The excited hadron spectrum in lattice QCD using a new variance reduction method

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Overview

- overarching goal: obtain stationary state energies of QCD in cubic boxes (periodic b.c.) of various sizes using Monte Carlo method.

- key points of talk:
  - good single hadron operators for various momenta now selected in nearly all light baryon and meson sectors.
  - to get spectrum for lighter quark masses
    - multi-hadron operators needed → slice-to-slice quark propagators
    - recent technology breakthrough → new quark smearing with improved variance reduction

- interpretation of finite-volume energies
  - spectrum matching to construct effective hadron theory?
current collaborators:

- Justin Foley, David Lenkner, Colin Morningstar, Ricky Wong (CMU)
- Keisuke Jimmy Juge (U. of Pacific)
- John Bulava (DESY, Zeuthen)
- Mike Peardon, (Trinity Coll. Dublin)
- Steve Wallace (U. Maryland)
- B. Joo (JLab)
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
- calculations done in cubic box (periodic boundary conditions)
  - all energies are discrete
  - zero-momentum states labeled by irreps of $O_h$ point group even in continuum limit
Single-hadron operators

- covariantly-displaced quark fields as building blocks
- group-theoretical projections onto irreps of lattice symmetry group
- displacements of different lengths build up radial structure
- displacements in different directions build up orbital structure

Quark- and gauge-field smearing

- smeared quark and gluon fields fields $\rightarrow$ dramatically reduced coupling with short wavelength modes

- **link-variable** smearing (stout links PRD69, 054501 (2004))
  - define $C_\mu(x) = \sum_{\pm(\nu\neq\mu)} \rho_{\mu\nu} U_\nu(x) U_\mu(x+\hat{\nu}) U_\nu^+(x+\hat{\mu})$
  - 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
    $$U_\mu^{(n+1)} = \exp \left( i Q_\mu^{(n)} \right) U_\mu^{(n)}$$
    $$U_\mu \rightarrow U_\mu^{(1)} \rightarrow \cdots \rightarrow U_\mu^{(n)} \equiv \tilde{U}_\mu$$

- initial **quark**-field smearing (Laplacian using smeared gauge field)
  $$\tilde{\psi}(x) = \left( \sigma_s \frac{\Delta}{4n_\sigma} \right)^{n_\sigma} \psi(x)$$
Operator selection

- operator construction leads to very large number of operators
- 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
Nucleons

- $N_f=2$ on $24^3 \times 64$ anisotropic clover lattice, $a_s \sim 0.11$ fm, $a_s/a_t \sim 3$
- Left: $m_\pi = 578$ MeV  Right: $m_\pi = 416$ MeV   PRD 79, 034505 (2009)

- multi-hadron thresholds above show need for multi-hadron operators to go to lower pion masses!!

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Nucleon operator pruning

- $N_f=2+1$ on $16^3 \times 128$ lattice, $m_\pi = 380$ MeV (100 configs, 32 eigvecs)
Delta operator pruning

- $N_f=2+1$ on $16^3 \times 128$ lattice, $m_\pi = 380$ MeV (481 configs, 32 eigvecs)
Sigma operator pruning

- $N_f=2+1$ on $16^3 \times 128$ lattice, $m_\pi = 380$ MeV (100 configs, 32 eigvecs)
Isovector G-parity odd mesons

- $N_f=2+1$ on $16^3 \times 128$ lattice, $m_\pi = 380$ MeV (100 configs, 32 eigvecs)
Kaons

- $N_f=2+1$ on $16^3 \times 128$ lattice, $m_\pi = 380$ MeV (100 configs, 32 eigvecs)
Multi-hadron states

- to extract $n^{th}$ level using correlator matrix method, must first extract all levels 0, 1, ..., $n-1$ below it
- as quark mass gets lighter, more and more multi-hadron states lie below the resonance energies of interest
- need multi-hadron operators to reliably extract energies of the multi-hadron states
  - need the quark propagators from all sites on one time slice to all sites on another time slice
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
  \[ \langle 0 | B(\vec{p} = 0, t) B(\vec{p} = 0, 0) | 0 \rangle = \frac{1}{V^2} \sum_{\vec{x}, \vec{y}} \langle 0 | \phi_B(\vec{x}, t) \phi_B(\vec{y}, 0) | 0 \rangle \]

- Computing all elements of propagators exactly not feasible since Dirac matrix \( M \) is huge
  \[ N_{\text{rows}} = N_{\text{columns}} = N_x N_y N_z N_t \times N_{\text{spin}} \times N_{\text{color}} \]
  - for 32\(^3\) \times 128 lattice, \( N_{\text{rows}} > 50 \text{ million} \)
  - Compute solution vectors \( x \) in \( Mx = y \) for handful of source vectors \( y \)

