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# Introduction to QCD: basics

Sinéad M. Ryan Trinity College Dublin



#### PANDA Physics Winter School, GSI December 2017

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## OUTLINE OF THIS LECTURE

• Some introduction and background:

#### • QCD

- Theoretical details.
- Symmetries and conservation laws.
- Understanding the hadron spectrum: quark models and beyond.

#### • Summary

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# A roadmap to QCD

Motivated by the zoo of particles discovered in 1960s: p, n,  $\delta$ ,  $\Lambda$ ,  $\pi$ ,  $\rho$ , K,  $\phi$ , D, ... Led to postulate of **quarks** and **gluons**.



- Quarks and gluons carry colour: r,g,b [introduced to explain the  $\Delta^{++}$ ]
- Counting flavours and colours
  - Quarks carry indices for flavour, quark/antiquark, colour
  - Gluons carry colour

Three quarks for Muster Mark! Sure he hasn't got much of a bark ... [James Joyce's Finnegan's Wake]

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#### Colour: quarks

Motivated by discovery of the  $\Delta^{++}(1232)$  baryon. It's structure is  $|\Delta^{++}\rangle = |u^{\uparrow}u^{\uparrow}u^{\uparrow}\rangle$  and  $J^{P} = \frac{3}{2}^{+}$ .

Now, considering wavefunctions

$$\Psi(\Delta^{++}) = \underbrace{\Psi(r)}_{symmetric} \cdot \underbrace{\Psi_{spin}(J)}_{symmetric} \cdot \underbrace{\Psi_{flavour}}_{symmetric}$$

This contradicts the Pauli principle which demands the total wavefunction be antisymmetric.

Requires a new (and unobservable) quantum number - colour:

 $\Psi(\Delta^{++}) = \Psi(r) \cdot \Psi_{\rm spin}(J) \cdot \Psi_{\rm flavour} \cdot \Psi_{\rm colour}$ 

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### Colour: quarks

**Color Confinement Hypothesis** 

Only colour singlet states can exist as free particles.

- Colour is a conserved quantum number.
- Quark spinors in a colour triplet  $\Psi = \begin{pmatrix} \Psi_r \\ \Psi_g \\ \Psi_b \end{pmatrix}$  respecting SU(3) symmetry.
- And this also explains the absence of e.g. qq states, from group theory.
  - $3 \otimes 3 \otimes 3 \otimes 3 = 1 + 8 + 8 + 10$ : contains singlet
  - $3 \otimes \overline{3} = 1 + 8$ : contains singlet
  - $3 \otimes 3 = \overline{3} + 6$ : no singlet!
- Leptons and other gauge bosons don't carry colour charge don't participate in strong interaction.

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#### Colour: gluons

Gluons are massles, spin-1 bosons. Emission or absorption of gluons by quarks changes colour of quarks - color is conserved.



Naive counting:  $r\bar{b}$ ,  $r\bar{g}$ ,  $g\bar{b}$ ,  $g\bar{r}$ ,  $b\bar{r}$ ,  $b\bar{g}$ ,  $r\bar{r}$ ,  $b\bar{b}$ ,  $g\bar{g}$  ie 9.

And SU(3) symmetry

- octet:  $r\bar{b}$ ,  $r\bar{g}$ ,  $g\bar{b}$ ,  $g\bar{r}$ ,  $b\bar{r}$ ,  $b\bar{g}$ ,  $\frac{1}{\sqrt{2}}(r\bar{r}-g\bar{g})$ ,  $\frac{1}{\sqrt{6}}(r\bar{r}+g\bar{g}-2b\bar{b})$ . Realised in nature.
- singlet:  $\frac{1}{\sqrt{3}}(r\bar{r}+b\bar{b}+g\bar{g}).$
- No singlet gluon realised in nature. Why?

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#### COLOR FORCE AND QUARK POTENTIAL

2 quarks at distance  $r \sim O(1)$ fm) define a *string* of *tension* k, potential V(r) = kr. Stored energy/unit length is constant: separation of quarks requires infinite energy. **QCD Potential:** QED-like at  $r \leq 0.1$ fm but increases linearly at  $r \geq 1$ fm.



Force:  $\left|\frac{dV}{dr}\right| = k = 1.6 \times 10^{-10} \text{J}/10^{-15} \text{m} = 16000 \text{N}$  weight of a car!

This stored energy gives the proton most of its mass (and not the Higgs as you sometimes hear)! Recall  $m_u + m_d \sim 9$ MeV but  $m_{proton} = 938$ MeV

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# QUANTUM CHROMODYNAMICS (QCD)

The quantum field theory of the strong interaction that binds quarks and gluons to form hadrons.

1/2 Guy Guy + 5 \$; (18 m Du + m;) ;; where  $G_{\mu\nu}^{a} \equiv \partial_{\mu} \mathcal{A}_{\nu}^{a} - \partial_{\nu} \mathcal{A}_{\mu}^{a} + i f_{\mu}^{a} \mathcal{A}_{\mu}^{b} \mathcal{A}_{\nu}^{c}$ and  $D_{\mu} \equiv \partial_{\mu} + i t^{a} \mathcal{A}_{\mu}^{a}$ T hat's it !

