Excited-State Hadrons using the Stochastic LapH Method

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Objective

- **Goal**: compute energies of low-lying stationary states of QCD in a box using Monte Carlo method on space-time lattice
Key issues

- 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 “slice-to-slice” quark propagators.
-Disconnected diagrams.
Hadron Spectrum Collaboration

- spin-off from the Lattice Hadron Physics Collaboration which was spear-headed by Nathan Isgur and John Negele
- current members:
  - David Lenkner, Colin Morningstar, Ricky Wong (CMU)
  - Justin Foley (Utah)
  - John Bulava (DESY, Zeuthen)
  - Keisuke Jimmy Juge (U. of Pacific)
  - Mike Peardon (Trinity Coll. Dublin)
  - Steve Wallace (U. Maryland)
  - R. Edwards, B. Joo, D. Richards, C. Thomas (Jefferson Lab.)
  - H.W. Lin (U. Washington)
  - J. Dudek (Old Dominion)

Stochastic LapH team
Outline

- Operator selection
  - Single hadrons at rest
  - Single hadrons with momentum
- Slice-to-slice quark propagators
  - Stochastic LapH method  (arXiv:1002.0818 [hep-lat])
Quark propagation

- quark propagator is inverse of Dirac matrix $M^{-1}[x, \alpha, a | y, \beta, b]$
  - rows/columns involve lattice site, spin, color
  - very large $N_{tot} \times N_{tot}$ matrix for each flavor, where
    $N_{tot} = N_{sites} \times N_{spin} \times N_{color}$
  - for $24^3 \times 128$ lattice, one has $N_{tot} = 21.2$ million
- not feasible to compute (or store) all elements of inverse
- solve linear systems $Mx = y$ for variable source vectors $y$
  - more ill-conditioned as quark mass decreases
  - results first obtained for unphysically heavy quark masses
- key issue: find method requiring as few source vectors as possible
- our method:
  - Laplacian Heaviside (LapH) quark smearing
  - stochastic estimation with noise dilutions
Excited-state energies from Monte Carlo

- Extracting excited-state energies requires a 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.
- One 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 $m^{\text{eff}}_\alpha(t) = \ln\left( \frac{\lambda_\alpha(t,t_0)}{\lambda_\alpha(t+1,t_0)} \right)$ now tend (plateau) to the $N$ lowest-lying stationary-state energies.
- Standard analysis:
  - Fits to “rotated” matrix when off-diagonals zero.
  - Matrix fits to “rotated” matrix.
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)
Quantum numbers in toroidal box

- Periodic boundary conditions in cubic box
  - not all directions equivalent

- Label stationary states of QCD in a periodic cubic box by irreps of cubic space group even in the continuum limit
  - zero momentum states: little group $O_h$
    \[ A_{1a}, A_{2a}, E_a, T_{1a}, T_{2a}, \ G_{1a}, G_{2a}, H_a, \quad a = g, u \]
  - on-axis momenta: little group $C_{4v}$
    \[ A_1, A_2, B_1, B_2, E, \ G_1, G_2 \]
  - planar-diagonal momenta: $C_{2v}$
    \[ A_1, A_2, B_1, B_2, \ G \]
  - cubic-diagonal momenta: $C_{3v}$
    \[ A_1, A_2, E, \ F_1, F_2, G \]

- include G-parity in some meson sectors
Three stage approach (PRD72:094506,2005)

• (1) basic building blocks: smeared, covariant-displaced quark fields

\[
(\tilde{D}^{(p)}_j \tilde{\psi}(\vec{x},t))_{Aa} \quad p\text{-link displacement } (j = 0, \pm 1, \pm 2, \pm 3)
\]

• (2) construct elemental operators

\[
B^F(t) = \sum e^{-i\vec{p} \cdot \vec{x}} \phi^{F}_{ABC} \epsilon_{abc} (\tilde{D}^{(p)}_i \tilde{\psi}(\vec{x},t))_{Aa} (\tilde{D}^{(p)}_j \tilde{\psi}(\vec{x},t))_{Bb} (\tilde{D}^{(p)}_k \tilde{\psi}(\vec{x},t))_{Cc}
\]

\[
M^F(t) = \sum e^{-i\vec{p} \cdot \vec{x}} \phi^{F}_{AB} \delta_{ab} (\tilde{\psi}(\vec{x},t) \tilde{D}^{(p)}_i)_{Aa} (\tilde{D}^{(p)}_j \tilde{D}^{(p)}_k \tilde{\psi}(\vec{x},t))_{Bb}
\]