- Translational invariance can limit summation over source site to a single site for local operators
  \[ \langle 0 | B(\vec{p} = 0, t) B(\vec{p} = 0, 0) | 0 \rangle = \frac{1}{V} \sum_{\vec{x}} \langle 0 | \phi_B(\vec{x}, t) \phi_B(0, 0) | 0 \rangle \]
Slice-to-slice quark propagators

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

\[
B(\vec{p}, t)M(-\vec{p}, t) = \frac{1}{\sqrt{2}} \sum_{\vec{x}, \vec{y}} \varphi_B(\vec{x}, t) \varphi_M(\vec{y}, t) e^{i\vec{p}\cdot(\vec{x} - \vec{y})}
\]

- **cannot** limit source to single site for multi-hadron operators
- quark propagator elements from all spatial sites to all spatial sites are needed!
  - resort to stochastic estimations
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
  \[ M^{-1}_{ij} = M^{-1}_{ik} \delta_{kj} = \sum_a M^{-1}_{ik} P^{(a)} = \sum_a M^{-1}_{ik} P^{(a)} \delta_{kj} P^{(a)} \]
  \[ = \sum_a M^{-1}_{ik} P^{(a)} E(\eta_k^* \eta_{j'}) P^{(a)} = \sum_a M^{-1}_{ik} E(P^{(a)} \eta_k^* \eta_{j'}^* P^{(a)}) \]

- define
  \[ \eta_k^{[a]} = P^{(a)}_{kk'} \eta_k', \quad \eta_j^{[a]*} = \eta_j^* P^{(a)}_{jj'}, \quad X_j^{[a]} = M^{-1}_{kj} \eta_j^{[a]} \]
  so that
  \[ M_{ij}^{-1} = \sum_a E(X_i^{[a]} \eta_j^{[a]*}) \]

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

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

- Introduce $Z_N$ noise in color, spin, space, time

\[ \eta_{\alpha\alpha}(\tilde{x},t) \]

- Time dilution (particularly effective)

\[ P_{\alpha\alpha;\beta\beta}^{(B)}(\tilde{x},t;\tilde{y},t') = \delta_{ab} \delta_{\alpha\beta} \delta(\tilde{x},\tilde{y}) \delta_{Bt} \delta_{B't'}, \quad B = 0,1,\ldots,N_t - 1 \]

- Spin dilution

\[ P_{\alpha\alpha;\beta\beta}^{(B)}(\tilde{x},t;\tilde{y},t') = \delta_{ab} \delta_{B\alpha} \delta_{B\beta} \delta(\tilde{x},\tilde{y}) \delta_{t'}, \quad B = 0,1,2,3 \]

- Color dilution

\[ P_{\alpha\alpha;\beta\beta}^{(B)}(\tilde{x},t;\tilde{y},t') = \delta_{Ba} \delta_{Bb} \delta_{\alpha\beta} \delta(\tilde{x},\tilde{y}) \delta_{t'}, \quad B = 0,1,2 \]

- Spatial dilutions
  - even-odd
Dilution tests (old method)

- 100 quenched configs, $12^3 \times 48$ anisotropic Wilson lattice

![Graph showing $C(t=5)$ for single-site nucleon]
Laplacian Heaviside quark-field smearing

- new quark-field smearing method  \( \text{PRD80, 054506 (2009)} \)
- judicious choice of quark-field smearing makes exact computations with all-to-all quark propagators possible (on small volumes)
- to date, quark field smeared using covariant Laplacian

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

- express in term of eigenvectors/eigenvalues of Laplacian

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

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

- 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

![Graph showing the spectrum of the covariant Laplacian](image)

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Choosing the smearing cut-off

- Laplacian Heaviside (Laph) quark smearing

$$\tilde{\psi}(x) = \Theta\left(\sigma_s^2 + \tilde{\Delta}\right)\psi(x)$$

$$\approx \sum_{k=1}^{N_{\text{max}}} |\phi_k\rangle \langle \phi_k | \psi(x)$$

- 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 about 32 modes on $16^3$ lattice
- about 128 modes on $24^3$ lattice
new Laph quark smearing method allows exact computation of all-to-all quark propagators on small lattices

but number of Laplacian eigenvectors needed becomes prohibitively large on large lattices
  - 128 modes needed on 24$^3$ lattice

computational method is rather cumbersome, too

provides improved variance reduction of stochastic estimation
New stochastic Laph method

- Introduce $Z_N$ noise in Laph subspace
  $$\rho_{\alpha k}(t) \quad t = \text{time, } \alpha = \text{spin, } k = \text{eigenvector number}$$

