Exploring Excited Hadrons in Lattice QCD

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Excited QCD: Zakopane, Poland

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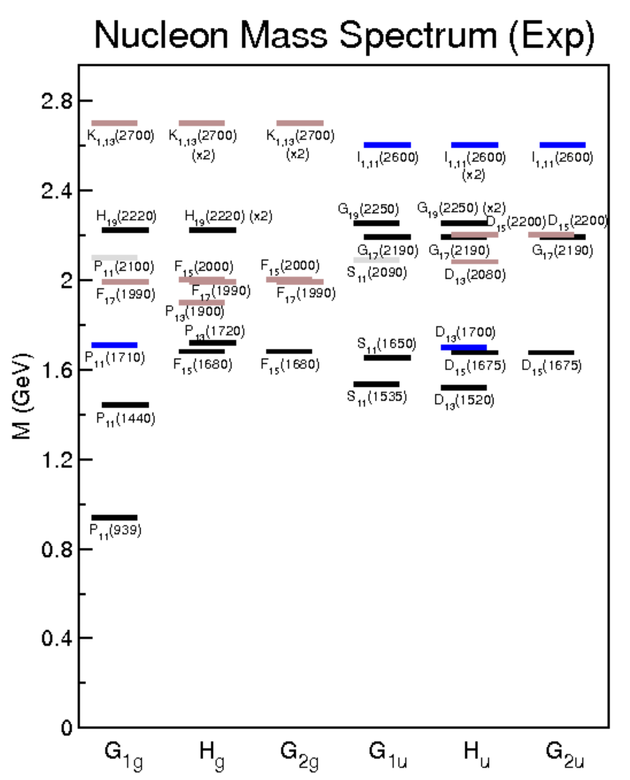
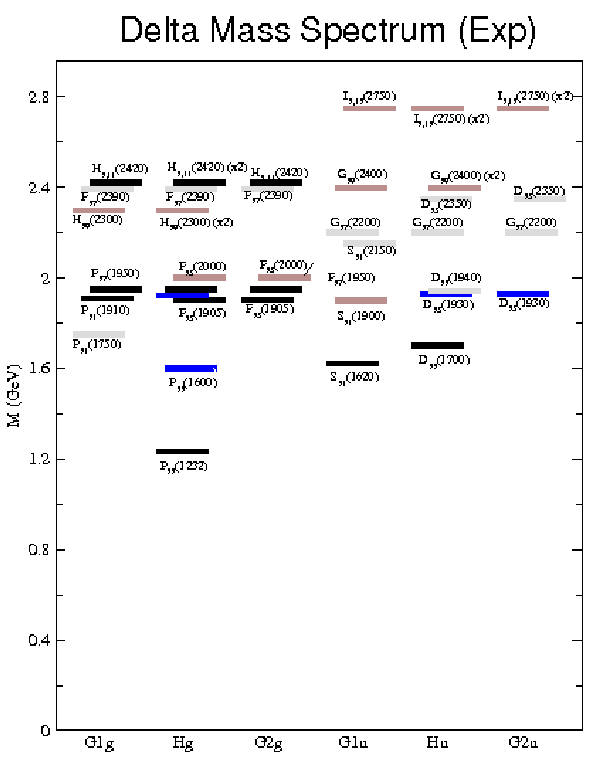
The frontier awaits

- 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)

- J. Bulava, C. Morningstar, J. Foley, Ricky Wong (Carnegie Mellon U.)
- 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 → done
  - 2nd milestone: N_f=2 excited states with heavy pion → done
  - 3rd milestone: N_f=2+1 excited states with light pion
    - unexplored territory in lattice QCD
    - multi-hadron operators needed → many-to-many quark propagators
    - recent technology breakthrough → 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 $\phi = \phi[\bar{\psi}, \psi, U]$ ψ =quark U =gluon field
- temporal correlations from path integrals

$$\langle \phi(t)\phi(0) \rangle = \frac{\int D[\bar{\psi},\psi,U]\ \phi(t)\phi(0)\, e^{-\bar{\psi}M[U]\psi - S[U]}}{\int D[\bar{\psi},\psi,U]\, e^{-\bar{\psi}M[U]\psi - S[U]}}$$

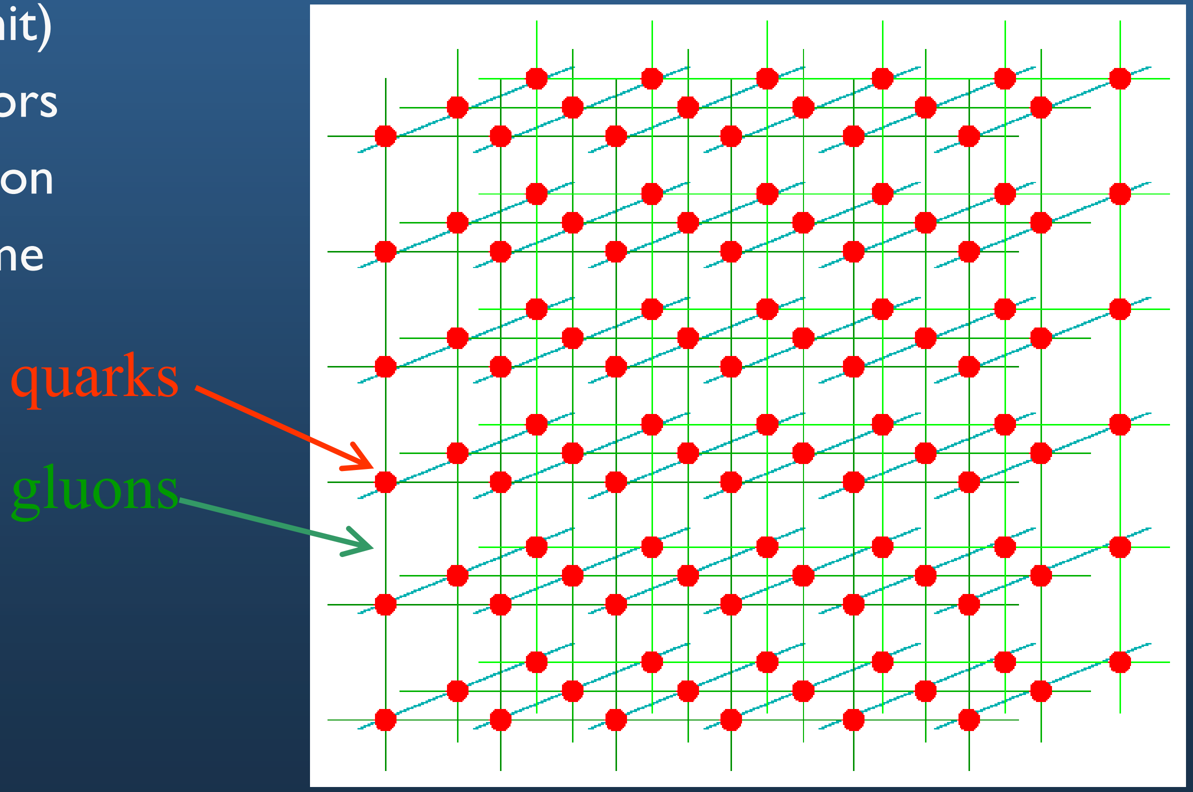
- integrate exactly over quark Grassmann fields

$$\langle \phi(t)\phi(0) \rangle = \frac{\int DU\ \det M[U] \left(M^{-1}[U] \cdots \right) e^{-S[U]}}{\int DU\ \det M[U]\, e^{-S[U]}}$$

- resort to Monte Carlo method to integrate over gluon fields
- generate sequence of field configurations $U_1, U_2, U_3, \cdots, U_N$ 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 $m^{\text{eff}}_\alpha(t) = \ln\left(\frac{\lambda_\alpha(t, t_0)}{\lambda_\alpha(t+1, t_0)} \right)$ now tend (plateau) to the N lowest-lying stationary-state energies
- analysis:
  - fit each principal correlator to single exponential
  - optimize on earlier time slice, matrix fit to optimized matrix
  - both methods as consistency check

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

$$(\tilde{D}_j^{(p)}\tilde{\psi}(x))_{Aa\alpha} \qquad p\text{-link displacement } (j = 0, \pm 1, \pm 2, \pm 3)$$

- (2) construct elemental operators (translationally invariant)

$$B^F(x) = \phi^F_{ABC}\varepsilon_{abc}(\tilde{D}_i^{(p)}\tilde{\psi}(x))_{Aa\alpha}(\tilde{D}_j^{(p)}\tilde{\psi}(x))_{Bb\beta}(\tilde{D}_k^{(p)}\tilde{\psi}(x))_{Cc\gamma}$$

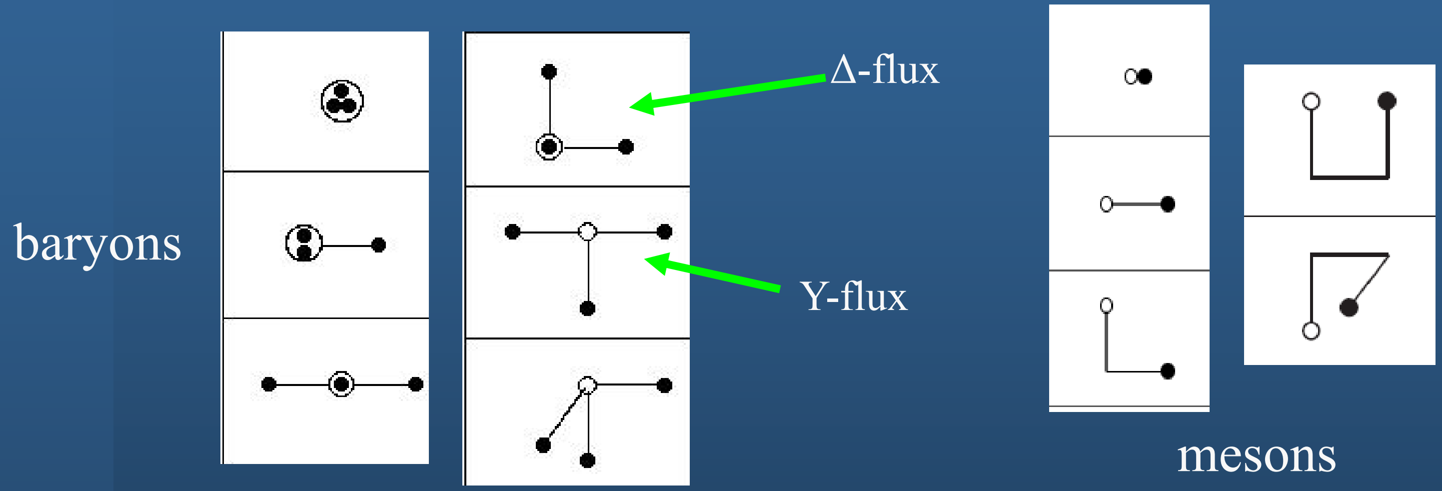
  - flavor structure from isospin
  - color structure from gauge invariance

