

# Introduction to Lattice QCD



**Constantia Alexandrou**  
*University of Cyprus and The Cyprus Institute*

# Lecture 1: Introduction to the lattice formulation

## Outline

- 1 Motivation**
  - Standard Model of Elementary Particles
  - QCD versus QED
- 2 Scalar field theory on a lattice**
- 3 Coherent States**
  - Bosons
  - Fermions
- 4 Formulation of Lattice Gauge Theories**
  - Local Gauge Symmetry
  - U(1) gauge theory
  - SU(N) Gauge Theory on a lattice
  - String tension
- 5 Continuum limit and Renormalization**
  - Asymptotic Freedom
- 6 Exercises**

## Standard model

The Standard Model (SM) is a synthesis of three of the four forces of nature described by gauge theories with coupling constants:

- Strong Interactions:  $\alpha_s \sim 1$
- Electromagnetic interactions:  $\alpha_{em} \approx 1/137$
- Weak interactions:  $G_F \approx 10^{-5} \text{ GeV}^{-2}$ .

Basic constituents of matter:

- Six quarks,  $u, d, s, c, b, t$ , each in 3 colors, and six leptons  $e, \nu_e, \mu, \nu_\mu, \tau, \nu_\tau$
- The quarks and leptons are classified into 3 generations of families.
- The interactions between the particles are mediated by vector bosons: the 8 gluons mediate strong interactions, the  $W^\pm$  and  $Z$  mediate weak interactions, and the electromagnetic interactions are carried by the photon  $\gamma$ .
- The weak bosons acquire a mass through the Higgs mechanism.
- The SM is a local gauge field theory with the gauge group  $SU(3) \times SU(2) \times U(1)$  specifying the interactions among these constituents.

### Masses in the Standard Model

Parameters	Number	Comments
Masses of quarks	6	$u, d, s$ light $c, b$ heavy $t = 175 \pm 6 \text{ GeV}$
Masses of leptons	6	$e, \mu, \tau$ $M_{\nu_e, \nu_\mu, \nu_\tau}$ non-zero
Mass of $W^\pm$	1	80.3 GeV
Mass of $Z$	1	91.2 GeV
Mass of gluons, $\gamma$		0 (Gauge symmetry)
Mass of Higgs	1	125.35(15) GeV

Three Generations of Matter (Fermions)				
	I	II	III	
mass	2.4 MeV	1.27 GeV	171.2 GeV	0
charge	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0
spin	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
name	u up	c charm	t top	$\gamma$ photon
Quarks	4.8 MeV	104 MeV	4.2 GeV	0
	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
	d down	s strange	b bottom	g gluon
Leptons	<2.2 eV	<0.17 MeV	<15.5 MeV	91.2 GeV
	0	0	0	0
	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	1
	$\nu_e$ electron neutrino	$\nu_\mu$ muon neutrino	$\nu_\tau$ tau neutrino	Z weak force
	e electron	$\mu$ muon	$\tau$ tau	W weak force

Bosons (Forces)

## QCD – Gauge theory of the strong interaction

- Lagrangian: formulated in terms of **quarks** and **gluons**

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{4}F_{\mu\nu}^a F^{a\mu\nu} + \sum_f \bar{\psi}_f (i\gamma^\mu D_\mu - m_f) \psi_f, \quad f = u, d, s, c, b, t$$

$$D_\mu = \partial_\mu - ig\left(\frac{1}{2}\lambda^a\right)A_\mu^a$$



Harald Fritzsch



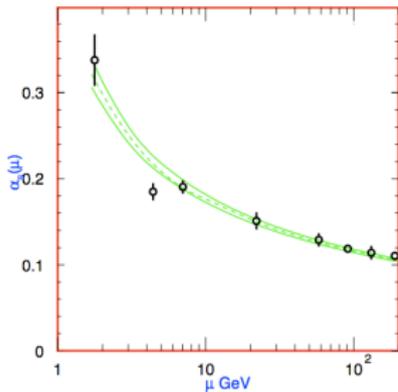
Murray Gell-Mann



Heinrich Leutwyler

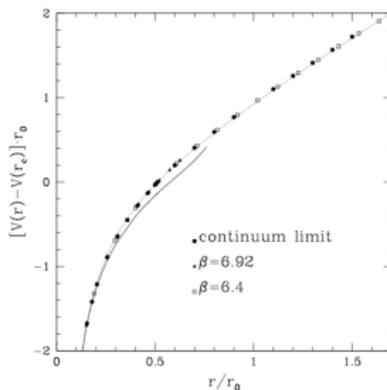
# Properties of QCD

## Asymptotic freedom: $g(\mu)$



[Yao et al., PDG 2006]

## Confinement



[Necco & Sommer, Nucl Phys B622 (2002) 328]

## Nobel Prize in Physics 2004

“...for the discovery of asymptotic freedom in the theory of the strong interaction”



David Gross



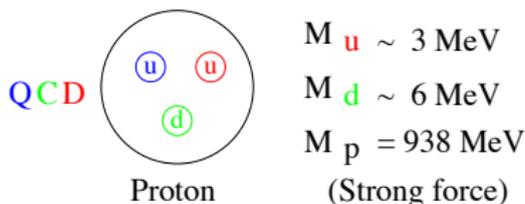
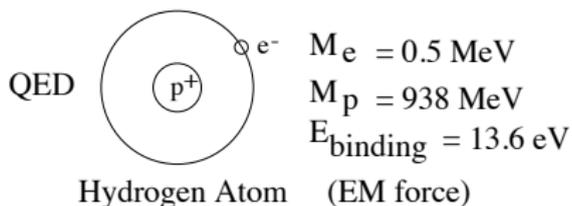
Frank Wilczek



David Politzer

## QCD versus QED

- QCD is the theory of strong interactions formulated in terms of quarks and gluons as the basic degrees of freedom of hadronic matter.
- Conventional perturbative approach cannot be applied for hadronic process at scales  $\lesssim 1$  GeV since the strong coupling constant  $\alpha_s \sim 1$   
 $\Rightarrow$  we cannot calculate the masses of mesons and baryons from QCD even if we are given  $\alpha_s$  and the masses of quarks.
- Bound state in QCD very different from QED e.g. the binding energy of a hydrogen atom is to a good approximation the sum of its constituent masses. Similarly for nuclei the binding energy is  $\mathcal{O}(\text{MeV})$ . For the proton almost all the mass is attributed to the strong non-linear interactions of the gluons.



### Why Lattice QCD?

- Discrete space-time lattice acts as a non-perturbative regularization scheme with the lattice spacing  $a$  providing an ultraviolet cutoff at  $\pi/a \rightarrow$  no infinities. Furthermore, renormalized physical quantities have a finite well behaved limit as  $a \rightarrow 0$ .
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems. These simulations allow us to calculate correlation functions of hadronic operators and matrix elements of any operator between hadronic states in terms of the fundamental quark and gluon degrees of freedom.

Like continuum QCD lattice QCD has as unknown input parameters the coupling constant  $\alpha_s$  and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).

⇒ Lattice QCD provides a well-defined approach to calculate observables non-perturbative starting directly from the QCD Lagrangian.

## Scalar field theory

Let the continuum  $\vec{r}$  be defined on lattice points i.e.  $\vec{r} \rightarrow \vec{n} \equiv (n_1, n_2, n_3)a$  where  $a$  is the lattice spacing.  
 $\Rightarrow$  equivalent to many-body problem where:

$$\hat{x}_i, \hat{p}_i \rightarrow \hat{\phi}(\vec{n}), \hat{\pi}(\vec{n}) \quad \hat{x}_i |x\rangle = x_i |x\rangle \rightarrow \hat{\phi}(\vec{n}) = \phi(\vec{n}) |\phi\rangle.$$

We then have

$$\int d^3r \left\{ \frac{1}{2} \pi^2(\vec{r}) + \frac{1}{2} |\vec{\nabla} \phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\} \rightarrow \sum_{\vec{n}} a^3 \left\{ \frac{1}{2} \pi^2(\vec{n}) + \frac{1}{2a^2} \sum_{i=1}^3 |\phi(\vec{n} + a\mu_i) - \phi(\vec{n})|^2 + V(\phi(\vec{n})) \right\}$$

where  $\mu_i$  denotes a displacement by one lattice site in the  $i^{\text{th}}$  direction.  
 The evolution operator in Euclidean time:

$$e^{-t \sum_{\vec{n}} a^3 \left\{ \frac{1}{2} \pi^2(\vec{n}) + F(\phi(\vec{n})) \right\}} = \int \mathcal{D}[\phi(\vec{n})] e^{-\Delta t a^3 \sum_{\vec{n}, k} \left[ \frac{1}{2\Delta t^2} (\phi_{k+1}(\vec{n}) - \phi_k(\vec{n}))^2 + F(\phi_k(\vec{n})) \right]}$$

Take isotropic lattice i.e.  $\Delta t = a$

$\Rightarrow$  time slicing replaces  $\hat{p}^2(\vec{n})$  by  $\frac{1}{\Delta t} (\phi_{k+1}(\vec{n}) - \phi_k(\vec{n}))^2 \equiv \frac{1}{\Delta t} (\phi(n + a\mu_0) - \phi(n))^2$  which has the same structure as the discrete spatial derivative and where  $n = (n_0, n_1, n_2, n_3)a$ .

$$\Rightarrow \mathcal{O}(\phi) e^{-t \int d^3r \left\{ \frac{1}{2} \pi^2(\vec{r}) + \frac{1}{2} |\vec{\nabla} \phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\}} \rightarrow \int \mathcal{D}[\phi(n)] \mathcal{O}(\phi) e^{-S_{\text{cl}}[\phi]}$$

where  $S_{\text{cl}}[\phi] = \sum_n a^4 \left\{ \sum_{i=0}^3 \frac{(\phi(n+a\mu_i) - \phi(n))^2}{a^2} + V(\phi(n)) \right\}$ .

Note that  $S_{\text{cl}}$  is completely symmetric in time and space  $\rightarrow$  if we choose periodic b.c. then the shortest dimension acts as a finite temperature.

## Coherent States for bosons

For the Feynman path integral of the 1-d QM example we needed:

- Eigenstates of  $\hat{x}$ ,  $\hat{x} |x\rangle = x |x\rangle$  and
- Unity:  $\int dx |x\rangle \langle x| = 1$

The analogs for creation and annihilation operators are provided by boson coherent states.

Consider a creation operator  $\hat{a}^\dagger$  then

$$\left[ \hat{a}, \hat{a}^\dagger \right] = 1 \quad \hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle \quad |n\rangle = \frac{1}{\sqrt{n!}} \left( \hat{a}^\dagger \right)^n |0\rangle$$

Define the coherent state  $|z\rangle$  by

$$|z\rangle \equiv e^{z\hat{a}^\dagger} |0\rangle = \sum_n \frac{z^n}{n!} \left( \hat{a}^\dagger \right)^n |0\rangle = \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle$$

Properties:

$$\begin{aligned} \hat{a} |z\rangle &= \sum_n \frac{z^n}{\sqrt{n!}} \hat{a} |n\rangle = z \sum_n \frac{z^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle = z |z\rangle \\ \langle z | z' \rangle &= \sum_{mn} \langle m | \frac{z^{*m}}{\sqrt{m!}} \frac{z'^n}{\sqrt{n!}} |n\rangle = e^{z^* z'} \\ \langle z | : A(\hat{a}^\dagger \hat{a}) : |z' \rangle &= e^{z^* z'} A(z^*, z') \\ 1 &= \int \frac{dz dz^*}{2\pi i} e^{-z^* z'} |z\rangle \langle z| \end{aligned} \tag{1}$$

## Coherent States for bosons

For the Feynman path integral of the 1-d QM example we needed:

- Eigenstates of  $\hat{x}$ ,  $\hat{x} |x\rangle = x |x\rangle$  and
- Unity:  $\int dx |x\rangle \langle x| = 1$

The analogs for creation and annihilation operators are provided by boson coherent states.

Consider a creation operator  $a^\dagger$  then

$$\left[ \hat{a}, \hat{a}^\dagger \right] = 1 \quad \hat{a}^\dagger |n\rangle = \sqrt{n+1} |n+1\rangle \quad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle \quad |n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle$$

Define the coherent state  $|z\rangle$  by

$$|z\rangle \equiv e^{z\hat{a}^\dagger} |0\rangle = \sum_n \frac{z^n}{n!} (\hat{a}^\dagger)^n |0\rangle = \sum_n \frac{z^n}{\sqrt{n!}} |n\rangle$$

Generalize for a set of creation operators  $\hat{a}_\alpha^\dagger$

$$\begin{aligned} |z\rangle &= e^{\sum_\alpha z_\alpha \hat{a}_\alpha^\dagger} |0\rangle \\ \hat{a}_\alpha |z\rangle &= z_\alpha |z\rangle \\ \langle z| : A(\hat{a}^\dagger \hat{a}) : |z'\rangle &= e^{\sum_\alpha z_\alpha z'_\alpha} A(z^*, z') \\ 1 &= \int \prod_\alpha \frac{dz_\alpha z_\alpha^*}{2\pi i} e^{-z_\alpha^* z'_\alpha} |z\rangle \langle z| \equiv \int d\mu(z) |z\rangle \langle z| \end{aligned}$$

## Path integral using coherent states

Time slicing the evolution operator:

$$\langle z_f | e^{-tH} | z_i \rangle = \langle z_f | e^{-\Delta t H} \int d\mu(z_{N-1}) | z_{N-1} \rangle \langle z_{N-1} | e^{-\Delta t H} \int d\mu(z_{N-2}) \cdots e^{-\Delta t H} | z_i \rangle$$

The matrix element of the infinitesimal evolution operator is

$$d\mu(z_k) \langle z_k | e^{-tH} | z_{k-1} \rangle = \prod_{\alpha} \frac{dz_{k,\alpha}^* dz_{k,\alpha}}{2i\pi} e^{-\sum_{\alpha} z_{k,\alpha}^* (z_{k,\alpha} - z_{k-1,\alpha}) - \Delta t H(z_{k,\alpha}^*, z_{k-1,\alpha})}$$

resulting in

$$\langle z_f | e^{-tH} | z_i \rangle = \int \mathcal{D}[z_{k,\alpha}^*, z_{k,\alpha}] e^{-S(z_{k,\alpha}^*, z_{k,\alpha})}$$
$$S(z^*, z) = \sum_k \Delta t \left\{ \sum_{\alpha} z_{k,\alpha}^* \left( \frac{z_{k,\alpha} - z_{k-1,\alpha}}{\Delta t} \right) + H(z_{k,\alpha}^*, z_{k-1,\alpha}) \right\}$$

## Coherent states for fermions

Fermions are represented by anti-commuting creation and annihilation operators  $c_\alpha^\dagger$  and  $c_\alpha \rightarrow$  need to introduce anti-commuting Grassmann variables  $\xi$  such that

$$\hat{c}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle \quad \hat{c}_\alpha \hat{c}_\beta |\xi\rangle = \xi_\alpha \xi_\beta |\xi\rangle = -\xi_\beta \xi_\alpha |\xi\rangle = -\hat{c}_\beta \hat{c}_\alpha |\xi\rangle$$

Since  $\xi_\alpha^2 = 0$  (Pauli principle) the only functions allowed are monomials. The rules for integration over a Grassmann variable  $\xi$  and  $\xi^*$  are

$$\int d\xi_\alpha = \int d\xi_\alpha^* = 0, \quad \int d\xi_\alpha \xi_\alpha = \int d\xi_\alpha^* \xi_\alpha^* = 1$$

A fermion coherent state is defined by

$$|\xi\rangle \equiv e^{-\sum_\alpha \xi_\alpha c_\alpha^\dagger} |0\rangle$$

with similar properties to bosons. The path integral have similar form to that for bosons with some minus signs that distinguish between bosons and fermions.

## Integration over fermions

For numerical evaluation we can not have the path integrals in terms of Grassmann variables. Fortunately for normalizable field theories we can integrate analytically over the fermionic degrees of freedom  
Recall Gaussian integral

$$\int \prod_i \frac{dz_i^* dz_i}{2i\pi} e^{-z_i^* H_{ij} z_j + J_i^* z_i + z_i^* J_j} = [\det H]^{-1} e^{J_i^* H_{ij}^{-1} J_j}$$

An analogous result is obtained for Grassmann "Gaussian": For one pair of Grassmann variables we have

$$\int d\xi^* d\xi e^{-\xi^* a \xi} = \int d\xi^* d\xi (1 - \xi^* a \xi) = a$$

This generalizes to

$$\int \prod_i d\xi_i^* d\xi_i e^{-\xi_i^* H_{ij} \xi_j + \eta_i^* \xi_i + \xi_i^* \eta_i} = [\det H] e^{\eta_i^* H_{ij}^{-1} \eta_j}$$

i.e. the only difference is that  $\det H$  appears in the numerator  $\rightarrow$  accounts for the minus sign of fermion loops.  
If our action is of the form  $S(\xi^*, \xi, \phi) = \xi_i^* M(\phi)_{ij} \xi_j + S_B(\phi)$  then

$$\int d\xi^* d\xi d\phi e^{\xi_i^* M(\phi)_{ij} \xi_j + S_B(\phi)} = \int d\phi \det M(\phi) e^{S_B(\phi)}$$

i.e.  $S_{\text{eff}}(\phi) = \ln \det M(\phi) + S_B(\phi)$

## Fermion propagators

Consider the time ordered product of field creation and annihilation operators at space-time points  $j = (x_j, t_j)$  and  $i = (x_i, t_i)$  respectively:

$$\langle \hat{T} \psi_i \bar{\psi}_j \rangle = \text{Tr} \hat{T} \psi_i \bar{\psi}_j e^{-\bar{\psi} M(\phi) \psi + S_B(\phi)} = \int \mathcal{D}[\phi] \mathcal{D}[\bar{\xi} \xi] \xi_i \bar{\xi}_j e^{-\bar{\xi} M(\phi) \xi + S_B(\phi)} = \int \mathcal{D}[\phi] M_{ij}^{-1}(\phi) e^{S_{\text{eff}}(\phi)}$$

In general for  $n$  pairs of creation and annihilation operators

$$\begin{aligned} & \int \mathcal{D}(\xi^*, \xi) \xi_{i_1} \cdots \xi_{i_n} \xi_{j_n}^* \cdots \xi_{j_1}^* e^{-\xi^* M \xi} \\ &= \frac{\delta^{2n}}{\delta \eta_{i_1}^* \cdots \delta \eta_{i_n}^* \delta \eta_{j_n} \cdots \delta \eta_{j_1}} \int \mathcal{D}(\xi^*, \xi) e^{-\xi_i^* M_{ij} \xi_j + \eta_i^* \xi_i + \xi_i^* \eta_j} \Big|_{\eta = \eta^* = 0} \\ &= \frac{\delta^{2n}}{\delta \eta_{i_1}^* \cdots \delta \eta_{i_n}^* \delta \eta_{j_n} \cdots \delta \eta_{j_1}} \det M e^{\eta_i^* M_{ij}^{-1} \eta_j} \Big|_{\eta = \eta^* = 0} \\ &= \sum_P (-1)^P M_{i_{P_n} j_n}^{-1} \cdots M_{i_{P_1} j_1}^{-1} e^{\ln \det M} \end{aligned}$$

where  $P$  denotes a permutation of the indices. This is nothing else but **Wick's theorem**.