• this doesn't look too bad - a bit like QED which we have a well-developed toolkit to deal with

from F.A. Wilczek

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QCD - THE THEORY OF THE STRONG INTERACTION

$$\mathcal{L}_{\text{QCD}} = -\frac{1}{4} F^{a}_{\mu\nu}(x) F^{a\,\mu\nu}(x) + \sum_{c=1}^{N_{c}} \sum_{f=1}^{N_{f}} \bar{\psi}_{c,f}(x) (i\gamma^{\mu} D_{\mu} - m_{f}) \psi(x)$$

#### The ingredients are:

Quark fields:  $\psi_{\alpha,c,f}(x)$ 

 $\alpha = 1, \dots, 4$  spinor index c = 1, 2, 3 colour index f = u, d, s, c, b, t flavour index

Field strength:

 $F^{a}_{\mu\nu} = \partial_{\mu}A^{a}_{\nu} - \partial_{\nu}A^{a}_{\mu} - gf_{abc}A^{b}_{\mu}A^{c}_{\nu}$ 

Covariant derivatives:

 $D_{\mu} = \partial_{\mu} - igT^{q}A^{a}_{\mu}(x)$ 

Parameters:

coupling,  $\alpha_s$  and quark masses,  $m_f$ .

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### CONSERVATION: QUARKS

- Relative Charge: quarks and anti-quarks carry fractional charge. Charge is conserved in all interactions
- Baryon Number: quarks have baryon number  $+\frac{1}{3}$  and anti-quarks  $-\frac{1}{3}$ . Baryon number is conserved in all interactions.
- Strangeness:  $s = -(n_s \bar{n}_s)$ . Quarks and anti-quarks have strangeness = 0 except for the strange quark (strangeness = -1) and anti-strange (strangeness=+1). In all strong (and EM) interactions strangeness is conserved. In weak interactions strangeness *may* be conserved or may *change* by  $\pm 1$ .

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# Symmetries

SU(2) and SU(3) play an important role in particle physics

Hadron symmetries that play a key role are:

- Chiral symmetry
- Approximate SU(3) uds flavour symmetry
- SU(2) and SU(3) colour symmetry
- SU(2) isospin symmetry:

Experimentally the strong interaction is isospin invariant, so e.g. I=1 meson cannot decay to states with total I=0. Note, em interaction is not isospin invariant. Combined with charge conjugation – G-parity

• Parity:

Experimentally strong interaction is parity invariant, once an intrinsic parity is assigned to hadrons.  $\mathcal{P}|p\rangle = +|p\rangle; \mathcal{P}|\pi\rangle = -|\pi\rangle$ 

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Hadrons, eg mesons labelled by the strong-interaction conserving quantum numbers:  $I^{G}I^{PC}$ .

States fall into 2 categories

- fermionic baryons with  $J = \frac{1}{2}, \frac{3}{2}, \ldots$
- bosonic mesons with  $J = 0, 1, 2, \ldots$

Was used to explain the observed hadrons and successfully predict others. Define the allowed states of **QCD** :

- *qq* mesons; *qqq* baryons
- qqqqq, qqqqq Exotic states e.g. pentaquarks

*Exercise: use the SU(3) colour symmetry to explain e.g. why only*  $q\bar{q}$  *mesons and not* qq *are allowed; and why*  $qqq(\bar{q}\bar{q}\bar{q})$  *baryons (antibaryons) allowed and not*  $qq\bar{q}$ .

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# QED AND QCD BY FEYNMAN DIAGRAMS

#### The fundamental vertices are the analogous:



charge leading to



#### probing small distance scales (x) $\rightarrow$



- QED: *α* varies with distance ie runs and the bare *e*<sup>-</sup> is screened, reducing *α*
- QCD: screening as in QED but gluon loops create same-charge gluonic cloud and antiscreening dominates!
  - *α<sub>s</sub>* ~ 1 at hadronic scales, perturbation theory fails.

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# VACUUM POLARISATION IN QCD (AND QED)



- Vacuum polarisation diagrams in QED have QCD analogues
- In QCD there are additional vacuum polarisation diagrams arising from gluon loops
- Quark loops lead to screening as in QED. The gluon loops lead to anti-screening.
- Net effect is the strong coupling is large at long distance, small at short distance



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#### RENORMALISATION AND QCD

$$\sim \int \frac{d^4k}{(2\pi)^4} \frac{(p_2\mu + k_\mu)\gamma^\mu + m}{p_2^2 + 2p_2k + k^2 - m^2} \frac{(p_1\mu - k_\mu)\gamma^\mu + m}{p_1^2 - 2p_1k + k^2 - m^2}$$