- flavor structure from isospin
- color structure from gauge invariance

• (3) group-theoretical projections onto irreps of \( G = O_h, C_{4v}, C_{3v}, C_{2v} \)

\[
H_i^{\Lambda \Lambda F}(t) = \frac{d_\Lambda}{g_G} \sum_{R \in G} D^{(\Lambda)}_{\lambda \lambda}(R)^* U_R H_i^{F}(t) U_R^+
\]

• (4) momenta: zero, on-axis, planar-diagonal, cubic-diagonal
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

baryons

Δ-flux

Y-flux

mesons

reference: PRD 72, 094506 (2005)

similar for nonzero-momentum operators, but must distinguish transverse and longitudinal displacements
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 $C_\mu(x) = \sum_{\nu \neq \mu} \rho_{\mu\nu} U_\nu(x) U_\mu(x + \hat{\nu}) U_\nu^+(x + \hat{\mu})$
  - spatially isotropic $\rho_{jk} = \rho, \rho_{4k} = \rho_{k4} = 0$
  - exponentiate traceless Hermitian matrix
    \[ \Omega_\mu = C_\mu U_\mu^+, \quad Q_\mu = \frac{i}{2} \Omega_\mu^+ - \Omega_\mu - \frac{i}{2N} \text{Tr} \left( \Omega_\mu^+ - \Omega_\mu \right) \]
  - iterate $U^{(n+1)}_{\mu} = \exp \left( iQ_{\mu}^{(n)} U_{\mu}^{(n)} \right)$
    $U_{\mu}^{(1)} \rightarrow \cdots \rightarrow U_{\mu}^{(n)} \equiv \tilde{U}_\mu$

- initial **quark**-field smearing (Laplacian using smeared gauge field)
  \[ \tilde{\psi}(x) = \left( 1 + \frac{\sigma_s}{4n_\sigma \tilde{\Delta}} \right)^{n_\sigma} \psi(x) \]
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
  \[ \sigma_s = 4.0, \quad n_\sigma = 32 \]
  \[ n_{\rho \rho} = 2.5, \quad n_\rho = 16 \]
- Less noise in excited states using $\sigma_s = 3.0$

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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
Nucleon $G_{1g}$ effective masses

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

- 200 quenched configs, $12^3 \times 48$ 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
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!!
**Spatial summations**

- Baryon at rest is operator of form
  \[ B(\vec{p} = 0, t) = \frac{1}{V} \sum_{\vec{x}} \varphi_B(\vec{x}, t) \]

- Baryon correlator has a double spatial sum
  \[ \langle 0 \mid \overline{B}(\vec{p} = 0, t) B(\vec{p} = 0, 0) \mid 0 \rangle = \frac{1}{V^2} \sum_{\vec{x}, \vec{y}} \langle 0 \mid \overline{\varphi}_B(\vec{x}, t) \varphi_B(\vec{y}, 0) \mid 0 \rangle \]

- Computing all elements of propagators exactly not feasible

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

  \[ \langle 0 \mid \overline{B}(\vec{p} = 0, t) B(\vec{p} = 0, 0) \mid 0 \rangle = \frac{1}{V} \sum_{\vec{x}} \langle 0 \mid \overline{\varphi}_B(\vec{x}, t) \varphi_B(0, 0) \mid 0 \rangle \]
Slice-to-slice quark propagators

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

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

- **cannot** limit source to single site for multi-hadron operators
- 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!
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

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

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

- 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

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

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

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

![Graphs showing behavior of nucleon t=1 effective masses](image-url)
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 112 modes on $24^3$ lattice, 256 modes on $32^3$ lattice
Nucleon operator pruning

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

- $G_g$ using 10x10 matrix: off-diagonals are zero

- $H_g$ using 10x10 matrix: off-diagonals are zero
Delta operator pruning

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

$\text{Delta Mass Spectrum (Exp)}$

$I = \frac{3}{2}, S=0$  
($\Delta$ baryons)

$G_{1g}, H_g, G_{2g}, G_{1u}, H_u, G_{2u}$

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Sigma operator pruning

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

$\left| I=1, S=-1 \right>$

\[(\Sigma \text{ baryons})\]
Sigma rotated effective masses

- $G_{1g}$

- $H_u$

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Lambda operator pruning

- \( N_f=2+1 \) on \( 16^3 \times 128 \) lattice, \( m_\pi = 380 \text{ MeV} \) (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)
Isovector G-parity odd rotated effective masses

- $A_{\text{lum}}$

- $T_{\text{lum}}$
Isovector G-parity even mesons

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

- $N_f=2+l$ on $16^3\times128$ lattice, $m_\pi = 380$ MeV (100 configs, 32 eigvecs)
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
Moving isovector mesons