⇒ **fermions can be integrated out and we left only with an effective action with the bosonic degrees of freedom.**

Boundary conditions:

$$\text{Tr} e^{-tH} = \int dz_0^* dz_0 e^{-z_0^* z_0} \langle \pm z_0 | e^{-tH} | z_0 \rangle = \int dz_0^* dz_0 e^{-z_0^* z_0} \int d\mathcal{D}[z^*, z] e^{-S(z^*, z)}$$

where the plus is for bosons and minus for fermions and

$$S(z^*, z) = \pm z_0^* (\pm z_0 - z_{N-1}) + H_{0, N-1} + z_{N-1}^* (z_{N-1} - z_{N-2}) + H_{N-1, N-2} + \cdots + z_1^* (z_1 - z_0) H_{1, 0}.$$

## Lattice Gauge theories

- K. Wilson: 1974 formulated Euclidean gauge theories on the lattice as a tool for the study of confinement and non-perturbative properties of QCD.
- M. Creutz: 1980 perform the first numerical implementation of the path integral for gauge theories.

The set-up for the numerical evaluation requires

- Discretization of space-time: Discretize space-time in 4 Euclidean dimensions  $\rightarrow$  simplest isotropic hypercubic grid with spacing  $a = a_S = a_T$  and size  $N_S \times N_S \times N_S \times N_T$
- Definition of the gauge and fermion degrees on the discrete space-time: The quark field is represented by anticommuting Grassmann variables defined at each site of the lattice. They belong to the fundamental representation of SU(3). The gauge field is discussed below.
- Construction of an appropriate action
- Definition of the measure of integration in the path integral.
- Construction of the operators used to probe the physics

## Gauge degrees of freedom

In the continuum a fermion moving from site  $x$  to  $y$  in the presence of a gauge field  $A_\mu(x)$  picks up a phase factor given by the path ordered product

$$\psi(y) = \mathcal{P} e^{i \int_x^y g A_\mu(x) dx^\mu} \psi(x) .$$

$\implies$  associate gauge fields with links that connect sites on the lattice. So, with each link associate a discrete version of the path ordered product:

$$U(x; x + \hat{\mu}) \equiv U_\mu(x) = e^{iagA_\mu(x)} ,$$

$U$  is a  $3 \times 3$  unitary matrix with unit determinant. It follows that

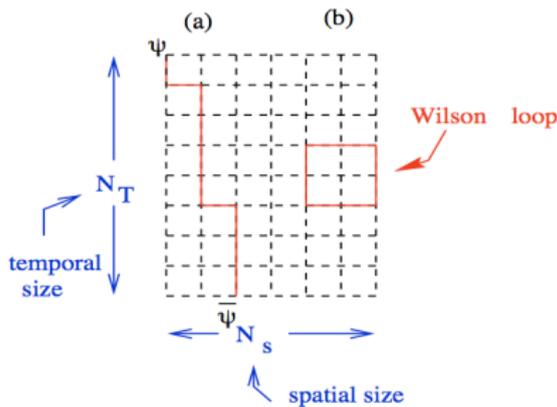
$$U(x; x - \hat{\mu}) \equiv U_{-\mu}(x) = e^{-iagA_\mu(x)} = U^\dagger(x - \hat{\mu}; x) .$$

## Local gauge symmetry

The effect of a local gauge transformation  $V(x)$  on the variables  $\psi(x)$  and  $U$  is defined as

$$\begin{aligned}\psi(x) &\rightarrow V(x)\psi(x) \\ \bar{\psi}(x) &\rightarrow \bar{\psi}(x)V^\dagger(x) \\ U_\mu(x) &\rightarrow V(x)U_\mu(x)V^\dagger(x + \hat{\mu})\end{aligned}$$

where  $V(x)$  is in the same representation as the  $U_\mu(x)$ , *i.e.*, it is an  $SU(3)$  matrix. With these definitions there are two types of gauge invariant objects that one can construct on the lattice.



- A string consisting of a path-ordered product of links capped by a fermion and an antifermion e.g.

$$\text{Tr } \bar{\psi}(x) U_\mu(x) U_\nu(x + \hat{\mu}) \dots U_\rho(y - \hat{\rho}) \psi(y)$$

where the trace is over the color indices.

If the string stretches across the lattice and is closed by the periodicity are called Polyakov lines.

- The simplest example of closed Wilson loops is the plaquette, a  $1 \times 1$  loop,

$$W_{\mu\nu}^{1 \times 1} = P_{\mu\nu}(x) = \text{Re Tr } (U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x)) .$$

Preserve gauge invariance at all  $a \rightarrow$  protects from having many more parameters to tune (the zero gluon mass, and the equality of the quark-gluon, 3-gluon, and 4-gluon couplings) and there would arise many more operators at any given order in  $a$ .

## U(1) gauge theory

Consider a Lagrangian of a complex field  $\phi$ :  $L = \partial_\mu \phi^* \partial^\mu \phi - V(\phi^*, \phi)$ . If we require that the Lagrangian is invariant under a local gauge transformation  $\phi'(x) = e^{-i\alpha(x)} \phi(x)$  then we need a field  $A_\mu(x)$  to compensate the change in the derivative  $\partial_\mu \phi$  that transforms as

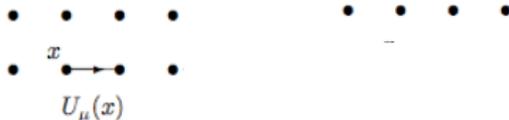
$$A'_\mu(x) = A_\mu(x) + \frac{1}{g} \partial_\mu \alpha(x) \quad \partial_\mu \rightarrow D_\mu \equiv \partial_\mu + igA_\mu(x)$$

The gauge invariant Lagrangian is written as

$$L = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + (D_\mu \phi)^* D_\mu \phi - V(\phi^*, \phi)$$

A scalar moving from site  $x$  to  $y$  in the presence of a gauge field  $A_\mu(x)$  picks up a phase factor given by

$$U(x; y) = e^{ig \int_x^y dx_\mu A^\mu(x)}$$



which removes the phase between the value of the field at the two points and yields a gauge invariant result.

The action is defined in terms of link variables assigned to links between sites of the space-time lattice.

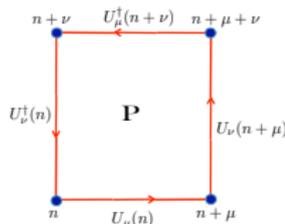
The link variable from site  $n$  in the  $\mu$  direction to site  $n + a\hat{e}_\mu$  is defined as the discrete approximation to the integral  $e^{ig \int_n^{n+\mu} dx_\mu A^\mu}$ :  $U_\mu(n) = e^{i\theta_\mu(n)}$  with  $\theta_\mu(n)$  the approximation of  $g \int_n^{n+\mu} dx_\mu A^\mu(x)$ .

The integral over the field variables is the invariant group measure for U(1):

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta.$$

The action is the sum of all plaquettes  $P_{\mu\nu} = U(n)_\mu U_\nu(n + \mu) U_\nu^\dagger(n + \mu + \nu) U_\mu^\dagger(n)$ .

For U(1):  $P_{\mu\nu}(n) = e^{i\theta_\mu(n)} e^{i\theta_\nu(n+\mu)} e^{-i\theta_\nu(n+\mu+\nu)} e^{-i\theta_\mu(n)} \equiv e^{iB_{\mu\nu}}$ ,  $B_{\mu\nu} = \Delta_\mu \theta_\nu - \Delta_\nu \theta_\mu \xrightarrow{a \rightarrow 0} F_{\mu\nu}$ .



## Lattice action of U(1)

Since a plaquette produces  $F_{\mu\nu}$  the action can be constructed by choosing a function of the plaquette such that it generates  $F_{\mu\nu}^2$  in the continuum limit.

$$S = \beta \sum_n \sum_{\mu > \nu} (1 - \text{Re } P_{\mu\nu}(n)) = \beta \sum_n \sum_{\mu > \nu} (1 - \cos B_{\mu\nu}),$$

where  $\beta = \frac{1}{g^2}$  and  $B_{\mu\nu} = \Delta_\mu \theta_\nu - \Delta_\nu \theta_\mu \xrightarrow{a \rightarrow 0} F_{\mu\nu}$ .

In the limit  $a \rightarrow 0$  we recover continuum QED:

Taking  $\theta_\mu(n) = agA_\mu(n)$  and expanding  $\theta_\nu(n + \hat{e}_\mu a) = \theta_\nu(n) + a\partial_\mu \theta_\nu(n) + \mathcal{O}(a^2)$

$$\begin{aligned} S &\sim \frac{1}{g^2} \sum_P [1 - \cos(a\partial_\mu \theta_\nu - a\partial_\nu \theta_\mu)] = \frac{1}{g^2} \sum_P [1 - \cos(a^2 g F_{\mu\nu})] = \frac{1}{g^2} \sum_n \sum_{\mu > \nu} \left[ \frac{a^4 g^2}{2} F_{\mu\nu}^2 + \dots \right] \\ &\rightarrow \frac{1}{4} \int d^4x F_{\mu\nu}^2(x) \end{aligned}$$

## SU(N) Gauge Theory on a lattice

The generalization to non-Abelian gauge theory is straightforward. The link variable is

$$U_\mu(n) = e^{iag\lambda^c A_\mu^c(n)} = e^{iagA_\mu(n)} \quad \text{and} \quad U_{-\mu}(n) = e^{-iag\lambda^c A_\mu^c(n)} = U_\mu^\dagger(n - \mu)$$

For SU(3)  $\lambda^c$  are the Gell-Mann matrices and  $c = 1, \dots, 8$  is a color label. The 8 group generators are normalized as  $\text{Tr} \lambda_a \lambda_b = 2\delta_{ab}$  and  $U$  is a  $3 \times 3$  unitary matrix with unit determinant.

The action is given in terms of the product of SU(N) group elements around an elementary plaquette

$$P_{\mu\nu}(n) = U_\mu(n)U_\nu(n + \mu)U_\mu^\dagger(n + \nu)U_\nu^\dagger(n) = e^{iagA_\mu(n)} e^{iagA_\nu(n+\mu)} e^{-iagA_\mu(n+\nu)} e^{-igA_\nu(n)}$$

In order to find the continuum limit of this plaquette we expand  $A$  by applying the Baker-Hausdorff identity

$$e^X e^Y = e^{X+Y + \frac{1}{2}[X, Y] + \dots}$$

$$\begin{aligned} P_{\mu\nu} &\sim e^{iagA_\mu(n)} e^{iag(A_\nu(n) + a\partial_\mu A_\nu(n))} e^{-iag(A_\mu(n) + a\partial_\nu A_\mu(n))} e^{-iagA_\nu(n)} \\ &\sim e^{iag(A_\mu(n) + A_\nu(n) + a\partial_\mu A_\nu(n) + \frac{1}{2}iag[A_\mu, A_\nu])} e^{-iag(A_\mu(n) + A_\nu(n) + a\partial_\nu A_\mu(n) - \frac{1}{2}iag[A_\mu, A_\nu])} \\ &\sim e^{ia^2g(\partial_\mu A_\nu(n) - \partial_\nu A_\mu(n) + ig[A_\mu, A_\nu])} = e^{ia^2gF_{\mu\nu}} \end{aligned}$$

and therefore we may define the SU(N) action by choosing a function of the plaquette which yields  $F_{\mu\nu}^2$ :

$$S(U) = \beta \sum_n \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \text{Re Tr} P_{\mu\nu} \right), \quad \beta = \frac{2N}{g^2},$$

## SU(N) Gauge Theory

$$S(U) = \beta \sum_n \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \text{Re Tr } P_{\mu\nu} \right), \quad \beta = \frac{2N}{g^2},$$

Using the continuum limit of the plaquette we can easily obtain the continuum limit of the above action:

$$\begin{aligned} S(U) &= \beta \sum_n \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \text{Re Tr} \left( 1 + ia^2 F_{\mu\nu} - \frac{1}{2} a^4 g^2 F_{\mu\nu}^2 + \dots \right) \right) \\ &\sim \frac{1}{2} \beta a^4 g^2 \sum_n \sum_{\mu > \nu} \frac{1}{N} \text{Tr} \left( \frac{1}{2} \lambda^c F_{\mu\nu}^c(n) \frac{1}{2} \lambda^b F_{\mu\nu}^b(n) \right) \sim \beta \frac{g^2}{2N} \sum_n a^4 \sum_{\mu\nu} \frac{1}{2} F_{\mu\nu}^c F_{\mu\nu}^c(n) \\ &\rightarrow \frac{1}{4} \int d^4x F_{\mu\nu}^c(x) F_{\mu\nu}^c \end{aligned}$$

The fact that the generators  $\lambda^c$  are traceless is used to eliminate linear terms. The relation  $\text{Tr} \lambda^b \lambda^c = 2\delta^{bc}$  has been used to get the diagonal piece.

There is a great freedom to construct other expressions with the same continuum limit. E.g. considering a product of link variables around a larger rectangle  $ja \times ka$  we obtain

$$\frac{1}{a^4} \left( 1 - \frac{1}{N} \text{Re Tr } W^{j \times k} \right) = c_{jk} F_{\mu\nu}^2 + a^2 \sum_m d_{jk}^m I^m(D_\mu, D_\nu, F_{\alpha\beta}, F_{\gamma\delta}) + \mathcal{O}(a^4)$$

where  $I^m$  denotes an invariant from two derivatives and two  $F$ 's and the coefficients  $c$  and  $d$  are calculable  $\rightarrow$  we can construct improved actions by taking linear combinations for various rectangles.

## Gauge action

There are four important points to note based on the above construction of the lattice action.

- 1 The leading correction is  $O(a^2)$ : The term  $\frac{a^2}{6} F_{\mu\nu} (\partial_\mu^3 A_\nu - \partial_\nu^3 A_\mu)$  is present in the expansion of all planar Wilson loops. Thus at the classical level it can be gotten rid of by choosing an action that is a linear combination of say  $1 \times 1$  and  $1 \times 2$  Wilson loops with the appropriate relative strength given by the Taylor expansion
- 2 Quantum effects will give rise to corrections, *i.e.*  $a^2 \rightarrow X(g^2)a^2$  where in perturbation theory  $X(g^2) = 1 + c_1 g^2 + \dots$ , and will bring in additional non-planar loops. Improvement of the action will consequently require including these additional loops, and adjusting the relative strengths which become functions of  $g^2$ .
- 3 The reason for defining the action in terms of small loops is computational speed and reducing the size of the discretization errors. For example the leading correction to  $1 \times 1$  loops is proportional to  $a^2/6$  whereas for  $1 \times 2$  loops it increases to  $5a^2/12$ . Also, the cost of simulation increases by a factor of 2 – 3.
- 4 The electric and magnetic fields  $E$  and  $B$  are proportional to  $F_{\mu\nu}$ . They are given in terms of the imaginary part of Wilson loops:  $\text{Im}P_{\mu\nu} \stackrel{a \rightarrow 0}{\approx} a^2 g F_{\mu\nu}$ .

## Wilson loops

In the pure gauge theory the only gauge invariant objects are closed loops. The Wilson loop

$$W = \text{Tr} U_i(x) U_k(x + ja) \cdots U_i(x - ia)$$

Consider a space-time Wilson loop: Under a gauge transformation a product of gauge links becomes

$$U_i(x) \cdots U_j(x + ka) \rightarrow V(x) U_i(x) \cdots U_j(x + ka) V^\dagger(x + ka)$$

whereas

$$\psi(x) \bar{\psi}(x + ka) \rightarrow V(x) \psi(x) \bar{\psi}(x + ka) V^\dagger(x + ka).$$

i.e. as far as the gauge fields are concerned the ends of a chain of link variables are equivalent to an external quark-antiquark source  $\rightarrow$  response of system to an external quark-antiquark source.

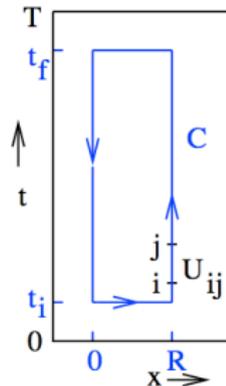
The expectation of the space-time Wilson loop

$$\langle W \rangle = \frac{\int \mathcal{D}U e^{-S(U)} W}{\int \mathcal{D}U e^{-S(U)}}$$

gives the time evolution of the system: Prior to  $t_i$  there are no color sources  $\rightarrow |0\rangle = e^{-t_i H} |Q=0\rangle$ .

- At time  $t_i$  the line of link variables between 0 and  $R$  creates an external antiquark source at 0 and a quark source at  $R$ .
- The links in the time direction between  $t_i$  and  $t_f$  maintain these sources at 0 and  $R$   $\rightarrow$  state evolves to the lowest gluon state in the presence of a quark-antiquark source.
- The  $q - \bar{q}$  pair is annihilated at time  $t_f$ .

$\Rightarrow \langle W \rangle \propto e^{-(t_f - t_i)V(R)}$  where  $V(R)$  is the potential between two static quarks.



## Wilson loops

In the pure gauge theory the only gauge invariant objects are closed loops. The Wilson loop

$$W = \text{Tr} U_i(x) U_k(x + ja) \cdots U_i(x - ia)$$

Consider a space-time Wilson loop: Under a gauge transformation a product of gauge links becomes

$$U_i(x) \cdots U_j(x + ka) \rightarrow V(x) U_i(x) \cdots U_j(x + ka) V^\dagger(x + ka)$$

whereas

$$\psi(x) \bar{\psi}(x + ka) \rightarrow V(x) \psi(x) \bar{\psi}(x + ka) V^\dagger(x + ka).$$

i.e as far as the gauge fields are concerned the ends of a chain of link variables are equivalent to an external quark-antiquark source  $\rightarrow$  response of system to an external quark-antiquark source.

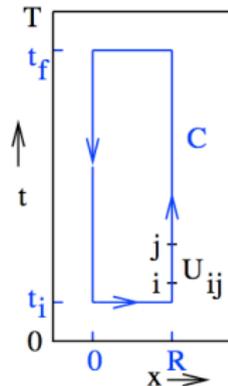
The expectation of the space-time Wilson loop

$$\langle W \rangle = \frac{\int \mathcal{D}U e^{-S(U)} W}{\int \mathcal{D}U e^{-S(U)}}$$

gives the time evolution of the system: Prior to  $t_i$  there are no color sources  $\rightarrow |0\rangle = e^{-t_i H} |Q=0\rangle$ .

- At time  $t_i$  the line of link variables between 0 and  $R$  creates an external antiquark source at 0 and a quark source at  $R$ .
- The links in the time direction between  $t_i$  and  $t_f$  maintain these sources at 0 and  $R \rightarrow$  state evolves to the lowest gluon state in the presence of a quark-antiquark source.
- The  $q - \bar{q}$  pair is annihilated at time  $t_f$ .

$\Rightarrow \langle W \rangle \propto e^{-(t_f - t_i)V(R)}$  where  $V(R)$  is the potential between two static quarks.



## Area law

Consider a non-relativistic particle

$$H = \frac{p^2}{2m} + V(r)$$

Propagator:

$$G(\vec{r}', t; \vec{r}, 0) = \langle r' | e^{-iHt} | r \rangle \xrightarrow{m \rightarrow \infty} \delta^3(r' - r) e^{-iV(r)t}$$

Wick rotation:  $t \rightarrow -it$

$$\Rightarrow G_E(r', t; r, 0) \xrightarrow{m \rightarrow \infty} \delta^3(r' - r) e^{-V(r)t}$$

i.e. the potential is determined by the exponential behavior of the propagator of a static particle.