- Calculations beyond tree-level incur UV-divergent integrals over loop momenta
- $\bullet\,$  Cured by regularisation, imposing a cutoff  $\Lambda\,$
- Physical meaning assigned to renormalised quantities:  $m^0 = Z_m m$  with  $Z_M(\Lambda/\mu)$
- Dimensional transmutation a dimensionful parameter in  $\mathcal{L}$  after renormalisation

$$\stackrel{k \to \infty}{\longrightarrow} \int d^4k \frac{k^2}{k^6} \sim \ln(k) \to \infty$$

$$\int^{\Lambda} d^4k \frac{k^2}{k^6} \sim \ln \Lambda$$

$$\alpha_s^{\text{bare}} = Z_i \left(\frac{\Lambda}{\mu}\right) \alpha_s \left(\frac{\mu}{\Lambda_{\text{QCD}}}\right)$$

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# QCD: MAKING CALCULATIONS

#### Deep inside the proton

- at short distances quarks behave as free particles
- weak coupling

Perturbation theory appropriate.

#### At "observable" distances

- at long distance (1fm) quarks confined
- strong coupling

Perturbation theory fails: nonperturbative approach needed.



+ Effects due to the complicated QCD vacuum

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#### The secret life of hadrons



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### A CONSTITUENT MODEL

- Understan QCD in terms of fundamental objects: quarks (in 6 flavours) and gluons
- Fields of the lagrangian are combined in colorless combinations: the mesons and baryons. Confinement.

quark model object	structure
meson	$3 \otimes \overline{3} = 1 \oplus 8$
baryon	$3 \otimes 3 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 10$
hybrid	$\overline{3} \otimes 8 \otimes 3 = 1 \oplus 8 \oplus 8 \oplus 8 \oplus 10 \oplus 10$
glueball	8 <b>8</b> 8 = 1 <b>9</b> 8 <b>9</b> 8 <b>9</b> 10 <b>9</b> 10
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• This is a model. QCD does not always respect this constituent picture! There can be strong mixing.

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### HADRON TAXONOMY

- Recall that states are classified by J<sup>PC</sup> multiplets (representations of the Poincaré symmetry)
- Recall the naming scheme:  $n^{2S+1}L_J$  with  $S = \{0, 1\}$  and  $L = \{0, 1, ...\}$
- Angular Momentum:  $|L S| \le J \le |L + S|$
- Parity:  $P = (-1)^{(L+1)}$
- Charge Conjugation:  $C = (-1)^{(L+S)}$ . Only for  $q\bar{q}$  states of same quark and antiquark flavour. So, not a good quantum number for e.g. heavy-light mesons  $(D_{(s)}, B_{(s)})$ .

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# Mesons

- Two spin-half fermions: <sup>25+1</sup>LJ
- S = 0 for antiparallel quark spins and S = 1 for parallel quark spins;
- *G*-parity =  $(-1)^{l+L+S}$  also for charged states eg  $u\bar{d}$ .



- Natural spin-parity series:  $P = (-1)^J$  so S = 1 and CP = +1:
  - $J^{PC} = 0^{-+}, 0^{++}, 1^{--}, 1^{+-}, 2^{--}, 2^{-+}, \dots$  allowed.
- States with  $P = (-1)^{j}$  but CP = -1 forbidden by rules of the  $q\bar{q}$  model of mesons. Allowed by QCD!
  - $J^{PC} = 0^{+-}, 0^{--}, 1^{-+}, 2^{+-}, 3^{-+}, \dots$  forbidden.

These are **EXOTIC** states: not just a  $q\bar{q}$  pair ...

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# Baryons

Baryon number B = 1: three quarks in colourless combination

- J is half-integer, C not a good quantum number: states classified by  $J^P$
- spin-statistics: a baryon wavefunction must be antisymmetric under exchange of any 2 quarks.
- totally antisymmetric combinations of the colour indices of 3 quarks
- the remaining labels: flavour, spin and spatial structure must be in totally symmetric combinations

 $|qqq\rangle_A = |color\rangle_A \times |space, spin, flavour\rangle_S$ 

With three flavours, the decomposition in flavour is

 $3 \otimes 3 \otimes 3 = 10_S \oplus 8_M \oplus 8_M \oplus 1_A$ 

#### Many more states predicted than observed: missing resonance problem

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### Exercise

Verify the following statements, using the quark model

- Baryons won't have spin 1
- What is the quark combination of an antibaryon of electric charge +2
- Why are mesons with charge +1 and strangeness -1 not possible?

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### BEYOND QUARK MODELS

• Hugely successful - predictions verified by experiment and a useful phenomenological picture.





Predicted  $m_{\Omega} \sim 1670 \text{MeV}$ ; Experiment  $m_{\Omega} = 1672.45 \pm 0.29 \text{MeV}$ 

Describes ground states.

- Ultimately not the fully picture and cannot accommodate exotics; explain XYZs etc
- Ab initio methods better.

