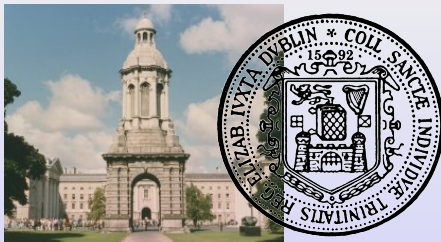


Lattice QCD and the Hadron Spectrum

Mike Peardon

School of Mathematics, Trinity College Dublin, Ireland



Heidelberg — 5th September 2013



- Essentials
 - QCD and the lattice
 - Quark and gluon actions
 - The path integral and Monte Carlo
- Spectroscopy on the lattice
 - Correlation functions
 - Variational method
 - Making measurements
 - Spin
- Measurements
 - Glueballs
 - Charmonium
 - Light quarks
 - Scattering, phase shifts and resonances

A constituent picture of hadrons

- QCD has **quarks** (in six flavours) and **gluons**
- **The confinement conjecture:** fields of the QCD lagrangian must be combined into colourless combinations: the **mesons** and **baryons**

A constituent model

constituents		quark model label
$3 \otimes \bar{3}$	=	$1 \oplus 8$ meson
$3 \otimes 3 \otimes 3$	=	$1 \oplus 8 \oplus 8 \oplus 10$ baryon
$8 \otimes 8$	=	$1 \oplus 8 \oplus 8 \oplus 10 \oplus 10$ glueball
$\bar{3} \otimes 8 \otimes 3$	=	$1 \oplus 8 \oplus 8 \oplus 8 \oplus 10 \oplus 10$ hybrid
\vdots		\vdots

- QCD does not always respect this constituent labelling!
There can be strong mixing.

Lattice Hadron Spectroscopy

- Significant experimental effort hoping to understand light hadron and charm spectroscopy
 - Are there resonances that don't fit in the quark model?
 - Are there gluonic excitations in this spectrum?
 - What structure does confinement lead to?
 - How do resonances decay?
- To use LQCD to address these questions means:
 - identifying continuum properties of states
 - computing scattering and resonance widths
- To achieve this we need
 - Techniques that give statistical precision
 - Spin identification
 - Control over extrapolations ($m_q \rightarrow 0, V \rightarrow \infty, a \rightarrow 0$).

Essential properties of QCD

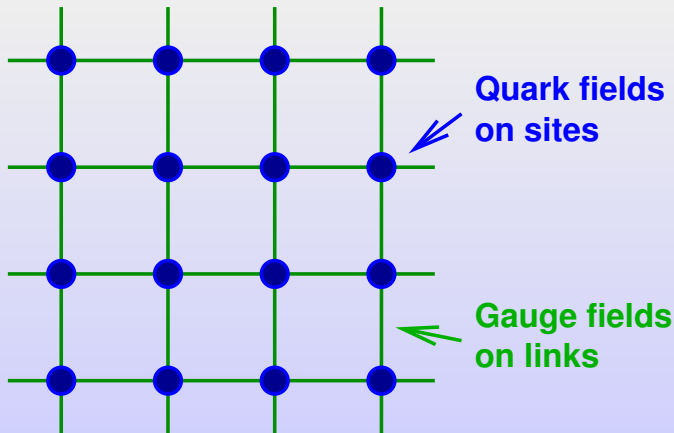
- To discretise theory and write useful lattice representation, important to do best possible job of respecting symmetries of theory.
- Symmetries define universality classes and ensure approach to continuum as we (try to) take $a \rightarrow 0$

Symmetries of QCD

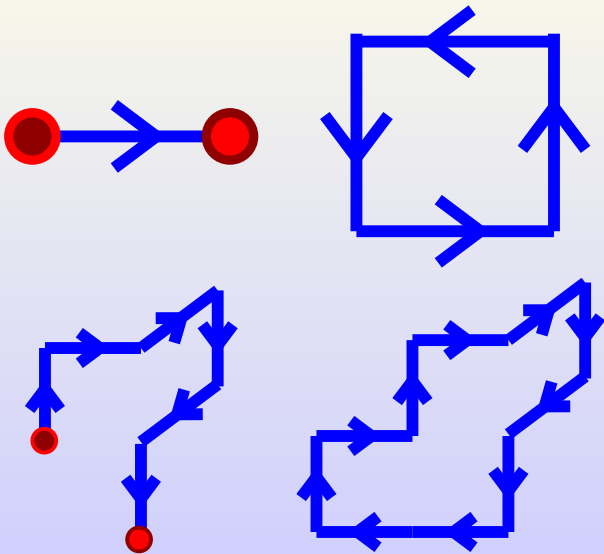
- Poincaré invariance (Lorentz and translation invariance)
- Gauge invariance - $SU(3)$ gauge group
- Discrete symmetries: parity, time-reversal, charge conjugation
- (Near) chiral symmetry (for massless quarks).
- (Near) flavour symmetry (for mass-degenerate quarks).
- The QCD path integral is written in terms of the two fundamental fields, the quarks and the gluons.

Wilson's big idea...

- Wilson realised that ensuring **gauge invariance** means the gluon fields have to be given special treatment:



Lattice gauge invariants



Lattice action - the gluons

- To define a path integral, we also need an action
- The simplest gauge invariant function of the gauge link variables alone is the **plaquette** (the trace of a path-ordered product of links around a 1×1 square).

$$S_G[U] = \frac{\beta}{N_c} \sum_{x, \mu < \nu} \text{ReTr} (1 - U_\mu(x)U_\nu(x + \hat{\mu})U_\mu^\dagger(x + \hat{\nu})U_\nu^\dagger(x))$$

This is the **Wilson gauge action**

- A path integral for the Yang-Mills theory of gluons would be

$$Z_{\text{YM}} = \int \prod_{\mu, x} \mathcal{D}U_\mu(x) e^{-S_G[U]}$$

- The coupling constant, g appears in $\beta = \frac{2N_c}{g^2}$
- No need to fix gauge; the gauge orbits can be trivially integrated over and the group manifold is compact.