- (3) group-theoretical projections onto irreps of O_h

$$B_i^{\Lambda\lambda F}(t) = \frac{d_\Lambda}{g_{O_h^D}} \sum_{R \in O_h^D} D_{\lambda\lambda}^{(\Lambda)}(R)^* U_R B_i^F(t) U_R^+$$

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 assuming two different displacement lengths

Irrep	Δ, Ω	N	Σ, Ξ	Λ
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

- total numbers of operators is huge → uncharted territory
- ultimately must face two-hadron scattering states

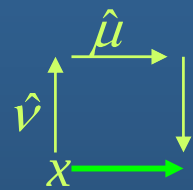
Quark- and gauge-field smearing

- smeared quark and gluon fields fields → dramatically reduced coupling with short wavelength modes
- link-variable smearing (stout links PRD**69**, 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 $\rho_{jk} = \rho, \quad \rho_{4k} = \rho_{k4} = 0$
  - exponentiate traceless Hermitian matrix

$$\Omega_\mu = C_\mu U_\mu^+ \qquad Q_\mu = \frac{i}{2}\left(\Omega_\mu^+ - \Omega_\mu\right) - \frac{i}{2N}\mathrm{Tr}\left(\Omega_\mu^+ - \Omega_\mu\right)$$

  - iterate $U_\mu^{(n+1)} = \exp\left(iQ_\mu^{(n)}\right) U_\mu^{(n)}$

$$U_\mu \to U_\mu^{(1)} \to \cdots \to U_\mu^{(n)} \equiv \widetilde{U}_\mu$$



- quark-field smearing (covariant Laplacian uses smeared gauge field)

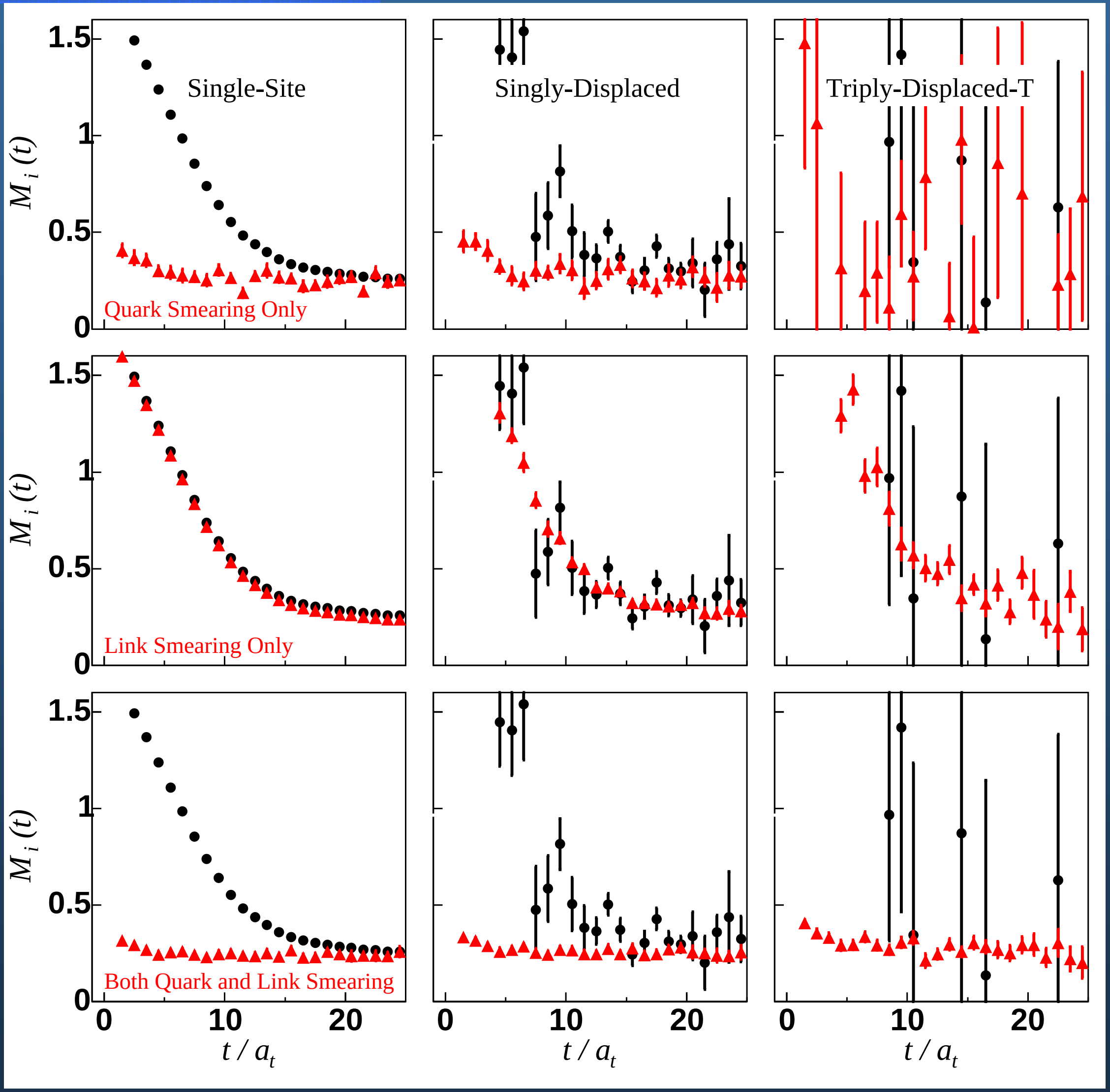
$$\tilde{\psi}(x) = \left(1 + \frac{\sigma_s}{4n_\sigma}\tilde{\Delta}\right)^{n_\sigma} \psi(x)$$

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

$$\sigma_s = 4.0, \quad n_\sigma = 32$$
$$n_\rho \rho = 2.5, \quad n_\rho = 16$$

- less noise in excited states using $\sigma_s = 3.0$



Operator selection

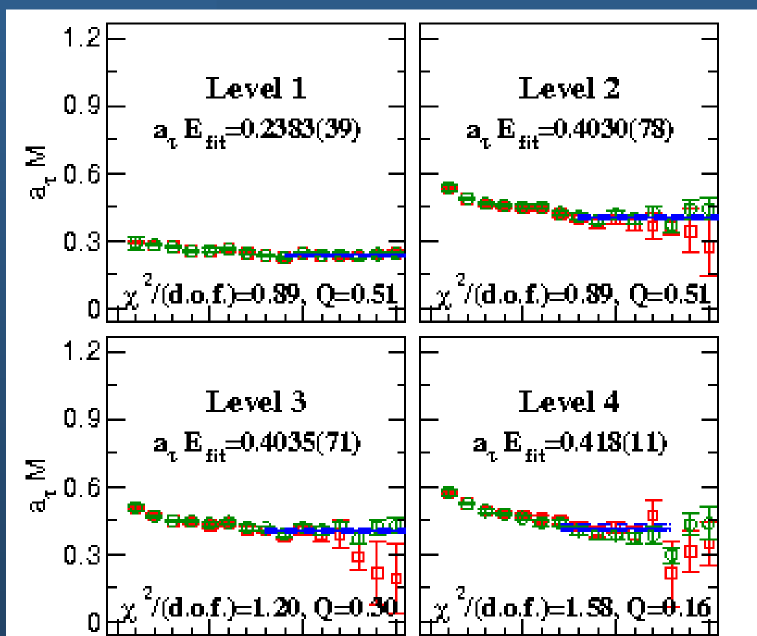
- rules of thumb for "pruning" operator sets
  - noise is the enemy!
  - prune first using intrinsic noise (diagonal correlators)
  - prune next within operator *types* (single-site, singly-displaced, *etc.*) based on condition number of
  - prune across all operators based on condition number
- best to keep a variety of different types of operators, as long as condition numbers maintained

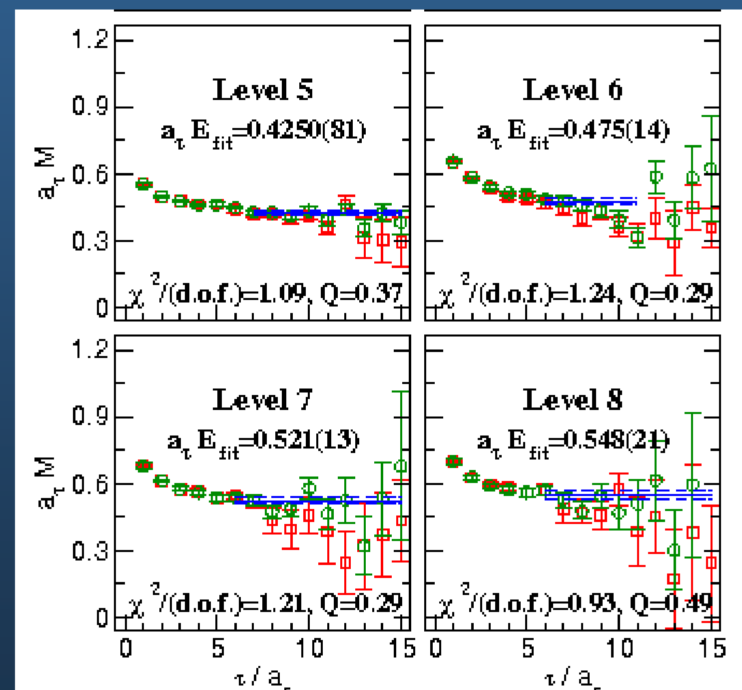
$$\hat{C}_{ij}(t) = \frac{C_{ij}(t)}{\sqrt{C_{ii}(t)C_{jj}(t)}}, \qquad t = 1$$

