Introduction to Lattice QCD

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Lecture 3: Hadron spectrum

Outline

1. **Spectrum calculations**
   - Introduction to the basic techniques
   - Smearing techniques
   - Stochastic sources
2. **Low-lying hadrons**
   - Comparison of results
3. **Excited states**
   - Variational principle
   - Anisotropic lattices
   - Excited states of the Nucleon
4. **Exotics**
   - Glueballs
   - Multi-quark states
5. **Resonances**

Introduction to the basic techniques

Successful calculations of the masses of low-lying baryons is a prerequisite for the validity of lattice QCD.

- Choose the set of input parameters i.e. the bare quark masses and coupling constant
- Choose lattice size
- Create initial state of the hadron $J_h^\dagger |0\rangle$. Some standard interpolating fields:

$$J_\pi = \bar{d}\gamma_5 u\,, \quad J_\rho = \bar{d}\gamma_\mu u\,, \quad J_N = \epsilon^{abc}(u^{aT} C\gamma_5 d^b)u^c\,, \quad J_\Delta = \epsilon^{abc}(u^{aT} C\gamma_\nu d^b)u^c$$

We can make the following observations for J_N:

- The combination $u^{aT}(C\gamma_5 d^b)u^c$ transforms like a Lorentz scalar $\rightarrow J_N$ transform like u and thus is a spin 1/2 Dirac spinor.
- The color variables are antisymmetrized
- The non-relativistic limit of J_N agrees with the non-relativistic quark model: The upper components of $uC\gamma_5 d = u(-i\sigma^2)d = -u_\uparrow d_\downarrow + u_\downarrow d_\uparrow \rightarrow$ produces the SU(6) proton wave function.

Consider the pion two-point function:

$$C_{\pi\pi}(t) = \int d^3x \, \langle 0| J_\pi(\vec{x},t) J_\pi^\dagger(\vec{0},0) |0\rangle$$

It is calculated by evaluating

$$\begin{aligned} C_{\pi\pi}(t) &= \int d^3x \int \mathcal{D}[\bar\psi\psi]\mathcal{D}[U]\, e^{-\bar\psi D(U)\psi - S[U]} \bar{d}(\vec{x},t)\gamma_5 u(\vec{x},t)\bar{u}(\vec{0},0)\gamma_5 d(\vec{0},0) \\ &= \int d^3x \int \mathcal{D}[U]\, e^{-\ln \mathrm{Det} D(U) - S[U]}\, D_u^{-1}(U)(\vec{x},t;\vec{0},0)\gamma_5 D_d^{-1}(\vec{0},0;\vec{x},t)\gamma_5 \\ &\overset{N\to\infty}{=} \frac{1}{N}\sum_U \mathrm{Tr}|G(U)(\vec{x},y;\vec{0},0)|^2 \end{aligned}$$

where $G = D^{-1}$ and we assume that u and d are degenerate.

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\end{aligned}$$

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Effective mass

The physical content of $C_{ki}(t)$ can be seen as follows:

$$C_{ki}(t) = \int d^3x e^{i\vec{p}.\vec{x}} \langle 0| e^{tH-i\vec{x}.\vec{q}} J_k(\vec{0},0)\, e^{-tH+i\vec{x}.\vec{q}} \sum_n \int d^3q \frac{|n,\vec{q}\rangle\langle n,\vec{q}|}{2E_n(\vec{q})} J_i^\dagger(\vec{0},0)|0\rangle$$

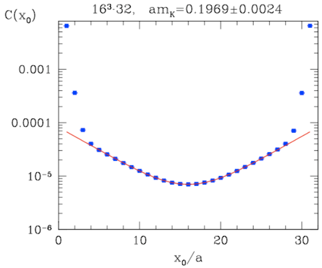
The integral over x projects onto momentum $\vec{p}$ and for large t only the lowest state of the quantum numbers of J contributes

$\rightarrow C_{ki}(\vec{p},t) \overset{t\to\infty}{=} \langle 0| J_k |\vec{p},h\rangle \langle \vec{p},h| J_i^\dagger |0\rangle \frac{e^{-E_h(\vec{p})t}}{2E_h(\vec{p})}$

- The mass of a given state is determined from the rate of exponential fall-off of $C_{kk}(\vec{0},t)$. Define an effective mass

$$m_{\rm eff}(t) \;=\; -\log\left(\frac{C_{kk}(\vec{0},t)}{C_{kk}(\vec{0},t-1)}\right) \overset{t\to\infty}{\longrightarrow} m$$

  which, in the limit $t\to\infty$, converges to the desired value.
- Optimize J_k to get a large overlap with the wave function, *i.e.* make $w_n(\vec{p}) \equiv \frac{|\langle 0|J_k|n\rangle|^2}{2E_n(\vec{p})}$: spectral weight of $n^{\rm th}$ state, large for the state of interest and the small for the rest
- Use enough statistics so that the signal extends to large enough t at which any remaining contamination from higher states is negligible
- Because of the finite extent of the lattice one usually imposes (anti)-periodic b.c. $\Longrightarrow$ meson correlators are symmetric in t and $e^{-mt} \rightarrow e^{-mt} + e^{-m(T-t)}$ where T is the time extent of the lattice



Comments on the behavior of the effective mass

- The convergence of $m_{\rm eff}(t)$ to the asymptotic value m can be from above or below depending on the choice of the interpolating field J. Only for $J_k = J_i$ is the correlation function positive definite and the convergence is monotonically and from above.
- Interpolating fields project to all states with the same quantum numbers. For large t the ground state dominates
  $i.e\ m_{\rm eff}(t) \rightarrow {\rm constant}$: plateau region
  The onset and the length of the plateau region depends on the interpolating operators.
- The statistical errors grow exponentially with t, except for the case of the pion.
- For extracting higher states number of methods are developed: A common approach is to use $k \neq i$ and study the generalized eigenvalue equations.