Lattice action - the gluons

- A Taylor expansion in a shows that

$$\begin{aligned} S_G[U] &= \frac{\beta}{N_c} \sum_{x, \mu < \nu} \text{ReTr} \left(1 - U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x) \right) \\ &= \int d^4x \left[-\frac{1}{4} \text{Tr} F_{\mu\nu} F_{\mu\nu} + \mathcal{O}(a^2) \right] \end{aligned}$$

- All terms proportional to odd powers in the lattice spacing vanish because the lattice action preserves a discrete parity symmetry.
- The action is also invariant under a charge-conjugation symmetry, which takes $U_\mu(x) \rightarrow U_\mu^*(x)$.
- We have kept almost all of the symmetries of the Yang-Mills sector, but broken the $SO(4)$ rotation group down to the discrete group of rotations of a hypercube.

Lattice actions - the quarks

- Continuum action:

$$S_Q = \int d^4x \bar{\psi} (\gamma_\mu D_\mu + m) \psi$$

- When $m = 0$, the action has an extra, chiral symmetry:

$$\psi \longrightarrow \psi(x) = e^{i\alpha\gamma_5} \psi, \bar{\psi} \longrightarrow \bar{\psi}(x) = \bar{\psi} e^{i\alpha\gamma_5}$$

- Central difference:

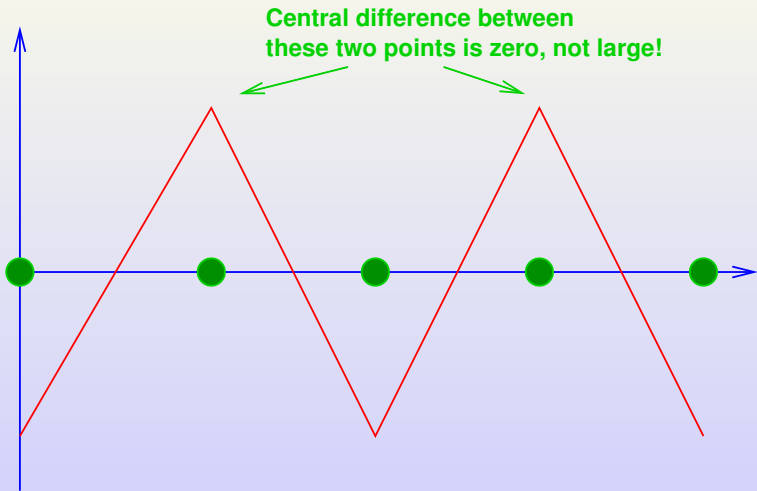
$$\partial_\mu \psi(\mathbf{x}) = \frac{1}{2a} (\psi(\mathbf{x} + \hat{\mu}) - \psi(\mathbf{x} - \hat{\mu}))$$

- Can be made gauge covariant by including the gauge links:

$$D_\mu \psi(\mathbf{x}) = \frac{1}{2a} (U_\mu(\mathbf{x}) \psi(\mathbf{x} + \hat{\mu}) - U_\mu(\mathbf{x} - \hat{\mu}) \psi(\mathbf{x} - \hat{\mu}))$$

- **BUT** on closer inspection - more minima to action. With no gauge fields and $\psi(\mathbf{x}) = e^{i\mathbf{k}\mathbf{x}}$ with $\mathbf{k} = \{\pi, 0, 0, 0\}$ or $\{\pi, \pi, 0, 0\}$ or $\{\pi, \pi, \pi, 0\}$ or ...

Lattice doubling



Lattice actions - the quarks (3)

- This is the (in)famous **doubling problem**.

The Nielsen-Ninomiya “no-go” theorem

There are **no** chirally symmetric, local, translationally invariant doubler-free fermion actions on a regular lattice.

- To put quarks on the lattice, more symmetry must be broken or else a theory with extra flavours of quarks must be simulated.
- A number of solutions are used, each with their advantages and disadvantages.
- The most commonly used are:
 - Wilson fermions
 - Kogut-Susskind (staggered) fermions
 - Ginsparg-Wilson fermions (overlap, domain wall, perfect...)
 - Twisted mass

QCD on the computer - Monte Carlo integration

- Finite lattice with $a \neq 0$, number of degrees of freedom is finite.
- The path integral is “ordinary” high-dimensional integral. Can be estimated stochastically by Monte Carlo.
- Variance reduction is crucial. Can only be done effectively if theory simulated in Euclidean space-time metric.
- No useful importance sampling weight for the theory in Minkowski space.
- Euclidean path-integral:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \mathcal{O}[U, \bar{\psi}, \psi] e^{-S[U, \bar{\psi}, \psi]}$$

- e^{-S} varies enormously; sample only the tiny region of configuration space that contributes significantly.

Dynamical quarks in QCD

- Monte Carlo with $N_f = 2$ degenerate quarks. Quark fields obey a grassmann algebra – difficult to manipulate in the computer.
- Quark action is bilinear; integrals done analytically:

$$Z_Q[U] = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} e^{-\sum_f \bar{\psi}_f M[U] \psi} = \det M^{N_f}[U]$$

- Including the gauge fields:

$$Z = \int \mathcal{D}U Z_Q[U] e^{-S_G[U]} = \int \mathcal{D}U \det M^{N_f}[U] e^{-S_G[U]}$$

- For $N_f = 2$ $\det M^2 \geq 0$ so can be included in importance sampling (but expensive).
- Using $M^\dagger = \gamma_5 M \gamma_5$, $\det M^2$ is re-written

$$Z_Q[U] = \int \mathcal{D}\phi \mathcal{D}\phi^* e^{-\phi^* [M^\dagger M]^{-1} \phi}$$