- typically use 16 operators to get 8 lowest lying levels

Nucleon G_{1g} effective masses

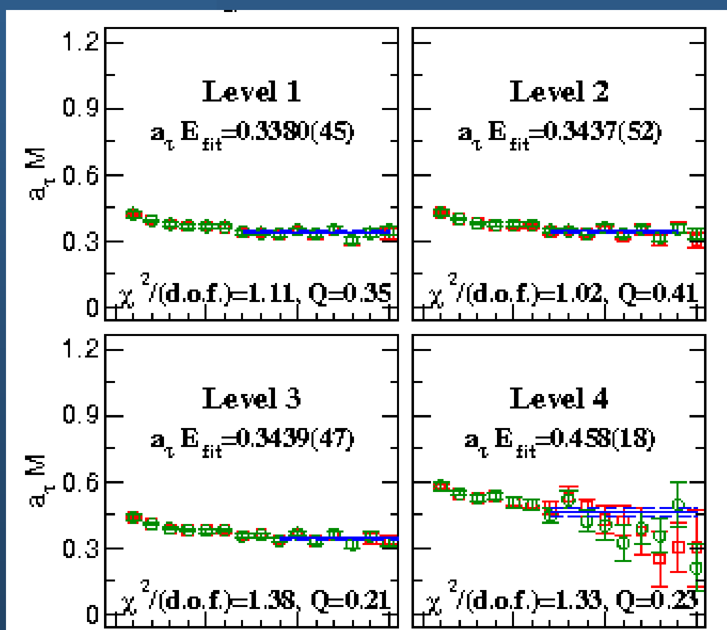
- 200 quenched configs, $12^3 \times 48$ anisotropic Wilson lattice, $a_s \sim 0.1$ fm, $a_s/a_t \sim 3$, $m_\pi \sim 700$ MeV
- nucleon G_{1g} channel
- green=fixed coefficients, red=principal

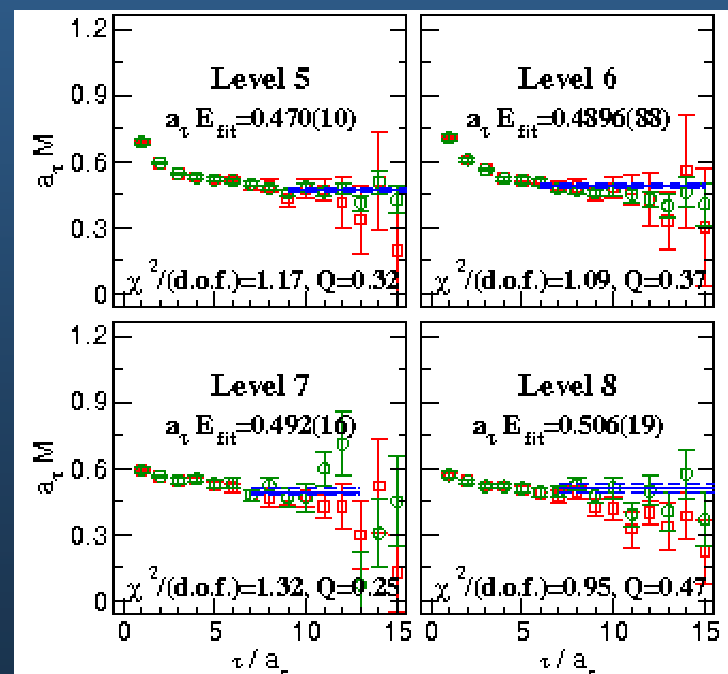




Nucleon H_u effective masses

- 200 quenched configs, 12^3 48 anisotropic Wilson lattice, a_s~0.1 fm, a_s/a_t~3, m_π~700 MeV
- nucleon H_u channel
- green=fixed coefficients, red=principal