Summary: Extract the mass as described above.
If computation is done with physical values of the quark masses, then study its dependence as a function of a, and L before we can compare to experimental data.
If the computation is not done with physical values of the quark masses then study quark mass dependence.

Exercise:
Convince yourself that the statistical errors grow exponentially with t, except for the case of the pion.

Current challenges

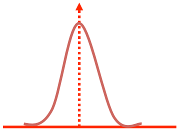
- Construct optimized interpolating fields which maximize the spectral weight w_n for a given state
- Develop techniques to extract excited states from the two-point correlators
- Develop techniques to study the internal structure of hadrons *e.g.* "molecular" versus multi-quark nature, radial excitation, etc.
- Develop techniques to study resonances and decay widths
- At the **physical point**, it is crucial to combine optimized methods to keep statistical noise small

Smearing techniques

Hadrons are extended objects having size $\mathcal{O}(1\text{ fm})$. The interpolating fields create point sources
$\rightarrow$ they have a small overlap with the hadron state we want to study
$\Longrightarrow$ Optimize projection to the state of interest:

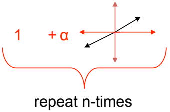
Employ "gauge invariant smearing" of quark fields:

$$\psi^{\text{smear}}(\vec{x}, t) = \sum_{\vec{y}} F(\vec{x}, \vec{y}, U(t))\psi(\vec{y}, t)$$



- To enhance ground state dominance use Gaussian smearing

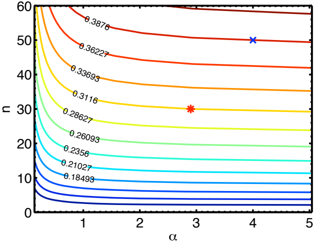
$$F(\vec{x}, \vec{y}, U(t)) = (\mathbb{1} + \alpha H)^{n_\sigma}$$
$$H(\vec{x}, \vec{y}; U(t)) = \sum_{i=1}^{3} \left(U_i(x)\delta_{x,y-\hat{i}} + U_i^\dagger(x - \hat{i})\delta_{x,y+\hat{i}} \right)$$



- Exponential smearing:

$$F(\vec{x}, \vec{y}, U(t)) = (D^2 + m_{sc}^2)^{-n_{sc}}(\vec{x}, \vec{y})$$

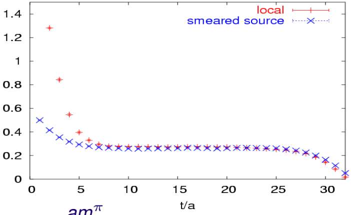
where one computes the propagator of a scalar particle propagating in the 3-dimensional space of the same background gauge field $U(t)$



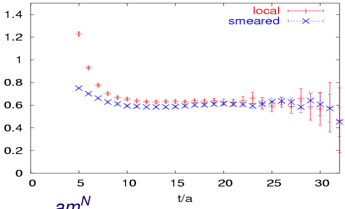
Adjust the smearing parameters α (m_{sc}) and n_σ (n_{sc}) so that $r.m.s$ radius of the initial state made of the smeared quarks has a value close to the experimental value.

Examples of effective mass plots

- Quenched at about 550 MeV pions:

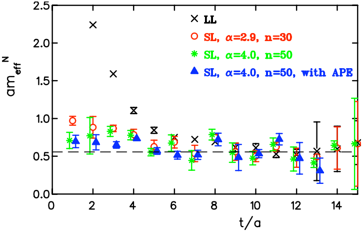


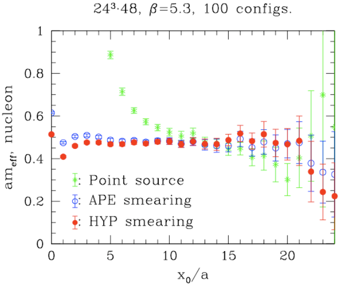
$am^{\pi}_{\rm eff}$



$am^{N}_{\rm eff}$

- Reduce gauge noise by using APE, hypercubic or stout smearing on the links U that enter the smearing function $F(\vec{x},\vec{y},U(t))$.
- $N_F = 2$



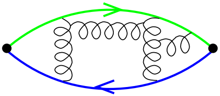


H. Wittig, SFB/TR16, August, 2009

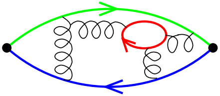
Stochastic sources

The calculation of hadron masses involves the computation of the point-to-all propagator:

$G(\vec{x},t;\vec{x}_0,t_0)^{aa_0}_{\mu\mu_0}$ obtained from solving $DG = \delta^4(\vec{x}_0,t_0)\delta_{aa_0}\delta_{\mu\mu_0}$



(A) Quenched QCD: quark loops neglected



(B) Full QCD

In order to reduce statistical noise as we approach the physical pion mass one may want to sum over the source coordinates as well. This requires a new inversion for each lattice point!
$\Longrightarrow$ replace point source by stochastic noise vector such that:

$$\frac{1}{N_r}\sum_{r=1}^{N_r}\zeta^a_\mu(x)_r \equiv \langle\zeta^a_\mu\rangle_r = 0\,,\quad \frac{1}{N_r}\sum_{r=1}^{N_r}\zeta^a_\mu(x')_r\zeta^{*a'}_{\mu'}(x)_r = \delta^4(x-x')\delta_{\mu\mu'}\delta_{aa'}$$