Dynamical quarks in QCD

- Requires applying inverse of M – very large matrix, so takes a lot of computer time.
- Where most computing power in lattice simulations goes; computing the effect of the quark fields acting on the gluons in the Monte Carlo updates.
- Alternative: quenched approximation to QCD. Ignore fermion path integral completely - unphysical approximation so effects are hard to quantify.
- Inversion is needed again in the measurement stage too;

$$\langle \psi(\mathbf{x}) \bar{\psi}(\mathbf{y}) \rangle = M^{-1}[U](\mathbf{x}, \mathbf{y})$$

Markov Chain Monte Carlo

- How is the configuration space sampled?
- All techniques use a **Markov process**: stochastic transition taking current state of the system randomly to a new state, such that probability of jump is independent of past states/
- Ergodic (positive recurrent, irreducible) Markov chains have unique stationary distributions; build the Markov process so it has our importance sampling distribution as its stationary state.
- If this can be done, then the **sequence of configurations generated by the process is our importance sampling ensemble!**
- Almost all algorithms exploit **detailed balance** to achieve this.

Variational method in Euclidean QFT

- Ground-state energies found from $t \rightarrow \infty$ limit of:

Euclidean-time correlation function

$$\begin{aligned} C(t) &= \langle 0 | \Phi(t) \Phi^\dagger(0) | 0 \rangle \\ &= \sum_{k,k'} \langle 0 | \Phi | k \rangle \langle k | e^{-\hat{H}t} | k' \rangle \langle k' | \Phi^\dagger | 0 \rangle \\ &= \sum_k |\langle 0 | \Phi | k \rangle|^2 e^{-E_k t} \end{aligned}$$

- So $\lim_{t \rightarrow \infty} C(t) = Z e^{-E_0 t}$
- Variational idea: find operator Φ to maximise $C(t)/C(t_0)$ from sum of basis operators $\Phi = \sum_a v_a \phi_a$

[C. Michael and I. Teasdale. NPB215 (1983) 433]

[M. Lüscher and U. Wolff. NPB339 (1990) 222]

Variational method

If we can measure $C_{ab}(t) = \langle 0 | \phi_a(t) \phi_b^\dagger(0) | 0 \rangle$ for all a, b and solve generalised eigenvalue problem:

$$C(t) \underline{v} = \lambda C(t_0) \underline{v}$$

then

$$\lim_{t-t_0 \rightarrow \infty} \lambda_k = e^{-E_k t}$$

For this to be practical, we need:

- a ‘good’ basis set that **resembles the states** of interest
- **all elements** of this correlation matrix measured

[see Blossier et.al. JHEP 0904 (2009) 094]

Fermions in the path integral

- In path integral, fermions are represented using **Grassmann** algebra.

$$\int d\eta = 0, \quad \int d\eta \eta = 1, \quad \eta^2 = 0$$

- Higher dimensions - anticommutation rule:

$$\eta_i \eta_j = -\eta_j \eta_i$$

- Expensive to manipulate directly by computer ...

Fermions in the path integral

- In QCD the action is (usually) bilinear.
- Consider computing a correlation function for the ρ -meson in 2-flavour QCD:

$$C_\rho(t_1, t_0) = \frac{\int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \bar{\psi}_u \gamma_i \psi_d(t_1) \bar{\psi}_d \gamma_i \psi_u(t_0) e^{-S_G[U] + \bar{\psi}_f M_f[U] \psi_f}}{\int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S_G[U] + \bar{\psi}_f M_f[U] \psi_f}}$$

- Integrate the grassmann fields analytically, giving:

$$C_\rho(t_1, t_0) = \frac{\int \mathcal{D}U \text{Tr} \gamma_i M_d^{-1}(t_1, t_0) \gamma_i M_u^{-1}(t_0, t_1) \det M^2[U] e^{-S_G[U]}}{\int \mathcal{D}U \det M^2[U] e^{-S_G[U]}}$$

- Fermions in lagrangian \rightarrow fermion determinant
- Fermions in measurement \rightarrow propagators

Fermions in the path integral

- With more insertions, need **Wick's theorem**
- Example — four field insertions:

$$\langle \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \rangle$$

- and the pairwise contraction can be done in two ways:

$$\psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \quad \text{and} \quad \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l$$

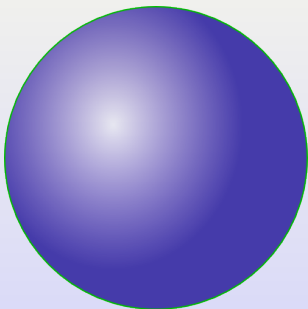
- ...giving the propagator combination

$$M_{ij}^{-1} M_{kl}^{-1} - M_{jk}^{-1} M_{il}^{-1}$$

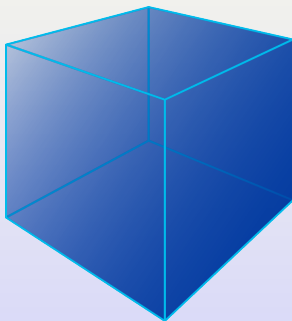
- the minus-sign comes from the anti-commutation needed in the second term.
- More fields means more combinations
- This is important in (eg.) isoscalar meson spectroscopy.

A tale of two symmetries

- Continuum: states classified by J^P irreducible representations of $O(3)$.



