Lattice QCD: a theoretical femtoscope for non-perturbative strong dynamics

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# Outline

Introduction to (lattice) QCD:

\* Asymptotic freedom and dimensional transmutation

\* Quantum chromodynamics on a lattice

Spontaneous symmetry breaking:

- \* Banks–Casher relation
- \* Renormalization of the spectral density
- \* Exploratory numerical study

**\square** Witten–Veneziano solution to the  $U(1)_A$  problem:

- \* Definition of the topological susceptibility
- \* Non-perturbative computation



Quantum chromodynamics (QCD)

QCD is assumed to be the quantum field theory of strong interactions in Nature. Its action [Fritzsch, Gell-Mann, Leutwyler 73; Gross, Wilczek 73; Weinberg 73]

 $S[A, \bar{\psi}_i, \psi_i; \boldsymbol{g}, \boldsymbol{m}_i, \boldsymbol{\theta}]$ 

is fixed by few simple principles:

\* SU(3)<sub>c</sub> gauge (local) invariance

\* Quarks in fundamental representation  $\psi_i = u, d, s, c, b, t$ 

\* Renormalizability

**Present experimental results compatible with**  $\theta = 0$ 

• It is fascinating that such a simple action and few parameters  $[g, m_i]$  can account for the variety and richness of strong-interaction physics phenomena



### Asymptotic freedom

• Quantization breaks scale invariance at  $m_i = 0$ 

The renormalized coupling constant is scale dependent

$$\mu \frac{d}{d\mu}g = \beta(g)$$

and QCD is asymptotically free [ $b_0 > 0$ ] [Gross, Wilczek 73; Politzer 73]

$$\beta(g) = -b_0g^3 - b_1g^5 + \dots$$

The theory develops a fundamental scale

$$\Lambda = \mu \left[ b_0 g^2(\mu) \right]^{-b_1/2b_0^2} e^{-\frac{1}{2b_0 g^2(\mu)}} e^{-\int_0^{g(\mu)} dg \left[ \frac{1}{\beta(g)} + \frac{1}{b_0 g^3} - \frac{b_1}{b_0^2 g} \right]}$$

which is a non-analytic function of the coupling constant at  $g^2 = 0$ 



#### Perturbative corner: hard processes



Experimental results significantly prove the logarithmic dependence in  $\mu/\Lambda$  predicted by perturbative QCD



 $\Lambda \sim 0.2 \ \mathrm{GeV} \qquad 1/\Lambda \sim 1 \ \mathrm{fm} = 10^{-15} \ \mathrm{m}$ 

- At these distances the dynamics of QCD is non-perturbative
- A rich spectrum of hadrons is observed at these energies. Their properties such as the mass

 $M_n = b_n \Lambda$ 

need to be computed non-perturbatively

• The theory is highly predictive: in the (interesting) limit  $m_{u,d,s} = 0$  and  $m_{c,b,t} \to \infty$ , for instance, dimensionless quantities are parameter-free numbers





- QCD can be defined on a discretized space-time so that gauge invariance is preserved
- Quark fields reside on a four-dimensional lattice, the gauge field  $U_{\mu} \in SU(3)$  resides on links

The Wilson action for the gauge field is

$$S_G[U] = \frac{\beta}{2} \sum_x \sum_{\mu,\nu} \left[ 1 - \frac{1}{3} \operatorname{ReTr} \left\{ U_{\mu\nu}(x) \right\} \right]$$

where  $\beta=6/g^2$  and the plaquette is defined as

$$U_{\mu\nu}(x) = U_{\mu}(x) U_{\nu}(x+\hat{\mu}) U_{\mu}^{\dagger}(x+\hat{\nu}) U_{\nu}^{\dagger}(x)$$

Popular discretizations of fermion action: Wilson, Domain-Wall-Neuberger, perfect actions, tmQCD





The lattice provides a non-perturbative definition of QCD. The path integral at finite spacing and volume is mathematically well defined (Euclidean time)

$$Z = \int DU D\bar{\psi}_i D\psi_i \ e^{-S[U,\bar{\psi}_i,\psi_i;g,m_i]}$$

Nucleon mass, for instance, can be extracted from the behaviour of a suitable two-point correlation function at large time-distance

$$\langle O_N(x)\bar{O}_N(y)\rangle = \frac{1}{Z} \int DUD\bar{\psi}_i D\psi_i \ e^{-S} \ O_N(x)\bar{O}_N(y) \longrightarrow R_N \ e^{-M_N} |x_0 - y_0|$$