Inverting using these $\zeta's$ as sources one obtains a set of solutions vectors

$$\phi^a_\mu(x)_r = \sum_y G^{ab}\mu\nu(x,y)\,\zeta^b_\nu(y)_r \quad \to G^{ab}_{\mu\nu}(x,y) = \langle\phi^a_\mu(x)\zeta^{*b}(y)\rangle_r$$

A common choice for the noise vectors is Z(2) noise. These satisfy only approximately the above relations and so one introduces stochastic noise needing a large number of N_r.
$\Longrightarrow$ reduce N_r by employing "dilution schemes"
For mesons one can apply the 'one-end' trick that combines appropriately solution vectors to obtain the two-point correlators. E.g. for the pion:

$$\frac{1}{N_r}\sum_{\vec{x},r}\phi^\dagger_r(\vec{x},t;t_0)\phi_r(\vec{x},y;t_0) = \sum_{\vec{x},\vec{x}_0}\mathrm{Tr}|G(x,x_0)|^2$$

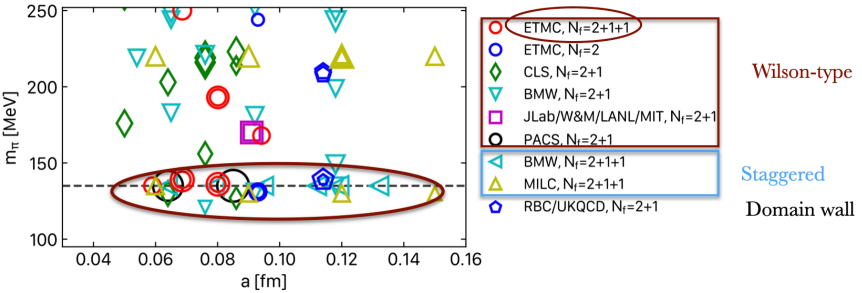
Systematic effects

- Cut-off effects

$$\frac{m_N}{m_\Omega}\Big|^{\rm lat} = \frac{m_N}{m_\Omega}\Big|^{\rm exp} + \mathcal{O}(a/r_0)^p,\ \ p \geq 1$$

  where r_0 some length scale e.g. determined from the force between a static quark and anti-quark.
  $\Longrightarrow$ we need to extrapolate to the continuum limit i.e. take $a \to 0$
- Finite volume effects: Use $Lm_\pi > 3.5$
- Larger light quark masses:
  Use chiral perturbation theory to extrapolate. Most collaborations are now simulating at pion masses below 200 MeV or at the physical point.

$\Longrightarrow$ Calculation of the ground state of mesons and baryons checks lattice artifacts, finite volume effects and chiral extrapolations.



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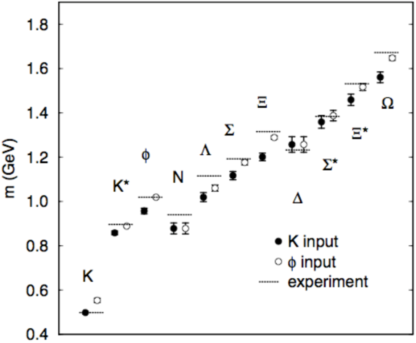
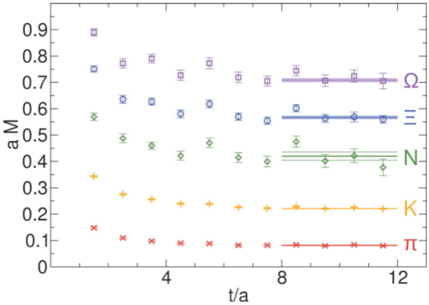


Quenched calculation with Wilson fermions CP-PACS Collaboration, S. Aoki et al. Phys. Rev. D 67 (2003)

- Calculation done at 4 values of $a \to$ take continuum limit
- The scale is set using m_ρ
- The strange quark mass is set by the kaon mass and by the ϕ mass
- Established that the quenched approximation reproduces the experimental spectrum with up to 15% deviations

Unquenched calculations

$N_f = 2 + 1$ smeared Clover fermions BMW Collaboration, S. Dürr et al. Science 322 (2008)



- 3 lattice spacing: $a \sim 0.125, 0.085, 0.065$ fm set by m_Ξ
- Pion masses: $m_\pi \stackrel{\sim}{>} 190$ MeV
- Volume:$m_\pi^{\min} L \stackrel{\sim}{>} 4$

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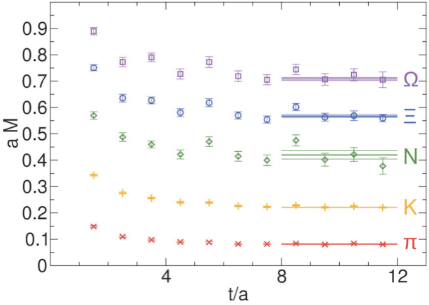