$O(3)$



O_h

- Lattice regulator breaks $O(3) \rightarrow O_h$
- Lattice: states classified by R^P “quantum letter” labelling irrep of O_h

Irreps of O_h

- O has 5 conjugacy classes (so O_h has 10)
- Number of conjugacy classes = number of irreps
- Schur: $24 = 1^2 + 1^2 + 2^2 + 3^2 + 3^2$
- These irreps are labelled A_1, A_2, E, T_1, T_2

	E	$8C_3$	$6C_2$	$6C_4$	$3C_2$
A_1	1	1	1	1	1
A_2	1	1	-1	-1	1
E	2	-1	0	0	2
T_1	3	0	-1	1	-1
T_2	3	0	1	-1	-1

Spin on the lattice

- O_h has 10 irreps: $\{A_1^{g,u}, A_2^{g,u}, E^{g,u}, T_1^{g,u}, T_2^{g,u}\}$, where $\{g, u\}$ label even/odd parity.
- Link to continuum: subduce representations of $O(3)$ into O_h

	A_1	A_2	E	T_1	T_2
$J = 0$	1				
$J = 1$				1	
$J = 2$			1		1
$J = 3$		1		1	1
$J = 4$	1		1	1	1
\vdots	\vdots	\vdots	\vdots	\vdots	\vdots

- Enough to search for degeneracy patterns in the spectrum?

$$4 \equiv 0 \oplus 1 \oplus 2$$

Operator basis – derivative construction

- A closer link to the continuum is needed
- Start with continuum operators, built from n derivatives:

$$\Phi = \bar{\psi} \Gamma (D_{i_1} D_{i_2} D_{i_3} \dots D_{i_n}) \psi$$

- Construct irreps of $SO(3)$, then subduce these representations to O_h
- Now replace the derivatives with lattice finite differences:

$$D_j \psi(\mathbf{x}) \rightarrow \frac{1}{a} \left(U_j(\mathbf{x}) \psi(\mathbf{x} + \hat{j}) - U_j^\dagger(\mathbf{x} - \hat{j}) \psi(\mathbf{x} - \hat{j}) \right)$$

Example: $J^{PC} = 2^{++}$ meson creation operator

- Need more information to discriminate spins. Consider continuum operator that creates a 2^{++} meson:

$$\Phi_{ij} = \bar{\psi} \left(\gamma_i D_j + \gamma_j D_i - \frac{2}{3} \delta_{ij} \gamma \cdot D \right) \psi$$

- Lattice: Substitute gauge-covariant lattice finite-difference D_{latt} for D
- A reducible representation:

$$\Phi^{T_2} = \{ \Phi_{12}, \Phi_{23}, \Phi_{31} \}$$

$$\Phi^E = \left\{ \frac{1}{\sqrt{2}} (\Phi_{11} - \Phi_{22}), \frac{1}{\sqrt{6}} (\Phi_{11} + \Phi_{22} - 2\Phi_{33}) \right\}$$

- Look for signature of continuum symmetry:

$$\langle 0 | \Phi^{(T_2)} | 2^{++(T_2)} \rangle = \langle 0 | \Phi^{(E)} | 2^{++(E)} \rangle$$

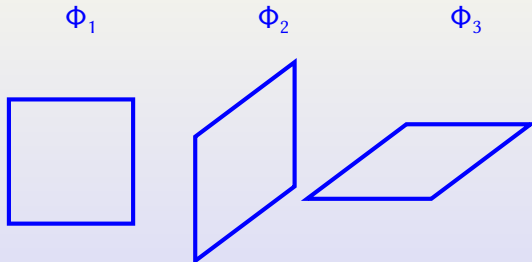
Glueballs

Creation operators: glueballs

- To measure the correlation functions, we need to measure appropriate creation operators on our ensemble.
- The operators should be functions of the fields on a time-slice and transform irreducibly according to an irrep of O_h (as well as isospin, charge conjugation etc.)
- First example: the glueball. An appropriate operator would be a gauge invariant function of the gluons alone: a closed loop trace.
- Link smearing greatly improved ground-state overlap.
- Apply smoothing filters to the links to extract just slowly varying modes that then have better overlap with the lowest states.

Creation operators: glueballs

- What do operators that transform irreducibly under O_h look like?

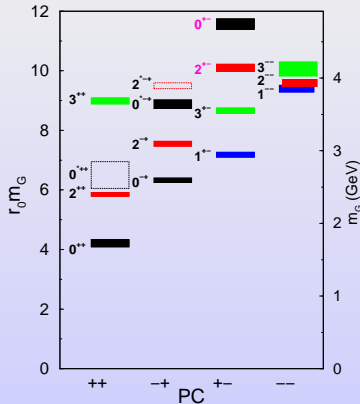
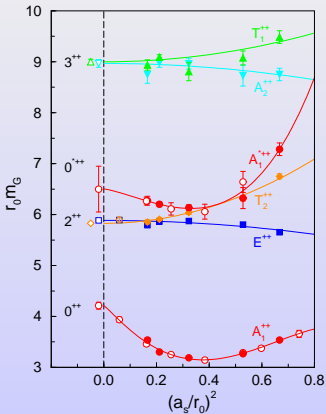


- Can make three operators by taking linear combinations of these loops.
- They form two irreducible representations (A_1^g and E_g).

$$\begin{array}{l} \Phi_{A_1^g} = \Phi_1 + \Phi_2 + \Phi_3 \\ \Phi_{E_g}^{(1)} = \Phi_1 - \Phi_2 \\ \Phi_{E_g}^{(2)} = \frac{1}{\sqrt{3}}(\Phi_1 + \Phi_2 - 2\Phi_3) \end{array}$$

Creation operators: glueballs

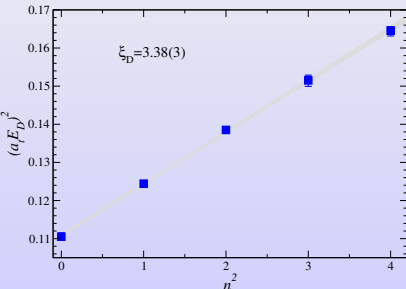
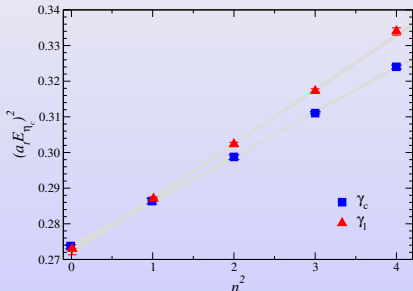
- After running simulations at more than one lattice spacing, a **continuum extrapolation** ($a \rightarrow 0$) can be attempted.
- The expansion of the action can suggest the appropriate choice of extrapolating function.