**P** For small gauge fields, the perturb. expansion differs from the usual one for terms of O(a)

$$= -igT^{a} \left\{ \gamma_{\mu} - \frac{i}{2}(p_{\mu} + p'_{\mu})a + O(a^{2}) \right\}$$

Consistency of lattice QCD with the standard perturbative approach is thus guaranteed

Continuum and infinite-volume limit of LQCD is the non-perturbative definition of QCD

Details of the discretization become irrelevant in the continuum limit, and any reasonable lattice formulation tends to the same continuum theory

 $M_N(a) = M_N + c_N a + \dots$ 

• Continuum and infinite-volume limit of LQCD is the *non-perturbative definition* of QCD

Details of the discretization become irrelevant in the continuum limit, and any reasonable lattice formulation tends to the same continuum theory

$$M_N(a) = M_N + d_N a^2 + \dots$$

By a proper tuning of the action and operators, convergence to continuum can be accelerated without introducing extra free-parameters [Symanzik 83; Sheikholeslami Wohlert 85; Lüscher et al. 96]

• Finite-volume effects are proportional to  $exp(-M_{\pi}L)$  at asymptotically large volumes

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
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| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | • | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | • | 0 | 0 | ٠ | • | • | • | 0 | 0 | ٠ | • | • | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | • | ٠ | • | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

Correlation functions at *finite volume* and *finite lattice spacing* can be computed by Monte Carlo techniques *exactly* up to statistical errors



#### **•** Typical lattice parameters:

- $a = 0.05 \text{ fm} \qquad (a\Lambda)^2 \sim 0.25\%$   $L = 3.2 \text{ fm} \implies M_{\pi}L \ge 4, \ M_{\pi} \ge 0.25 \text{ GeV}$   $V = 2L \times L^3 \qquad \text{\#points} = 2^{25} \sim 3.4 \cdot 10^7$
- Monte Carlo algorithms integrate over 10<sup>7</sup>-10<sup>9</sup>
   SU(3) link variables
- A typical cluster of PCs:
  - \* Standard CPUs [AMD, Intel]
  - \* Fast connection [40Gbit/s]
- Lattice partitioned in blocks which are distributed over the nodes (128 a good example)
- Data exchange among nodes minimized thanks to the locality of the action

| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | • | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | • | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 | 0 | ٠ | ٠ | ٠ | ٠ | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |



- Extraordinary algorithmic progress over the last 30 years, keywords:
  - \* Hybrid Monte Carlo (HMC) Duane et al. 87
  - \* Multiple time-step integration Sexton, Weingarten 92
  - \* Frequency splitting of determinant Hasenbusch 01
  - \* Domain Decomposition Lüscher 04
  - \* Mass preconditioning and rational HMC Urbach et al 05; Clark, Kennedy 06
  - \* Deflation of the low quark modes Lüscher 07
- Light dynamical quarks can be simulated (continuum limit still problematic). Chiral regime of QCD is becoming accessible
- Algorithms are designed to produce exact results up to statistical errors



- Lattice QCD is the femtoscope for studying strong dynamics. Its lenses are made of quantum field theory, numerical techniques and computers
- It allows us to look also at quantities not accessible to experiments which may help understanding the underlying mechanisms
- Femtoscope still rather crude. Often we compute what we can and not what would like to
- An example: the signal-to-noise ratio of the nucleon two-point correlation function

$$\frac{\langle O_N \bar{O}_N \rangle^2}{\Delta^2} \propto n \, e^{-(2M_N - 3M_\pi)|x_0 - y_0|}$$

decreases exp. with time-distance of sources. At physical point  $2M_N$ - $3M_\pi \simeq 7 \text{ fm}^{-1}$ 



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Analogous problem for glueballs in Yang–Mills theory solved by decomposing the path integral and by enforcing the global symmetries of the theory into the Monte Carlo [Della Morte, LG 08-10]



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- Femtoscope still rather crude. Often we compute what we can and not what would like to
- A rather general strategy is emerging: design special purpose algorithms which exploit known math. and phys. properties of the theory to be faster
- Results from first-principles when all syst. uncertainties quantified. This achieved without introducing extra free parameters or dynamical assumptions but just by improving the femtoscope