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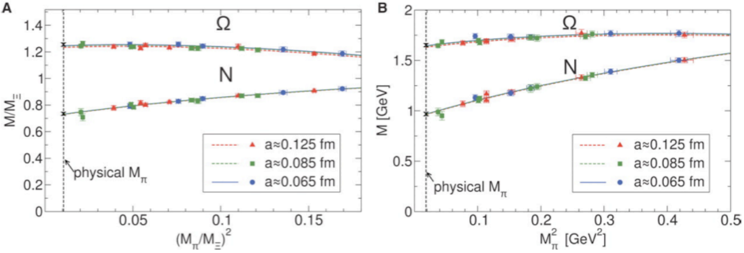
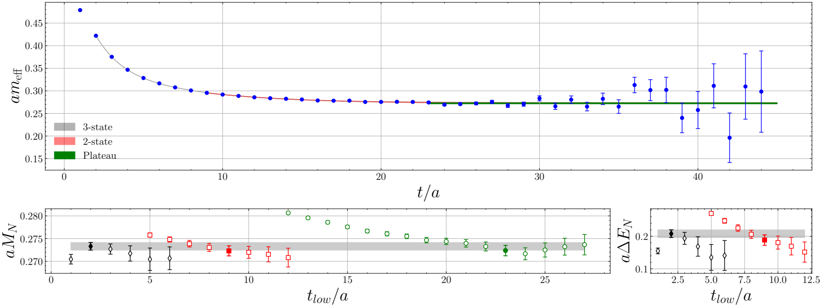


Low-lying hadron masses

Simulation parameters used by the Extended Twisted Mass Collaboration (ETMC)

Ensemble	V	β	μ_l	μ_σ	μ_δ	$L \cdot m_\pi$	m_π [MeV]
cB211.072.64	128×64^3	1.778	0.00072	0.1246826	0.1315052	3.62	140.1 (0.2)
cC211.060.80	160×80^3	1.836	0.00060	0.106586	0.107146	3.78	136.7 (0.2)
cD211.054.96	192×96^3	1.900	0.00054	0.087911	0.086224	3.9	140.8 (0.2)



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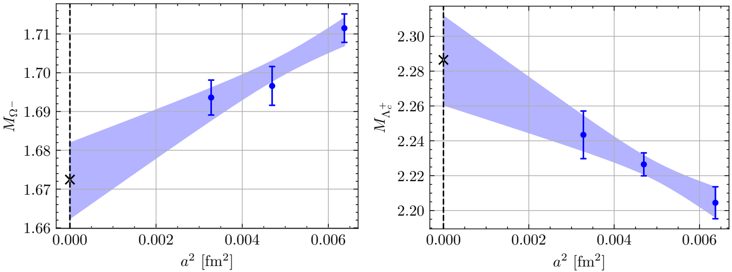
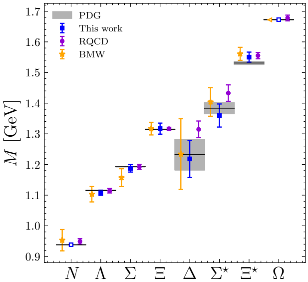
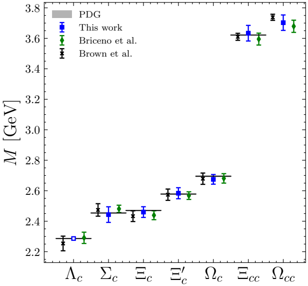
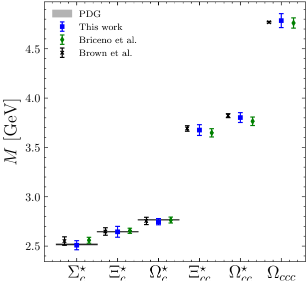


Continuum limit extrapolation for the mass of the Ω^- (top) and the Λ_c^+ (bottom)

Comparison of results using different actions







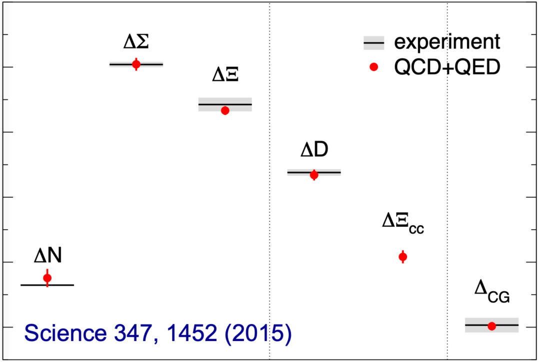
ETMC, C. Alexandrou *et al.* Phys. Rev. D 108 (2023) 9, 094510, arXiv: 2309.04401 [hep-lat]

Good agreement between different discretization schemes

$\Longrightarrow$ Significant progress in understanding the masses of low-lying mesons and baryons

Isospin and QED corrections to masses

BMW collaboration computed isospin and QED corrections determining the mass splitting for the low-lying baryons, Sz. Borsanyi et al., Science 347 (2015) 1452



	mass splitting [MeV]	QCD [MeV]	QED [MeV]
$\Delta N = n - p$	1.51(16)(23)	2.52(17)(24)	-1.00(07)(14)
$\Delta\Sigma = \Sigma^- - \Sigma^+$	8.09(16)(11)	8.09(16)(11)	0
$\Delta\Xi = \Xi^- - \Xi^0$	6.66(11)(09)	5.53(17)(17)	1.14(16)(09)
$\Delta D = D^\pm - D^0$	4.68(10)(13)	2.54(08)(10)	2.14(11)(07)
$\Delta\Xi_{cc} = \Xi_{cc}^{++} - \Xi_{cc}^{+}$	2.16(11)(17)	-2.53(11)(06)	4.69(10)(17)
$\Delta_{\mathrm{CG}} = \Delta N - \Delta\Sigma + \Delta\Xi$	0.00(11)(06)	-0.00(13)(05)	0.00(06)(02)