Charmonium and D/D_s

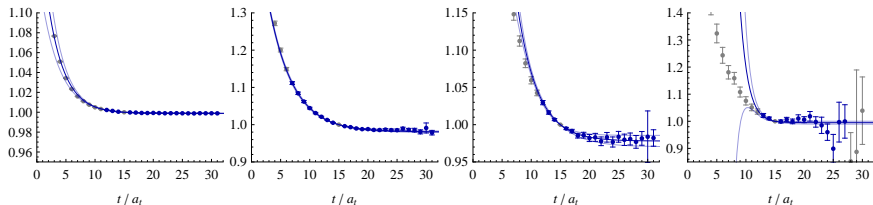
Dispersion relations - η_c and D mesons

- Action parameters for charm quark tuned to ensure dispersion relation for η_c is relativistic
- Using these tuned parameters, D meson also has relativistic dispersion relation



Fits to $\lambda_k(t)$

- Variational basis, so can access excited states
- Fit $\lambda_k(t)$ to one or two exponentials
- Second exponential to stabilise some fits - value not used
- Plots show $\lambda_k(t) \times e^{E_k(t-t_0)}$



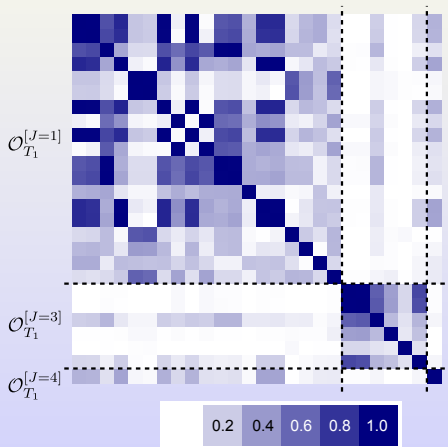
- Data from T_1^- channel ($J = 1, 3, 4, \dots$)

Subduction of derivative-based operators

- T_1^- variational basis
- 26 operators, up to $D_i D_j D_k$
- Correlation matrix at $t/a_t = 5$, $\mathcal{O}_{T_1}^{[J=1]}$ normalised:

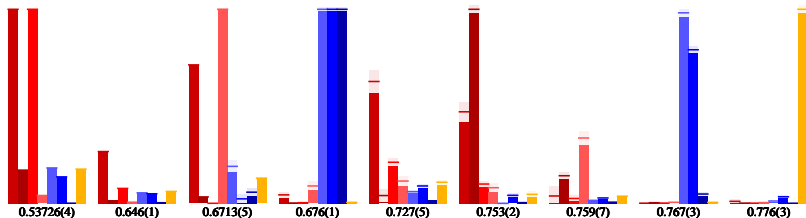
$$Q_{ij} = \frac{C_{ij}}{\sqrt{C_{ii}C_{jj}}}$$

- Reasonable **spin separation** seen



Spin identification

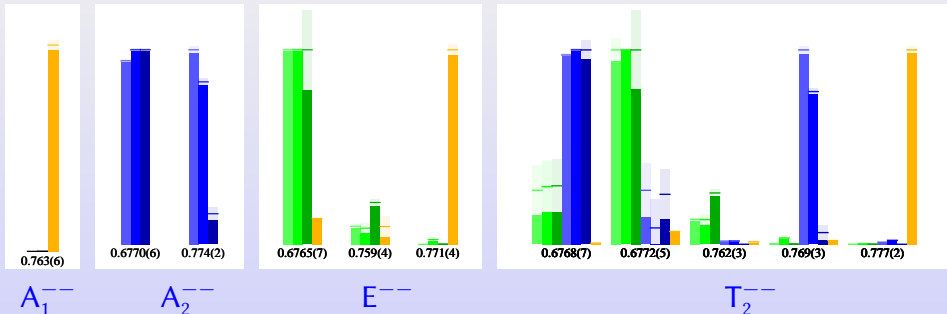
- Using $Z = \langle 0|\Phi|k\rangle$, helps to identify continuum spins
- For high spins, can look for agreement between irreps
- Data below for T_1^- irrep, colour-coding is **Spin 1**, **Spin 3** and **Spin 4**.



- Can help identify glue-rich states, using operators with $[D_i, D_j]$

... the rest of the spin-4 state

- All polarisations of the spin-4 state are seen
- Spin labelling: **Spin 2**, **Spin 3** and **Spin 4**.

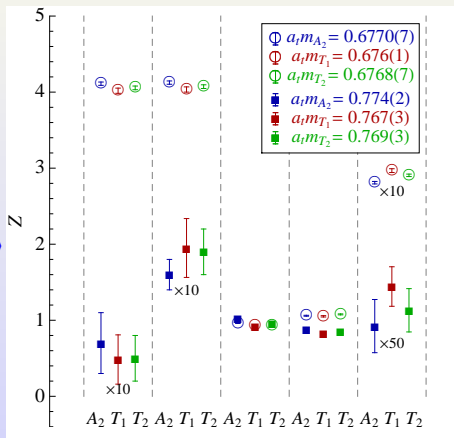


Identifying spin - operator overlaps

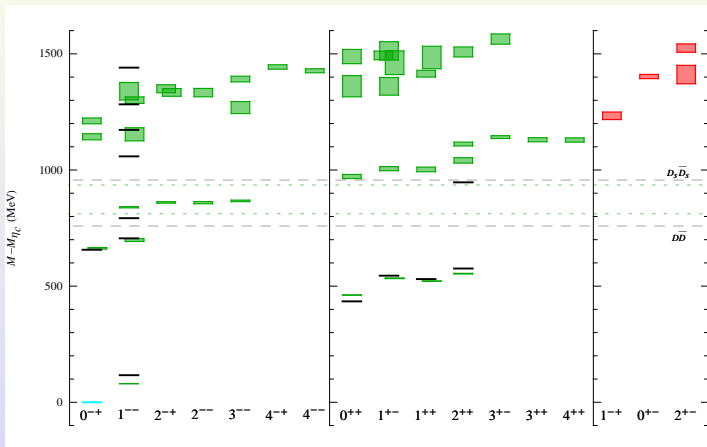
- Example — 3^{--} continuum
- Look for remnant of continuum symmetry:

$$\langle 0 | \Phi_{A_2^{--}}^{[J=3]} | k \rangle = \langle 0 | \Phi_{T_1^{--}}^{[J=3]} | k \rangle = \langle 0 | \Phi_{T_2^{--}}^{[J=3]} | k \rangle$$

- Can identify two spin-3 states.

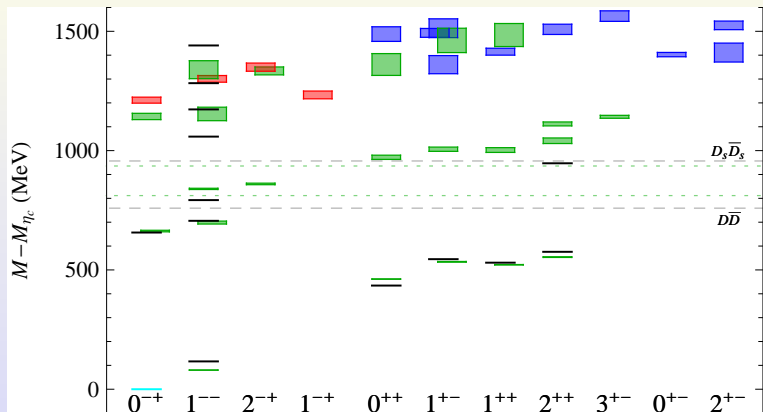


Excitation spectrum of charmonium



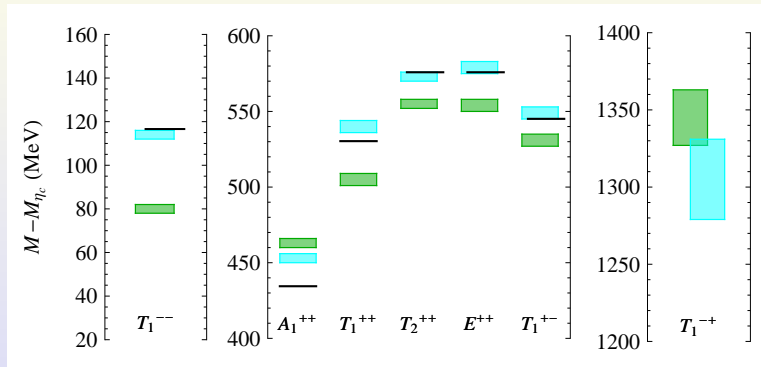
- Quark model: $1S, 1P, 2S, 1D, 2P, 1F, 2D, \dots$ all seen.
- Not all fit quark model: spin-exotic (and non-exotic) hybrids seen

Gluonic excitations in charmonium?



- See states created by operators that excite intrinsic gluons
- **two-** and **three-**derivatives create states in the open-charm region.

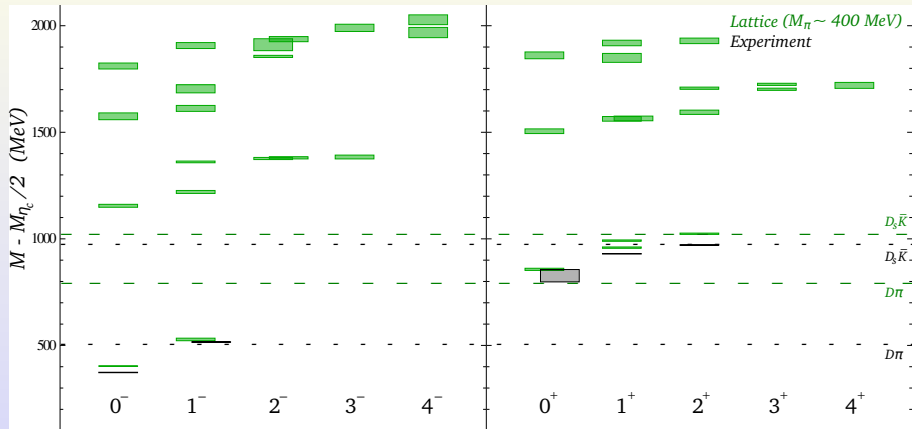
Lattice artefacts in charmonium



- Hyperfine structure sensitive to lattice artefacts. Boost co-efficient of action term to suppress these.
- green \rightarrow light blue. Shifts are ≈ 40 MeV.

[Liu et al. arXiv:1204.5425]

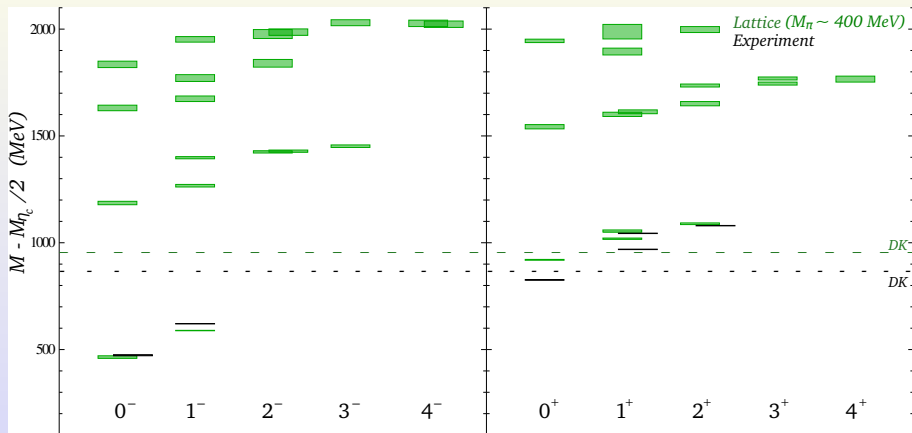
Excitation spectrum of D



- Subtract $\frac{1}{2}M_{\eta_c}$ to reduce systematic error
- Thresholds for both physical M_π and $M_\pi \approx 400$ MeV