In the gauge theory we need to generate the eigenstate of the QCD Hamiltonian for static quark-antiquark  $\rightarrow$  e.g. time evolving the Wilson loop or correlation between two Polyakov loops.

If there are  $J$  links in the time direction and  $K$  links in the space direction then

$$\langle W^{J \times K} \rangle \xrightarrow{J \rightarrow \infty} e^{-aJV(aK)} \xrightarrow{K \rightarrow \infty} e^{-a^2 \sigma JK}$$

where we used the fact that at large distances the potential is linear since in pure gauge no quark-antiquark can be produced.

$\Rightarrow$  **Area law - Signature of confinement**

Note that this holds in the limit of large Wilson loops and for the Wilson loops considered one has corrections that are proportional to the perimeter of the loop as well as a constant term. Take ratios to eliminate these:

$$\Rightarrow \chi(l, J) = -\log \left( \frac{W^{l \times J} W^{J-1 \times J-1}}{W^{l \times J-1} W^{J-1 \times J}} \right) \sim a^2 \sigma.$$

## Area law

Consider a non-relativistic particle

$$H = \frac{p^2}{2m} + V(r)$$

Propagator:

$$G(\vec{r}', t; \vec{r}, 0) = \langle r' | e^{-iHt} | r \rangle \xrightarrow{m \rightarrow \infty} \delta^3(r' - r) e^{-iV(r)t}$$

Wick rotation:  $t \rightarrow -it$

$$\Rightarrow G_E(r', t; r, 0) \xrightarrow{m \rightarrow \infty} \delta^3(r' - r) e^{-V(r)t}$$

i.e. the potential is determined by the exponential behavior of the propagator of a static particle.

In the gauge theory we need to generate the eigenstate of the QCD Hamiltonian for static quark-antiquark  $\rightarrow$

e.g. time evolving the Wilson loop or correlation between two Polyakov loops.

If there are  $J$  links in the time direction and  $K$  links in the space direction then

$$\langle W^{J \times K} \rangle \xrightarrow{J \rightarrow \infty} e^{-aJV(aK)} \xrightarrow{K \rightarrow \infty} e^{-a^2 \sigma JK}$$

where we used the fact that at large distances the potential is linear since in pure gauge no quark-antiquark can be produced.

$\Rightarrow$  **Area law - Signature of confinement**

Note that this holds in the limit of large Wilson loops and for the Wilson loops considered one has corrections that are proportional to the perimeter of the loop as well as a constant term. Take ratios to eliminate these:

$$\Rightarrow \chi(l, J) = -\log \left( \frac{W^{l \times J} W^{J-1 \times J-1}}{W^{l \times J-1} W^{J-1 \times J}} \right) \sim a^2 \sigma.$$

## Wilson loop revisited

Consider a heavy quark  $Q$  and a heavy antiquark  $\bar{Q}$ . Construct a gauge invariant state at  $t = 0$

$$|\phi_{\alpha,\beta}\rangle(\vec{x}, \vec{y}) = \bar{Q}_{\alpha}(\vec{x}, 0)U(\vec{x}, 0; \vec{y}, 0)Q_{\beta}(\vec{y}, 0)|\Omega\rangle$$

Propagate at later time  $t$  and annihilate the  $Q\bar{Q}$ :

$$\begin{aligned} G_{\beta',\alpha';\alpha,\beta}(y'x';x,y) &\equiv \langle\Omega|\hat{T}\bar{Q}_{\beta'}(\vec{y}',t)U(\vec{y}',t;\vec{x}',t)Q_{\alpha'}(\vec{x}',t)\bar{Q}_{\alpha}(\vec{x},0)U(\vec{x},0;\vec{y},0)Q_{\beta}(\vec{y},0)|\Omega\rangle \\ &= \frac{1}{Z}\int\mathcal{D}U\mathcal{D}(\bar{Q},Q)\bar{Q}_{\beta'}(y')\cdots Q_{\beta}(x)e^{iS} \end{aligned}$$

where  $x = (\vec{x}, 0)$ ,  $y = (\vec{y}, 0)$ ,  $x' = (\vec{x}', t)$  and  $y' = (\vec{y}', t)$ .

Do in the continuum theory, *i.e.*

$$S = S_G(A) + S_Q(\bar{Q}, Q, A), \quad S_Q = \int d^4x \bar{Q}(x)(i\gamma_{\mu}D^{\mu} - M_Q)Q(x)$$

Integrate over heavy fermions:

$$\begin{aligned} G_{\beta',\alpha';\alpha,\beta}(y'x';x,y) &= \frac{1}{Z}\int\mathcal{D}(A)[S_{\beta\beta'}(y,y';A)S_{\alpha'\alpha}(x',x;A) - S_{\alpha'\beta'}(x',y';A)S_{\beta\alpha}(y,x;A)] \\ &\quad U(x;y)U(y';x')\text{Det}D^Q(A)e^{iS_G} \end{aligned}$$

$S(z, z'; A)$  is the quark propagator in an external field  $A_{\mu}$  *i.e.*

$$(i\gamma^{\mu}D_{\mu} - M_Q)S(z, z'; A) = \delta^4(z - z')$$

Take  $M_Q \rightarrow \infty$ :

$$S(z, z'; A) = P e^{ig \int_0^t dt' A_0(\vec{x}, t')} S(z - z'), \quad (i\gamma_0 \partial_0 - M_Q) S(z - z') = \delta^4(z - z')$$

$$\begin{aligned} \Rightarrow iS(z, z'; A) = \delta^{(3)}(\vec{z} - \vec{z}') P e^{ig \int_0^t dt' A_0(\vec{x}, t')} & \left\{ \Theta(z_0 - z'_0) \left( \frac{1 + \gamma_0}{2} \right) e^{-iM_Q(z_0 - z'_0)} \right. \\ & \left. + \Theta(z'_0 - z_0) \left( \frac{1 - \gamma_0}{2} \right) e^{iM_Q(z_0 - z'_0)} \right\} \end{aligned}$$

$$G_{\beta', \alpha'; \alpha, \beta}(y' x'; x, y) \xrightarrow{M_Q \rightarrow \infty} \delta^{(3)}(\vec{x} - \vec{x}') \delta^{(3)}(\vec{y} - \vec{y}') \left( \frac{1 + \gamma_0}{2} \right)_{\alpha' \alpha} \left( \frac{1 - \gamma_0}{2} \right)_{\beta \beta'} e^{-2iM_Q t} \langle P e^{ig \oint dx^\mu A_\mu} \rangle$$

Rotate in Euclidean time and discretize:

$$G_{\beta', \alpha'; \alpha, \beta}(y' x'; x, y) \xrightarrow{M_Q \rightarrow \infty} \delta^{(3)}(\vec{x} - \vec{x}') \delta^{(3)}(\vec{y} - \vec{y}') \left( \frac{1 + \gamma_0}{2} \right)_{\alpha' \alpha} \left( \frac{1 - \gamma_0}{2} \right)_{\beta \beta'} e^{-2M_Q t} \langle W_C(U) \rangle$$

where  $W_C$  is the Wilson loop:  $\langle W_C \rangle = \frac{1}{Z} \int \mathcal{D}(U) W_C(U) e^{-S_G(U)} \rightarrow e^{-V(R)t}$ .

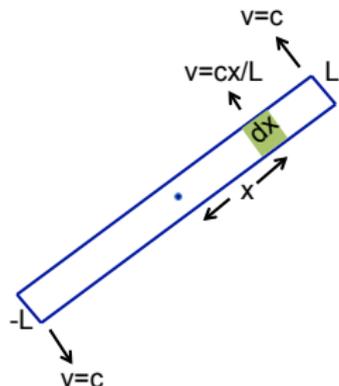
## String tension

Can we relate the string tension extracted from the Wilson loop to a quantity measured in experiment?  
Families of mesons with a given set of quantum numbers have masses obeying the Regge formula

$$M_J^2 = \frac{1}{\alpha} J, \quad \alpha = 0.9 \text{ GeV}^{-1}$$

Consider a simple model: [J. W. Negele]

- A massless quark and an antiquark connected by a string of length  $2L$ .
- Since they are massless they are moving with the speed of light and the speed of a segment of string a distance  $x$  from the origin is  $v = \frac{x}{L}c$
- $\sigma$ =energy per unit length of the flux in its rest frame
- Contribution to energy and angular momentum of the element  $dx$ :



$$dE = \gamma \sigma dx, \quad dJ = \gamma \sigma v x dx$$

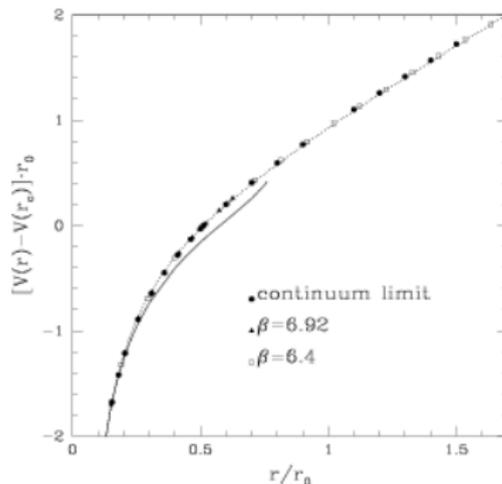
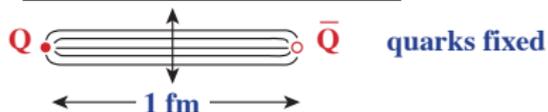
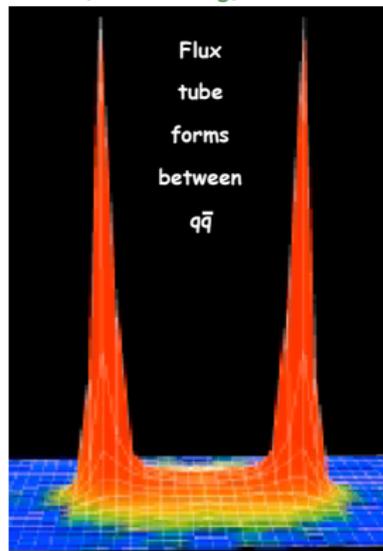
$$\Rightarrow M = \int_{-L}^L dx \frac{\sigma}{\sqrt{1 - (\frac{x}{L})^2}} = \pi \sigma L, \quad J = \int_{-L}^L dx \frac{\sigma x^2 / L}{\sqrt{1 - (\frac{x}{L})^2}} = \frac{\pi}{2} \sigma L^2 \Rightarrow M^2 = 2\pi \sigma J$$

$$\text{or } \sqrt{\sigma} = 2\pi\alpha^{-1/2} = 420 \text{ MeV.}$$

Note that this is a rough model and disagreement to the 10% level will not come as a surprise.

# Results

G. Bali, K. Schilling, C. Schlichter, 1995



[S. Necco and R. Sommer, NPB622 (2002)]

$r_0$  extracted from the  $q\bar{q}$  force:  $r^2 \frac{\partial V(r)}{\partial r} \Big|_{r=r_0} = 1.65$ .

## Continuum limit

Pure gauge on a lattice has only two parameters: the dimensionless bare coupling constant  $g$  and the lattice spacing  $a$ .

As we change  $a$ ,  $g$  must be adjusted to keep physical quantities fixed.

The renormalization procedure is in principle simple:

- Pick an initial value of  $g$
- Calculate a set of dimensionful physical quantities  $\langle \mathcal{O}_i \rangle$ . These can be written in the form:

$$\langle \mathcal{O}_i \rangle = a^{-d_i} \langle \mathcal{O}_i^L(g) \rangle, \quad d_i = \text{dimension of operator, and } \mathcal{O}_i^L \text{ dimensionless.}$$

e.g. the string tension has the form  $\sigma = a^{-2} \chi$

- Use the physical value of one operator, e.g.  $\mathcal{O}_1$  to determine  $a$  that corresponds to the particular value of  $g$  e.g. if we choose  $\sigma$  then  $a = \sqrt{\chi}/0.420 \text{ GeV}^{-1}$
- All other observables are then determined

One should then repeat the above steps for smaller values of  $g$  to determine  $g(a)$  and the physical quantities  $\langle \mathcal{O}_2 \rangle \cdots \langle \mathcal{O}_N \rangle$ .

The existence of a continuum limit implies that

$$\langle \mathcal{O}_i(g(a), a) \rangle = a^{-d_i} \langle \mathcal{O}_i^L(g) \rangle \xrightarrow{a \rightarrow 0} \mathcal{O}_i^{\text{phys.}}$$

*i.e.* the values of these observables should approach a limit as  $g \rightarrow 0$  and agree with experiment.

All dimensionful quantities in lattice simulations are measured in units of the lattice spacing e.g. for masses one measures  $m^L \equiv Ma$  and not  $M$ . As  $a \rightarrow 0$   $Ma \rightarrow 0$  or the correlation length  $\xi^L \equiv 1/Ma$  diverges. This is precisely what one wants to happen so that the system loses memory of the lattice.

## Continuum limit

Pure gauge on a lattice has only two parameters: the dimensionless bare coupling constant  $g$  and the lattice spacing  $a$ .

As we change  $a$ ,  $g$  must be adjusted to keep physical quantities fixed.

The renormalization procedure is in principle simple:

- Pick an initial value of  $g$
- Calculate a set of dimensionful physical quantities  $\langle \mathcal{O}_i \rangle$ . These can be written in the form:

$$\langle \mathcal{O}_i \rangle = a^{-d_i} \langle \mathcal{O}_i^L(g) \rangle, \quad d_i = \text{dimension of operator, and } \mathcal{O}_i^L \text{ dimensionless.}$$

e.g. the string tension has the form  $\sigma = a^{-2} \chi$

- Use the physical value of one operator, e.g.  $\mathcal{O}_1$  to determine  $a$  that corresponds to the particular value of  $g$  e.g. if we choose  $\sigma$  then  $a = \sqrt{\chi}/0.420 \text{ GeV}^{-1}$
- All other observables are then determined

One should then repeat the above steps for smaller values of  $g$  to determine  $g(a)$  and the physical quantities  $\langle \mathcal{O}_2 \rangle \cdots \langle \mathcal{O}_N \rangle$ .

The existence of a continuum limit implies that

$$\langle \mathcal{O}_i(g(a), a) \rangle = a^{-d_i} \langle \mathcal{O}_i^L(g) \rangle \xrightarrow{a \rightarrow 0} \mathcal{O}_i^{\text{phys.}}$$

*i.e. the values of these observables should approach a limit as  $g \rightarrow 0$  and agree with experiment.*

All dimensionful quantities in lattice simulations are measured in units of the lattice spacing e.g. for masses one measures  $m^L \equiv Ma$  and not  $M$ . As  $a \rightarrow 0$   $Ma \rightarrow 0$  or the correlation length  $\xi^L \equiv 1/Ma$  diverges. This is precisely what one wants to happen so that the system loses memory of the lattice.

## Asymptotic freedom

Asymptotic freedom: the running coupling  $g \rightarrow 0$  as the momentum scale of the probe  $\mu$  or  $1/a \rightarrow \infty$ . It is characterized by renormalization group function  $a \frac{dg}{da}$  or the  $\beta$ -function

$$-a \frac{\partial g}{\partial a} \equiv \beta(g) = -\beta_0 g^3 - \beta_1 g^5 + \dots$$

The perturbative  $\beta$ -function satisfies for  $N$  colors and  $n_f$  active flavors [t Hooft, Politzer, Gross and Wilczek]

$$\beta_0 = \left( \frac{11N - 2n_f}{3} \right) \frac{1}{16\pi^2}, \beta_1 = \left( \frac{34N^2}{3} - \frac{10Nn_f}{3} - \frac{n_f(N^2 - 1)}{N} \right) \frac{1}{(16\pi^2)^2}.$$

The point is that these two leading terms in the expansion of  $\beta(g)$  are gauge and regularization scheme invariant  $\rightarrow$  can be used in lattice regularization.

Integration of this relation yields

$$a(g^2) = \frac{1}{\Lambda_L} \left( \beta_0 g^2 \right)^{-\frac{\beta_1}{2\beta_0^2}} e^{-\frac{1}{2\beta_0 g^2}} \equiv \frac{1}{\Lambda_L} f(g),$$

where  $n_f = 0$  for pure gauge and  $\Lambda_L$  is an integration constant which is regularization scheme dependent. Inverting we obtain:

$$g(a)^{-2} = \beta_0 \ln(a^{-2} \Lambda_L^{-2}) + \frac{\beta_1}{\beta_0} \ln \left( \ln(a^{-2} \Lambda_L^{-2}) \right) + \dots$$

i.e. changing  $a$  one must tune  $g$  such that physical observables remain independent. Vanishing  $a$  corresponds to vanishing  $g \rightarrow$  **asymptotic freedom**.

From our lattice calculation we can calculate  $a(g^2)$  e.g.

$$a(g^2) = \left[ \frac{a^2 \sigma |g^2}{\sigma_{\text{exper.}}} \right]^{1/2} = \frac{\sqrt{\chi}}{0.42 \text{ GeV}}$$

should coincide with the perturbative result as  $a \rightarrow 0$  and be independent of the observable used. This is called **asymptotic scaling**.

## Mass scale $\Lambda_{QCD}$

Asymptotic freedom implies that QCD dynamically generates a mass scale.

Consider:  $\mu \frac{\partial g}{\partial \mu} = \beta = -\beta_0 g^3 - \beta_1 g^5$ .

Integrate from momentum scale  $\mu_1$  to  $\mu_2$  with  $\mu_2 > \mu_1$  keeping only the  $\beta_0$  term:

$$\frac{1}{2\beta_0 g^2(\mu_2)} - \frac{1}{2\beta_0 g^2(\mu_1)} = \log \frac{\mu_2}{\mu_1},$$

*i.e.* the coupling constant of non-abelian gauge theories depends logarithmically on the momentum scale of the process. Equivalently:

$$\begin{aligned} \frac{1}{2\beta_0 g^2(\mu)} - \log \mu &= \log \Lambda_{QCD} \implies \exp \left\{ \frac{1}{2\beta_0 g^2(\mu)} \right\} = \frac{\mu}{\Lambda_{QCD}} \\ \implies \alpha_s(\mu) &= \frac{g^2(\mu)}{4\pi} = \frac{1}{8\pi\beta_0 \log \frac{\mu}{\Lambda_{QCD}}} \end{aligned}$$

introduces  $\Lambda_{QCD}$ , the invariant scale of the theory with dimensions of mass.

$\implies$  QCD in pure gauge with  $g$  dimensionless dynamically generates a mass scale.

This happens because to specify  $g$  we need a momentum scale at which it is defined.

## Mass scale $\Lambda_{QCD}$

Extending the above analysis to include  $\beta_1$  gives

$$\Lambda_{QCD} = \lim_{\mu \rightarrow \infty} \mu \left( \frac{1}{\beta_0 g^2(\mu)} \right)^{\frac{\beta_1}{2\beta_0^2}} \exp\left[-\frac{1}{2\beta_0 g^2(\mu)}\right] \equiv \mu f(g(\mu)) .$$

This 2-loop definition of  $\Lambda_{QCD}$  is not unique; the value of  $\Lambda_{QCD}$  depends on the precise relation between  $g$  and  $\mu$ . However, once the value of  $\Lambda$  is determined in one scheme it can be related to that in any other perturbative scheme. For example, in the lattice regularized theory  $\Lambda_{latt}$  is also defined by the same equation but with  $\mu$  replaced by  $1/a$ . Then to 1-loop

$$\frac{\Lambda_{QCD}}{\Lambda_{latt}} = \mu a \exp\left\{-\frac{1}{2\beta_0} \left[ \frac{1}{g^2(\mu)} - \frac{1}{g^2(a)} \right]\right\} .$$

In perturbation theory the two coupling constants are related as

$$g^2(\mu) = g^2(a) \left\{ 1 - \beta_0 g^2(a) \left( \log(\mu a)^2 - \log C^2 \right) + O(g^4) \right\}$$

and

$$\Lambda_{QCD} = C \Lambda_{latt}$$

*i.e.* the two constants,  $\Lambda_{QCD}$  and  $\Lambda_{latt}$ , are related by a multiplicative constant. To calculate  $C$  requires knowing the finite part of the coupling constant renormalization to 1-loop in both the lattice and continuum regularization schemes.