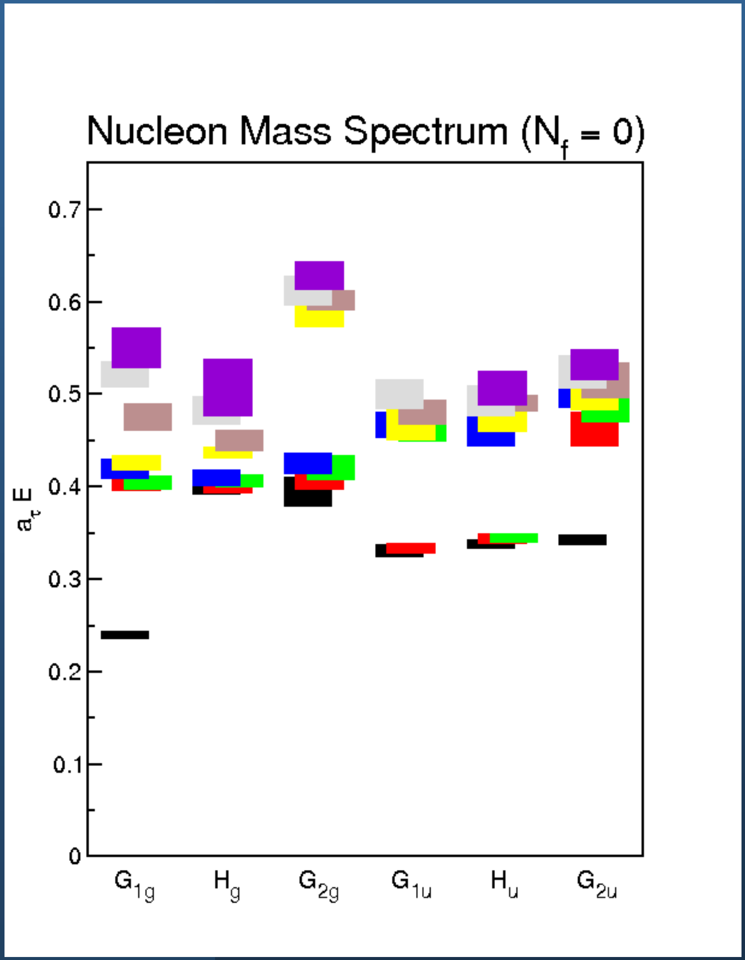


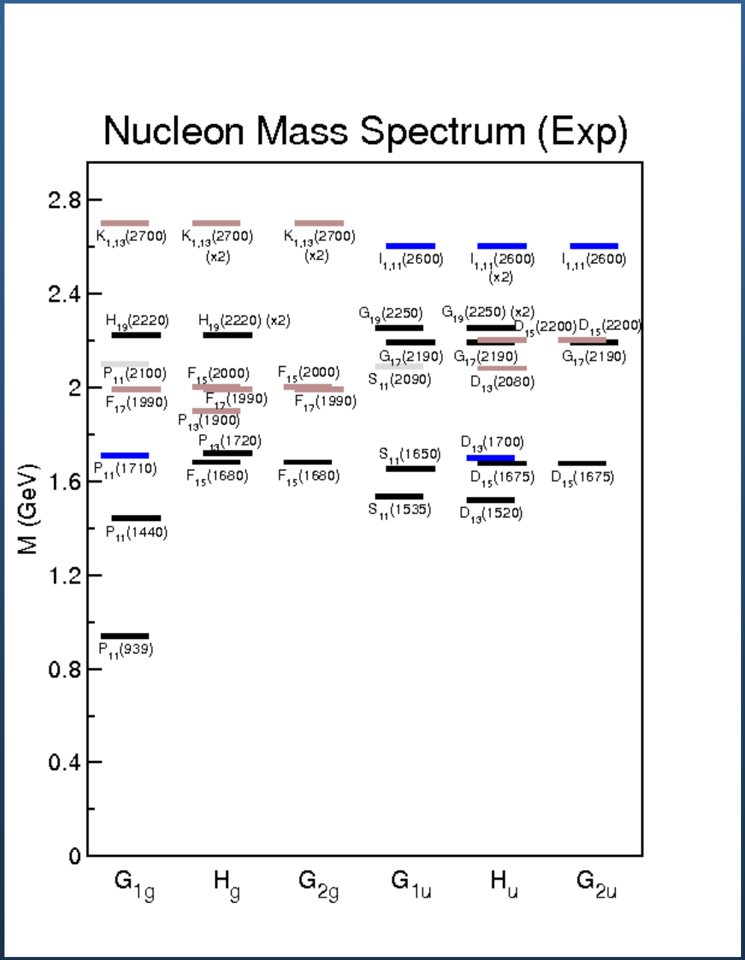
MILESTONE 1

Single-hadron excitations in quenched approximation

Nucleon spectrum: first results

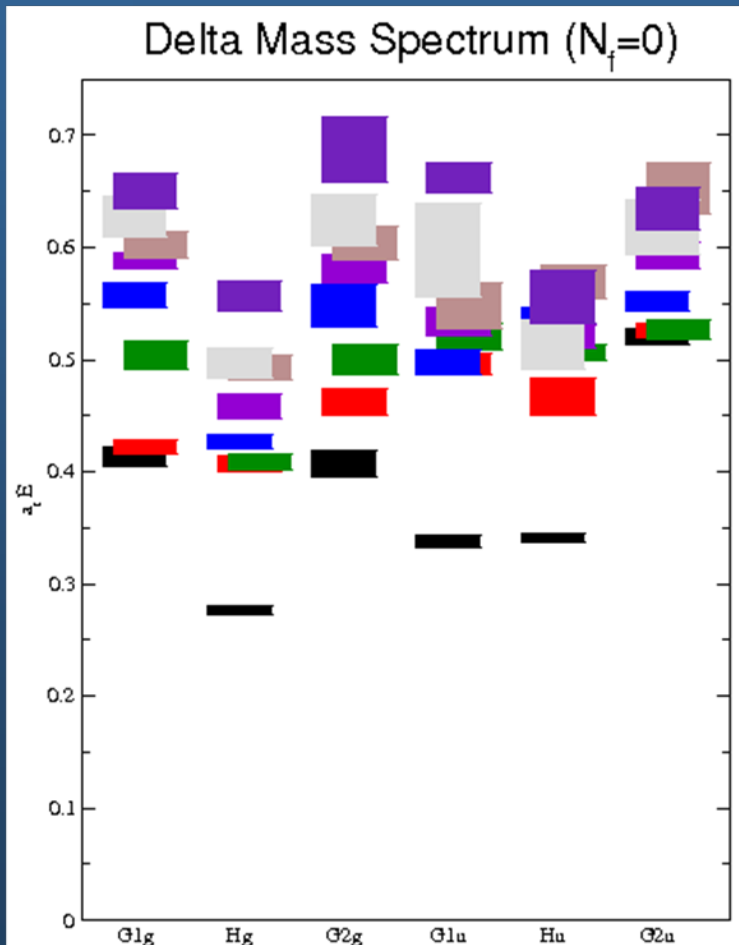
- 200 quenched configs, 12^3 48 anisotropic Wilson lattice, a_s~0.1 fm, a_s/a_t~3, m_π~700 MeV (A. Lichtl thesis)

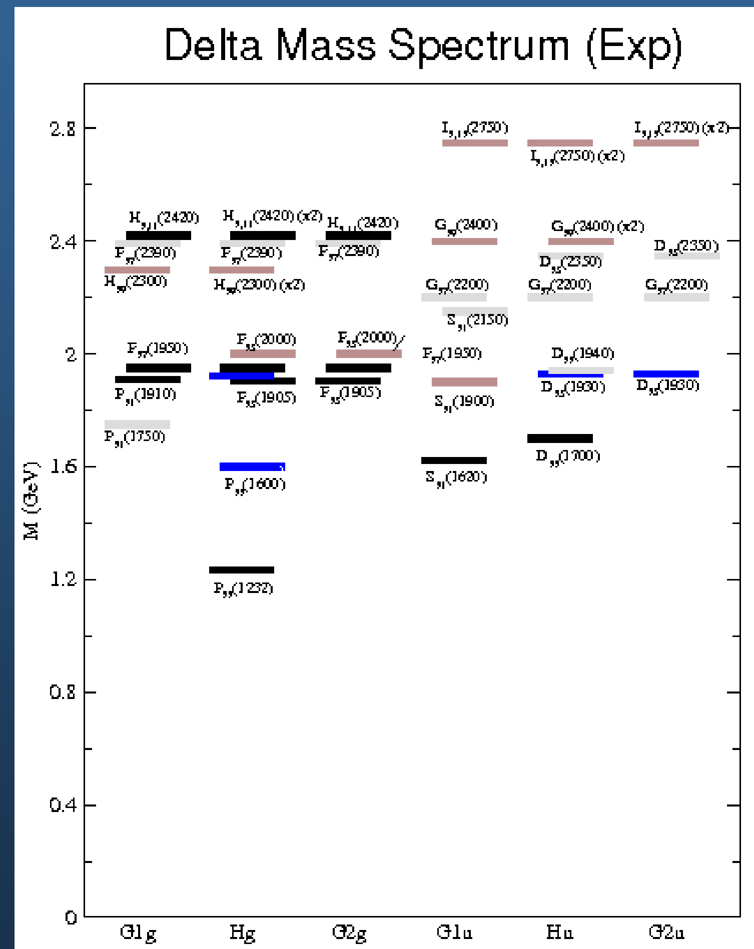




Delta spectrum: first results

- 200 quenched configs, 12^3 48 anisotropic Wilson lattice, a_s~0.1 fm, a_s/a_t~3, m_π~700 MeV (J. Bulava)