QCD action and its (broken) symmetries

• QCD action for 
$$N_f = 3$$
,  $M = \operatorname{diag}(m_u, m_d, m_s)$   
 $S = S_G + \int d^4x \left\{ \bar{\psi} D\psi + \bar{\psi} M\psi \right\}$ ,  $D = \gamma_\mu (\partial_\mu + iA_\mu)$   
• For  $M = 0$  chiral symmetry  $SU(3)_c \times SU(3)_L \times SU(3)_L \times U(1)_L \times U(1)_R \times \mathcal{R}_{scale}$   
 $\psi_{R,L} \rightarrow V_{R,L} \psi_{R,L}$   $\psi_{R,L} = \left(\frac{1 \pm \gamma_5}{2}\right) \psi$   $(\operatorname{dim. transm., chiral anomaly)}$   
Chiral anomaly: measure not invariant SSB: vacuum not symmetric  $SU(3)_c \times SU(3)_L \times SU(3)_L \times SU(3)_R \times U(1)_{B=L+R}$   
 $\psi(x) \rightarrow G(x)\psi(x)$   $SU(3)_c \times SU(3)_{L+R} \times U(1)_R$ 

Confinement: no isolated coloured charge

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 $SU(3)_{\tiny L+R} \times U(1)_{\tiny B}$ 

QCD action and its (broken) symmetries

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• QCD action for 
$$N_f = 3$$
,  $M = \text{diag}(m_u, m_d, m_s)$   
 $S = S_G + \int d^4x \left\{ \bar{\psi} D\psi + \bar{\psi} M\psi \right\}$ ,  $D = \gamma_\mu (\partial_\mu + iA_\mu)$   
 $SU(3)_c \times SU(3)_n \times U(1)_n \times U(1)_n \times \mathcal{R}_{\text{scale}}$   
 $\downarrow$  (dim. transm., chiral anomaly)  
• Confinement and SSB due to non-perturbative  
dynamics  $SU(3)_c \times SU(3)_n \times U(1)_{n-t_i + n}$   
 $SU(3)_c \times SU(3)_n \times SU(3)_n \times U(1)_{n-t_i + n}$   
 $\downarrow$  (Spont. Sym. Break.)  
• Today focus on SSB and chiral anomaly  
 $\downarrow$  (Confinement)

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 ${\rm SU}(3)_{\scriptscriptstyle L+R} \times {\rm U}(1)_{\scriptscriptstyle B}$ 

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- \* Banks–Casher relation
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**\square** Witten–Veneziano solution to the  $U(1)_A$  problem:

- \* Definition of the topological susceptibility
- \* Non-perturbative computation



• An axial Ward identity of the chiral group is [for simplicity M = diag(m, m, m)]

$$\langle \bar{\psi}_1 \psi_1 \rangle = m \int d^4 x \left\langle P_{12}(x) P_{21}(0) \right\rangle \,, \qquad P_{ij} = \bar{\psi}_i \gamma_5 \psi_j \label{eq:phi_star}$$

 $\checkmark$  In the limit  $m \rightarrow 0$ 

$$\Sigma = -\lim_{m \to 0} \langle \bar{\psi}_1 \psi_1 \rangle \neq 0 \qquad \Longrightarrow \qquad M^2 = \frac{2m\Sigma}{F^2} \qquad \text{[Gell-Mann, Oakes, Renner 68]}$$

where the decay constant is defined as

$$|\langle 0|\hat{A}_{12,\mu}|\pi^{-},p\rangle| = \sqrt{2} F_{\pi} p_{\mu} , \qquad F = \lim_{m \to 0} F_{\pi}$$

|   | Ostat as manatible with CCD nottons                                   |   |                |
|---|---|---|----------------|
| _ | Octet compatible with SSB pattern                                     | I I $_3$ S Me                                   | sor            |
|   |   |   |                |
|   | $SU(3)_{L} \times SU(3)_{R} \rightarrow SU(3)_{L+R}$                  | 1 1 0 π   | +              |
|   |   | <b>1 -1 0</b> π                                 | _              |
|   | and soft explicit symmetry breaking                                   | 100 π   | 0              |
|   |   |   |                |
|   | $m_u, m_d \ll m_s < \Lambda$  | $\frac{1}{2}$ $\frac{1}{2}$ +1 K                | +              |
|   |   | $\frac{1}{2} - \frac{1}{2} + 1$ K               | 0              |
|   |   | $\frac{1}{2} - \frac{1}{2} - 1$ K               | _              |
|   |   | $\frac{1}{12}$ $\frac{1}{12}$ -1 $\overline{K}$ | <del>.</del> 0 |
|   |   | 2 2   | -              |
| _ | $m_u, m_d \ll m_s \Longrightarrow m_\pi \ll m_{\rm K}$                | $\overline{000}$                                | <u>ן</u>       |
|   |   |   |                |
|   |   | 000 m   | /              |
|   | $\Delta 0^{\text{th}}$ pseudoscalar with $m \to \mathcal{O}(\Lambda)$ |   |                |
| - | $\pi$ 9 poeudoscalar with $m_{\eta'} \sim O(\Lambda)$                 | $n_{\circ}$ =                                   | (              |