The results are listed in the following Table for  $\Lambda_{MOM}$  and  $\Lambda_{\overline{MS}}$ .

$n_f$	0	1	2	3	4
$\Lambda_{\overline{MS}}/\Lambda_{latt}$	28.8	34.0	41.1	51.0	65.5
$\Lambda_{MOM}/\Lambda_{latt}$	83.4	89.4	96.7	105.8	117.4

## Exercises

- 1 Using fermion coherent states find the path integral representation of the evolution operator. Then find the partition function and propagator for a non-interacting many particle system.
- 2 Using the SPA evaluate the 1-D integral

$$I(I) = \int_{-\infty}^{\infty} dx e^{-If(x)}$$

to  $\mathcal{O}(1/I)$  assuming  $I \gg 1$  and  $f(x)$  a real function with a minimum at  $x = x_0$ . Try to use a diagrammatic expression and then give the diagrams for the  $\mathcal{O}(1/I^2)$ -terms.

- 3 Write a computer program to implement the Metropolis Monte Carlo algorithm for the one dimensional harmonic oscillator  $V(x) = \frac{x^2}{2}$  with  $m = 1$ . Compare your results with those of standard quantum mechanics:

$$\langle x | e^{-HT} | x \rangle \approx |\langle x | E_0 \rangle|^2 e^{-E_0 T}$$

where  $E_0 = 1/2$  and  $\langle x | E_0 \rangle = \frac{e^{-x^2/2}}{\pi^{1/4}}$ .

Extract the energy and wave-function from your numerical result. In addition calculate

$$G(t) = \frac{1}{N} \sum_j \langle x(t_j + t)x(t_j) \rangle$$

for all  $t = 0, a, 2a \dots (N-1)a$ ; i.e. calculate  $G_n = \frac{1}{N} \sum_j \langle x_{(j+n) \bmod N} x_j \rangle$  for  $n = 0 \dots N-1$  with periodic boundary conditions. Try  $N = 20$  lattice sites with lattice spacing  $a = 1/2$ , and set  $\epsilon = 1.4$  and  $N_{cor} = 20$ . Try  $N_{cf}$ 's of 25, 100, 1000 and 10000. Use the results to compute the excitation energy from

$$\Delta E_n \equiv \log(G_n/G_{n+1}) \xrightarrow{n \text{ large}} (E_1 - E_0)a$$

Repeat this exercise for  $V(x) = x^4/2$ .

# 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

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

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

## 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

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

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

## Effective mass

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

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

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

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

- 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

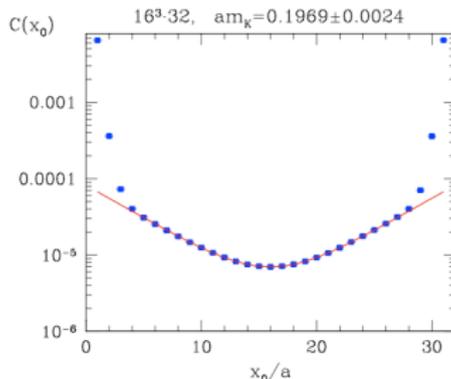
$$m_{\text{eff}}(t) = -\log\left(\frac{C_{kk}(\vec{0}, t)}{C_{kk}(\vec{0}, t-1)}\right) \stackrel{t \rightarrow \infty}{\rightarrow} m$$

which, in the limit  $t \rightarrow \infty$ , 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  $n^{\text{th}}$  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.  
 $\Rightarrow$  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  $m_{\text{eff}}(t)$  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.*  $m_{\text{eff}}(t) \rightarrow \text{constant}$  : 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.

# Lecture 4: Hadron spectrum

## Outline

- 1 Spectrum calculations**
  - Introduction to the basic techniques
  - Smearing techniques
  - Stochastic sources
- 2 Low-lying hadrons**
  - Setting the scaling
  - Comparison of results
- 3 Excited states**
  - Variational principle
  - Anisotropic lattices
  - $\chi^2$ -method
  - 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

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

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

## 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

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

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

## Effective mass

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

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

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

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

- 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

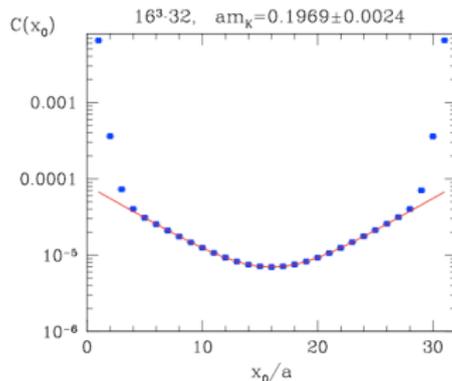
$$m_{\text{eff}}(t) = -\log\left(\frac{C_{kk}(\vec{0}, t)}{C_{kk}(\vec{0}, t-1)}\right) \stackrel{t \rightarrow \infty}{\rightarrow} m$$

which, in the limit  $t \rightarrow \infty$ , 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  $n^{\text{th}}$  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.  
 $\Rightarrow$  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  $m_{\text{eff}}(t)$  to the asymptotic value  $m$  can be from above or below depending on the choice of the interpolating field  $J$ . Only for  $J_k = J_j$  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*  $m_{\text{eff}}(t) \rightarrow \text{constant}$  : 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.

Extracting the mass as described above, we then study its dependence as a function of quark masses,  $a$ ,  $L$ , before we can compare to experimental data.

### 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
- Near chiral regime it is crucial to combine optimized methods to keep statistical noise small

## Smearing techniques

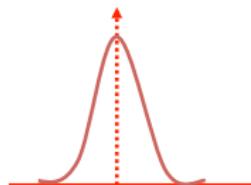
Hadrons are extended objects having size  $\mathcal{O}(1 \text{ fm})$ . The interpolating fields create point sources

→ they have a small overlap with the hadron state we want to study

⇒ Optimize projection to the state of interest:

Employ "gauge invariant smearing" of quark fields:

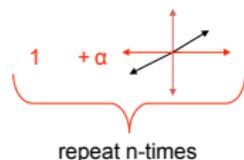
$$\psi^{\text{smear}}(\vec{x}, t) = \sum_{\vec{y}} F(\vec{x}, \vec{y}, U(t)) \psi(\vec{y}, t)$$



- To enhance ground state dominance use Gaussian smearing

$$F(\vec{x}, \vec{y}, U(t)) = (\mathbb{1} + \alpha H)^{n_\sigma}$$

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

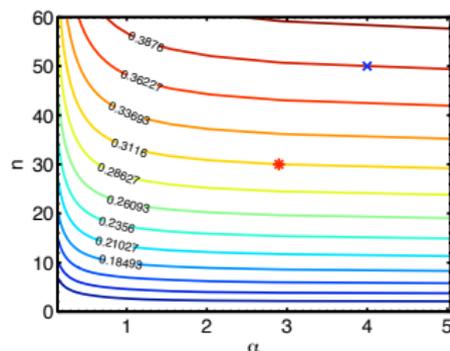


- Exponential smearing:

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

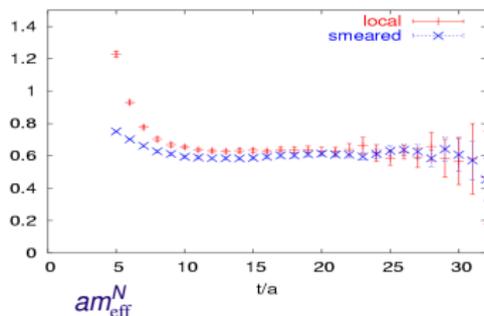
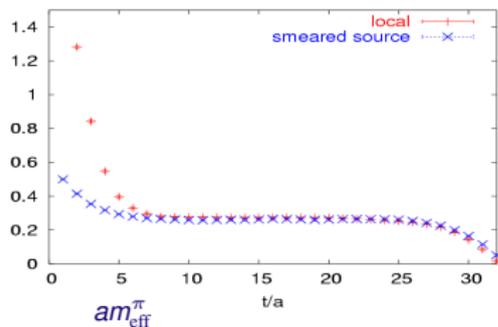
where one computes the propagator of a scalar particle propagating in the 3-dimensional space of the same background gauge field  $U(t)$

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

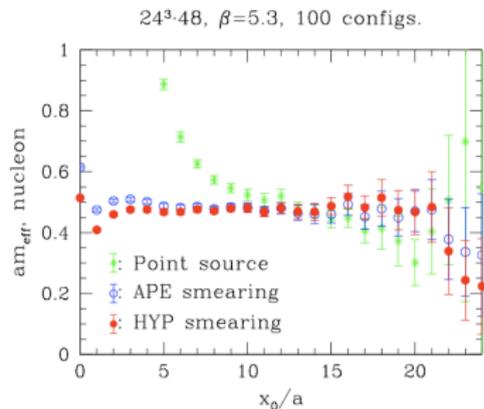
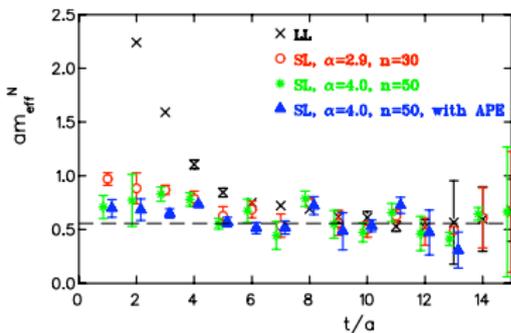


## Examples of effective mass plots

- Quenched at about 550 MeV pions:



- 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:

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

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!

⇒ replace point source by stochastic noise vector such that:

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

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

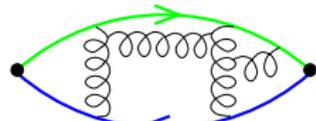
$$\phi_{\mu}^a(x)_r = \sum_y G_{\mu\nu}^{ab}(x, y) \zeta_{\nu}^b(y)_r \rightarrow G_{\mu\nu}^{ab}(x, y) = \langle \phi_{\mu}^a(x) \zeta_{\nu}^{*b}(y) \rangle_r$$

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  $N_r$ .

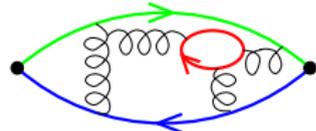
⇒ reduce  $N_r$  by employing "dilution schemes"

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:

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



(A) Quenched QCD: quark loops neglected



(B) Full QCD

## Systematic effects

- Cut-off effects

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

where  $r_0$  is determined from the force between a static quark and anti-quark.

⇒ we need to extrapolate to the continuum limit i.e. take  $a \rightarrow 0$

- 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.

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

## Systematic effects

- Cut-off effects

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

where  $r_0$  is determined from the force between a static quark and anti-quark.

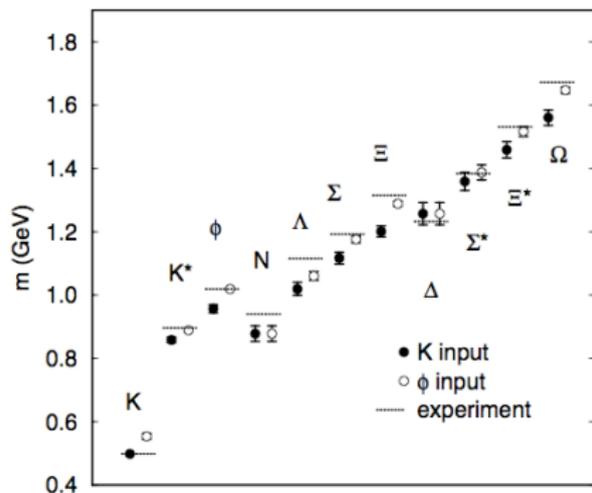
⇒ we need to extrapolate to the continuum limit i.e. take  $a \rightarrow 0$

- 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.

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

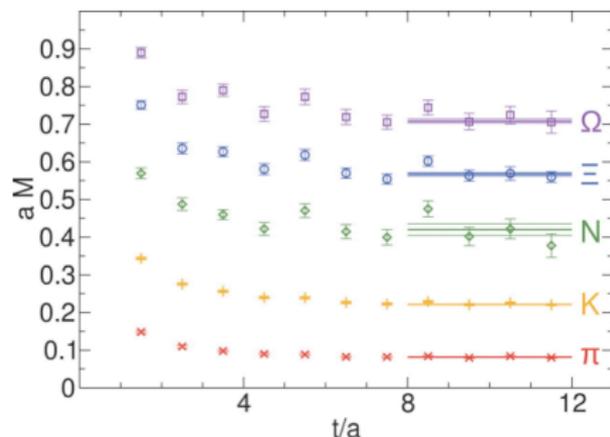


Quenched calculation with Wilson fermions CP-PACS Collaboration, S. Aoki et al. Phys. Rev. D 67 (2003)

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

# Unquenched calculations

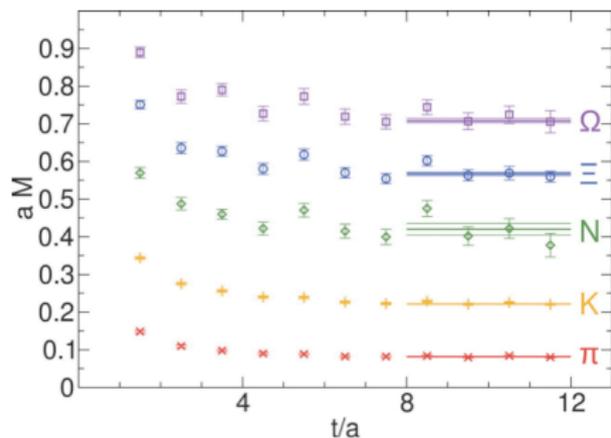
$N_f = 2 + 1$  smeared Clover fermions BMW Collaboration, S. Dürr et al. Science 322 (2008)



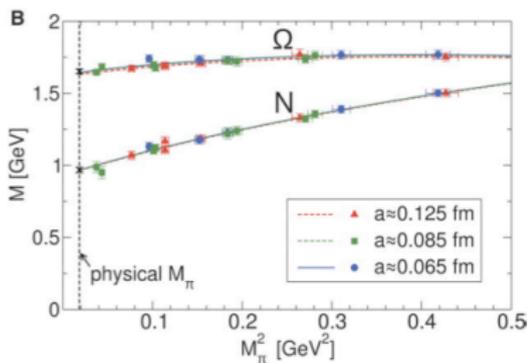
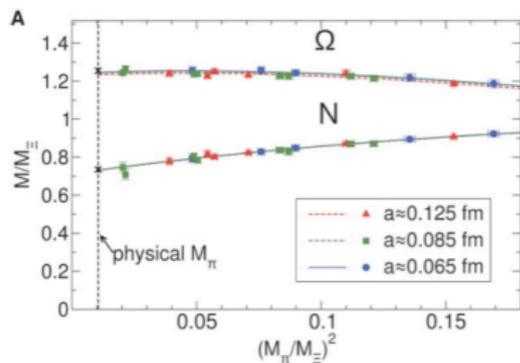
- 3 lattice spacing:  $a \sim 0.125, 0.085, 0.065$  fm set by  $m_{\Xi}$
- Pion masses:  $m_{\pi} \gtrsim 190$  MeV
- Volume:  $m_{\pi}^{\min} L \gtrsim 4$

# Unquenched calculations

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

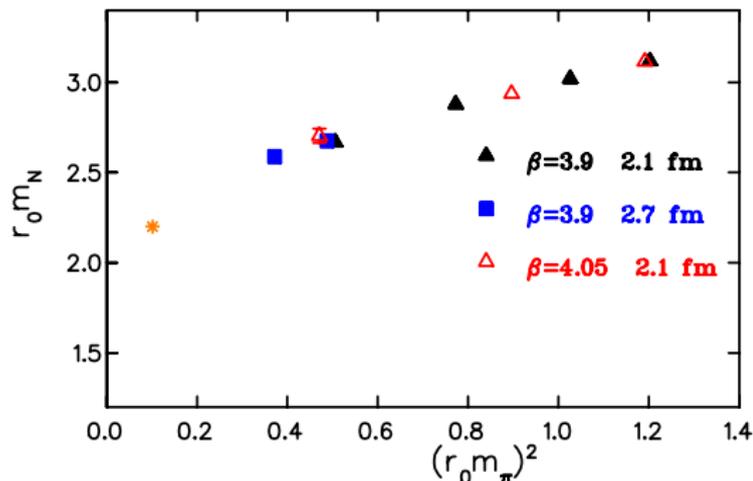


- 3 lattice spacing:  $a \sim 0.125, 0.085, 0.065$  fm set by  $m_\pi$
- Pion masses:  $m_\pi \gtrsim 190$  MeV
- Volume:  $m_\pi^{\min} L \gtrsim 4$



## Nucleon mass

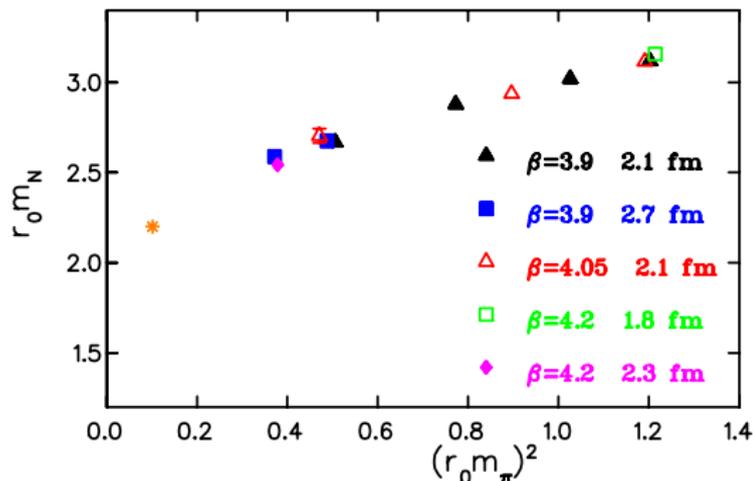
- Use nucleon mass at physical limit
- Cut-off effects negligible  $\Rightarrow$  use continuous chiral perturbation.
- Correct for volume dependence coming from pions propagating around the lattice [A. Ali Khan *et al.* (QCDSF) NPB689, 175 (2004)]



$N_f = 2$  twisted mass,  $m_\pi^{\min} \sim 270$  MeV,  $Lm_\pi^{\min} \sim 3.3$  [C. Alexandrou *et al.* (ETMC) PRD78 (2008) 014509]

## Nucleon mass

- Use nucleon mass at physical limit
- Cut-off effects negligible  $\Rightarrow$  use continuous chiral perturbation.
- Correct for volume dependence coming from pions propagating around the lattice [A. Ali Khan *et al.* (QCDSF) NPB689, 175 (2004)]