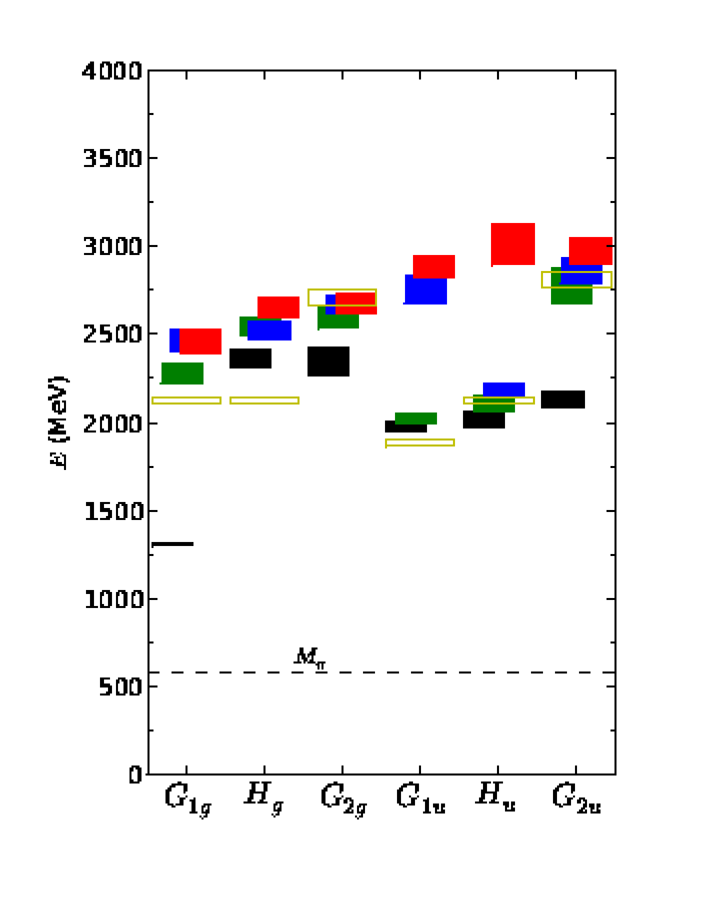


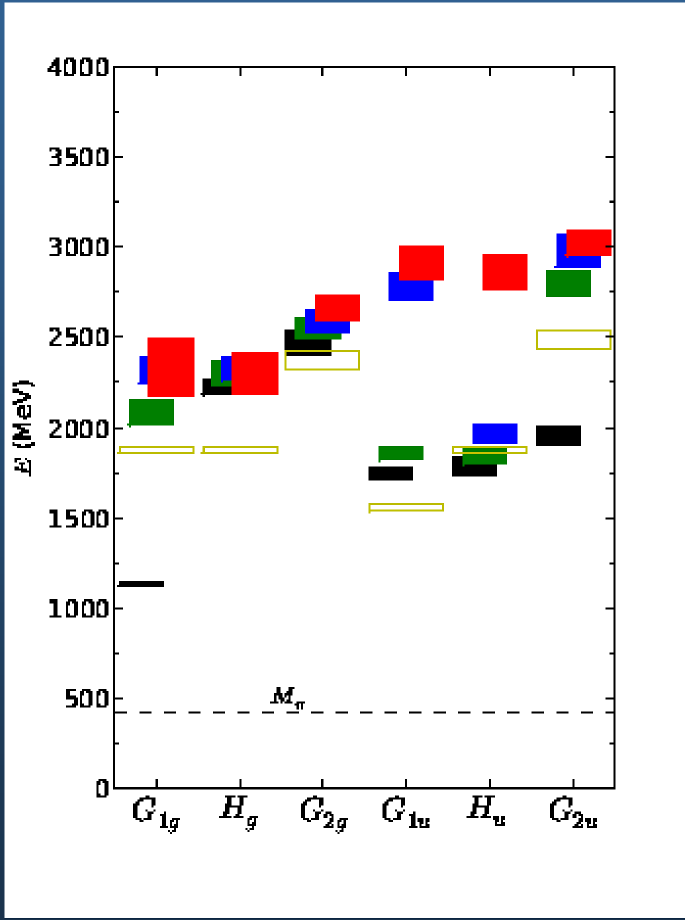
MILESTONE 2

Single-hadron excitations for $N_f = 2$

Inclusion of quark loops

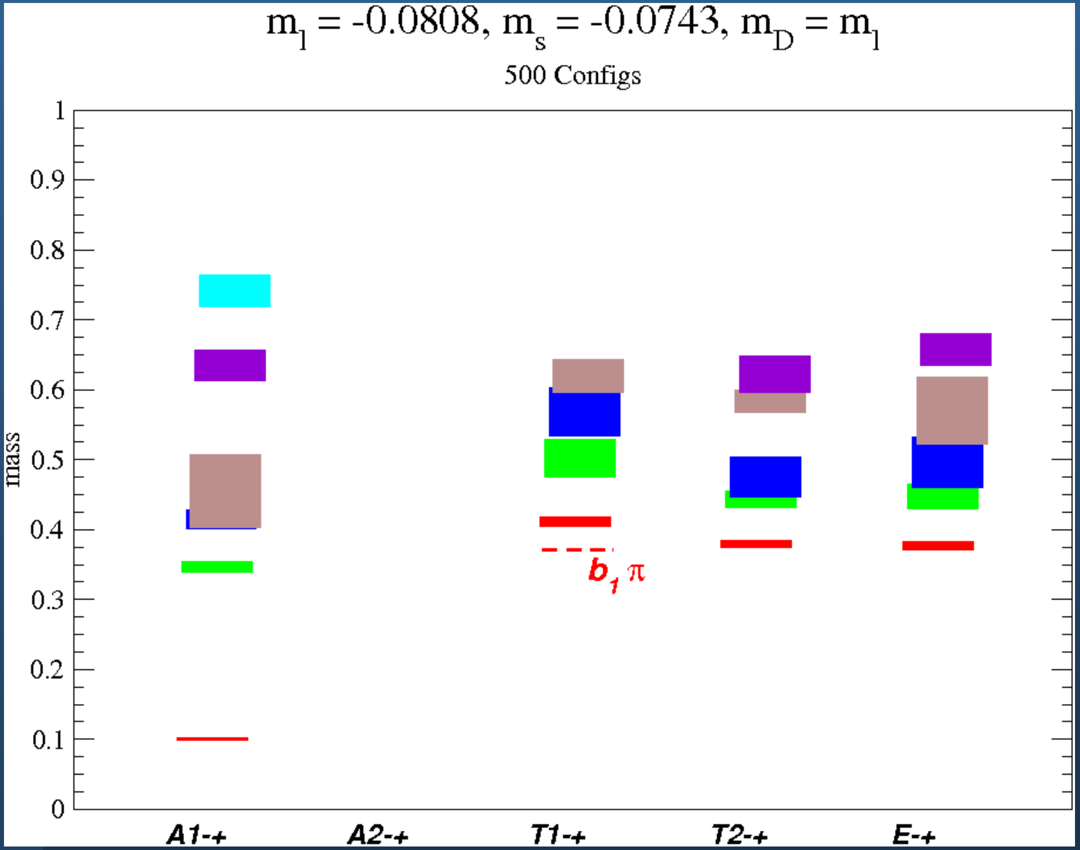
- N_f=2 on 24^3 64 anisotropic clover lattice, a_s~0.11 fm, a_s/a_t~3
- Left: m_π=578 MeV Right: m_π=416 MeV (PRD 2009, to appear)





Mesons

- N_f=2+1 on 16^3 128 anisotropic clover lattice, a_s~0.1 fm, a_s/a_t~3.5
- m_π=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

$$B(\vec{p}=0,t)=\frac{1}{V}\sum_{\vec{x}}\varphi_B(\vec{x},t)$$

- baryon correlator has a double spatial sum

$$\left\langle 0\middle|\overline{B}(\vec{p}=0,t)\;B(\vec{p}=0,0)\middle|0\right\rangle=\frac{1}{V^2}\sum_{\vec{x},\vec{y}}\left\langle 0\middle|\overline{\varphi}_B(\vec{x},t)\;\varphi_B(\vec{y},0)\middle|0\right\rangle$$

- computing all elements of propagators exactly not feasible
- translational invariance can limit summation over source site to a single site for local operators

$$\left\langle 0\middle|\overline{B}(\vec{p}=0,t)\;B(\vec{p}=0,0)\middle|0\right\rangle=\frac{1}{V}\sum_{\vec{x}}\left\langle 0\middle|\overline{\varphi}_B(\vec{x},t)\;\varphi_B(0,0)\middle|0\right\rangle$$

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!
  - new territory → exploration

Initial stochastic estimation

- quark propagator is just inverse of Dirac matrix M
- noise vectors η 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

$$E(X_i\eta_j^*) = E\left(\sum_k M_{ik}^{-1}\eta_k\eta_j^*\right) = \sum_k M_{ik}^{-1} E\left(\eta_k\eta_j^*\right) = \sum_k M_{ik}^{-1}\delta_{kj} = M_{ij}^{-1}$$

- 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}:

$$M_{ij}^{-1} \approx \frac{1}{N_R}\sum_{r=1}^{N_R} X_i^{(r)}\eta_j^{(r)*}$$

- 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:

$$P^{(a)}P^{(b)}=\delta^{ab}P^{(a)},\qquad \sum_a P^{(a)}=1,\qquad P^{(a)\dagger}=P^{(a)}$$

- observe that

$$M^{-1}_{ij}=M^{-1}_{ik}\delta_{kj}=\sum_a M^{-1}_{ik}P^{(a)}_{kj}=\sum_a M^{-1}_{ik}P^{(a)}_{kk'}\delta_{k'j'}P^{(a)}_{j'j}$$

$$=\sum_a M^{-1}_{ik}P^{(a)}_{kk'}E\left(\eta_{k'}\eta^*_{j'}\right)P^{(a)}_{j'j}=\sum_a M^{-1}_{ik}E\left(P^{(a)}_{kk'}\eta_{k'}\eta^*_{j'}P^{(a)}_{j'j}\right)$$

- define $\eta^{[a]}_k=P^{(a)}_{kk'}\eta_{k'},\qquad \eta^{[a]*}_j=\eta^*_{j'}P^{(a)}_{j'j},\qquad X^{[a]}_k=M^{-1}_{kj}\eta^{[a]}_j$

  so that $$M^{-1}_{ij}=\sum_a E\left(X^{[a]}_i\eta^{[a]*}_j\right)$$

- Monte Carlo estimate is now

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

- $\sum_a \eta^{[a]}_i\eta^{[a]*}_j$ has same expected value as $\eta_i\eta^*_j$, but reduced variance (statistical zeros → exact)

Dilution schemes for spectroscopy

- Time dilution (particularly effective)

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{ab}\delta_{\alpha\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{Bt}\delta_{Bt'},\qquad B=0,1,\ldots,N_t-1$$

- Spin dilution

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{ab}\delta_{B\alpha}\delta_{B\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{tt'},\qquad B=0,1,2,3$$

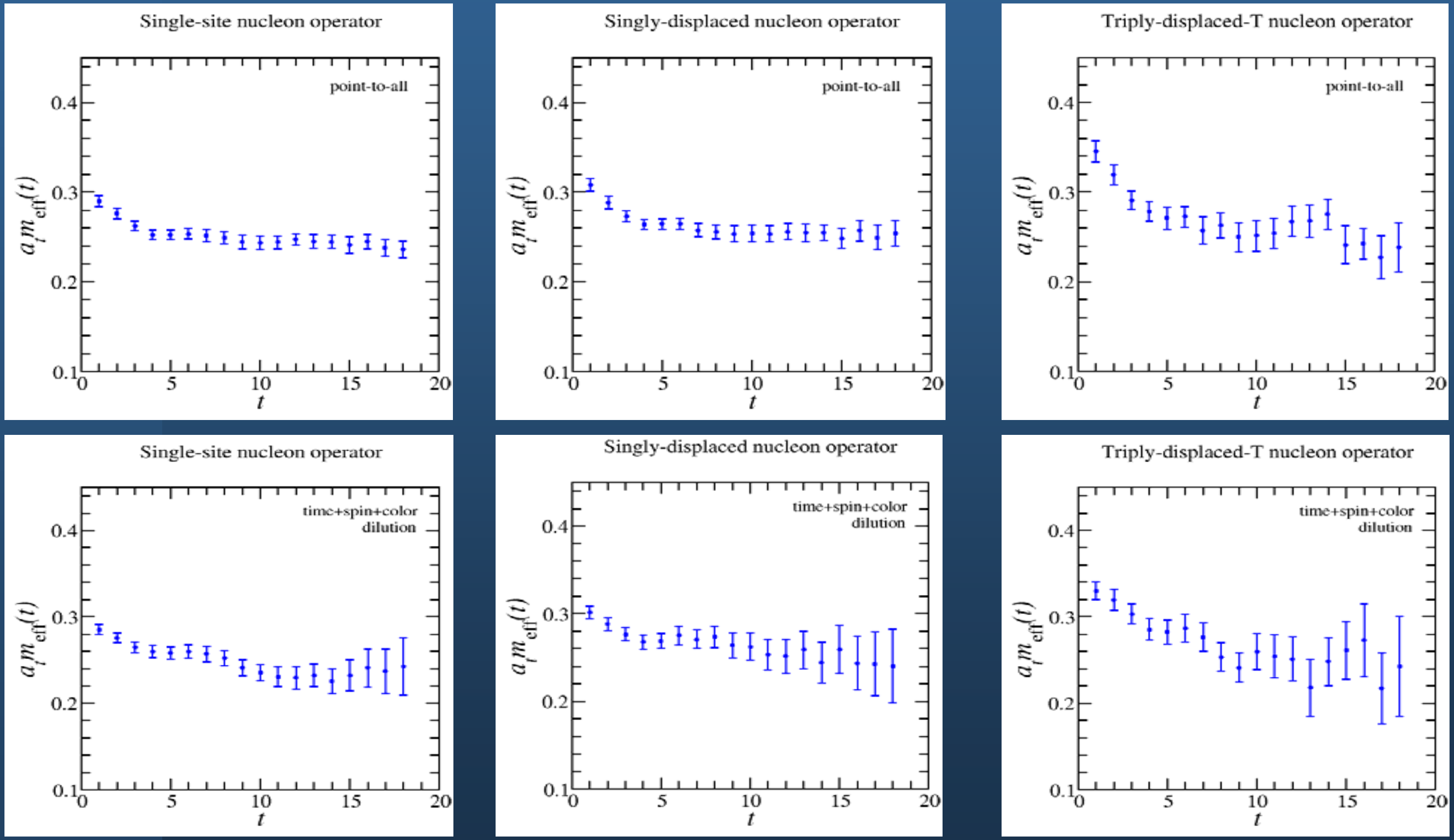
- Color dilution

$$P^{(B)}_{a\alpha;b\beta}\left(\vec{x},t;\vec{y},t'\right)=\delta_{Ba}\delta_{Bb}\delta_{\alpha\beta}\delta\left(\vec{x},\vec{y}\right)\delta_{tt'},\qquad B=0,1,2$$

