\Lambda F}(t) = \sum_{R \in O_h} \frac{1}{g_{O_h}^{DP}} D_{\Lambda\Lambda}^{(\Lambda)}(R)^* \{ U_R B_i^{F}(t) \} U_R^+$$
Incorporating orbital and radial structure

- displacements of different lengths build up radial structure
- displacements in different directions build up orbital structure

- operator design minimizes number of sources for quark propagators
- useful for mesons, tetraquarks, pentaquarks even!
- can even incorporate **hybrid meson** operators
Spin identification and other remarks

- spin identification possible by pattern matching

| $J$ | $n^J_{G_1}$ | $n^J_{G_2}$ | $n^J_H$ |
|-----|-------------|-------------|---------|
| $\frac{1}{2}$ | 1 | 0 | 0 |
| $\frac{3}{2}$ | 0 | 0 | 1 |
| $\frac{5}{2}$ | 0 | 1 | 1 |
| $\frac{7}{2}$ | 1 | 1 | 1 |
| $\frac{9}{2}$ | 1 | 0 | 2 |
| $\frac{11}{2}$ | 1 | 1 | 2 |
| $\frac{13}{2}$ | 1 | 2 | 2 |
| $\frac{15}{2}$ | 1 | 1 | 3 |
| $\frac{17}{2}$ | 2 | 1 | 3 |

- total numbers of operators is huge $\Rightarrow$ uncharted territory

- ultimately must face two-hadron scattering states

| Irrep | $\Delta, \Omega$ | $N$ | $\Sigma, \Xi$ | $\Lambda$ |
|-------|------------------|-----|--------------|---------|
| $G_{1g}$ | 221 | 443 | 664 | 656 |
| $G_{1u}$ | 221 | 443 | 664 | 656 |
| $G_{2g}$ | 188 | 376 | 564 | 556 |
| $G_{2u}$ | 188 | 376 | 564 | 556 |
| $H_g$ | 418 | 809 | 1227 | 1209 |
| $H_u$ | 418 | 809 | 1227 | 1209 |
Quark- and gauge-field smearing

- smeared quark and gluon fields fields → dramatically reduced coupling with short wavelength modes
- **link-variable** smearing (stout links PRD69, 054501 (2004))
  - define $C_{\mu}(x) = \sum_{\pm(\nu \neq \mu)} \rho_{\mu\nu} U_\nu(x) U_\mu(x + \mathbf{v}) U^+_\nu(x + \mathbf{\mu})$
  - spatially isotropic $\rho_{jk} = \rho$, $\rho_{4k} = \rho_{k4} = 0$
  - exponentiate traceless Hermitian matrix
    $$\Omega_\mu = C_{\mu} U^+_\mu$$
    $$Q_\mu = \frac{i}{2} \left( \Omega^+_\mu - \Omega_\mu \right) - \frac{i}{2N} \text{Tr} \left( \Omega^+_\mu - \Omega_\mu \right)$$
  - iterate
    $$U^{(n+1)}_\mu = \exp \left( i Q^{(n)}_\mu \right) U^{(n)}_\mu$$
  - quark-field smearing (covariant Laplacian uses smeared gauge field)
    $$\tilde{\psi}(x) = \left( 1 + \frac{\sigma_s}{4n_\sigma} \tilde{\Delta} \right)^{n_\sigma} \psi(x)$$
Importance of smearing

- Nucleon G_{1g} channel
- Effective masses of 3 selected operators
- Noise reduction from link variable smearing, especially for displaced operators
- Quark-field smearing reduces couplings to high-lying states
  \[ \sigma_s = 4.0, \quad n_\sigma = 32 \]
  \[ n_\rho = 2.5, \quad n_\rho = 16 \]
- Less noise in excited states using \( \sigma_s = 3.0 \)
Operator selection

- rules of thumb for “pruning” operator sets
  - noise is the enemy!
  - prune first using intrinsic noise (diagonal correlators)
  - prune next within operator types (single-site, singly-displaced, etc.) based on condition number of
  - prune across all operators based on condition number
- best to keep a variety of different types of operators, as long as condition numbers maintained
  \[
  \hat{C}_{ij}(t) = \frac{C_{ij}(t)}{\sqrt{C_{ii}(t)C_{jj}(t)}}, \quad t = 1
  \]
- typically use 16 operators to get 8 lowest lying levels
Nucleon $G_{1g}$ effective masses

- 200 quenched configs, $12^3$ 48 anisotropic Wilson lattice, $a_s \sim 0.1 \text{ fm}$, $a_s/a_t \sim 3$, $m_\pi \sim 700 \text{ MeV}$
- nucleon $G_{1g}$ channel
- green=fixed coefficients, red=principal
Nucleon $H_u$ effective masses