$N_f = 2$  twisted mass,  $m_\pi^{\min} \sim 270$  MeV,  $Lm_\pi^{\min} \sim 3.3$  [C. Alexandrou *et al.* (ETMC) PRD78 (2008) 014509]

## Lattice spacing determination

- Use nucleon mass at physical limit
- Cut-off effects negligible  $\Rightarrow$  use continuous chiral perturbation.
- Correct for volume dependence coming from pions propagating around the lattice [A. Ali Khan \*et al.\* \(QCDSF\) NPB689, 175 \(2004\)](#)
- Extrapolate using LO expansion:  $m_N = m_N^0 - 4c_1 m_\pi^2 - \frac{3g_A^2}{16\pi f_\pi^2} m_\pi^3$
- Simultaneous fits to  $\beta = 3.9$ ,  $\beta = 4.05$  and  $\beta = 4.2$  results

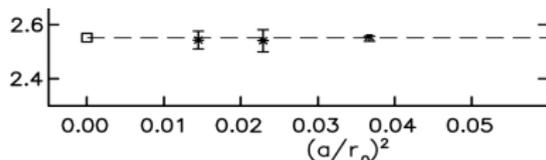
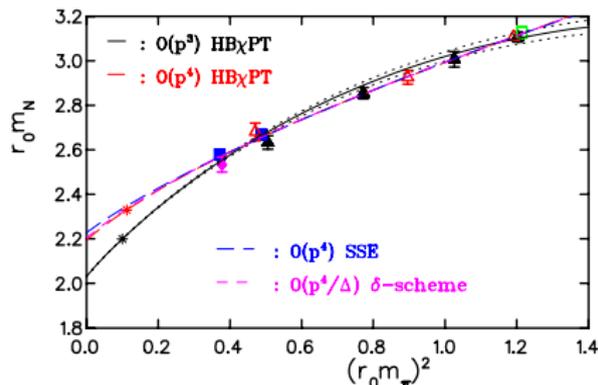
- We find  $r_0 = 0.462(5)(27)$  fm where the systematic error is estimated using  $\text{HB}\chi\text{PT}$  to  $\mathcal{O}(p^4)$

$$\Rightarrow a_{\beta=3.9} = 0.089(1)(5) \text{ fm},$$

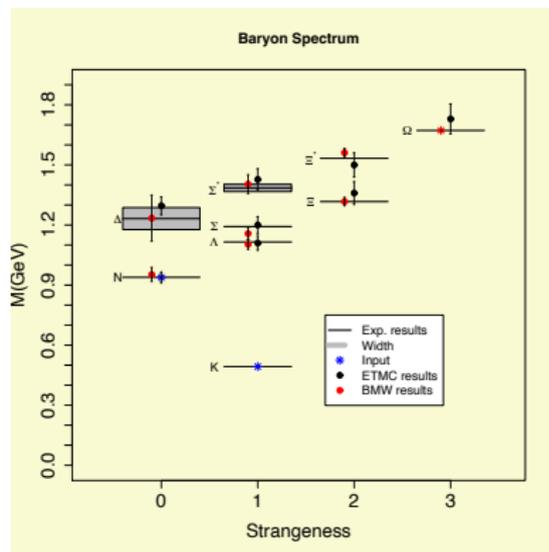
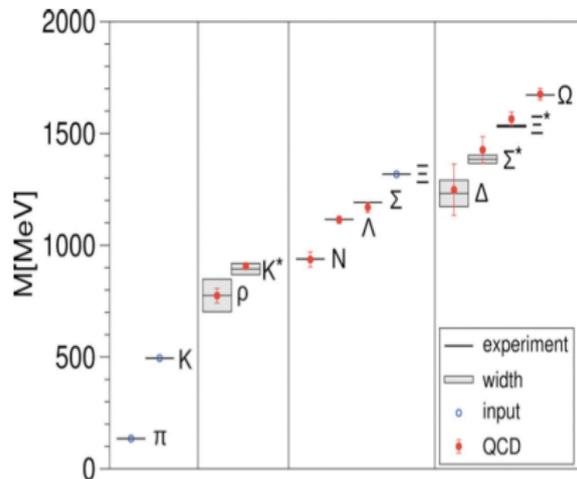
$$a_{\beta=4.05} = 0.070(1)(4) \text{ fm and}$$

$$a_{\beta=3.9} = 0.056(1)(4) \text{ fm}$$

- These are consistent with the lattice spacings from  $f_\pi$ .
- We use the lattice spacing determined from the nucleon mass for converting to physical units for baryon structure.



## Comparison of results using different actions



Good agreement between different discretization schemes

⇒ Significant progress in understanding the masses of low-lying mesons and baryons

## Excited states

Lattice calculations of excited states are much less advanced:

- Usually calculations are done on coarse lattices and at one lattice spacing → no continuum extrapolations
  - Up to very recently only in quenched QCD
  - Chiral extrapolations are scarce
  - The width of resonances is mostly ignored
- 1 One major challenge is to isolate the sub-leading contributions to the two-point correlator. Various methods are used:
- ▶ Variational
  - ▶ Bayesian
  - ▶  $\chi^2$ -histogram searches
- 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  $J_i$ ,  $i = 1, \dots, N$  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  $n^{\text{th}}$  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]

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

## Anisotropic lattices

Use a different lattice space  $a_t$  for time direction as that for the spatial directions  $a_s$

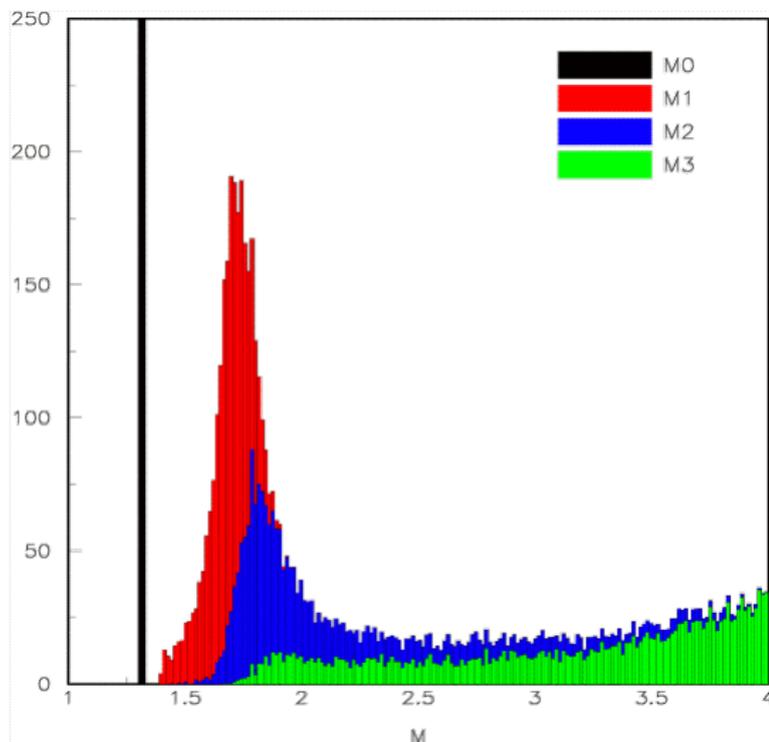
⇒ this is advantageous for studying excitations which have larger masses since the two-point correlation function fall off rapidly:

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

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)

## $\chi^2$ -method

- Assign to each solution  $\{A_1, \dots, A_n\}$  a  $\chi^2$  and a probability.
- Construct an ensemble of solutions.
- The probability distribution for any parameter assuming a given value is the solution.
- Assume a maximum number of  $L$  excited states in the spectral decomposition of the correlator  $C(t) = \sum_{i=0}^L A_i e^{-m_i t}$  and select a suitable range of values for each of the parameters  $A_i > 0$  and  $m_0 < m_1 < m_2 < \dots$ .
- Evaluate the  $\chi^2(1+L, j)$  corresponding to the particular solution using our lattice data. We repeat this procedure a large number, typically a few hundred thousand, generating an ensemble of solutions.

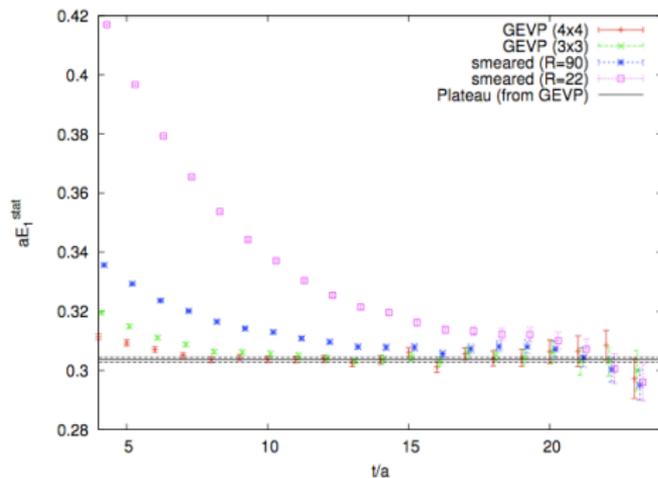


We find  $m_0 = 1.3171(13)$ ,  $m_1 = 1.608(9)$ ,  $m_2 = 2.010(11)$  as compared to 1.3169(1), 1.62(2) and 1.98(22) from a Bayesian analysis, [G. P. Lepage *et al.*, NP109A (2002) 185]

[C. A., C.N. Papanicolas and E. Stiliaris, PoS LAT2008, arXvi:0810.3882]

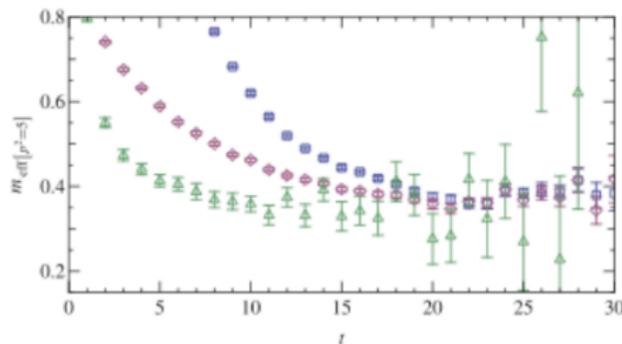
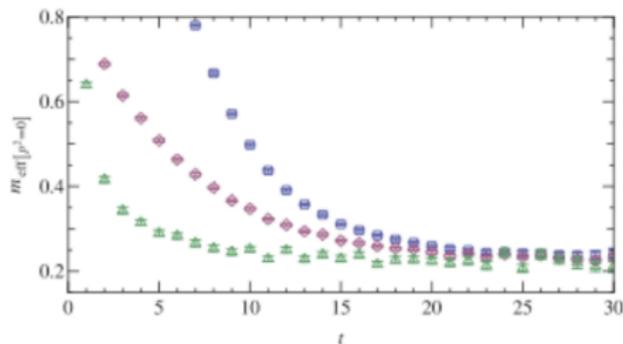
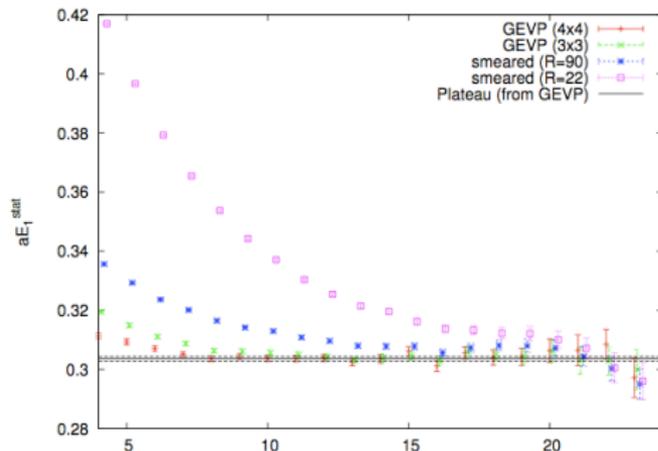
## Results using the variational principle

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



## Results using the variational principle

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

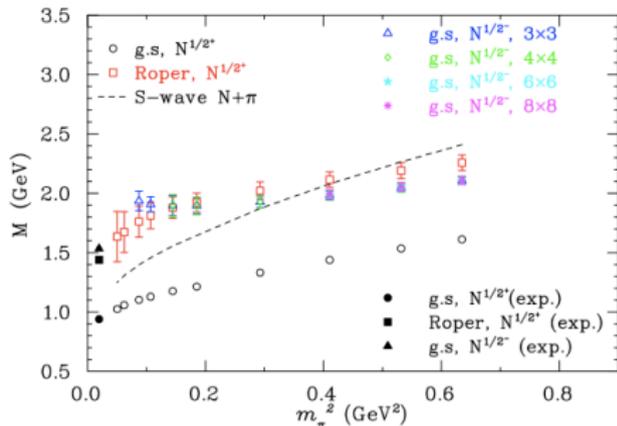
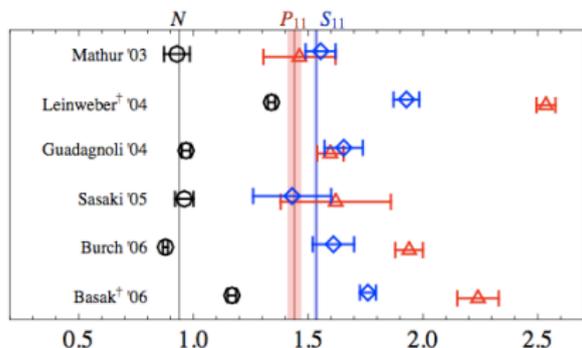


Nucleon effective mass plots with  $m_{\pi} = 450$  MeV using differing Gaussian smearings

## 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

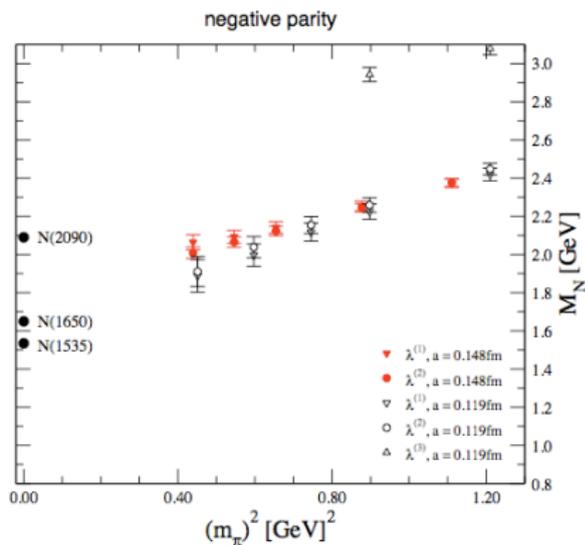
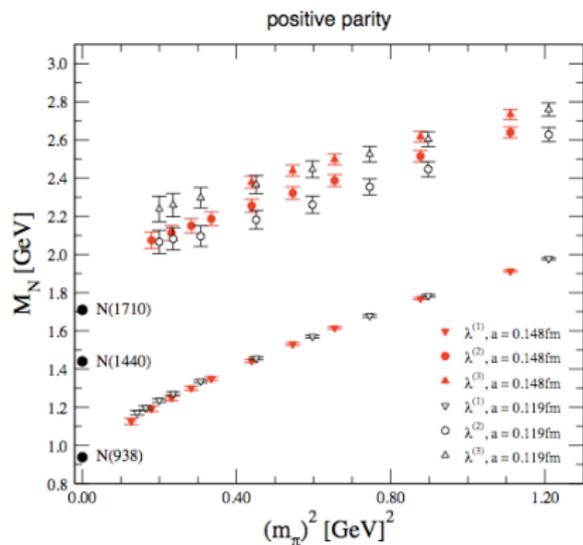


Quenched calculation, using variational principle [M. S. Mahbub *et al.*, arXiv:1007.4871]

## Excited states of the Nucleon/ $\Delta$

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

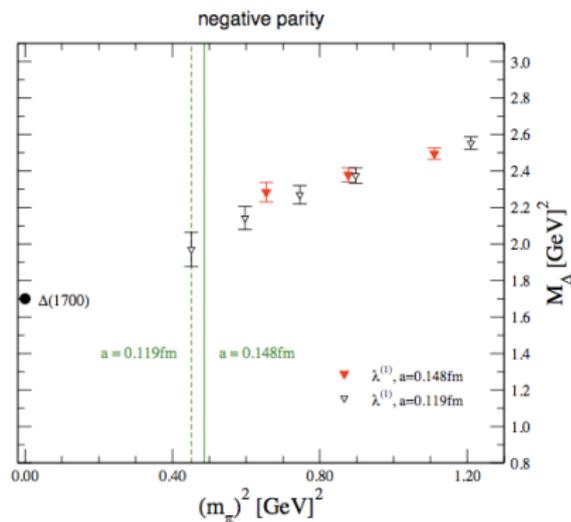
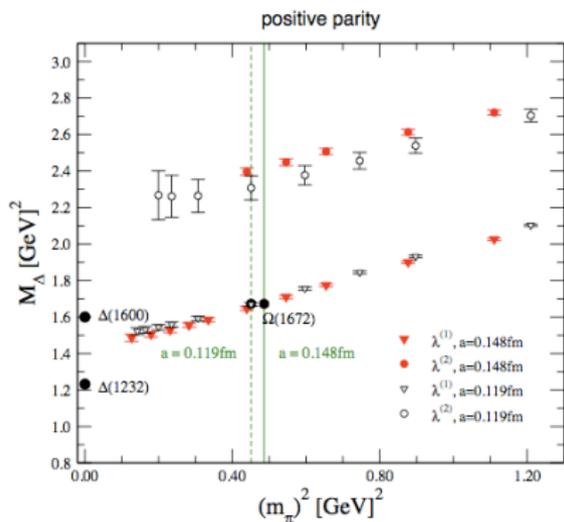
- Two lattice spacings:  $a = 0.15$  fm,  $a = 0.12$  fm
- $m_\pi \gtrsim 350$  MeV and lattice sizes  $16^3 \times 32$  and  $20^3 \times 32$  with  $m_\pi^{\min} L \sim 4$
- Variational approach using different levels of Gaussian smearing;  $6 \times 6$  correlation matrix



## Excited states of the Nucleon/ $\Delta$

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

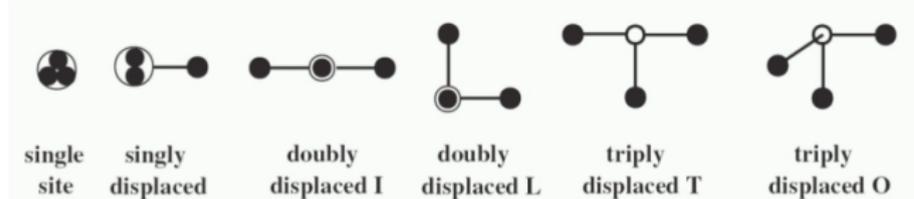
- Two lattice spacings:  $a = 0.15$  fm,  $a = 0.12$  fm
- $m_\pi \gtrsim 350$  MeV and lattice sizes  $16^3 \times 32$  and  $20^3 \times 32$  with  $m_\pi^{\min} L \sim 4$
- Variational approach using different levels of Gaussian smearing;  $6 \times 6$  correlation matrix



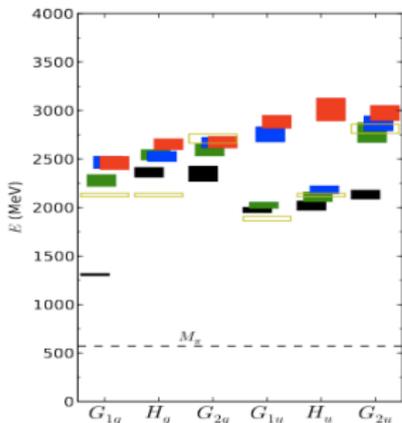
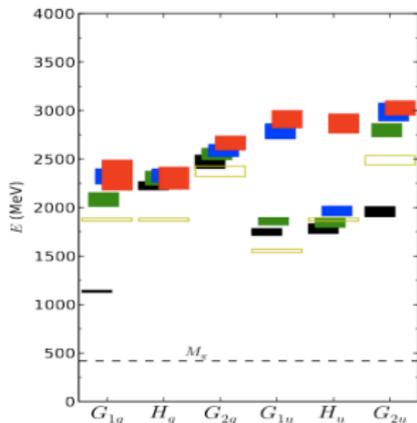
## Results using variational method and anisotropic lattices

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  $\rightarrow m_\pi^{\min} \sim 5.6$ .