- Spatial dilutions?
  - even-odd

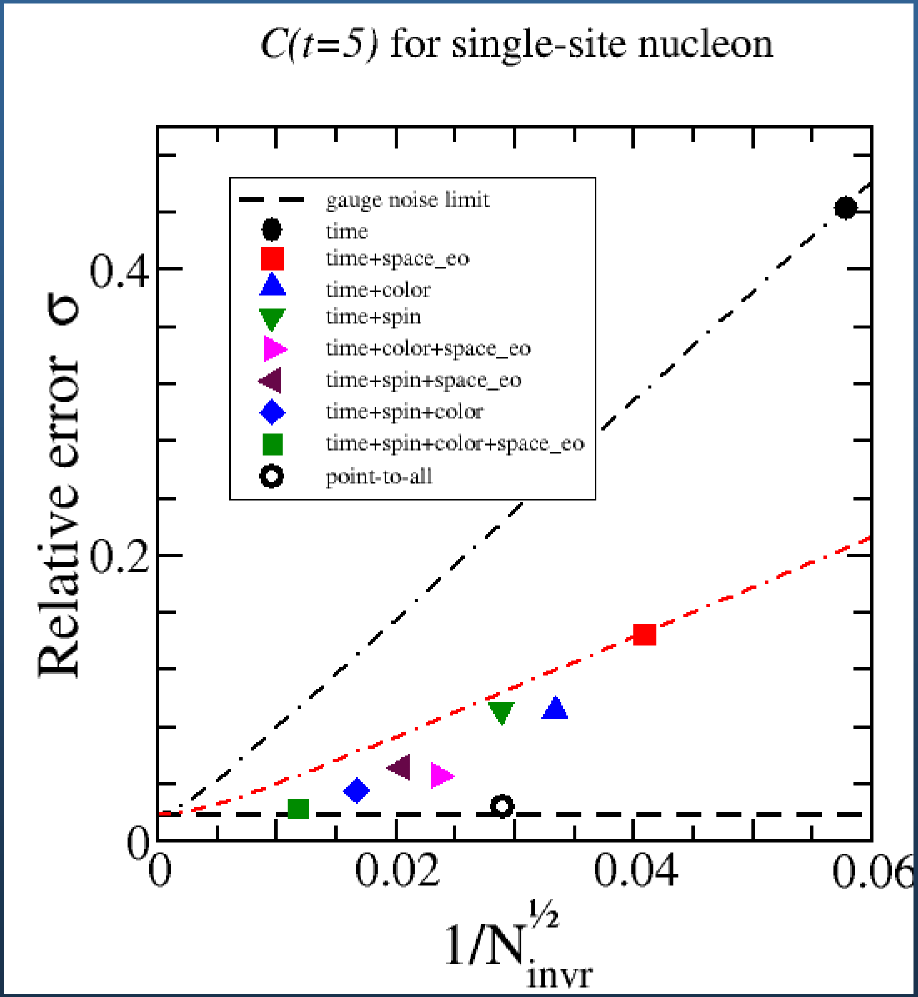
Dilution tests

- 100 quenched configs, 12^3 48 anisotropic Wilson lattice, a_s~0.1 fm, a_s/a_t~3, m_π~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

$$C_{l\bar{l}} = c_{ijk}^{(l)} c_{\bar{i}\bar{j}\bar{k}}^{(\bar{l})*} Q_{i\bar{i}}^{A} Q_{j\bar{j}}^{B} Q_{k\bar{k}}^{C}$$

- stochastic estimates with dilution

$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} c_{ijk}^{(l)} c_{\bar{i}\bar{j}\bar{k}}^{(\bar{l})*} \left(\varphi_i^{(Ar)[d_A]} \eta_{\bar{i}}^{(Ar)[d_A]*} \right) \times \left(\varphi_j^{(Br)[d_B]} \eta_{\bar{j}}^{(Br)[d_B]*} \right) \left(\varphi_k^{(Cr)[d_C]} \eta_{\bar{k}}^{(Cr)[d_C]*} \right)$$

- define

$$\Gamma_l^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \varphi_i^{(Ar)[d_A]} \varphi_j^{(Br)[d_B]} \varphi_k^{(Cr)[d_C]}$$

$$\Omega_l^{(r)[d_A d_B d_C]} = c_{ijk}^{(l)} \eta_i^{(Ar)[d_A]} \eta_j^{(Br)[d_B]} \eta_k^{(Cr)[d_C]}$$

- correlator becomes dot product of source vector with sink vector

$$C_{l\bar{l}} \approx \frac{1}{N_R} \sum_{r} \sum_{d_A d_B d_C} \Gamma_l^{(r)[d_A d_B d_C]} \Omega_{\bar{l}}^{(r)[d_A d_B d_C]*}$$

- 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

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

- express in term of eigenvectors/eigenvalues of Laplacian

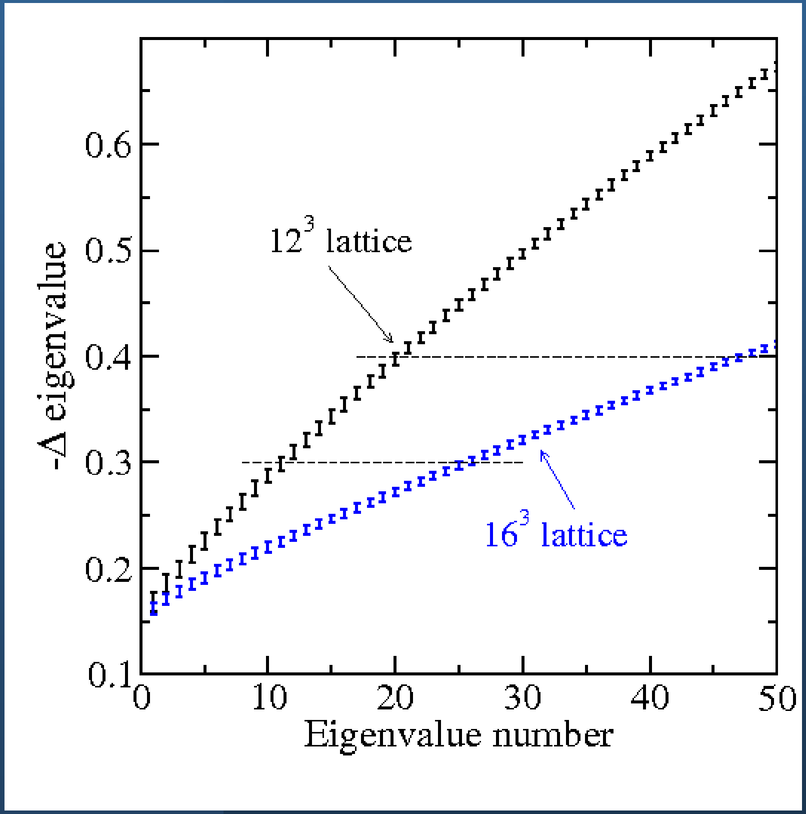
$$\tilde{\psi}(x) = \left(1 + \frac{\sigma_s}{4n_\sigma}\tilde{\Delta}\right)^{n_\sigma} \sum_k |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

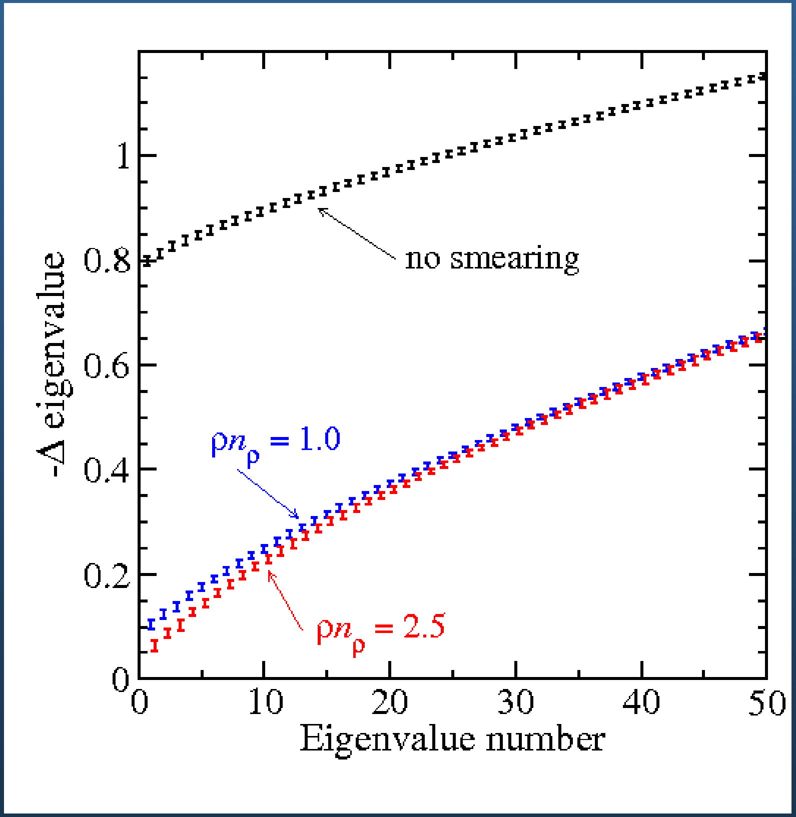
$$= \sum_k \left(1 + \frac{\sigma_s \lambda_k}{4n_\sigma}\right)^{n_\sigma} |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