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### Summary so far

#### • Considered some fundamentals of QCD including:

- Color charge and confinement
- Asymptotic freedom and the running coupling
- QCD renormalisation and perturbation theory
- Quark models and some motivation to go beyond.
- Next: focus on nonperturbative methods

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Verify/discuss the following statements, using the quark model

- Baryons won't have spin 1.
- What is the quark combination in an antibaryon of electruc charge +2?
- Why are mesons with charge +1 and strangeness -1 not possible?

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Verify/discuss the following statements, using the quark model

- Baryons won't have spin 1.
- What is the quark combination in an antibaryon of electruc charge +2?
- Why are mesons with charge +1 and strangeness -1 not possible?
- A baryon consists of 3 quarks. Since the spin of each is 1/2, they cannot combine to form a baryon of spin 1.
- An antibaryon comprises 3 antiquarks. To combine 3 antiquarks to make a baryon of charge +2 you need antiquarks of electric charge +2/3.
- A meson consists of a quark and an antiquark. Only the strange quark as non-zero strangeness so to form a meson of strangeness -1 and electric charge 1 you would need an a strange quark and an antiquark of electric charge 4/3.

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## Exercise

Use the SU(3) colour symmetry to explain e.g. why only  $q\bar{q}$  mesons and not qq are allowed; and why  $qqq(\bar{q}\bar{q}\bar{q})$  baryons (antibaryons) allowed and not  $qq\bar{q}$ .

\* Represent r, g, b SU(3) colour states by:  $r = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}; g = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; b = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ 

- \* Colour states can be labelled by two quantum numbers:
  - $I_3^c$  colour isospin
  - Y<sup>c</sup> colour hypercharge

Exactly analogous to labelling u,d,s flavour states by  $I_3$  and Y

\* Each quark (anti-quark) can have the following colour quantum numbers:



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Use the SU(3) colour symmetry to explain e.g. why only  $q\bar{q}$  mesons and not qq are allowed; and why  $qqq(\bar{q}\bar{q}\bar{q})$  baryons (antibaryons) allowed and not  $qq\bar{q}$ .

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Use the SU(3) colour symmetry to explain e.g. why only  $q\bar{q}$  mesons and not qq are allowed; and why  $qqq(\bar{q}\bar{q}\bar{q})$  baryons (antibaryons) allowed and not  $qq\bar{q}$ .

### **Meson Colour Wave-function**

- **★** Consider colour wave-functions for  $q\overline{q}$
- The combination of colour with anti-colour is mathematically identical to construction of meson wave-functions with uds flavour symmetry



 Colour confinement implies that hadrons only exist in colour singlet states so the colour wave-function for mesons is:

$$\boldsymbol{\psi}_{c}^{q\overline{q}} = \frac{1}{\sqrt{3}} (r\overline{r} + g\overline{g} + b\overline{b})$$

★ Can we have a  $qq\bar{q}$  state ? i.e. by adding a quark to the above octet can we form a state with  $Y^c = 0$ ;  $I_3^c = 0$ . The answer is clear no.

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1. There are 3 colours: red, green, blue; and 3 anti-colours: antired, antigreen, antiblue. Naively then one could expect 9 gluons. Discuss why there are in fact only 8.

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#### **EXERCISES AND DISCUSSION**

1. There are 3 colours: red, green, blue; and 3 anti-colours: antired, antigreen, antiblue. Naively then one could expect 9 gluons. Discuss why there are in fact only 8.

The 9 combinations one might expect are:  $r\bar{b}$ ,  $r\bar{g}$ ,  $g\bar{b}$ ,  $g\bar{r}$ ,  $b\bar{r}$ ,  $b\bar{g}$ ,  $r\bar{r}$ ,  $b\bar{b}$ ,  $g\bar{g}$ 8 gluons are realised in nature (in a colour octet) as  $r\bar{b}$ ,  $r\bar{g}$ ,  $g\bar{b}$ ,  $g\bar{r}$ ,  $b\bar{r}$ ,  $b\bar{g}$ ,  $\frac{1}{\sqrt{2}}(r\bar{r} - g\bar{g})$ ,  $\frac{1}{\sqrt{6}}(r\bar{r} + g\bar{g} - 2b\bar{b}$ .

A colour singlet gluon would be unconfined (colour confinement hypothesis) and would behave as a strongly-interacting photon, implying an infinite range strong force! Empirically, the strong force is short range so the singlet state not allowed.