| I                       | $I_3$          | S            | Meso                        | n Quark  | Mass  |  |
|-------------------------|----------------|--------------|-----------------------------|--|-------|--|
|                         | -              |              |                             | Content  | (GeV) |  |
| 1                       | 1              | 0            | $\pi^+$                     | $u ar{d}$  | 0.140 |  |
| 1                       | -1             | 0            | $\pi^{-}$                   | $dar{u}$   | 0.140 |  |
| 1                       | 0              | 0            | $\pi^0$                     | $(d\bar{d}-u\bar{u})/\sqrt{2}$   | 0.135 |  |
| $\frac{1}{2}$           | $\frac{1}{2}$  | +1           | K <sup>+</sup>              | $u\bar{s}$   | 0.494 |  |
| $\frac{2}{1}{2}$        | $-\frac{1}{2}$ | +1           | $\mathrm{K}^{\mathrm{0}}$   | $dar{s}$   | 0.498 |  |
| $\frac{\frac{2}{1}}{2}$ | $-\frac{1}{2}$ | -1           | $K^{-}$                     | $sar{u}$   | 0.494 |  |
| $\frac{1}{2}$           | $\frac{1}{2}$  | -1           | $\overline{\mathrm{K}}^{0}$ | $sar{d}$   | 0.498 |  |
| 0                       | 0              | 0            | $\eta$                      | $\cos\vartheta\eta_8 - \sin\vartheta\eta_0$  | 0.548 |  |
|                         |                |              |                             |  |       |  |
| 0                       | 0              | 0            | $\eta'$                     | $\sin\vartheta\eta_8 + \cos\vartheta\eta_0$  | 0.958 |  |
|                         | r<br>r         | 78<br>70     | =                           | $\frac{(d\bar{d} + u\bar{u} - 2s\bar{s})/\sqrt{6}}{(d\bar{d} + u\bar{u} + s\bar{s})/\sqrt{3}}$ |       |  |
|                         | ť              | <del>)</del> | $\sim$                      | $-10^{\circ}$  |       |  |

Chiral effective theory for pions

$$S_{\text{eff}} = S_{\text{eff}}^2(U; m, F, \Sigma) + S_{\text{eff}}^4(U; m, F, \Sigma, \Lambda_i) + \cdots$$

encodes spontaneous symmetry breaking

- For m = 0 pions can interact only if they carry momentum. Expansion in p and m
- Chiral dynamics parameterized by effective low-energy coupling constants

 $\checkmark$  For instance the pion mass and decay constant at  $\mathcal{O}(p^4)$  are given by

$$M_{\pi}^{2} = M^{2} \left\{ 1 + \frac{M^{2}}{32\pi^{2}F^{2}} \ln\left(\frac{M^{2}}{\Lambda_{3}^{2}}\right) \right\}, \qquad F_{\pi} = F \left\{ 1 - \frac{M^{2}}{16\pi^{2}F^{2}} \ln\left(\frac{M^{2}}{\Lambda_{4}^{2}}\right) \right\}$$

Analogous expressions for other quantities such as S-wave  $\pi\pi$  scattering lengths  $a_0^0$  and  $a_0^2$ 

#### [Colangelo, Gasser, Leutwyler 01; Leutwyler 09]



- Chiral regime is becoming accessible to lattice QCD simulations
- The pion mass squared is found to be a nearly linear function of quark mass up to (0.5 GeV)<sup>2</sup>.
   At smallest masses non-linear correction is 1 3%
- Non-Abelian chiral symmetry spontaneously broken as expected
- Compatible with the fact that the bulk of the mass is given by the leading term in standard ChPT
- Relations dictated by SSB can be verified quantitatively. GMOR is maybe the simplest to start with