[Moir et.al. JHEP 1305 (2013) 021]

Excitation spectrum of D_s

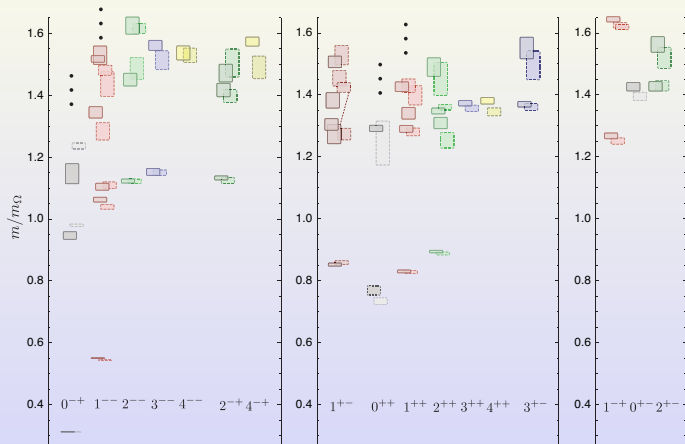


- Subtract $\frac{1}{2}M_{\eta_c}$ to reduce systematic error
- Thresholds for both physical M_π and $M_\pi \approx 400$ MeV

[Moir et.al. JHEP 1305 (2013) 021]

Light quark hadrons

Isvector meson spectroscopy

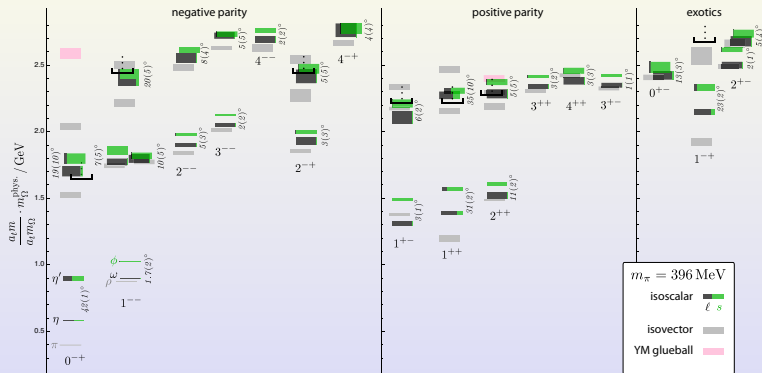


- $m_\pi = 400 \text{ MeV}$
- No 2-meson operators

- Spin-exotic states seen
- Non-exotic hybrids too?

[Dudek et.al. Phys.Rev.D82:034508,2010]

Isoscalar mesons



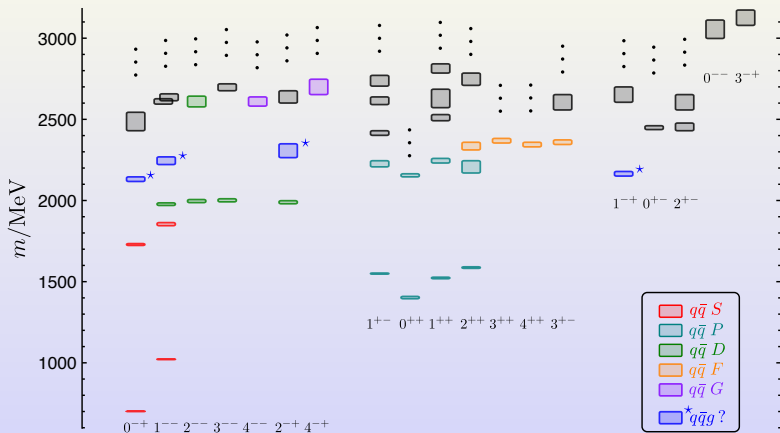
- $m_\pi = 400 \text{ MeV}$, finite a
- No 0^{++} data presented
- No glueball or two-meson operators

Statistical precision:

η 0.5 %

η' 1.9 %

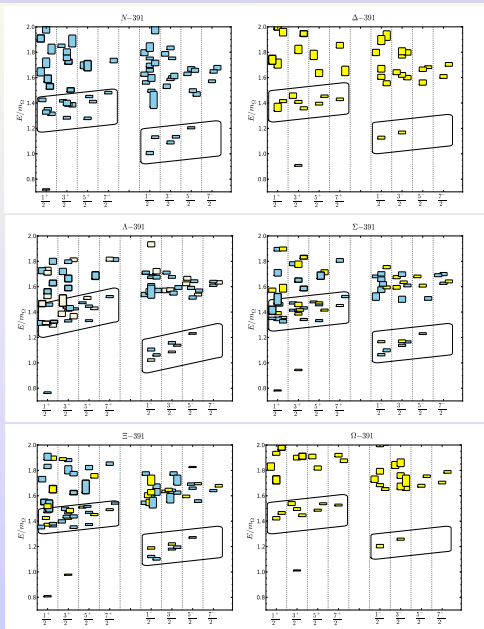
Hybrid excitations?