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Symmetries: isopin and light quarks, as an example

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#### Symmetries: isopin and light quarks, as an example

Consider  $\psi(x) = \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix}$  and the symmetry transformations acting on the fields

$$\begin{aligned} \psi' &= U\psi, \ U \in SU(2), \ UU^{\dagger} = 1\\ \bar{\psi}' &= \psi'^{\dagger}\gamma^{0} = \psi^{\dagger}U^{\dagger}\gamma^{0} = \psi^{\dagger}\gamma_{0}U^{\dagger}\end{aligned}$$

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#### Symmetries: isopin and light quarks, as an example

Consider  $\psi(x) = \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix}$  and the symmetry transformations acting on the fields

$$\begin{aligned} \boldsymbol{\psi}' &= \boldsymbol{U}\boldsymbol{\psi}, \ \boldsymbol{U} \in SU(2), \ \boldsymbol{U}\boldsymbol{U}^{\dagger} = 1\\ \boldsymbol{\bar{\psi}}' &= \boldsymbol{\psi}'^{\dagger}\boldsymbol{\gamma}^{0} = \boldsymbol{\psi}^{\dagger}\boldsymbol{U}^{\dagger}\boldsymbol{\gamma}^{0} = \boldsymbol{\psi}^{\dagger}\boldsymbol{\gamma}_{0}\boldsymbol{U}^{\dagger} \end{aligned}$$

Now, if  $m_u = m_d$
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### Exercises and discussion

#### Symmetries: isopin and light quarks, as an example

Consider  $\psi(x) = \begin{pmatrix} \psi_u \\ \psi_d \end{pmatrix}$  and the symmetry transformations acting on the fields

$$\begin{aligned} \boldsymbol{\psi}' &= \boldsymbol{U}\boldsymbol{\psi}, \ \boldsymbol{U} \in SU(2), \ \boldsymbol{U}\boldsymbol{U}^{\dagger} = 1\\ \bar{\boldsymbol{\psi}}' &= \boldsymbol{\psi}'^{\dagger}\boldsymbol{\gamma}^{0} = \boldsymbol{\psi}^{\dagger}\boldsymbol{U}^{\dagger}\boldsymbol{\gamma}^{0} = \boldsymbol{\psi}^{\dagger}\boldsymbol{\gamma}_{0}\boldsymbol{U}^{\dagger} \end{aligned}$$

Now, if  $m_u = m_d$ 

$$\bar{\psi}'(i\gamma^{\mu}D_{\mu}-m)\psi'=\bar{\psi}U^{\dagger}(i\gamma^{\mu}D_{\mu}-m)U\psi=\bar{\psi}(i\gamma^{\mu}d_{\mu}-m)U^{\dagger}U\psi.$$

For non-degenerate quark masses this does not work!

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## Introduction to QCD: methods for hadronic physics

Sinéad M. Ryan Trinity College Dublin



#### PANDA Physics Winter School, GSI December 2017

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## Outline

We've discussed QCD as the theoretical framework for the strong interaction, including comparison to QED and it's characteristic features.

#### Now:

- Understanding hadronic physics using nonperturbative approaches.
- Potential model.
- EFT see Christoph's lectures.
- Lattice QCD I'll spend most time here.
- Some results and challenges.
- Summary.

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## POTENTIAL MODELS



Many models exist, most have a similar set of ingredients:

The (confining) potl assumed from phenomenological arguments and might be extracted from data or a lattice.

A useful approach, albeit with limitations. Especially effective for understanding particular regimes (e.g. quarkonia) or states (e.g. XYZ)



#### Keep in mind

Relies on an assumed potential. There are many choices and some discrimination is needed. Not a systematic approach to full QCD

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### PREDICTIONS: QUARKONIA

c, b and t quarks are non-relativistic: solve Schrödinger equation with a potential



- Bottomonium below threshold reproduced
- Similarly charmonium
- Above threshold, explaining narrow XYZ difficult

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## EFT SUMMARY

- The basic ideas underpinning EFTs: separate physics at different scales; identify approprite degrees of freedom
- Implement the consequences of symmetries
- EFT allows you to compute using dimensional analysis even if the underlying theory is unknown
- EFT a powerful tool for probing **QCD** and hadron spectroscopy

#### Keep in mind ...

- in some cases the full theory (QCD) cannot be formally recovered i.e. the EFT is nonrenormalisable e.g. lattice NRQCD.
- the effective theory is a good description of some regime in **QCD** of interest but cannot predict/describe beyond that.
- accuracy/precision physics needs a robust expansion as well as a reliable estimate of systematic uncertainties.

## HQET AND CHPT

Exploit the symmetries of **QCD** and existing hierarchies of scales to write down effective lagrangians that are appropriate for the problem at hand.

- Using hadronic degrees of freedom:
  - Chiral perturbation theory, an EFT for light hadrons. Expansion parameter is the pion energy/momentum.
- Using quark and gluon degrees of freedom:
  - HQET an EFT for hadrons with 1 heavy quark. Expansion in powers of the quark mass. Spin and flavour symmetries emerge.
  - NRQCD an EFT for hadrons with 2 heavy quarks. Expansion in relative velocity of the heavy quarks.
- many others ... and effective theories can be a useful tool in combination with other methods e.g. LQCD

Lattice QCD: an overview for hadron spectroscopy

## Why Lattice **QCD**?

- A systematically-improvable non-perturbative formulation of QCD
  - Well-defined theory with the lattice a UV regulator
- Arbitrary precision is in principle possible
  - of course algorithmic and field-theoretic "wrinkles" can make this challenging!
- Starts from first principles i.e. from the QCD Lagrangian
  - inputs are quark mass(es) and the coupling can explore mass dependence and coupling dependence but getting to physical values can be hard!