Excited states

Lattice calculations of excited states are harder:

- Usually calculations are done on coarse lattices and at one lattice spacing $\rightarrow$ no continuum extrapolations
- Still done at larger than physical pion masses and the width of resonances is mostly ignored
- At the physical point most are resonances

1. One major challenge is to isolate the sub-leading contributions to the two-point correlator. Various methods are used:
   - Variational
   - Bayesian, see e.g. G. P. Lepage *at al,*, NP109A (2002) 185
   - χ^2-histogram searches, see [C. Alexandrou, C.N. Papanicolas and E. Stiliaris, PoS LAT2008, arXvi:0810.3882
2. Another major challenge is to distinguish resonances from multi-quark or multi-hadron states
   - Use scaling of spectral weight with the spatial volume
   - Dependence on boundary conditions

Variational principle

Consider a basis of interpolating fields J_i, $i = 1, \cdots, N$ having the same quantum numbers

- Define an $N \times N$ correlator matrix:

$$C_{kj}(t) = \langle J_k(t) J_j^\dagger \rangle = \sum_{n=1}^{\infty} \langle 0| J_k |n\rangle \langle n| J_j^\dagger |0\rangle \, e^{-E_n t}$$

- Define the N principal correlators $\lambda_k(t, t_0)$ as the eigenvalues of the generalized eigenvalue problem (GEVP):

$$C(t) v_n(t, t_0) = \lambda_n(t, t_0) C(t_0) v_n(t, t_0)$$

  where t_0 is some reference time separation.
- The vectors $\tilde{v}_n(t, t_0) \equiv C^{1/2}(t_0) v_n(t, t_0)$ diagonalize $C^{-1/2}(t_0) C(t) C^{-1/2}(t_0) \rightarrow$ use to define a basis of interpolating fields $\tilde{J}_n = \sum_{k=1}^{N} (\tilde{v}_n^*)_k J_k$
- $\tilde{J}_n{}^\dagger$ creates the n^{th} eigenstate: $|n\rangle = \tilde{J}_n^\dagger |0\rangle$.
  The N principal eigenvalues correspond to the N lowest-lying stationary-state energies [Lüscher and Wolff 1990]

$$E_n^{\text{eff}}(t, t_0) = -\partial_t \lambda_n(t, t_0) = E_n + \mathcal{O}\left(e^{-\Delta E_n t}\right) \ , \quad \Delta E_n = \overset{m \neq n}{\min} |E_m - E_n|$$

Anisotropic lattices

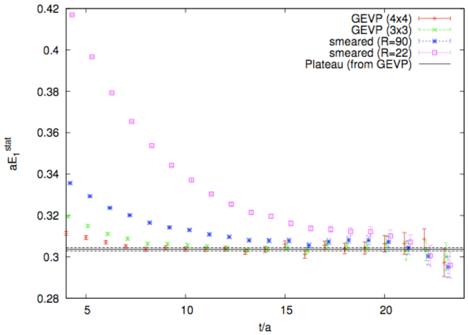
Use a different lattice space a_t for time direction as that for the spatial directions a_s
$\Longrightarrow$ this is advantageous for studying excitations which have larger masses since the two-point correlation function fall off rapidly:

$$C(\vec{0}, t) \stackrel{t \gg 0}{\to} e^{-a_t m(t/a_t)}$$

Typically $\xi \equiv \frac{a_s}{a_t} \sim 3$ and $a_s \sim 0.1 - 0.15$ fm (check for spatial lattice spacing effects)

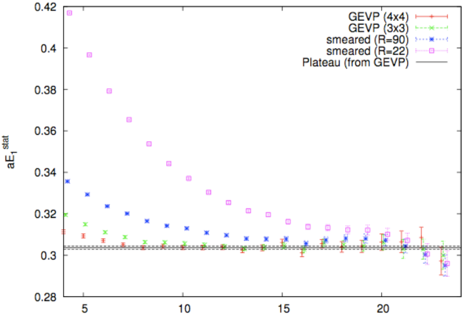
Results using the variational principle

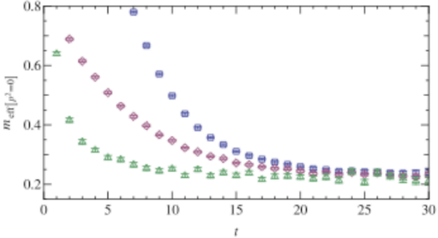
If $t_0 = t/2$ then correction is only $\mathcal{O}\left(e^{-\Delta E_{N+1} t}\right)$ [Blossier *et al.* (Alpha Collaboration), arXiv:0902.1265]

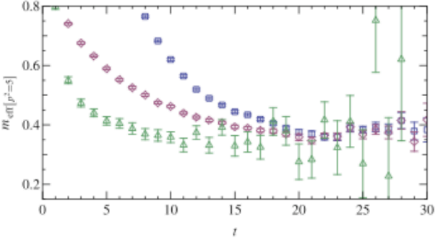


Results using the variational principle

If $t_0 = t/2$ then correction is only $\mathcal{O}\left(e^{-\Delta E_{N+1} t}\right)$ [Blossier *et al.* (Alpha Collaboration), arXiv:0902.1265]