- truncate sum and set weights to unity → Laplacian Heaviside

Getting to know the Laplacian

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





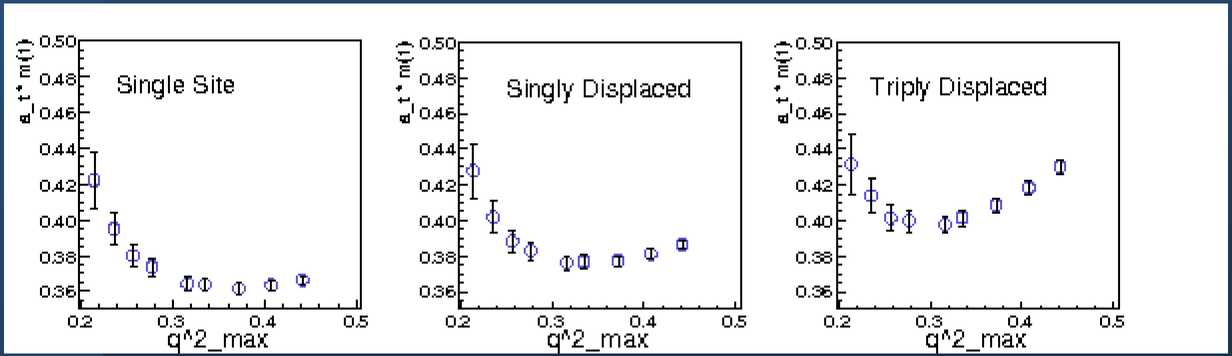
Choosing the smearing cut-off

- Laplacian Heaviside (LAPH) quark smearing

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

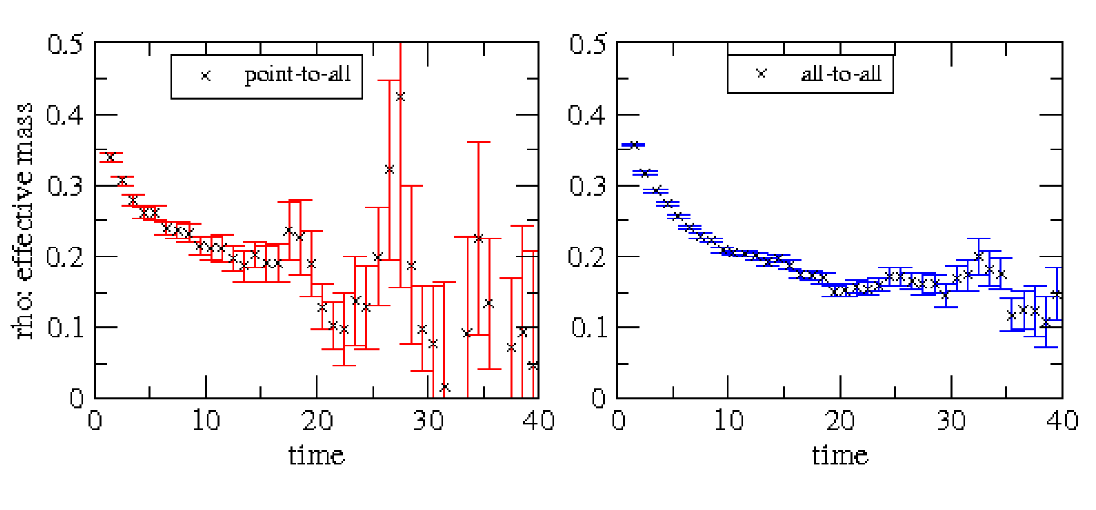
$$\approx \sum_{k=1}^{N_{\max}} |\varphi_k\rangle\langle\varphi_k|\psi(x)$$

- 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 ρ-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 → multi-hadron operators

Configuration generation

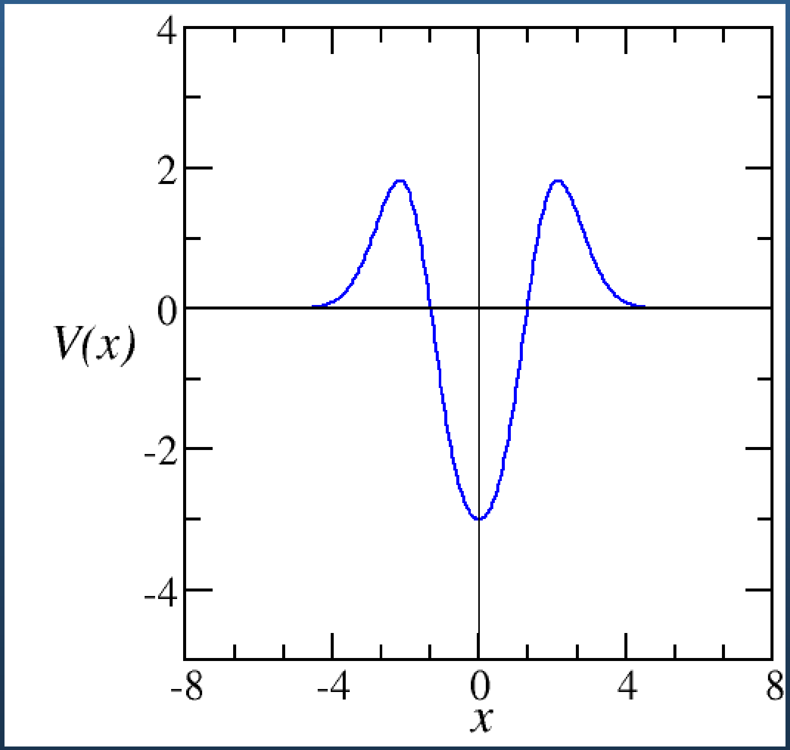
- significant time on USQCD (DOE) and NSF computing resources
- anisotropic clover fermion action (with stout links) and anisotropic improved gauge action
  - tunings of couplings, aspect ratio, lattice spacing done
- anisotropic Wilson configurations generated during clover tuning
- current goal:
  - three lattice spacings: a = 0.125 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, $m_\pi \sim$ 350 MeV, 220 MeV, 180 MeV
- USQCD Chroma software suite

Resonances in a box

Resonances in a box: an example

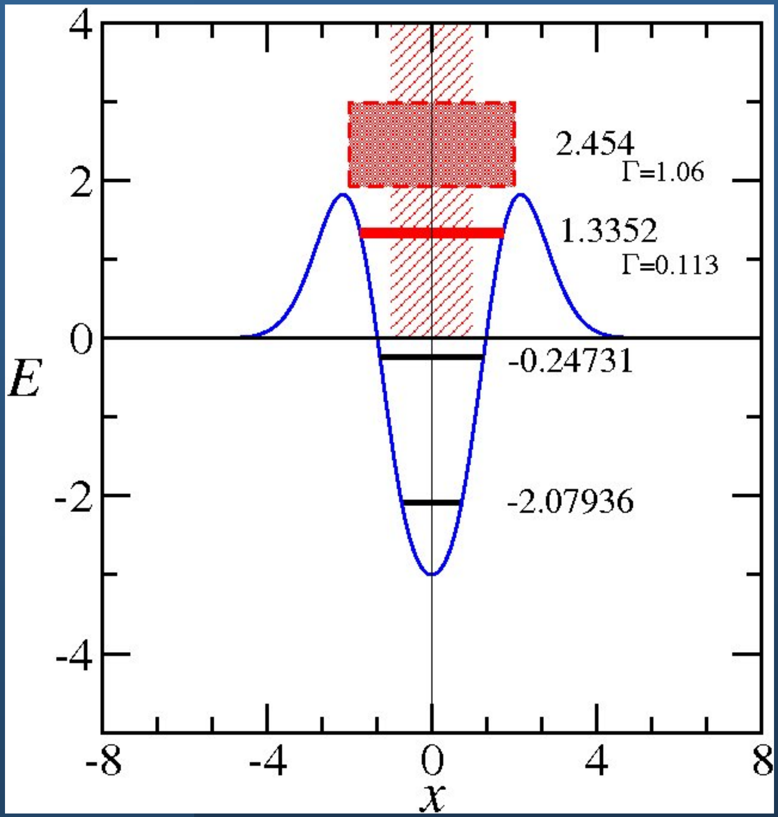
- Consider simple 1D quantum mechanics example
- Hamiltonian

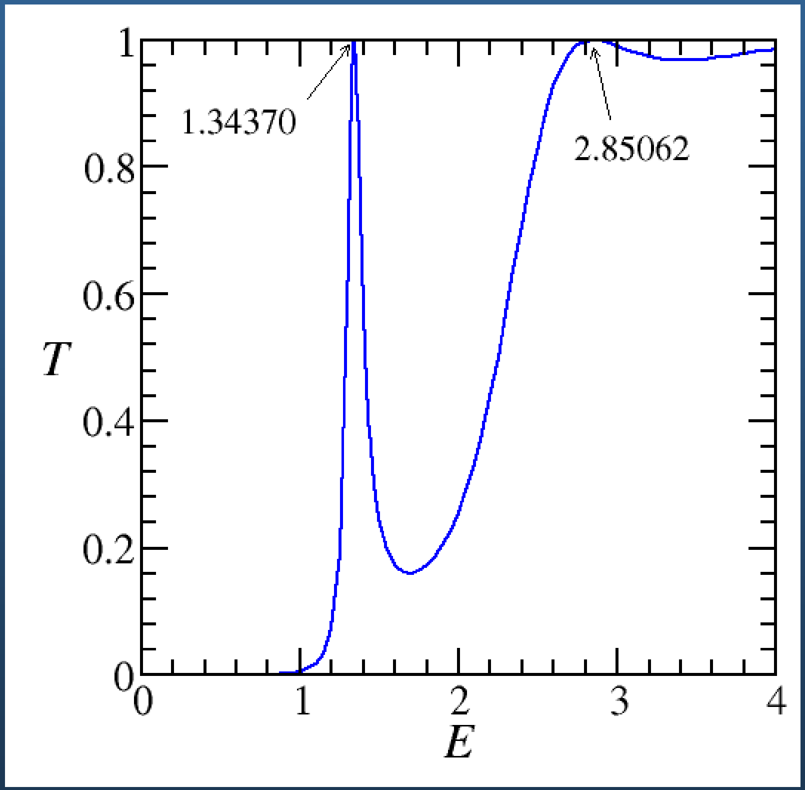
$$H = \frac{1}{2} p^2 + V(x) \qquad V(x) = (x^4 - 3)\, e^{-x^2/2}$$