- 200 quenched configs, $12^3$ 48 anisotropic Wilson lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3$, $m_\pi \sim 700$ MeV
- nucleon $H_u$ channel
- green=fixed coefficients, red=principal
MILESTONE 1

Single-hadron excitations in quenched approximation
Nucleon spectrum: first results

- 200 quenched configs, $12^3$ 48 anisotropic Wilson lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3$, $m_\pi \sim 700$ MeV (A. Lichtl thesis)
Delta spectrum: first results

- 200 quenched configs, $12^3$ 48 anisotropic Wilson lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3$, $m_\pi \sim 700$ MeV (J. Bulava)
MILESTONE 2

Single-hadron excitations for $N_f=2$
Inclusion of quark loops

- \( N_f=2 \) on \( 24^3 \) 64 anisotropic clover lattice, \( a_s \sim 0.11 \text{ fm}, a_s/a_c \sim 3 \)
- Left: \( m_\pi = 578 \text{ MeV} \) Right: \( m_\pi = 416 \text{ MeV} \) (PRD 2009, to appear)
Mesons

- $N_f=2+1$ on $16^3 \times 128$ anisotropic clover lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3.5$
- $m_\pi = 578$ MeV (preliminary… operators not optimized)
MILESTONE 3

Multi-hadron states for $N_f=2+1$
(in progress)
Spatial summations

- Baryon at rest is operator of form

\[ B(\vec{p} = 0, t) = \frac{1}{V} \sum_{\vec{x}} \phi_B(\vec{x}, t) \]

- Baryon correlator has a double spatial sum

\[ \langle 0 | \bar{B}(\vec{p} = 0, t) B(\vec{p} = 0, 0) | 0 \rangle = \frac{1}{V^2} \sum_{\vec{x}, \vec{y}} \langle 0 | \bar{\phi}_B(\vec{x}, t) \phi_B(\vec{y}, 0) | 0 \rangle \]

- Computing all elements of propagators exactly not feasible

- Translational invariance can limit summation over source site to a single site for local operators

\[ \langle 0 | \bar{B}(\vec{p} = 0, t) B(\vec{p} = 0, 0) | 0 \rangle = \frac{1}{V} \sum_{\vec{x}} \langle 0 | \bar{\phi}_B(\vec{x}, t) \phi_B(0, 0) | 0 \rangle \]
Slice-to-slice quark propagators

- **good** baryon-meson operator of total zero momentum has form

\[
B(\vec{p}, t)M(−\vec{p}, t) = \frac{1}{V^2} \sum_{\vec{x}, \vec{y}} \phi_B(\vec{x}, t)\phi_M(\vec{y}, t)e^{i\vec{p} \cdot (\vec{x}−\vec{y})}
\]

- **cannot** limit source to single site for multi-hadron operators
- disconnected diagrams (scalar mesons) will also need many-to-many quark propagators
- quark propagator elements from all spatial sites to all spatial sites are needed!
  - new territory → exploration
Initial stochastic estimation

- quark propagator is just inverse of Dirac matrix \( M \)
- noise vectors \( \eta \) satisfying \( E(\eta_i) = 0 \) and \( E(\eta_i\eta_j^*) = \delta_{ij} \) are useful for stochastic estimates of inverse of a matrix \( M \)
- \( Z_4 \) noise is used \{1, i, -1, -i\}
- define \( X(\eta) = M^{-1}\eta \) then
  \[
  E(X_i\eta_j^*) = E\left(\sum_k M^{-1}_{ik}\eta_k\eta_j^*\right) = \sum_k M^{-1}_{ik}E(\eta_k\eta_j^*) = \sum_k M^{-1}_{ik}\delta_{kj} = M^{-1}_{ij}
  \]
- if can solve \( M X^{(r)} = \eta^{(r)} \) for each of \( N_R \) noise vectors \( \eta^{(r)} \) then we have a Monte Carlo estimate of all elements of \( M^{-1} \):
  \[
  M^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_i^{(r)}\eta_j^{(r)*}
  \]
- variances in above estimates usually unacceptably large
- introduce variance reduction using source *dilution*
Source dilution for single matrix inverse

- dilution introduces a complete set of projections:
  \[ P^{(a)} P^{(b)} = \delta^{ab} P^{(a)}, \quad \sum_a P^{(a)} = 1, \quad P^{(a)\dagger} = P^{(a)} \]