Isovector $C_{4v}$ Meson Spectrum, $V=20^3$, $P=(0,0,1)$

Preliminary
Stochastic estimation of quark propagators

- new Laph quark smearing method allows exact computation of all-to-all quark propagators
- *but* number of Laplacian eigenvectors needed becomes prohibitively large on large lattices
  - 112 modes needed on $24^3$ lattice, 256 modes on $32^3$ lattice
- computational method is rather cumbersome, too
- need to resort to stochastic estimation
  - much more efficient
  - better source-sink factorization
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 $1, i, -1, -i$

- Solve $M X^{(r)} = \eta^{(r)}$ for each of $N_R$ noise vectors $\eta^{(r)}$ for Monte Carlo estimate of all elements of $M^{-1}$:

$$M^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X^{(r)}_i \eta^{(r)*}_j$$

- 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:
  \[ P^{(a)} P^{(b)} = \delta^{ab} P^{(a)} , \quad \sum_a P^{(a)} = 1 , \quad P^{(a)\dagger} = P^{(a)} \]

- Define
  \[ \eta^{[a]}_k = P^{(a)}_{kk} \eta_k , \quad \eta^{[a]*}_j = \eta_j^* P^{(a)}_{jj} , \quad X^{[a]}_k = M^{-1} \eta^{[a]}_j \]

- Monte Carlo estimate is now
  \[ M^{-1}_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a X^{(r)[a]}_i \eta^{(r)[a]*}_j \]

- Dramatically reduced variance
Earlier schemes

- Introduce $Z_N$ noise in color, spin, space, time
  
  $\eta_{\alpha\alpha} \tilde{x}, t$

- Time dilution (particularly effective)
  
  $P_{a\alpha; b\beta}^{(B)} \tilde{x}, t; \tilde{y}, t' = \delta_{ab} \delta_{\alpha\beta} \delta \tilde{x}, \tilde{y} \delta_{Bt} \delta_{Bt'}$, \hspace{1cm} $B = 0, 1, ..., N_t - 1$

- Spin dilution
  
  $P_{a\alpha; b\beta}^{(B)} \tilde{x}, t; \tilde{y}, t' = \delta_{ab} \delta_{B\alpha} \delta_{B\beta} \delta \tilde{x}, \tilde{y} \delta_{\nu}, \hspace{1cm} B = 0, 1, 2, 3$

- Color dilution
  
  $P_{a\alpha; b\beta}^{(B)} \tilde{x}, t; \tilde{y}, t' = \delta_{Ba} \delta_{Bb} \delta_{\alpha\beta} \delta \tilde{x}, \tilde{y} \delta_{\nu}$, \hspace{1cm} $B = 0, 1, 2$

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

- 100 quenched configs, $12^3 \times 48$ anisotropic Wilson lattice
New stochastic Laph method

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

- Four dilution schemes:
  \[ P_{ij}^{(a)} = \delta_{ij}, \quad a = 0 \quad \text{(none)} \]
  \[ P_{ij}^{(a)} = \delta_{ij} \delta_{ai}, \quad a = 0, 1, \ldots, N - 1 \quad \text{(full)} \]
  \[ P_{ij}^{(a)} = \delta_{ij} \delta_{a, Ki/N}, \quad a = 0, 1, \ldots, K - 1 \quad \text{(interlace-K)} \]
  \[ P_{ij}^{(a)} = \delta_{ij} \delta_{a, i \mod K}, \quad a = 0, 1, \ldots, K - 1 \quad \text{(block-K)} \]

- Apply dilutions to
  - Time indices  (full for fixed src, interlace-16 for relative src)
  - Spin indices  (full)
  - Laplacian eigenvector indices  (interlace-8)
Dilution projectors

- **Full dilution**
  
  \[
  P_1 = \begin{bmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 1 & 0 \\
  0 & 0 & 0 & 1 \\
  \end{bmatrix}
  \]

- **Block-3 dilution**
  
  \[
  P_1 = \begin{bmatrix}
  1 & 0 & 0 & 0 \\
  0 & 1 & 0 & 0 \\
  0 & 0 & 1 & 0 \\
  \end{bmatrix}
  \]

- **Interlace-3 dilution**
  
  \[
  P_1 = \begin{bmatrix}
  1 & 0 & 0 \\
  0 & 1 & 0 \\
  0 & 0 & 1 \\
  \end{bmatrix}
  \]

- Useful for evaluating sources on all time slices.