- $m_{\pi} = 700 \text{ MeV}$
- Complete hybrid supermultiplet seen

Light Baryon Spectra

- Baryon spectra using operators with $SU(3)_F$
- $m_\pi \approx 400$ MeV
- Blue - flavour octet
- Yellow - flavour decuplet
- White - flavour singlet
- Thick boxes - hybrid content



Scattering

Scattering matrix elements not directly accessible from Euclidean QFT [Maiani-Testa theorem]

- Scattering matrix elements: asymptotic $|\text{in}\rangle, |\text{out}\rangle$ states.
 $\langle \text{out} | e^{i\hat{H}t} | \text{in} \rangle \rightarrow \langle \text{out} | e^{-\hat{H}t} | \text{in} \rangle$
- Euclidean metric: project onto ground-state
- **Lüscher's formalism:** information on elastic scattering inferred from **volume dependence** of spectrum
- Requires precise data, resolution of two-hadron and excited states.



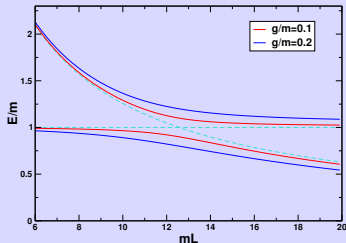
Hadrons in a finite box: scattering

- On a finite lattice with periodic b.c., hadrons have quantised momenta; $\underline{p} = \frac{2\pi}{L} \{n_x, n_y, n_z\}$
- Two hadrons with total $\mathbf{P} = \mathbf{0}$ have a discrete spectrum
- These states can have same quantum numbers as those created by $\bar{q}\Gamma q$ operators and QCD can mix these

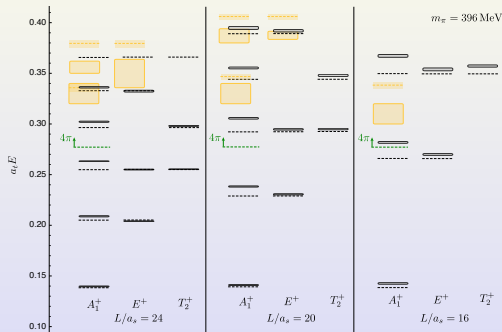
- This leads to shifts in the spectrum in finite volume
- This is the same physics that makes resonances in an experiment
- Lüscher's method - relate elastic scattering to energy shifts

Toy model

$$H = \begin{pmatrix} m & g \\ g & \frac{4\pi}{L} \end{pmatrix}$$



$l = 2$ $\pi - \pi$ phase shift

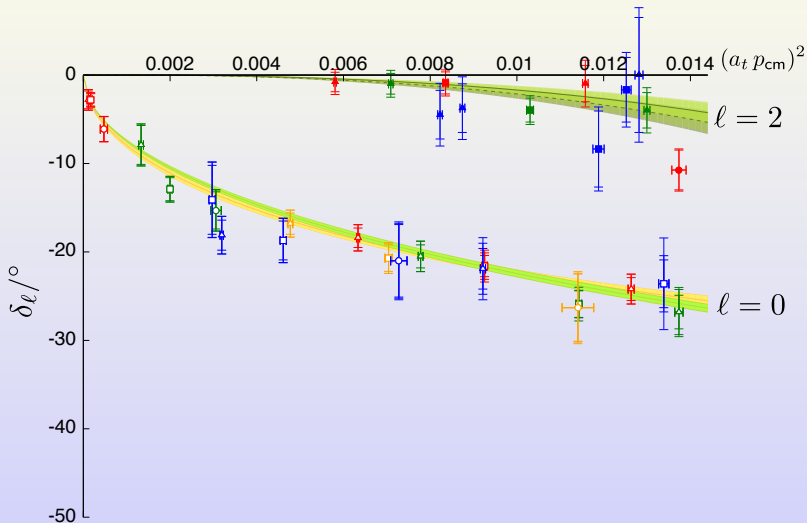


- Lüscher's method: first determine energy shifts as volume changes
- Data for $L = 16a_s, 20a_s, 24a_s$
- Small energy shifts are resolved

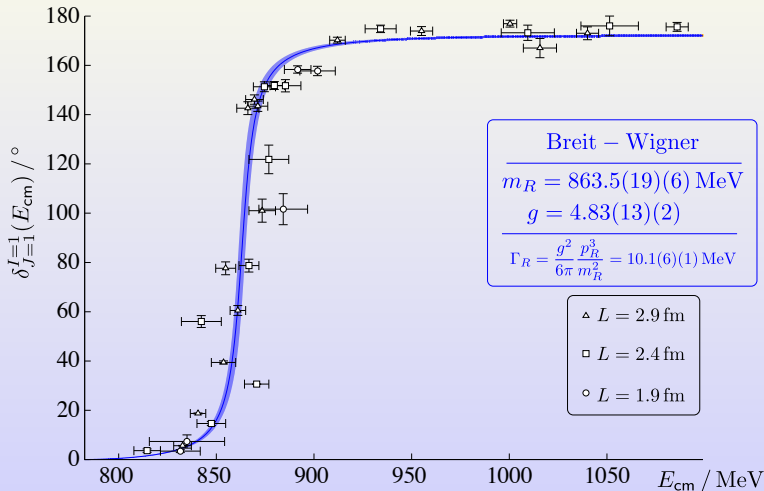
- Measured δ_0 and δ_2 (δ_4 is very small)
- $l = 2$ a useful first test - simplest Wick contractions

Dudek et.al. [Phys.Rev.D83:071504,2011, arXiv:1203.6041]

$l = 2 \quad \pi - \pi$ phase shift



$l = 1$ $\pi - \pi$ phase shift (near the ρ)



- The lattice provides a non-perturbative regularisation of the QCD path integral.
- Modern simulations include light quark dynamics close to the physical up and down mass.
- Excitation spectra can be computed using variational methods
- Scattering can not be directly computed - but can be inferred (below inelastic thresholds) using Lüscher's method.
- Inelastic scattering is a new field...
- Also: Matrix elements, distribution functions, production rates, ...