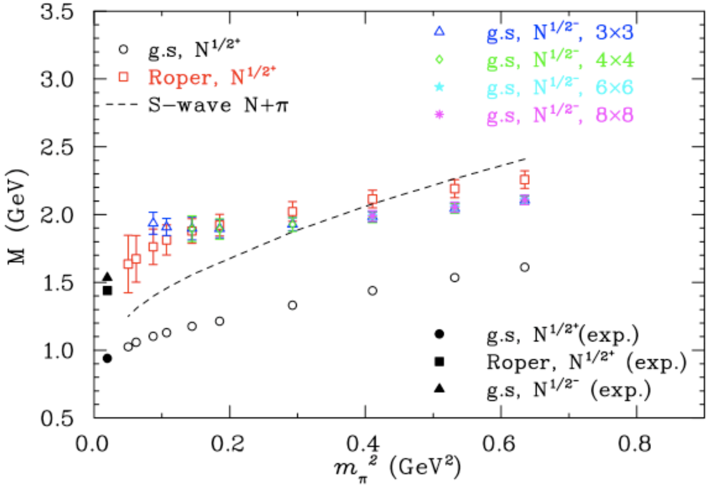




Nucleon effective mass plots with $m_\pi = 450$ MeV using differing Gaussian smearings

Excited states of the Nucleon

The first excited state of the nucleon is known as the Roper. It has a mass below the negative parity state of the nucleon.
It has been difficult to obtain the Roper in lattice calculations most of which are done in the quenched approximation

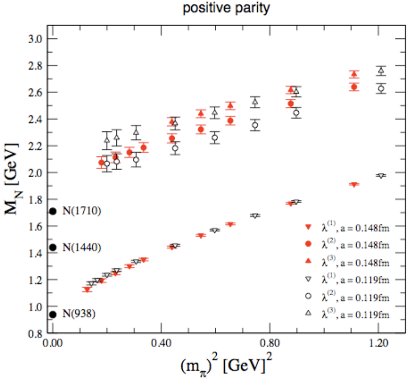


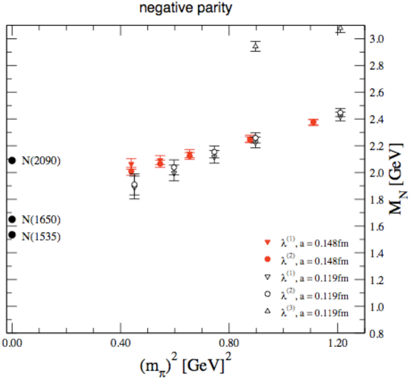
Quenched calculation, using variational principle [M. S. Mahbub *et al.*, arXiv:1007.4871]

Excited states of the Nucleon/Δ

BGR Collaboration, Quenched, domain wall fermions [Burch *et al.*, Phys. Rev. D74 (2006)]

- Two lattice spacings: $a = 0.15$ fm, $a = 0.12$ fm
- $m_\pi \gtrsim 350$ MeV and lattice sizes $16^3 \times 32$ and $20^3 \times 32$ with $m_\pi^{\text{min}} L \sim 4$
- Variational approach using different levels of Gaussian smearing; 6×6 correlation matrix





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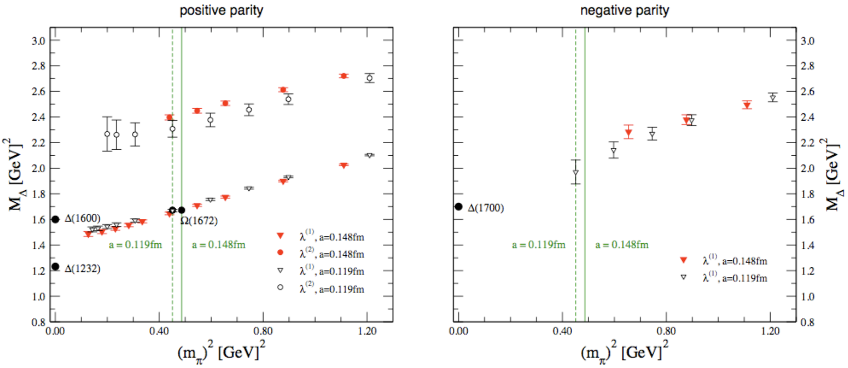
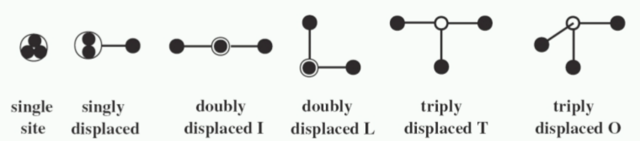
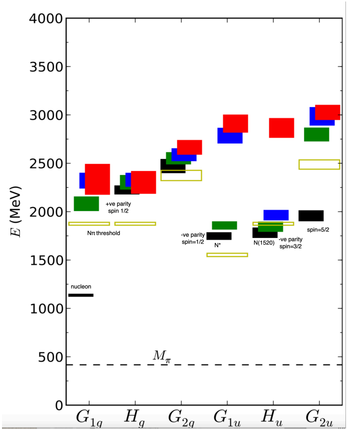


Results using variational method and anisotropic lattices

Hadron Spectrum Collaboration [Bulava *et al.*, Phys. Rev. D79 (2009) 034505]

Use extended fields operators in a variational approach $\rightarrow 16 \times 16$ correlator matrix