- observe that
  \[
  M_{ij}^{-1} = M_{ik}^{-1} \delta_{kj} = \sum_a M_{ik}^{-1} P^{(a)} = \sum_a M_{ik}^{-1} P^{(a)} \delta_{k'j'} P^{(a)}
  \]
  \[= \sum_a M_{ik}^{-1} P^{(a)} E(\eta_k \eta_j^*) P^{(a)} = \sum_a M_{ik}^{-1} E\left(P^{(a)} \eta_k \eta_j^* P^{(a)}\right)\]

- define
  \[
  \eta_{[a]}^k = P_{kk'}^{(a)} \eta_{k'}, \quad \eta_{[a]}^j = \eta_j^* P_{jj}^{(a)}, \quad X_{[a]}^k = M_{kj}^{-1} \eta_{[a]}^j
  \]
  so that
  \[
  M_{ij}^{-1} = \sum_a E\left( X_{[a]}^i \eta_{[a]}^j \right)
  \]

- Monte Carlo estimate is now
  \[
  M_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a X_{[a]}^{(r)[a]} \eta_{[a]}^{(r)[a]*}
  \]

- \[\sum_a \eta_{[a]}^i \eta_{[a]}^j \] has same expected value as \[\eta_i \eta_j^*\], but reduced variance
  (statistical zeros \(\rightarrow\) exact)
Dilution schemes for spectroscopy

- **Time dilution (particularly effective)**
  \[ P^{(B)}_{ab;\alpha\beta}(\bar{x},t;\bar{y},t') = \delta_{ab}\delta_{\alpha\beta}\delta(\bar{x},\bar{y})\delta_{Bt}\delta_{B't'}, \quad B = 0,1,\ldots, N_t - 1 \]

- **Spin dilution**
  \[ P^{(B)}_{ab;\alpha\beta}(\bar{x},t;\bar{y},t') = \delta_{ab}\delta_{B\alpha}\delta_{B\beta}\delta(\bar{x},\bar{y})\delta_{tt'}, \quad B = 0,1,2,3 \]

- **Color dilution**
  \[ P^{(B)}_{\alpha\alpha;\beta\beta}(\bar{x},t;\bar{y},t') = \delta_{Ba}\delta_{Bb}\delta_{\alpha\beta}\delta(\bar{x},\bar{y})\delta_{tt'}, \quad B = 0,1,2 \]

- **Spatial dilutions?**
  - even-odd
Dilution tests

- 100 quenched configs, $12^3$, 48 anisotropic Wilson lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3$, $m_\pi \sim 700$ MeV
- three representative operators: SS, SD, TDT nucleon operators
Dilution tests (continued)

- 100 quenched configs, $12^3$ 48 anisotropic Wilson lattice
Source-sink factorization

- baryon correlator has form
  \[ C_{ij} = c_{ijk}^{(l)} c_{ijk}^{(T)*} Q_{ii}^A Q_{jj}^B Q_{kk}^C \]

- stochastic estimates with dilution
  \[ C_{ij} \approx \frac{1}{N_R} \sum_r \sum_d A d_B d_C c_{ijk}^{(l)} c_{ijk}^{(T)*} \left( \phi_i^{(Ar)[d_A]} \eta_i^{(Ar)[d_A]*} \right) \]
  \[ \times \left( \phi_j^{(Br)[d_B]} \eta_j^{(Br)[d_B]*} \right) \left( \phi_k^{(Cr)[d_C]} \eta_k^{(Cr)[d_C]*} \right) \]

- define
  \[ \Gamma_{ij}^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \phi_i^{(Ar)[d_A]} \phi_j^{(Br)[d_B]} \phi_k^{(Cr)[d_C]} \]
  \[ \Omega_{ij}^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \eta_i^{(Ar)[d_A]} \eta_j^{(Br)[d_B]} \eta_k^{(Cr)[d_C]} \]

- correlator becomes dot product of source vector with sink vector
  \[ C_{ij} \approx \frac{1}{N_R} \sum_r \sum_d A d_B d_C \Gamma_{ij}^{(r)[d_A d_B d_C]} \Omega_{ij}^{(r)[d_A d_B d_C]*} \]

- store ABC permutations to handle Wick orderings
Laplacian Heaviside quark-field smearing

- new quark-field smearing method (summer 2008)
- clever choice of quark-field smearing makes exact computations with all-to-all quark propagators possible!!
  - will work for disconnected diagrams
  - preserves source-sink factorization
- to date, quark field smeared using covariant Laplacian

\[ \psi(x) = \left( 1 + \frac{\sigma_s}{4n_\sigma} \tilde{\Delta} \right)^{n_\sigma} \psi(x) \]