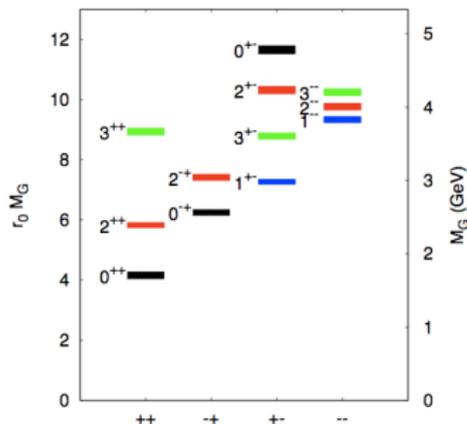
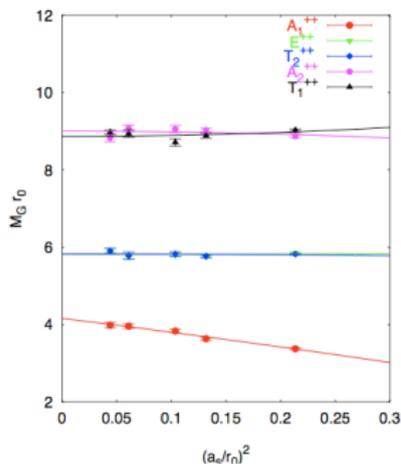
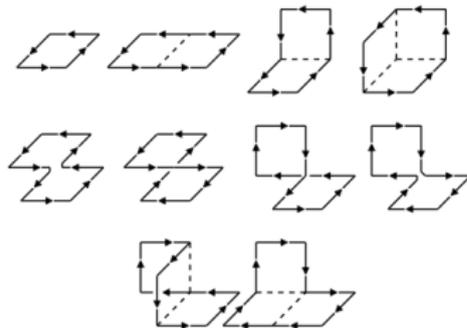
Extrapolation of the mass of the nucleon linearly in  $m_\pi^2$  yields  $m_N = 972(28)$  MeV

Excited states of nucleon:

$$\frac{m_{P_{11}}}{m_N} = 1.83 \text{ (experiment 1.53) and } \frac{m_{P_{11}}}{m_{S_{11}}} = 1.19 \text{ (experiment 0.94) i.e. wrong ordering}$$

# Glueballs

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



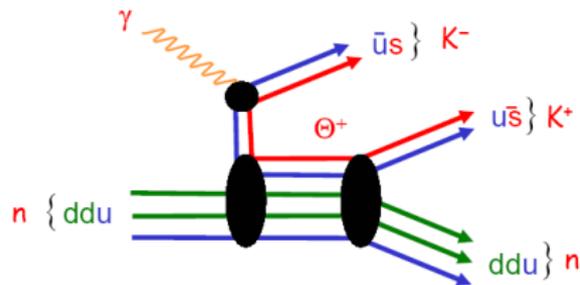
Quenched results:  $m_{0^{++}} = 1710(50)(80)$  MeV,  $m_{2^{++}} = 2390(30)(120)$  MeV [Chen *et al.*, hep-lat/0510074]

## Multi-quark states

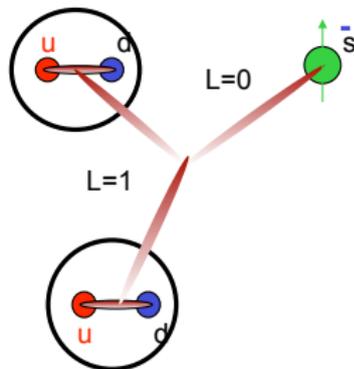
Up now only bound states of  $\bar{q}q$  and  $qqq$  have been clearly established  
 QCD predicts many more: quarks+glue, tetra-quarks (candidate  $\sigma$ -meson), molecular states of mesons, pentaquarks, etc

Example: Pentaquark state  $\Theta^+(1540)$ -experimental evidence faded away?

Very narrow resonance about 100 MeV above  $K - N$  threshold  $\implies$  presents a challenge for lattice QCD since we need to distinguish between a resonance and a 2-particle scattering state



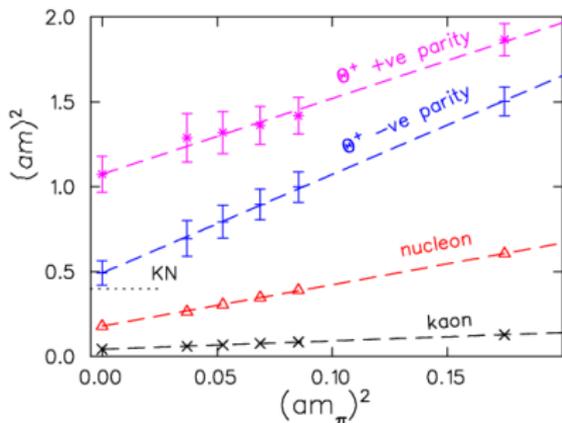
$\Theta^+$  is composed of  $(uudd\bar{s})$  quarks



## Lattice study of $\Theta^+$

Techniques developed:

- Identify the two lowest states and check for volume dependence of their mass: For scattering state  $E = \sqrt{m_n^2 + (2\pi\vec{n}/L)^2} + \sqrt{m_k^2 + (2\pi\vec{n}/L)^2}$ . For -ve parity channel we have S-wave KN scattering.
- Extract spectral weights and check their scaling with the spatial volume: Spectral weight for a resonance is independent of spatial volume whereas for a scattering state scales as  $\sim 1/L^3$
- Change from periodic to anti-periodic b.c. in the spatial directions and check if the mass in the negative parity channel changes: Use anti-periodic for light quarks and periodic for the strange  $\rightarrow \Theta^+$  is not affected since it has an even number of light quarks  
 $N$  has three and  $K$  one  $\rightarrow$  smallest allowed momentum for each quark id  $\pi/L$  and therefore the S-wave KN scattering energy is increased.
- Use interpolating fields in which the quarks are spatially separated
- Check whether the binding increases with quark mass



All lattice computations are done in the quenched theory using Wilson, domain wall or overlap fermions and a number of different actions. All groups but one agree that if the pentaquark exists it has negative parity

$\Rightarrow$  no real evidence for its existence

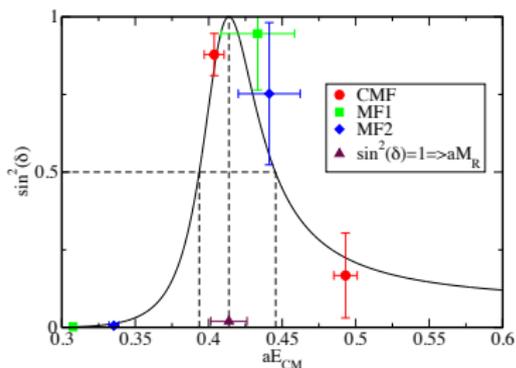
[C.A. & A. Tsapalis, PRD73 (2006) 014507]

## Resonances

As we approach the physical point it is important to develop techniques to study unstable particle  
 The favorite method is to study the energy of a two-particle state as a function of the spatial length of the box.  
 The  $\rho$ -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  $l = 1$ -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:  $\tan \delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E(m_R^2 - E^2)}$ ,  $k = \sqrt{E^2/4 - m_\pi^2} \rightarrow$  determine  $M_R$  and  $g_{\rho\pi\pi}$  and then extract  $\Gamma_\rho = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m_R^2}$ ,  $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

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

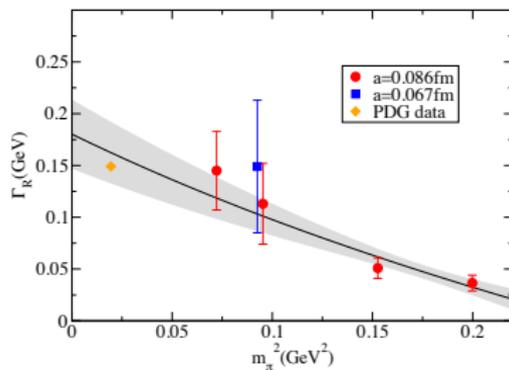
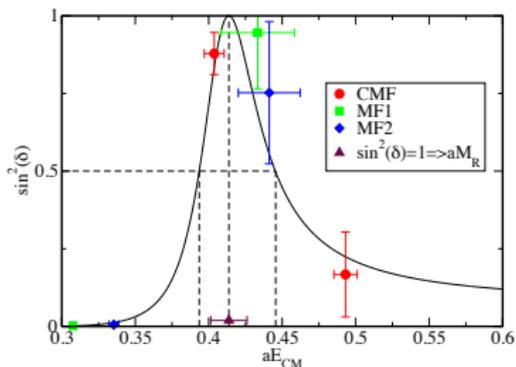


## Resonances

As we approach the physical point it is important to develop techniques to study unstable particle  
 The favorite method is to study the energy of a two-particle state as a function of the spatial length of the box.  
 The  $\rho$ -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  $l = 1$ -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:  $\tan\delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E(m_R^2 - E^2)}$ ,  $k = \sqrt{E^2/4 - m_\pi^2} \rightarrow$  determine  $M_R$  and  $g_{\rho\pi\pi}$  and then extract  $\Gamma_\rho = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m_R^2}$ ,  $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

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



## 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

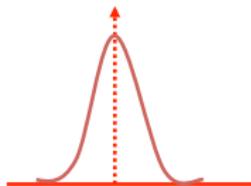
Hadrons are extended objects having size  $\mathcal{O}(1 \text{ fm})$ . The interpolating fields create point sources

→ they have a small overlap with the hadron state we want to study

⇒ Optimize projection to the state of interest:

Employ "gauge invariant smearing" of quark fields:

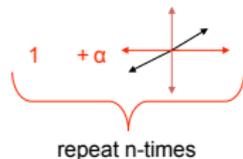
$$\psi^{\text{smear}}(\vec{x}, t) = \sum_{\vec{y}} F(\vec{x}, \vec{y}, U(t)) \psi(\vec{y}, t)$$



- To enhance ground state dominance use Gaussian smearing

$$F(\vec{x}, \vec{y}, U(t)) = (\mathbb{1} + \alpha H)^{n_\sigma}$$

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

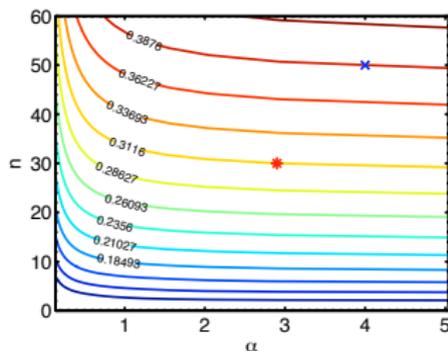


- Exponential smearing:

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

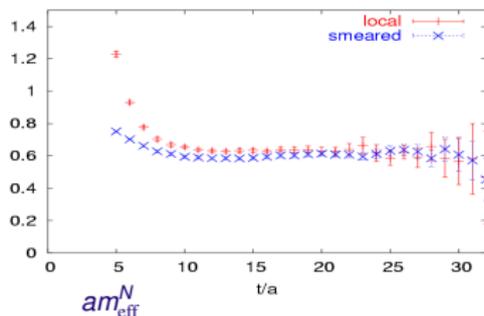
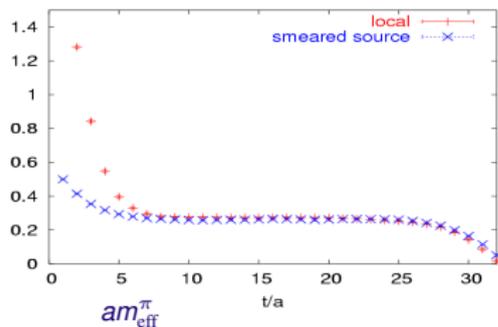
where one computes the propagator of a scalar particle propagating in the 3-dimensional space of the same background gauge field  $U(t)$

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

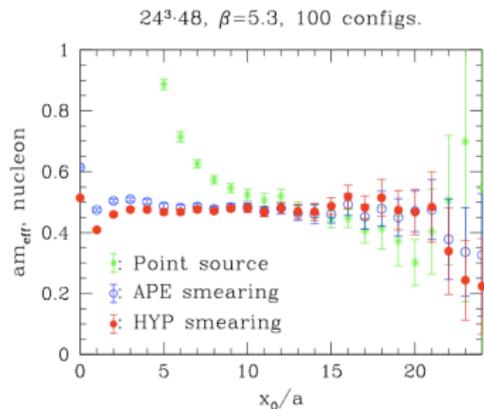
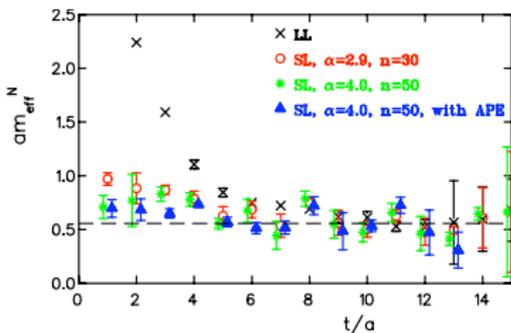


## Examples of effective mass plots

- Quenched at about 550 MeV pions:



- 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:

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

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!

⇒ replace point source by stochastic noise vector such that:

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

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

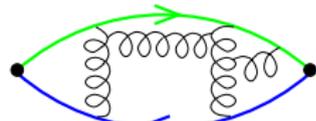
$$\phi_{\mu}^a(x)_r = \sum_y G_{\mu\nu}^{ab}(x, y) \zeta_{\nu}^b(y)_r \rightarrow G_{\mu\nu}^{ab}(x, y) = \langle \phi_{\mu}^a(x) \zeta_{\nu}^{*b}(y) \rangle_r$$

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  $N_r$ .

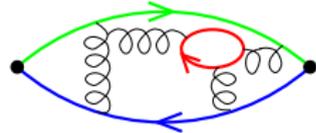
⇒ reduce  $N_r$  by employing "dilution schemes"

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:

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



(A) Quenched QCD: quark loops neglected



(B) Full QCD

## Systematic effects

- Cut-off effects

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

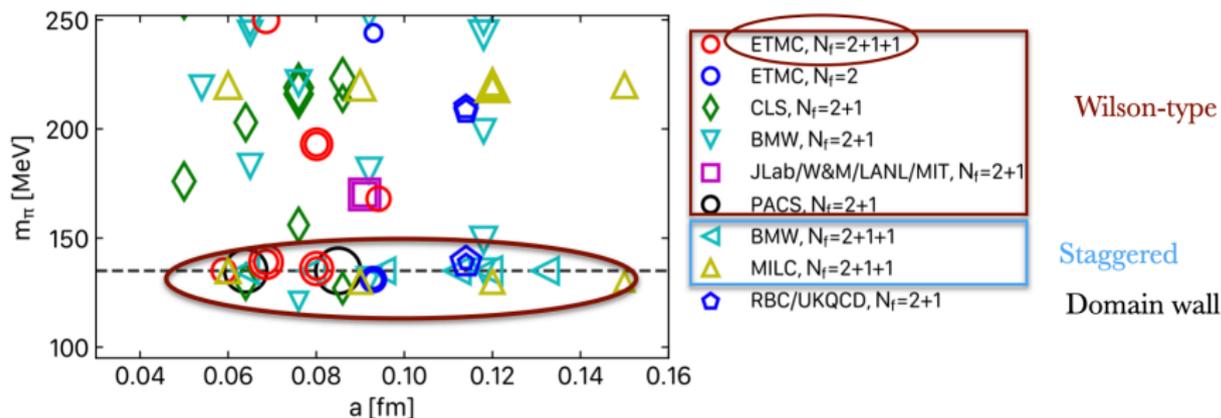
where  $r_0$  some length scale e.g. determined from the force between a static quark and anti-quark.  
⇒ we need to extrapolate to the continuum limit i.e. take  $a \rightarrow 0$

- 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.

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



Wilson-type

Staggered

Domain wall

## Systematic effects

- Cut-off effects

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

where  $r_0$  some length scale e.g. determined from the force between a static quark and anti-quark.

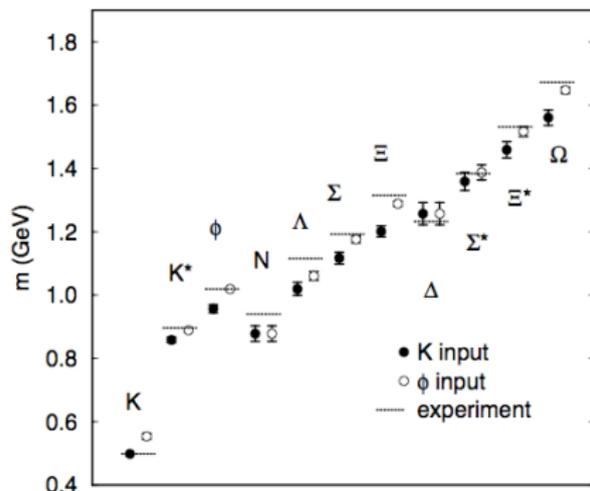
⇒ we need to extrapolate to the continuum limit i.e. take  $a \rightarrow 0$

- 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.