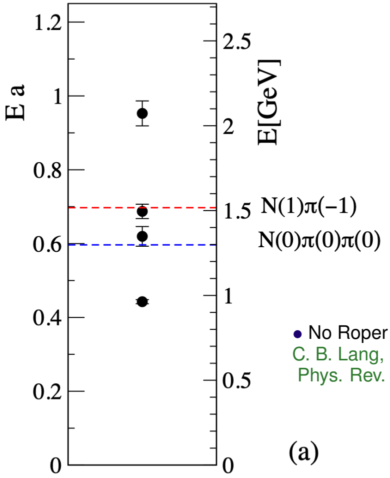




- $N_f = 2$ Wilson fermions with $\frac{a_t}{a_s} = 3$ and $a = 0.11$ fm at $m_\pi = 420$ MeV and 580 MeV on a volume of $L = 2.64$ fm $\rightarrow m_\pi^{\rm min} \sim 5.6$.
- Extrapolation of the mass of the nucleon linearly in m_π^2 yields $m_N = 972(28)$ Mev
- Excited states of nucleon: $\frac{m_{P_{11}}}{m_N} = 1.83$ (experiment 1.53) and $\frac{m_{P_{11}}}{m_{S_{11}}} = 1.19$ (experiment 0.94) i.e. wrong ordering

Recent results on nulceon excited states

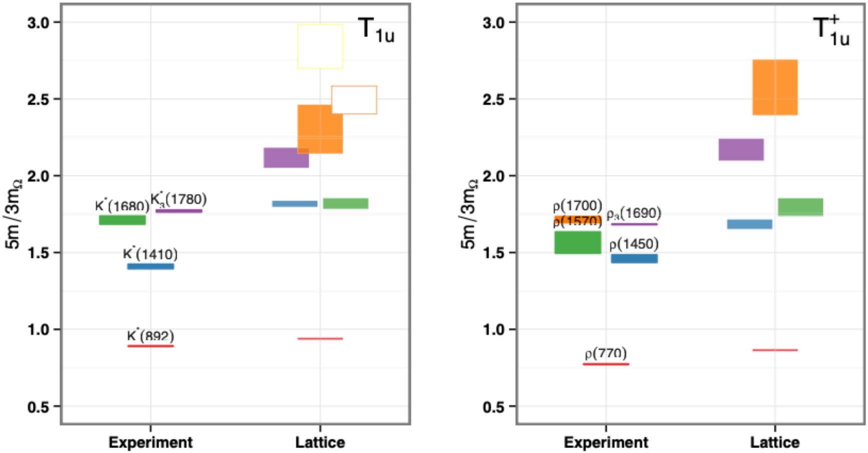
• $N_f = 2 + 1$ Wilson-clover dynamical fermions, $m_\pi = 156$ MeV
Variational basis: $N(0)$, $N(0)\sigma(0)$ and $N(p)\pi(-p)$ with $p = 2\pi/L$



• No Roper state observed
C. B. Lang, L. Leskovec, M. Padmanath and S. Prelovsek, Phys. Rev. D 95 (2017) 1, 014510, arXiv:1610.01422 [hep-lat]

Excited meson states

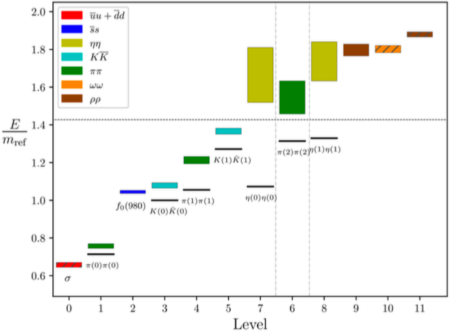
Analysis using $N_f = 2 + 1$ clover fermions on a $24^3 \times 128$ anisotropic lattice with a pion mass $m_\pi \sim$240 MeV.
A correlation matrix of 58 operators including extended operators



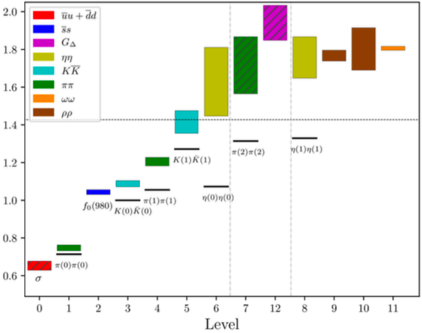
J. Bulava, et al., PoS(Lattice 2013):266 (2013) (arXiv:1310.7887 [hep-lat])

Excited meson states

Analysis using $N_f = 2 + 1$ clover fermions on a $24^3 \times 128$ anisotropic lattice with a pion mass m_π ~390 MeV.
A correlation matrix of 13×13 correlation matrix including the scalar gluon operator



Without the gluon operator

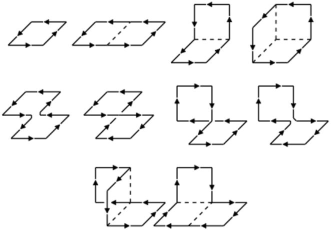


With gluon operator

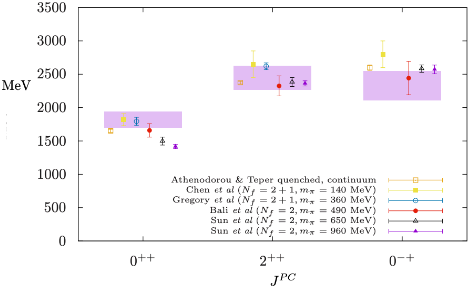
C. Morningstar, arXiv:2502.02547 [hep-lat])

Glueballs

- The non-Abelian nature of QCD allows bound states of gluon
  Candidate states observed experimentally: $f_0(1370)$, $f_0(1500)$, $f_0(1710)$, $f_0(222)$
  $\rightarrow$ can be calculated in lattice QCD
- Interpolating fields purely gluonic $\rightarrow J^{PC}$ assignment ambiguous
- Use variational approach using interpolating operators for given irreducible representation of the hypercubic group $\rightarrow$ recover spin-parity in the continuum limit



Computation with $N_f = 4$ and $N_f = 2+1+1$ twisted mass fermions with $m_\pi \sim$260 MeV.