### A typical road map:

- Develop methods and verify calculations through precision comparison with lattice and with experiment.
- Make predictions subsequently verified experimentally.
- Make robust, precise calculations of quantities not accessible to experiment.

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## A potted history

- 1974 Lattice QCD formulated by K.G. Wilson
- 1980 Numerical Monte Carlo calculations by M. Creutz
- **1989** "and extraordinary increase in computing power (10<sup>8</sup> is I think not enough) and equally powerful algorithmic advances will be necessary before a full interaction with experiment takes place." Wilson @ Lattice Conference in Capri.
- Now at 100TFlops 1PFlop
- Lattice QCD also contributing to development of computing QCDSP QCDOC BlueGene.



Learning from history ... better computers help but better ideaas are crucial! that's what we will focus on ...

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## A LATTICE **QCD** PRIMER

Start from the QCD Lagrangian:

$$\mathcal{L} = \bar{\psi} \left( i \gamma^{\mu} D_{\mu} - m \right) \psi - \frac{1}{4} G^{a}_{\mu\nu} G^{\mu\nu}_{a}$$

- Gluon fields are SU(3) matrices links of a hypercube.  $A\mu(x) \rightarrow U(x, \mu) = e^{-iagA^b_{\mu}(x)t^b}$
- Quark fields  $\psi(x)$  on sites with color, flavor, Dirac indices. Fermion discretisation - Wilson, Staggered, Overlap.
- Derivatives  $\rightarrow$  finite differences:  $\nabla_{\mu}^{\text{fwd}}\psi(x) = \frac{1}{a} \left[ U_{\mu}(x)\psi(x+a\hat{\mu}) - \psi(x) \right]$



Solve the QCD path integral on a finite lattice with spacing  $a \neq 0$  estimated stochastically by Monte Carlo. Can only be done effectively in a Euclidean space-time metric (no useful importance sampling weight for the theory in Minkowski space). Observables determined from (Euclidean) path integrals of the QCD action

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

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## Correlators in Lattice Euclidean Field Theory: I

 $\bullet\,$  Physical observables  ${\cal O}$  are determined from

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D} U \mathcal{D} \Psi \mathcal{D} \bar{\Psi} \mathcal{O} e^{-S_{QCD}}$$

- Analytically integrate Grassman fields  $(\Psi, \bar{\Psi}) \langle \mathcal{O} \rangle \stackrel{N_f=2}{=} \frac{1}{Z} \int \mathcal{D}U \det M^2 \mathcal{O}e^{-S_G}$ Calculated by importance sampling of gauge fields and averaging over ensembles.
- Simulate N<sub>cfg</sub> samples of the field configuration, then

$$\langle \mathcal{O} \rangle = \lim_{N_{cfg} \to \infty} \frac{1}{N_{cfg}} \sum_{i=1}^{N_{cfg}} \mathcal{O}_i[U_i]$$

- Correlation functions have improvable(!) statistically uncertainty ~  $1/\sqrt{N_{cfg}}$ .
- Calculating det *M* for *M* a large, sparse matrix with small eigenvalues takes > 80% of compute cycles in configuration generation. det *M* = 1 is the quenched approximation.
- $(\mathcal{O})$  brings  $M^{-1}$  via contractions of quark fields. Second computational overhead.
- Fermions in lagrangian: sea quarks → fermion determinant. Fermions in measurement: valence quarks → propagators

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## A RECIPE FOR ( MESON) SPECTROSCOPY

- Construct a basis of local and non-local operators  $\overline{\Psi}(x)\Gamma D_i D_j \dots \Psi(x)$  from distilled fields [PRD80 (2009) 054506].
- Build a correlation matrix of two-point functions

$$C_{ij} = \langle 0 | \mathcal{O}_i \mathcal{O}_j^{\dagger} | 0 \rangle = \sum_n \frac{Z_i^n Z_j^{n\dagger}}{2E_n} e^{-E_n t}$$

- Ground state mass from fits to  $e^{-E_n t}$
- Beyond ground state: Solve generalised eigenvalue problem  $C_{ij}(t)v_j^{(n)} = \lambda^{(n)}(t)C_{ij}(t_0)v_j^{(n)}$
- eigenvalues:  $\lambda^{(n)}(t) \sim e^{-E_n t} \left[1 + O(e^{-\Delta E t})\right]$  principal correlator
- eigenvectors: related to overlaps  $Z_i^{(n)} = \sqrt{2E_n} e^{E_n t_0/2} v_j^{(n)\dagger} C_{ji}(t_0)$

## **Lattice Calculations**

Compromises and the Consequences not an exhaustive list

#### 1. Working in a finite box at finite grid spacing

- Identify a "scaling window" where physics doesn't change/changes weakly with *a* or *V*. Recover continuum **QCD** by extrapolation.
- Lattice spacing small enough to resolve structures induced by strong dynamics
- Volume large enough to contain lightest particle in spectrum: mπL ≥ 2π



A costly procedure but a regular feature in lattice calculations now

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#### 2. Simulating at physical quark masses: light quarks

- Light quarks in gauge generation through fermion determinant *M*.
- Computational cost grows rapidly with decreasing quark mass → mq = mu, d costly.
- Many improvements over the years for all fermion discretisations
- The wall has come down Physical point can be reached!
- Still costly and intricate for resonance physics.