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

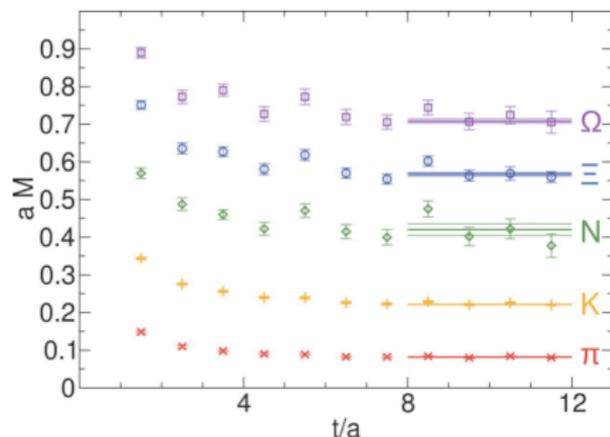


Quenched calculation with Wilson fermions CP-PACS Collaboration, S. Aoki et al. Phys. Rev. D 67 (2003)

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

# Unquenched calculations

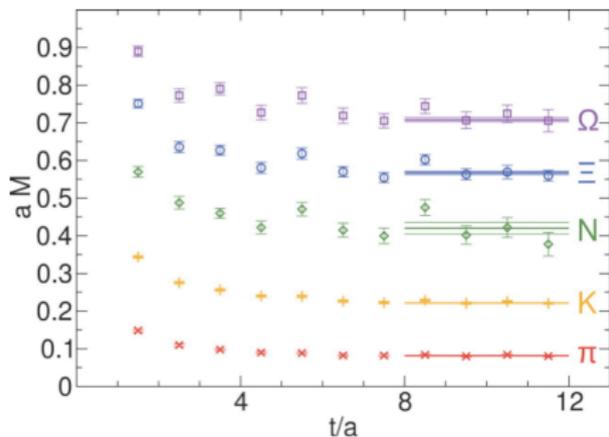
$N_f = 2 + 1$  smeared Clover fermions BMW Collaboration, S. Dürr et al. Science 322 (2008)



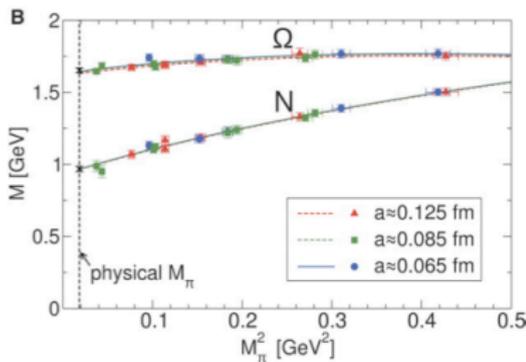
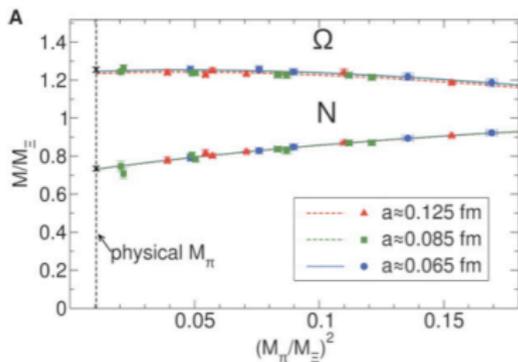
- 3 lattice spacing:  $a \sim 0.125, 0.085, 0.065$  fm set by  $m_{\Xi}$
- Pion masses:  $m_{\pi} \gtrsim 190$  MeV
- Volume:  $m_{\pi}^{\min} L \gtrsim 4$

# Unquenched calculations

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



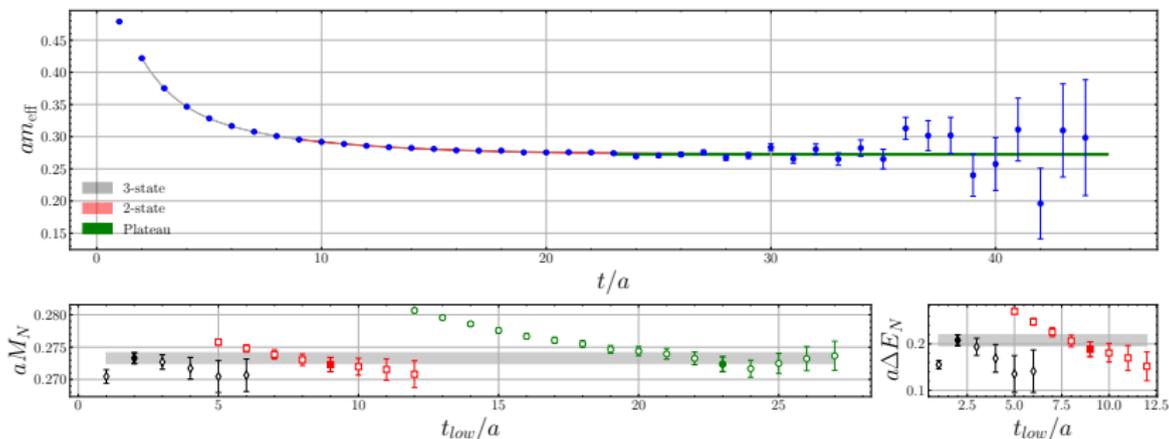
- 3 lattice spacing:  $a \sim 0.125, 0.085, 0.065$  fm set by  $m_\Xi$
- Pion masses:  $m_\pi \gtrsim 190$  MeV
- Volume:  $m_\pi^{\min} L \gtrsim 4$



# Low-lying hadron masses

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

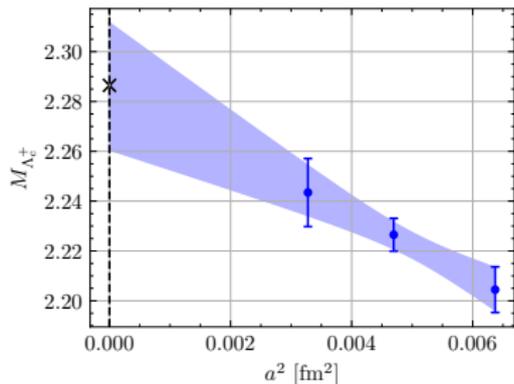
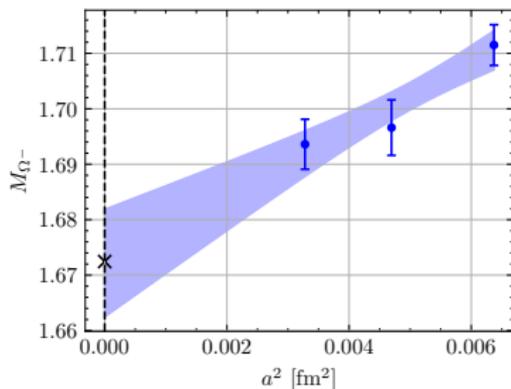
Ensemble	$V$	$\beta$	$\mu_l$	$\mu_\sigma$	$\mu_\delta$	$L \cdot m_\pi$	$m_\pi$ [MeV]
cB211.072.64	$128 \times 64^3$	1.778	0.00072	0.1246826	0.1315052	3.62	140.1 (0.2)
cC211.060.80	$160 \times 80^3$	1.836	0.00060	0.106586	0.107146	3.78	136.7 (0.2)
cD211.054.96	$192 \times 96^3$	1.900	0.00054	0.087911	0.086224	3.9	140.8 (0.2)



# Low-lying hadron masses

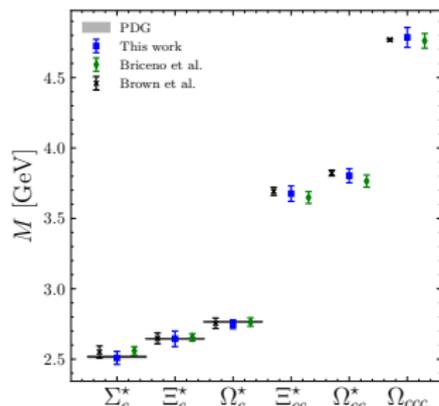
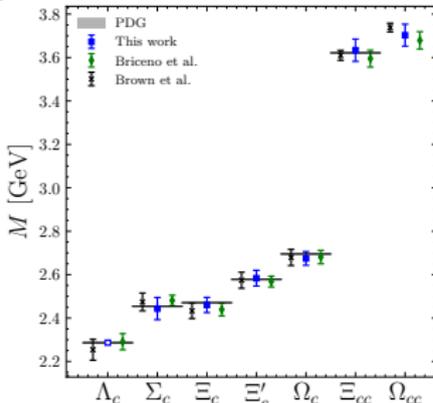
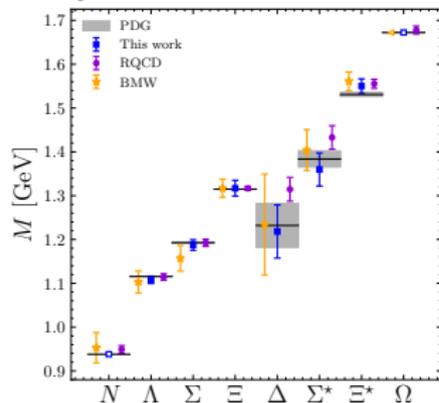
Simulation parameters used by the Extended Twisted Mass Collaboration (ETMC)

Ensemble	$V$	$\beta$	$\mu_l$	$\mu_\sigma$	$\mu_\delta$	$L \cdot m_\pi$	$m_\pi$ [MeV]
cB211.072.64	$128 \times 64^3$	1.778	0.00072	0.1246826	0.1315052	3.62	140.1 (0.2)
cC211.060.80	$160 \times 80^3$	1.836	0.00060	0.106586	0.107146	3.78	136.7 (0.2)
cD211.054.96	$192 \times 96^3$	1.900	0.00054	0.087911	0.086224	3.9	140.8 (0.2)



Continuum limit extrapolation for the mass of the  $\Omega^-$  (top) and the  $\Lambda_c^+$  (bottom)

## Comparison of results using different actions



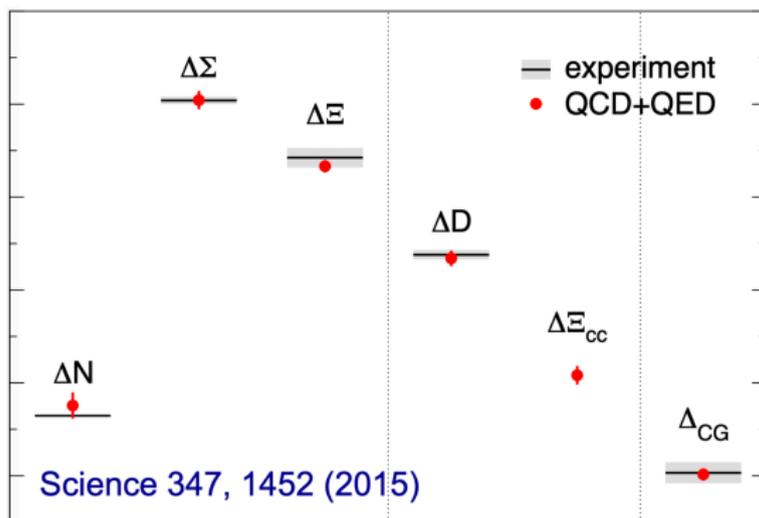
ETMC, C. Alexandrou *et al.* Phys. Rev. D 108 (2023) 9, 094510, arXiv: 2309.04401 [hep-lat]

Good agreement between different discretization schemes

⇒ 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)
$\Delta_{CG} = \Delta N - \Delta \Sigma + \Delta \Xi$	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 \*et al.\*, NP109A \(2002\) 185](#)
  - ▶  $\chi^2$ -histogram searches, see [[C. Alexandrou, C.N. Papanicolas and E. Stiliaris, PoS LAT2008, arXiv: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  $J_i$ ,  $i = 1, \dots, N$  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  $n^{\text{th}}$  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]

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

## Anisotropic lattices

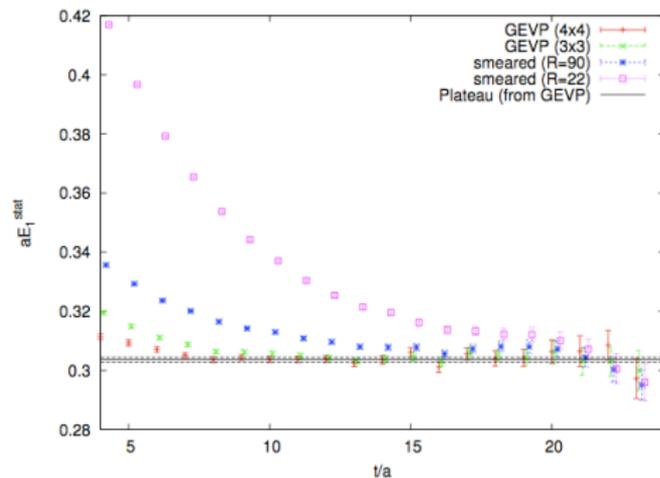
Use a different lattice space  $a_t$  for time direction as that for the spatial directions  $a_s$   
⇒ this is advantageous for studying excitations which have larger masses since the two-point correlation function fall off rapidly:

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

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)

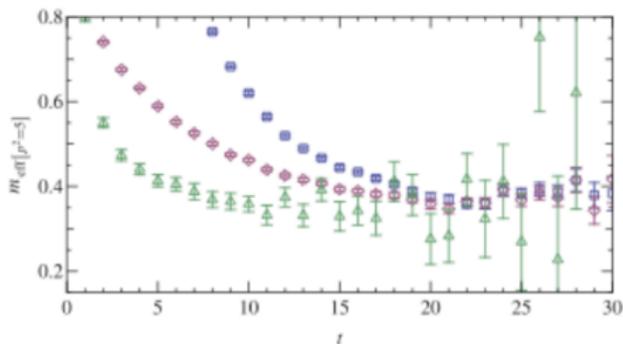
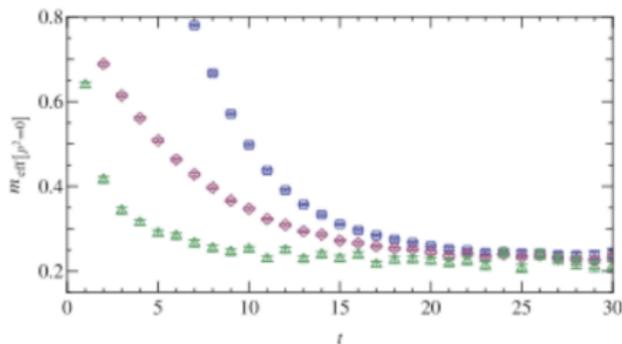
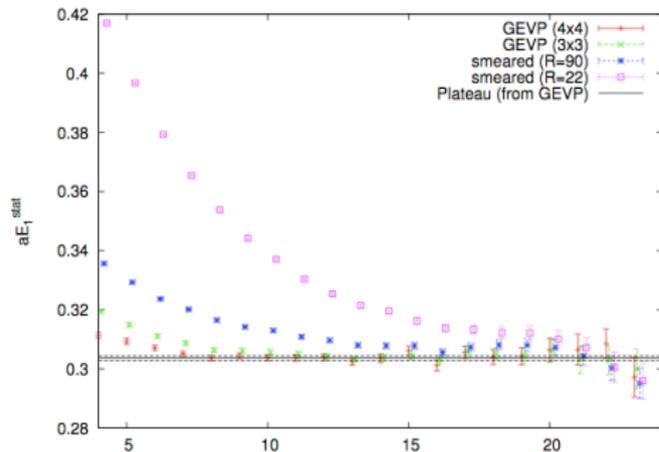
## Results using the variational principle

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



## Results using the variational principle

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

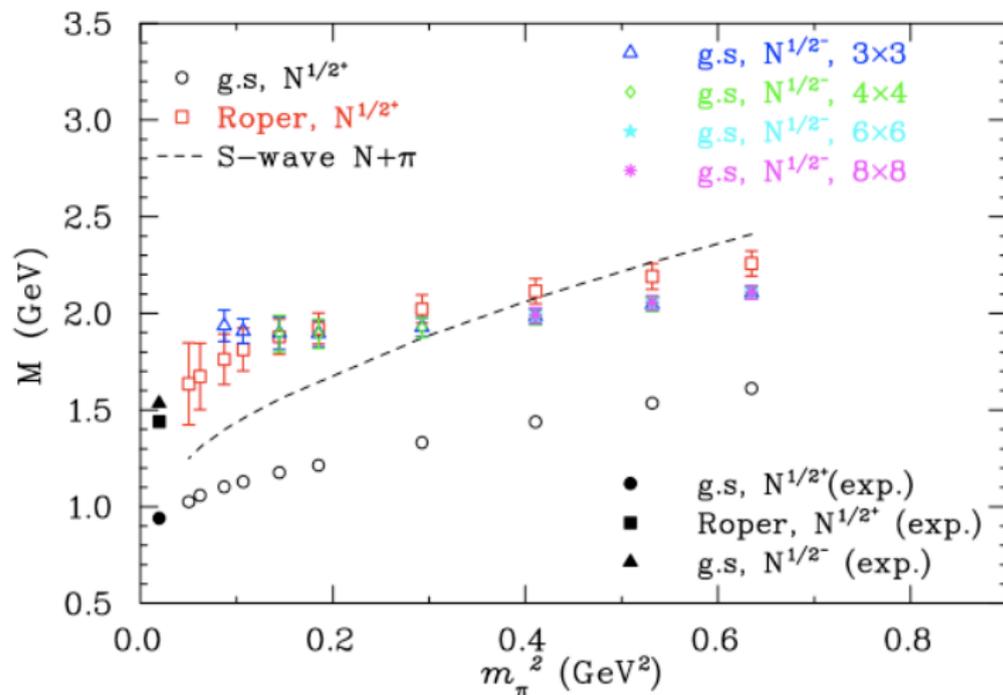


Nucleon effective mass plots with  $m_\pi = 450$  MeV using differing Gaussian smearings

## 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

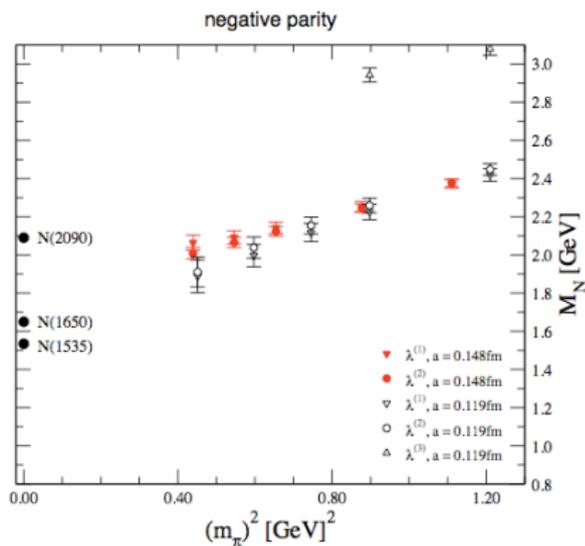
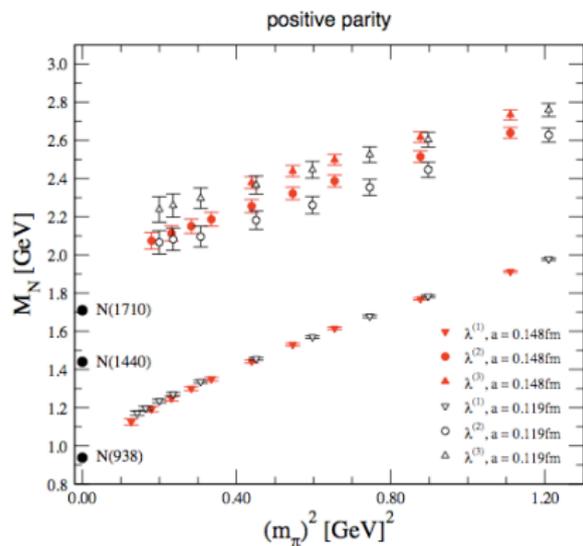


Quenched calculation, using variational principle [M. S. Mahbub *et al.*, arXiv:1007.4871]