- Time dilution (particularly effective)
  $$P_{\alpha k; \beta l}^{(B)}(t; t') = \delta_{kl} \delta_{\alpha \beta} \delta_{Bt} \delta_{B't'}, \quad B = 0, 1, \ldots, N_t - 1$$

- Spin dilution
  $$P_{\alpha k; \beta l}^{(B)}(t; t') = \delta_{kl} \delta_{B\alpha} \delta_{B\beta} \delta_{t't'}, \quad B = 0, 1, 2, 3$$

- Laplacian eigenvector dilution
  - define
    $$P_{\alpha k; \beta l}^{(B)}(t; t') = \delta_{Bk} \delta_{B l} \delta_{\alpha \beta} \delta_{t't'}, \quad B = 0, 1, 2, N_{\text{eig}} - 1$$
  - group projectors together
    - by blocking
    - as interlaced
Old stochastic versus new stochastic

- new method (open symbols) has dramatically decreased variance
- test using a triply-displaced-T nucleon operator
Old stochastic versus new stochastic (zoom in)

- zoom in of triply-displaced-T nucleon plot on last slide
Old stochastic versus new stochastic

- comparison using single-site $\pi$ operator
Old stochastic versus new stochastic

- Zoom in of $\pi$ plot on previous slide
Mild volume dependence

- $16^3$ lattice versus $20^3$ lattice, both old and new stochastic methods
- test using triply-displaced-T nucleon operator
Mild volume dependence

- zoom in of plot on previous slide
Source-sink factorization

- Baryon correlator has form

\[ C_{l\bar{l}} = c^{(l)}_{ijk} c^{(T)^*}_{ijk} Q^{A}_{ii} Q^{B}_{jj} Q^{C}_{kk} \]

- Stochastic estimates with dilution

\[ C_{l\bar{l}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} c^{(l)}_{ijk} c^{(T)^*}_{ijk} \left( \varphi^{(Ar)[d_A]}_i \eta^{(Ar)[d_A]^*}_i \right) \times \left( \varphi^{(Br)[d_B]}_j \eta^{(Br)[d_B]^*}_j \right) \left( \varphi^{(Cr)[d_C]}_k \eta^{(Cr)[d_C]^*}_k \right) \]

- Define

\[ \Gamma^{(r)[d_A d_B d_C]}_l = c^{(l)}_{ijk} \varphi^{(Ar)[d_A]}_i \varphi^{(Br)[d_B]}_j \varphi^{(Cr)[d_C]}_k \]
\[ \Omega^{(r)[d_A d_B d_C]}_l = c^{(l)}_{ijk} \eta^{(Ar)[d_A]}_i \eta^{(Br)[d_B]}_j \eta^{(Cr)[d_C]}_k \]

- Correlator becomes dot product of source vector with sink vector

\[ C_{l\bar{l}} \approx \frac{1}{N_R} \sum_r \sum_{d_A d_B d_C} \Gamma^{(r)[d_A d_B d_C]}_l \Omega^{(r)[d_A d_B d_C]^*}_l \]

- Store ABC permutations to handle Wick orderings
Moving $\pi$ and $a$ mesons

- first step towards including multi-hadron operators:
  - moving single hadrons
  - results below have one unit of on-axis momentum
  - projections onto space group irreps (see J. Foley talk)
Same-time quark lines

- Last step to finite-box spectra: same time $t$-to-$t$ quark lines
First results with t-to-t diagrams

- $24^3 \times 128$ lattice: dilution schemes (TF, SF, LI8) (TI16, SF, LI8)
- 112 eigenvectors, local operators only
Results at lighter pion mass

- $24^3 \times 128$ lattice: dilution schemes (TF, SF, LI8) (TI16, SF, LI8)
- 112 eigenvectors, local operators only

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**Isoscalar PseudoScalar ($\eta$)**

$V=24^3 \times 128, m_\pi = 220 \text{MeV}, 173 \text{ configs}$

- Connected
- Disconnected
- Combined

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**Isoscalar PseudoScalar ($\eta$)**

$V=24^3 \times 128, m_\pi = 220 \text{MeV}, 173 \text{ configs}$

- Connected
- Combined
Results at lighter pion mass (cont’d)

- $24^3 \times 128$ lattice: dilution schemes (TF, SF, LI8) (TI16, SF, LI8)
- 112 eigenvectors, local operators only
Summary

- goal → to wring out hadron spectrum from QCD Lagrangian using Monte Carlo methods on a space-time lattice
  - stationary state energies in cubic box
- good single hadron operator selected in nearly all baryon and meson channels
- 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
- new stochastic Laph method → dramatically reduced variances
- currently running two pion tests