#### 2001 - a Berlin wall

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#### 2. Simulating at physical quark masses: heavy quarks

- Discretisation errors grow as  $\mathcal{O}(am_q)$ : large for reasonable *a* and heavy quarks
- Bottom quarks treated with Effective Field Theories NRQCD, Fermilab etc
  - Continuum limits and EFTs can be tricky not always possible e.g. with NRQCD
  - Controlling systematics important for precision CKM physics
- Charm quarks can be handled relativistically
  - Anisotropic lattices useful here:  $a_s \neq a_t$  and  $a_t m_c < 1$ .

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Better algorithms for physical light quarks and/or chiral extrapolation. Relativistic  $m_b$  is in reach.



Turn a weakness into a strength by using lattice simulations to study *quark mass dependence*!

#### 3. Breaking symmetry



- Almost all symmetries of QCD are preserved. But Lorentz symmetry broken at *a* ≠ 0 so SO(4) rotation group broken to discrete rotation group of a hypercube.
- Angular momentum and parity  $J^{P}$  correspond to irreducible representations of the rotation group O(3).
- A spatially isotropic lattice breaks  $O(3) \rightarrow O_h$ , the cubic point group.
- Eigenstates of the lattice  $\mathcal{H}$  transform under irreps of  $O_h$  so states are classified by these irreps and not by  $J^P$ .
- Classify states by irreps of  $O_h$  and relate by subduction to J values of O(3).
- 5 irreps of O(3) and an infinite number for  $J^P$  so values are distributed across lattice irreps.
- Lots of degeneracies in subduction for  $J \ge 2$  and physical near-degeneracies. Complicates spin identification.

#### 4. Working in Euclidean time





- Scattering matrix elements not directly accessible from Euclidean QFT [Maiani-Testa theorem].
- Scattering matrix elements: asymptotic |in⟩, |out⟩ states: (out|e<sup>iĤt</sup>|in) → (out|e<sup>-Ĥt</sup>|in).
- Euclidean metric: project onto ground state.
- **Benefit:** can isolate lightest states in the spectrum (as we will see!). But to access radial and orbital excitations need additional ideas.
- Problem: direct information on scattering is lost and must be inferred indirectly.

**Scattering:** Lüscher method and generalisations give indirect access [later]. **Excited states:** use a variational method [C.Michael and I. Teasdale NPB215 (1983) 433, M. Lüscher and U. Wolff NPB339 (1990) 222]

#### 5. Setting the scale

Lattice quantities are computed in lattice units e.g.  $am_N$ . and converted to physical units to compare to experiment/make predictions e.g. masses and form factors.

Choose an observable O that is relatively easy to calculate and insensitive to e.g. up and down quark masses (which may not be correct in the simulation) and match to its experimental value to determine *a*. This quantity is no longer a prediction!

Many reasonable choices and discretisation errors mean there is some uncertainty from this procedure.

### 6. Quenching

- A computational expedient to set  $\det M = 1$  in gauge configuration generation.
- Rarely necessary now, results in a non-unitary theory so not a good approximation of nature.
- Sometimes useful for investigating new methods.

No longer an issue: Simulations with  $N_f = 2, 2 + 1, 2 + 1 + 1$ .

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## RECENT RESULTS: LATTICE CHARMONIUM SPECTROSCOPY



from the Hadron Spectrum Collaboration, 2012

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### **Resonances and scattering states**

- We have assumed that all states in the spectrum are stable
- Many (the majority) are not.
- A resonance is a state that forms e.g. when colliding two particles and then decays quickly to scattering states.
- These states respect conservation laws e.g. if isospin of the colliding particles is 3/2, resonance must have isospin 3/2 (△ resonance)
- Usually indicated by a sharp peak in a cross section as a function of c.o.m. energy of the collision.

#### How can lattice QCD identify resonances and scattering states?

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### **EXCITED HADRONS ARE RESONANCES**

#### Resonant phase shift



from Protopopescu et al (1972)



Resonances are pole singularites in complex  $s = E^2$ 



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### MAIANI-TESTA NO-GO THEOREM



- Monte-carlo simulations via importance sampling rely on a path integral with positive definite probability measure: Euclidean space.
- Maiani-Testa: scattering matrix (S-matrix) elements cannot be extracted from infinite-volume Euclidean-space correlation functions (except at threshold).
  - Minkowski space: S-matrix elements complex functions above kinematic thresholds.
  - Euclidean space: S-matrix elements are real for all kinematics phase information lost.