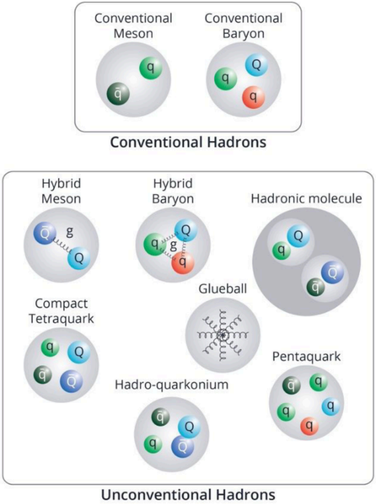


- The pseudoscalar and tensor glueball mass are not affected by including light quarks.
- A lowest state is observed in the scalar channel when introducing dynamical light quarks - multipion state.

A. Athenodorou *et al.*, 2308.10054 [hep-lat]

Multi-quark states

- Bound states of $\bar{q}q$ and qqq have been clearly established
- QCD predicts many more: quarks+glue, tetra-quarks, molecular states of mesons, pentaquarks, etc



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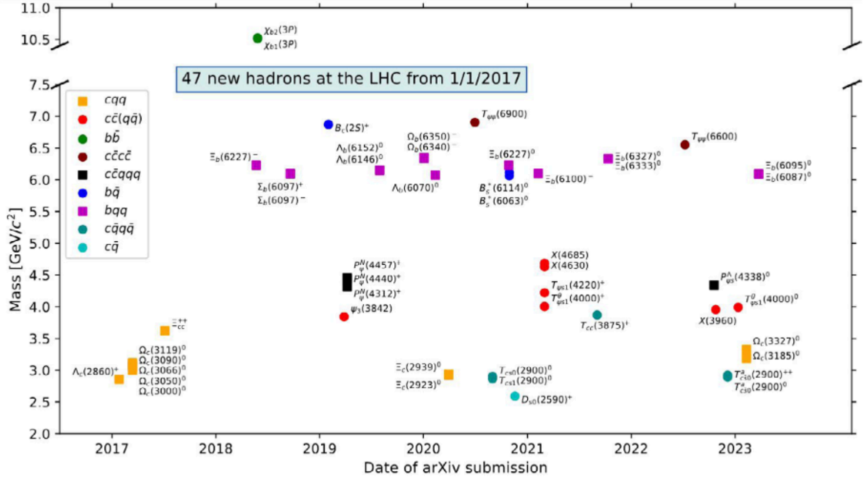
Examples are the recently discovered X, Y and Z states at LHCb and BESII
Very narrow resonances near threshold $\Longrightarrow$ presents a challenge for lattice QCD since we need to distinguish between a resonance and a 2-particle scattering state

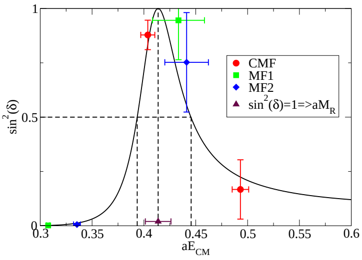


Resonances

At the physical point it is important to develop techniques to study unstable particle
Lüscher method: study the energy of a two-particle state as a function of the spatial length of the box.
The ρ-meson width was studied in $N_F = 2$ twisted mass fermions (ETMC) by Xu Feng, K. Jansen and D. Renner.

- Consider $\pi^+\pi^-$ in the $I = 1$-channel
- Estimate P-wave scattering phase shift $\delta_{11}(k)$ using finite size methods
- Use Lüscher's relation between energy in a finite box and the phase in infinite volume
- Use Center of Mass frame and Moving frame
- Use effective range formula: $tan\delta_{11}(k) = \frac{g^2_{\rho\pi\pi}}{6\pi}\frac{k^3}{E\left(m_R^2 - E^2\right)}$, $k = \sqrt{E^2/4 - m_\pi^2} \rightarrow$ determine M_R and $g_{\rho\pi\pi}$ and then extract $\Gamma_\rho = \frac{g^2_{\rho\pi\pi}}{6\pi}\frac{k_R^3}{m_R^2}$, $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

$m_\pi = 309$ MeV, $L = 2.8$ fm



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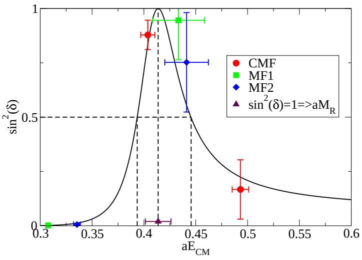

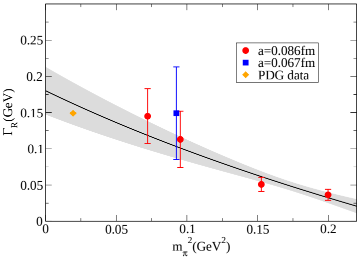

Resonances - Δ

Elastic pion-nucleon scattering in I=3/2 channel [S. Paul *el.* PoS LATTICE2018 (2018) 089]
Use $N_f = 2 + 1$ clover fermions with $m_\pi \approx 250$ MeV, and two volumes
Basis: Δ and $N\pi$