## Excited states of the Nucleon/ $\Delta$

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

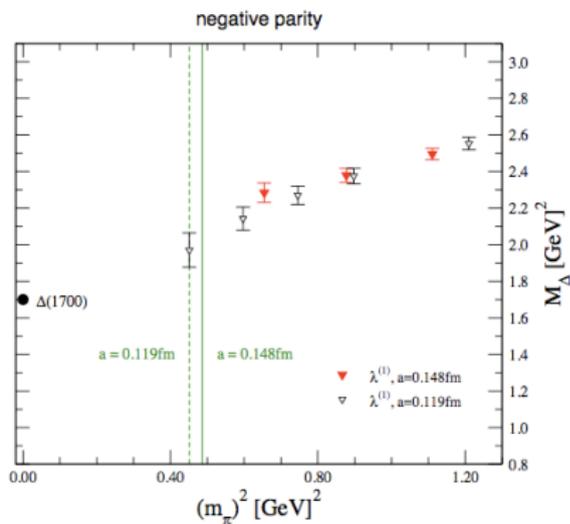
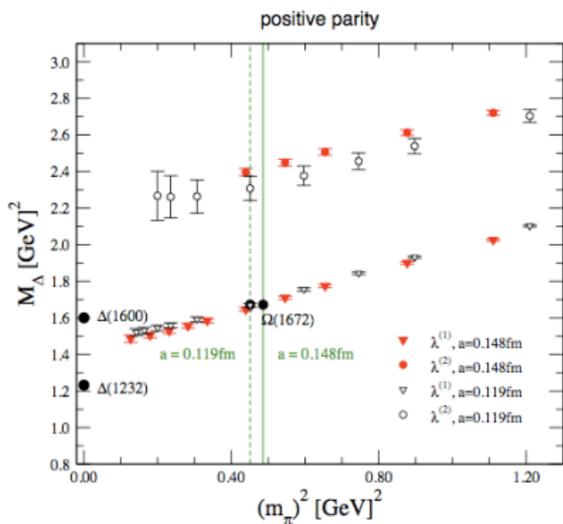
- Two lattice spacings:  $a = 0.15$  fm,  $a = 0.12$  fm
- $m_\pi \gtrsim 350$  MeV and lattice sizes  $16^3 \times 32$  and  $20^3 \times 32$  with  $m_\pi^{\min} L \sim 4$
- Variational approach using different levels of Gaussian smearing;  $6 \times 6$  correlation matrix



## Excited states of the Nucleon/ $\Delta$

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

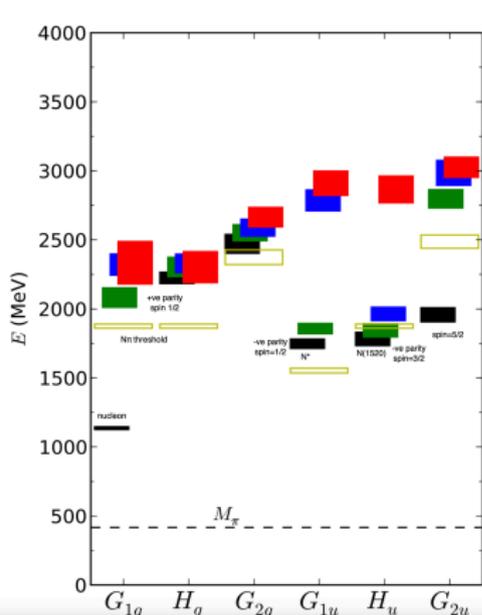
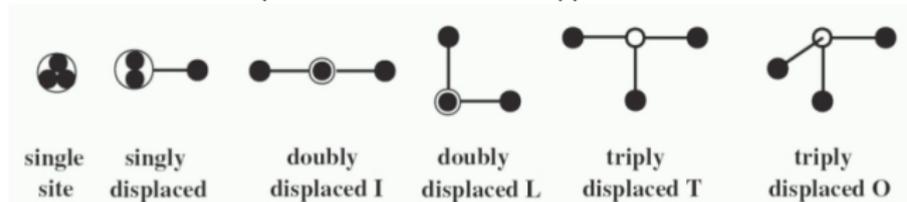
- Two lattice spacings:  $a = 0.15$  fm,  $a = 0.12$  fm
- $m_\pi \gtrsim 350$  MeV and lattice sizes  $16^3 \times 32$  and  $20^3 \times 32$  with  $m_\pi^{\min} L \sim 4$
- Variational approach using different levels of Gaussian smearing;  $6 \times 6$  correlation matrix



## 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

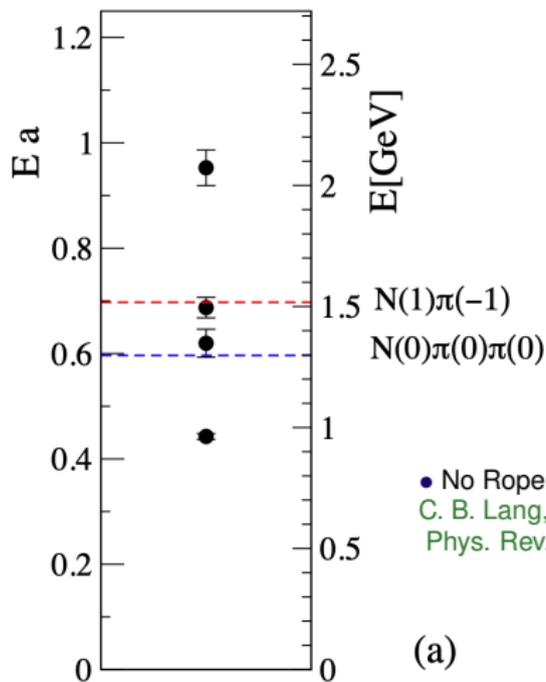


- $N_f = 2$  Wilson fermions with  $\frac{a_t}{a_s} = 3$  and  $a = 0.11$  fm at  $m_\pi = 420$  MeV and 580 MeV on a volume of  $L = 2.64$  fm  $\rightarrow m_\pi^{\min} \sim 5.6$ .
- Extrapolation of the mass of the nucleon linearly in  $m_\pi^2$  yields  $m_N = 972(28)$  MeV

- 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 nucleon 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  $p = 2\pi/L$



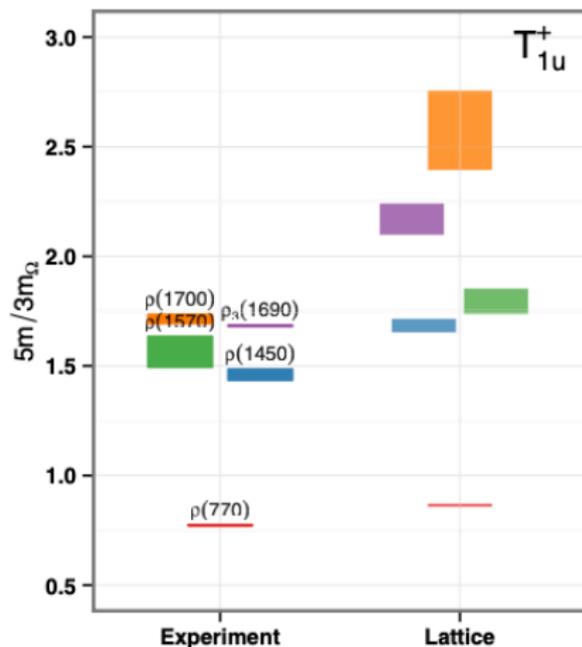
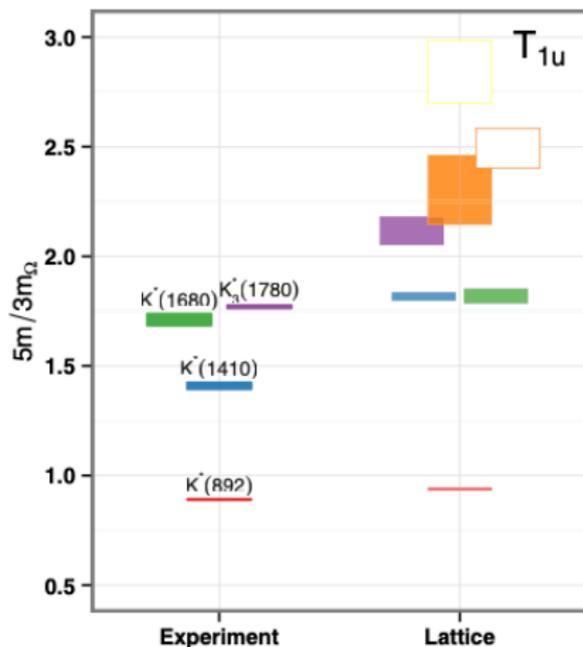
• No Roper state observed

C. B. Lang, L. Leskovec, M. Padmanath and S. Prelovsek,  
Phys. Rev. D 95 (2017) 1, 014510, arXiv:1610.01422 [hep-lat]

(a)

## Excited meson states

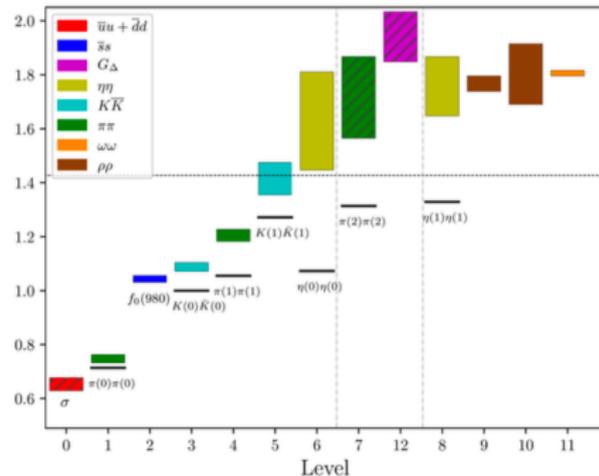
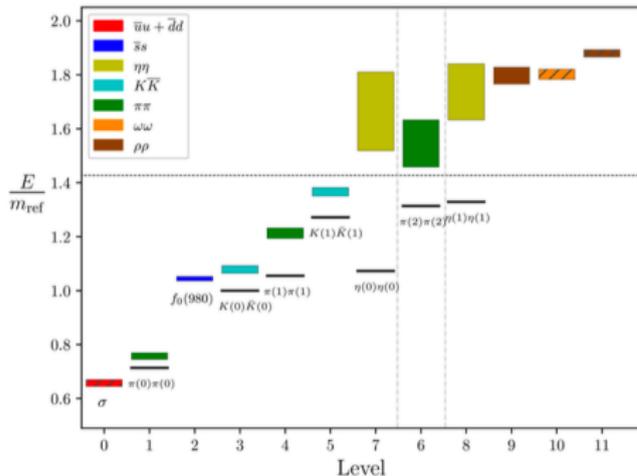
Analysis using  $N_f = 2 + 1$  clover fermions on a  $24^3 \times 128$  anisotropic lattice with a pion mass  $m_\pi \sim 240$  MeV. A correlation matrix of 58 operators including extended operators



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

## Excited meson states

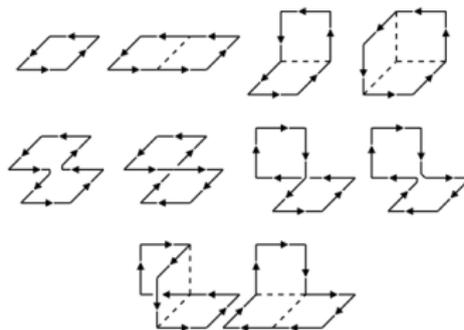
Analysis using  $N_f = 2 + 1$  clover fermions on a  $24^3 \times 128$  anisotropic lattice with a pion mass  $m_\pi \sim 390$  MeV. A correlation matrix of  $13 \times 13$  correlation matrix including the scalar gluon operator



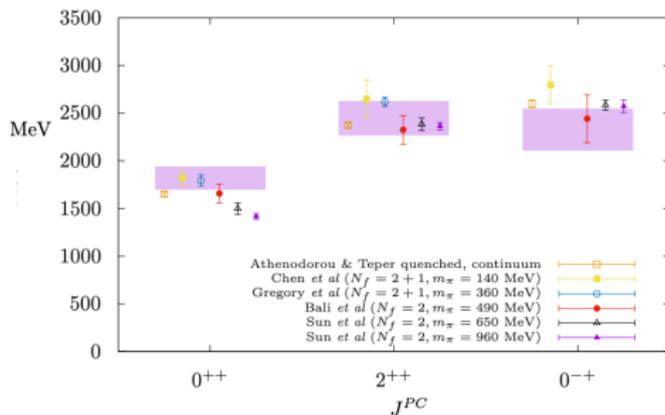
C. Morningstar, arXiv:2502.02547 [hep-lat]

## Glueballs

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

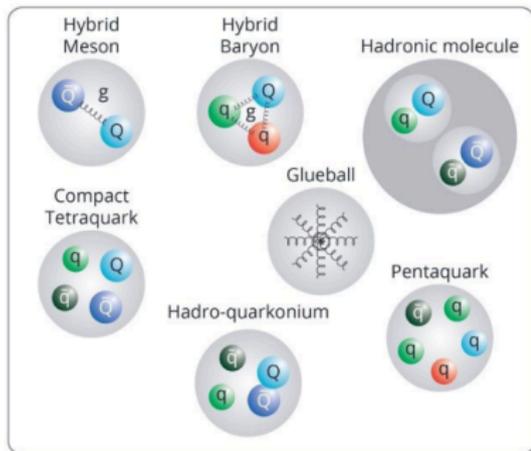
A. Athenodorou *et al.*, 2308.10054 [hep-lat]

# 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



Conventional Hadrons



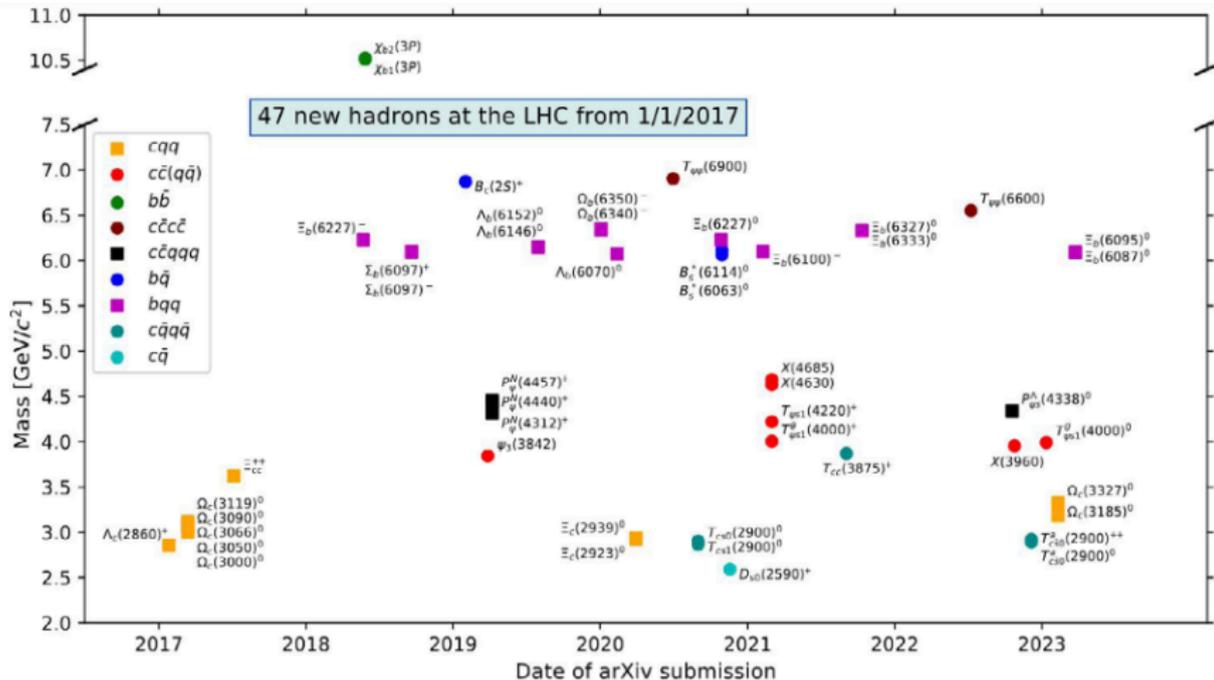
Unconventional Hadrons

## 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

Examples are the recently discovered X, Y and Z states at LHCb and BESII

Very narrow resonances near threshold  $\implies$  presents a challenge for lattice QCD since we need to distinguish between a resonance and a 2-particle scattering state

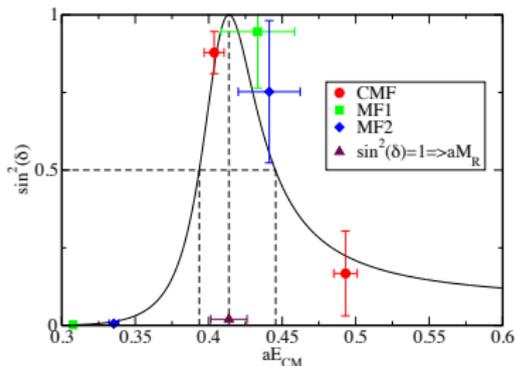


## Resonances

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  $\rho$ -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  $l = 1$ -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:  $\tan \delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E(m_R^2 - E^2)}$ ,  $k = \sqrt{E^2/4 - m_\pi^2} \rightarrow$  determine  $M_R$  and  $g_{\rho\pi\pi}$  and then extract  $\Gamma_\rho = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m_R^2}$ ,  $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

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

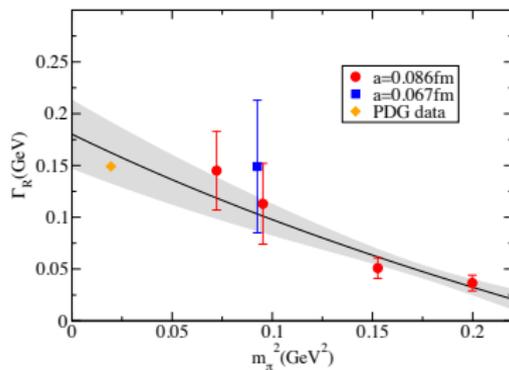
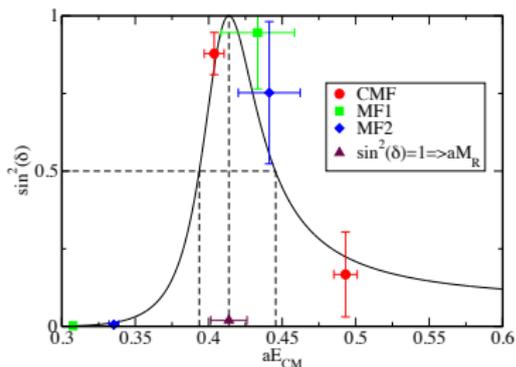


## Resonances

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  $\rho$ -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  $l = 1$ -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:  $\tan \delta_{11}(k) = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k^3}{E(m_R^2 - E^2)}$ ,  $k = \sqrt{E^2/4 - m_\pi^2} \rightarrow$  determine  $M_R$  and  $g_{\rho\pi\pi}$  and then extract  $\Gamma_\rho = \frac{g_{\rho\pi\pi}^2}{6\pi} \frac{k_R^3}{m_R^2}$ ,  $k_R = \sqrt{m_R^2/4 - m_\pi^2}$

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

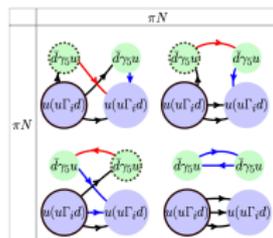
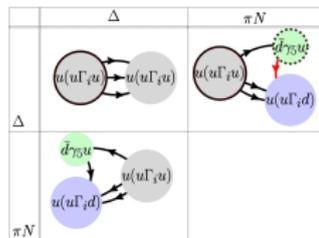


## Resonances - $\Delta$

Elastic pion-nucleon scattering in  $I=3/2$  channel [S. Paul *et al.* PoS LATTICE2018 (2018) 089]

Use  $N_f = 2 + 1$  clover fermions with  $m_\pi \approx 250$  MeV, and two volumes

Basis:  $\Delta$  and  $N\pi$



### J=3/2, P-wave Analysis