Michael 1989 and Maiani, Testa (1990)

## MAIANI-TESTA (2)

Can the lattice get around the no-go theorem to extract the masses and widths of such unstable particles? Yes - **use** the finite volume. Computations done in a periodic box

- momenta quantised
- discrete energy spectrum of stationary states → single hadron, 2 hadron ...
- scattering phase shifts → resonance masses, widths deduced from finite-box spectrum
- Two-particle states and resonances identified by examining the behaviour of energies in finite volume



#### For elastic two-body resonances (Lüscher): $\pi\pi \rightarrow \pi\pi$ scattering from LQCD

Discrete energy spectrum → Phase shift in infinite volume → Mass and width of resonance - parameterising the phase shift e.g. with Breit Wigner.

• Recent lectures on the physics of two particles in a box - covered by Lang and Detmold at TUM2017 Summer School and other refs (at the end).

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## Brief overview of Lüscher's formalism

**Finite Volume** Extract a discrete tower of energy levels

 $E_n(L, \vec{P})$ 

depends on the volume (L) and total momentum

Infinite Volume Decompose scattering amplitude in partial waves. One real observable

 $\delta_l(E^*)$ 

in each partial wave (I) and CM energy.

 $\det\left[\cot\delta(E_n^*)+\cot\phi(E_n,\vec{P},L)\right]=0$ 

with  $\cot \phi$  a known function (containing a generalised zeta function).

• To use this idea many technical improvements were needed - this is why it has taken a while ...

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# $\pi\pi$ in P-wave: $I^G J^{PC} = 1^+(1^{--})$

A relatively straightforward example

- consider the  $\rho$  on a lattices of different volumes
- at each volume extract the spectrum and use Lüscher formalism to deduce phase shift



• the more distinct spectrum points the better the phase shift picture

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### MAPPING OUT THE PHASE SHIFT

What sort of operators are needed? A good operator basis reflects the relevant physics.

- single hadron:  $\bar{\psi} \Gamma \psi$ ,  $\bar{\psi} \Gamma \overleftarrow{D} \dots \overleftarrow{D} \psi$  etc with the correct quantum numbers.
- multi-hadron: O<sub>ππ</sub>(|p|) = Σ<sub>p</sub> c(p)π(p)π(-p) where each π operator is a "variationally optimised" object, π = Σ<sub>i</sub> v<sub>i</sub>(ūΓ<sub>i</sub>d) for a range of |p|.
- form a correlator matrix with these operators and solve a GEVP extracting the spectrum of states.
- requires precision determinations of connected and disconnected diagrams.



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### $\pi\pi$ in P-wave I=1

#### A Breit-Wigner energy-dependent description



from Dudek, Edwards, Thomas in Phys. Rev. D87 (2013) 034505

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## $\pi\pi$ in P-wave, I=1

coupled  $\pi\pi$ ,  $K\bar{K}$  scattering in P-wave, PRD 92 (2015) 094592



• Includes **coupled channel**  $\pi\pi$ ,  $K\bar{K}$  at  $m_{\pi} = 236$ MeV.

- $m_R = 790(2)$  MeV;  $g_R = 5.688(70)(26)$
- Reducing  $m_{\pi}$  moves mass and width in the right direction.

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### HOW IMPORTANT ARE MULTI-HADRON OPERATORS?



Low-lying states overlap with both operator types Expected for a system with a resonance that is dominantly  $q\bar{q}$  but coupled to the decay channel  $\pi\pi$ . Phase shift from single hadron operators only. Suggests a narrow state present but no way to determine resonant properties.



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### Some open challenges

- No theoretical framework to handle beyond 2-final state coupled channels. Many are relevant in charmonium e.g.  $J/\psi\pi\pi$
- At physical pion masses many more decay channels open up:  $\pi\pi\pi$  etc
- Understanding the XYZs see Christoph's lectures coming next ... Probably needs a combination of methods and calculations.
- Scattering and spectroscopy of exotics in the Upsilon sector.
- Many more ...

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## SUMMARY

- It's a very exciting time in hadronic physics!
- From the theory perspective, there's been enormous progress in the last 5 years.
- Many open questions and unsolved problems phenomenological and theoretical remain.
- Lots to do!

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## SUMMARY

- It's a very exciting time in hadronic physics!
- From the theory perspective, there's been enormous progress in the last 5 years.
- Many open questions and unsolved problems phenomenological and theoretical remain.
- Lots to do!

Thanks for listening!

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### TYPICAL SIZE OF A LATTICE CALCULATION



[from D.Leinweber]

There are 2 compute intensive steps: **1. Generating Configurations snapshots of the QCD vacuum** Volume:  $32^3 \times 256$  (sites)  $U_{\mu}(x)$  defined by  $4 \times 8 \times 32^3 \times 256$  real numbers **2. Quark Propagation** 

Volume:  $32^3 \times 256$  (sites)  $\rightarrow M$  is a 100 million x 100 million sparse matrix with complex entries.

Solving QCD requires supercomputing resources worldwide.


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