- express in term of eigenvectors/eigenvalues of Laplacian

\[ \psi(x) = \left( 1 + \frac{\sigma_s}{4n_\sigma} \tilde{\Delta} \right)^{n_\sigma} \sum_k \langle \phi_k | \phi_k \rangle \psi(x) \]

\[ = \sum_k \left( 1 + \frac{\sigma_s \lambda_k}{4n_\sigma} \right)^{n_\sigma} \langle \phi_k | \phi_k \rangle \psi(x) \]

- truncate sum and set weights to unity \( \Rightarrow \) Laplacian Heaviside
Getting to know the Laplacian

- spectrum of the covariant Laplacian
- left: dependence on lattice size; right: dependence on link smearing
Choosing the smearing cut-off

- Laplacian Heaviside (LAPH) quark smearing

\[ \tilde{\psi}(x) = \Theta(Q_{\text{max}}^2 + \tilde{\Delta}) \psi(x) \]

\[ \approx \sum_{k=1}^{N_{\text{max}}} |\varphi_k\rangle \langle \varphi_k | \psi(x) \]

- choose smearing cut-off based on minimizing excited-state contamination, keep noise small
  - behavior of nucleon \( t=1 \) effective masses
Tests of Laplacian Heaviside smearing

- comparison of $\rho$-meson effective masses using same number of gauge-field configurations

- typically need $< 30$ modes on $16^3$ lattice
- about 100 modes on $24^3$ lattice
Advantages of new smearing

- source-sink factorization
- simpler expressions than stochastic method
- improved statistics
- slice-to-slice quark propagators $\Rightarrow$ multi-hadron operators
Configuration generation

- significant time on USQCD (DOE) and NSF computing resources
- anisotropic clover fermion action (with stout links) and anisotropic improved gauge action
  - tunings of couplings, aspect ratio, lattice spacing done
- anisotropic Wilson configurations generated during clover tuning
- current goal:
  - three lattice spacings: \( a = 0.125 \text{ fm}, 0.10 \text{ fm}, 0.08 \text{ fm} \)
  - three volumes: \( V = (3.2 \text{ fm})^4, (4.0 \text{ fm})^4, (5.0 \text{ fm})^4 \)
  - 2+1 flavors, \( m_\pi \sim 350 \text{ MeV}, 220 \text{ MeV}, 180 \text{ MeV} \)
- USQCD Chroma software suite
Resonances in a box
Resonances in a box: an example

- Consider simple 1D quantum mechanics example
- Hamiltonian

\[ H = \frac{1}{2} p^2 + V(x) \quad \text{where} \quad V(x) = (x^4 - 3) e^{-x^2/2} \]
1D example spectrum

- Spectrum has two bound states, two resonances for $E<4$
Scattering phase shifts

- define even- and odd-parity phase shifts $\delta_\pm$
- phase between transmitted and incident wave
Spectrum in box (periodic b.c.)

- spectrum is discrete in box (momentum quantized)
- narrow resonance is avoided level crossing, broad resonance?

Dotted curves are $V=0$ spectrum
Unstable particles (resonances)

- our computations done in a periodic box
  - momenta quantized
  - discrete energy spectrum of stationary states \( \rightarrow \) single hadron, 2 hadron, …
- how to extract resonance info from box info?
- **approach 1**: crude scan
  - if goal is exploration only \( \rightarrow \) “ferret” out resonances
  - spectrum in a few volumes
  - placement, pattern of multi-particle states known
  - resonances \( \rightarrow \) level distortion near energy with little volume dependence
  - short-cut tricks of McNeile/Michael, Phys Lett B556, 177 (2003)
Unstable particles (resonances)

- **approach 2**: phase-shift method
  - if goal is high precision $\Rightarrow$ work much harder!
  - relate finite-box energy of multi-particle model to infinite-volume phase shifts
  - evaluate energy spectrum in several volumes to compute phase shifts using formula from previous step
  - deduce resonance parameters from phase shifts
  - early references
    - B. DeWitt, PR 103, 1565 (1956) (sphere)
    - M. Luscher, NPB 364, 237 (1991) ($\rho\pi\pi$ in cube)

- **approach 3**: histogram method
  - recent work for pion-nucleon system:
    - V. Bernard et al, arXiv:0806.4495 [hep-lat]

- **new approach**: construct effective theory of hadrons?
Summary

- goal: to wring out hadron spectrum from QCD Lagrangian using Monte Carlo methods on a space-time lattice
  - baryons, mesons (and glueballs, hybrids, tetraquarks, …)
- discussed extraction of excited states in Monte Carlo calculations
  - correlation matrices needed
  - operators with very good overlaps onto states of interest
- must extract all states lying below a state of interest
  - as pion get lighter, more and more multi-hadron states
- multi-hadron operators → relative momenta
  - need for slice-to-slice quark propagators
- nearing final milestone!
- interpretation of finite-box energies