1D example spectrum

- Spectrum has two bound states, two resonances for *E*<4

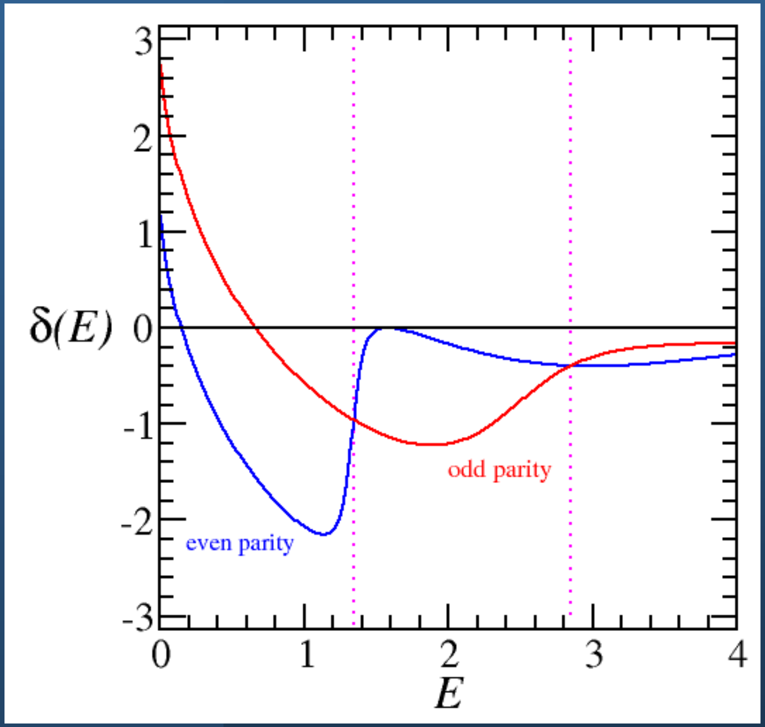


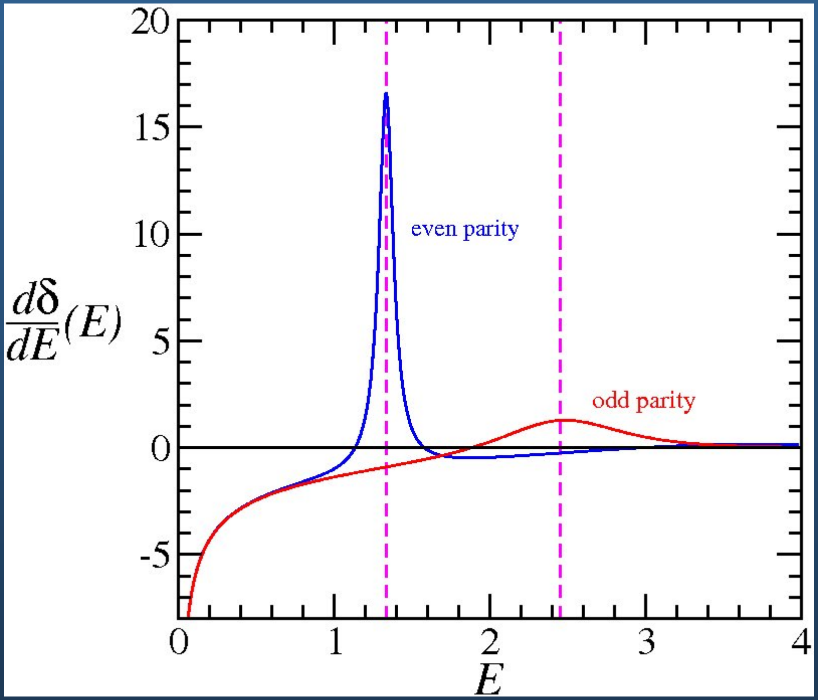


transmission coefficient

Scattering phase shifts

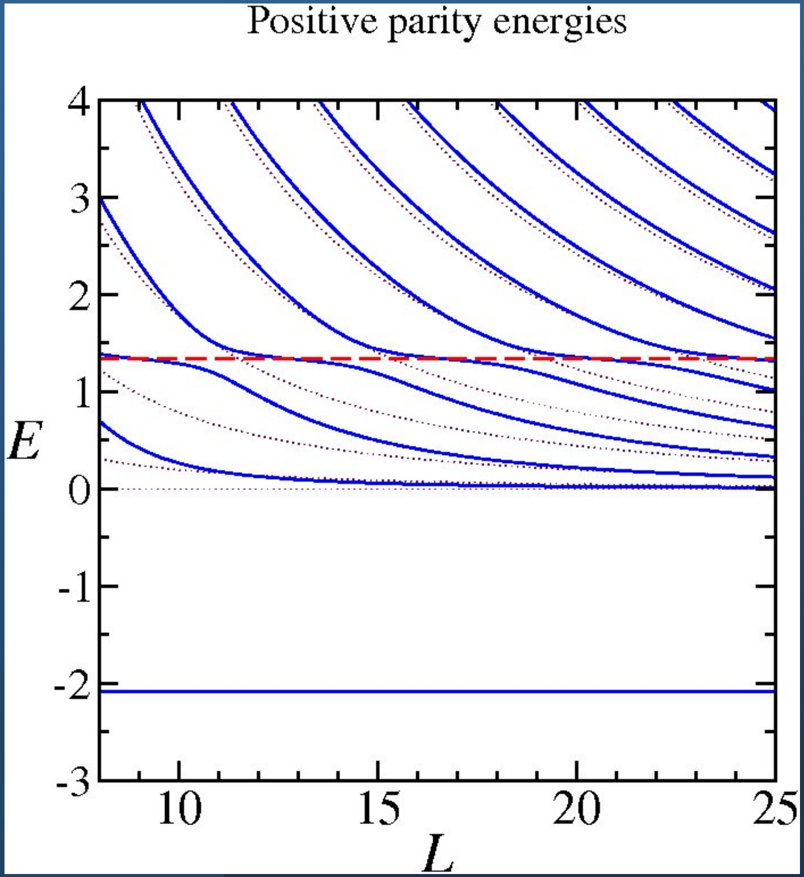
- define even- and odd-parity phase shifts $\delta_{\pm}$
  - phase between transmitted and incident wave

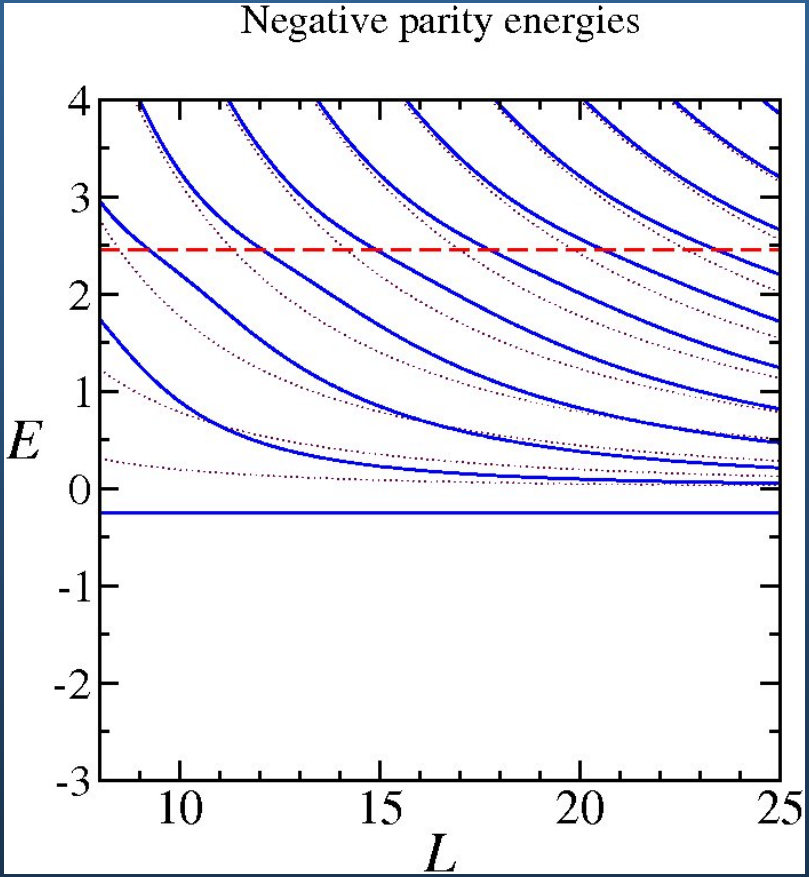




Spectrum in box (periodic b.c.)

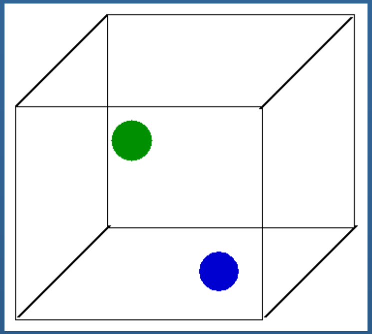
- spectrum is discrete in box (momentum quantized)
- narrow resonance is avoided level crossing, broad resonance?





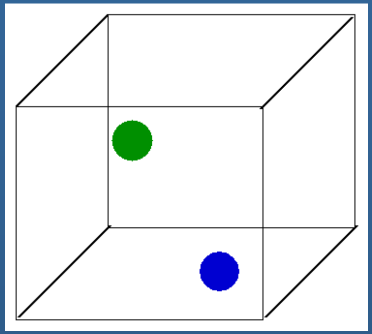
Dotted curves are V=0 spectrum

Unstable particles (resonances)



- our computations done in a periodic box
  - momenta quantized
  - discrete energy spectrum of stationary states → single hadron, 2 hadron, …
- how to extract resonance info from box info?
- approach 1: crude scan
  - if goal is exploration only → "ferret" out resonances
  - spectrum in a few volumes
  - placement, pattern of multi-particle states known
  - resonances → 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 → 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) (ρ-$\pi\pi$ 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