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Old stochastic versus new stochastic

- new method has dramatically decreased variance
- test using a triply-displaced-T nucleon operator
Mild volume dependence

- $16^3$ lattice versus $20^3$ lattice, both old and new stochastic methods
- test using triply-displaced-$T$ nucleon operator
Source-sink factorization

- Baryon correlator has form

\[ C_{\bar{l}l} = c_{ijk}^{(l)} c_{\bar{ijk}}^{(\bar{l})} Q_{i\overline{i}}^{A} Q_{j\overline{j}}^{B} Q_{k\overline{k}}^{C} \]

- Stochastic estimates with dilution

\[ C_{\bar{l}l} \approx \frac{1}{N_{R}} \sum_{r} \sum_{d_{A}d_{B}d_{C}} c_{ijk}^{(l)} c_{\bar{ijk}}^{(\bar{l})} \ast \phi_{i}^{(Ar)[d_{A}]} \eta_{i}^{(Ar)[d_{A}]\ast} \times \phi_{j}^{(Br)[d_{B}]} \eta_{j}^{(Br)[d_{B}]\ast} \phi_{k}^{(Cr)[d_{C}]} \eta_{k}^{(Cr)[d_{C}]\ast} \]

- Define

\[ \Gamma_{l}^{(r)[d_{A}d_{B}d_{C}]} = c_{ijk}^{(l)} \phi_{i}^{(Ar)[d_{A}]} \phi_{j}^{(Br)[d_{B}]} \phi_{k}^{(Cr)[d_{C}]} \]

\[ \Omega_{l}^{(r)[d_{A}d_{B}d_{C}]} = c_{ijk}^{(l)} \eta_{i}^{(Ar)[d_{A}]} \eta_{j}^{(Br)[d_{B}]} \eta_{k}^{(Cr)[d_{C}]} \]

- Correlator becomes dot product of source vector with sink vector

\[ C_{\bar{l}l} \approx \frac{1}{N_{R}} \sum_{r} \sum_{d_{A}d_{B}d_{C}} \Gamma_{l}^{(r)[d_{A}d_{B}d_{C}]} \Omega_{l}^{\ast (r)[d_{A}d_{B}d_{C}]} \]

- Store ABC permutations to handle Wick orderings
Same-time quark lines

- Last step to finite-box spectra: same time t-to-t quark lines

Interlace-16 time dilution (relative sources)
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

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Isoscalar PseudoScalar$(\eta)$

$v = 24^3 \times 128$, $m_\pi = 392\text{MeV}$, 210 configs

C(τ)

- Connected
- Disconnected 2
- Combined

Isoscalar PseudoScalar$(\eta)$

$v = 24^3 \times 128$, $m_\pi = 392\text{MeV}$, 210 configs

$\tau$

- Connected
- Combined

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Results at lighter pion mass

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

Isoscalar PseudoScalar($\eta$)

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

$C(\tau)$ vs $\tau$

$\text{m}_{\text{eff}}$ vs $\tau$
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
Multi-hadron diagrams

- Two-pion energy levels currently in progress
  - all needed quark propagators evaluated
  - moving pion sources/sink in progress
  - formation of correlators is final step
- Will then proceed to other moving mesons and baryons
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
- goal:
  - three lattice spacings: $a = 0.125$ fm, 0.10 fm, 0.08 fm
  - three volumes: $V = (3.2 \text{ fm})^4$, $(4.0 \text{ fm})^4$, $(5.0 \text{ fm})^4$
  - 2+1 flavors, $m_\pi \sim 390$ MeV, 220 MeV, 180 MeV
- USQCD Chroma software suite
- Progress
  - $24^3 \times 128$ lattice for $m_\pi \sim 390$ MeV, 220 MeV done
  - $32^3 \times 256$ lattice for $m_\pi \sim 390$ MeV, 220 MeV in progress
Resonances in a box: an example

- Consider simple 1D quantum mechanics example
- Hamiltonian

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

![Graphs showing even and odd parity phase shifts](image)

$\delta(E)$ and $\frac{d\delta}{dE}(E)$ graphs with even and odd parity markers.
Spectrum in box (periodic b.c.)

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

Positive parity energies

Negative parity energies

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

- our computations done in a periodic box
  - momenta quantized
  - discrete energy spectrum of stationary states → single hadron, 2 hadron, …
- how to extract resonance info from box info?
  - phase-shift methods
  - construct effective theory of hadrons?
Summary

- **goal**: compute energies of low-lying stationary states of QCD in a box using Monte Carlo method on space-time lattice
- single hadron operator construction
- need for multi-hadron operators as pion gets lighter
- slice-to-slice quark propagators
- new stochastic Laph method