Low-energy constants will finally be determined



For each gauge configuration

$$D_m \chi_k = (m + i\lambda_k)\chi_k$$

 $\blacksquare$  The spectral density of D is

$$\rho(\lambda, m) = \frac{1}{V} \sum_{k} \left\langle \delta(\lambda - \lambda_k) \right\rangle$$

where  $\langle \dots \rangle$  indicates path-integral average



The Banks–Casher relation

$$\lim_{\lambda \to 0} \lim_{m \to 0} \lim_{V \to \infty} \rho(\lambda, m) = \frac{\Sigma}{\pi}$$

provides a link between the condensate and the (non-zero) spectral density at the origin. To be compared, for instance, with the free case  $\rho(\lambda) \propto |\lambda^3|$  For each gauge configuration

$$D_m \chi_k = (m + i\lambda_k)\chi_k$$

 $\blacksquare$  The spectral density of D is

$$\rho(\lambda,m) = \frac{1}{V} \sum_{k} \left\langle \delta(\lambda - \lambda_k) \right\rangle$$

where  $\langle \dots \rangle$  indicates path-integral average

The number of modes in a given energy interval

$$\nu(\Lambda, m) = V \int_{-\Lambda}^{\Lambda} d\lambda \ \rho(\lambda, m) \qquad \nu(\Lambda, m) = \frac{2}{\pi} \Lambda \Sigma V + \dots$$

grows linearly with  $\Lambda,$  and they condense near the origin with values  $\propto 1/V$  In the free case  $\nu(\Lambda,m)\propto V\Lambda^4$ 



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Instead of the spectral density, consider the spectral sum

$$\sigma_k(m_v, m) = V \int_{-\infty}^{\infty} d\lambda \frac{\rho(\lambda, m)}{(\lambda^2 + m_v^2)^k}$$

$$= -a^{8k} \sum_{x_1...x_{2k}} \langle P_{12}(x_1) P_{23}(x_2) \dots P_{2k1}(x_{2k}) \rangle$$

\* Integral converges if  $k \geq 3$ 

\* The relation between  $\sigma_k(m_v,m)$  and  $ho(\lambda,m)$  invertible for every k

Senormalization properties of  $\rho(\lambda, m)$  can thus be inferred from those of  $\sigma_k$ 

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$$= -a^{8k} \sum_{x_1...x_{2k}} \langle P_{12}(x_1) P_{23}(x_2) \dots P_{2k1}(x_{2k}) \rangle$$

• Corr. functions of pseudoscalar densities at physical distance renormalized by  $(1/Z_m)^{2k}$ 

At short distance the flavour structure implies

$$P_{12}(x_1)P_{23}(x_2) \sim C(x_1 - x_2)S_{13}(x_1) \qquad S_{13} = \bar{\psi}_1\psi_3$$

where C(x) diverges like  $|x|^{-3}$  and it is therefore integrable. Analogous argument for all other short-distance singularities. No extra contact terms needed to renormalize  $\sigma_k$ 

Instead of the spectral density, consider the spectral sum

$$\sigma_k(m_v, m) = V \int_{-\infty}^{\infty} d\lambda \frac{\rho(\lambda, m)}{(\lambda^2 + m_v^2)^k}$$

$$= -a^{8k} \sum_{x_1...x_{2k}} \langle P_{12}(x_1) P_{23}(x_2) \dots P_{2k1}(x_{2k}) \rangle$$

Once the gauge coupling and the mass(es) are renormalized, the spectral sum

$$\sigma_{k,\mathrm{R}}(m_{v_{\mathrm{R}}},m_{\mathrm{R}}) = Z_m^{-2k} \sigma_k \left(\frac{m_{v_{\mathrm{R}}}}{Z_m},\frac{m_{\mathrm{R}}}{Z_m}\right)$$

is ultraviolet finite. Continuum limit universal (if same renormalization conditions are used)

### Renormalization and continuum limit [LG, Lüscher 09]

Instead of the spectral density, consider the spectral sum

$$\sigma_k(m_v, m) = V \int_{-\infty}^{\infty} d\lambda \frac{\rho(\lambda, m)}{(\lambda^2 + m_v^2)^k}$$

$$= -a^{8k} \sum_{x_1...x_{2k}} \langle P_{12}(x_1) P_{23}(x_2) \dots P_{2k1}(x_{2k}) \rangle$$

The spectral density thus renormalizes as

$$\rho_{\mathrm{R}}(\lambda_{\mathrm{R}},m_{\mathrm{R}}) = Z_m^{-1} \rho\left(\frac{\lambda_{\mathrm{R}}}{Z_m},\frac{m_{\mathrm{R}}}{Z_m}\right)$$

For Wilson fermions similar derivation but twisted-mass valence quarks

### Renormalization and continuum limit [LG, Lüscher 09]

Instead of the spectral density, consider the spectral sum

$$\sigma_k(m_v, m) = V \int_{-\infty}^{\infty} d\lambda \frac{\rho(\lambda, m)}{(\lambda^2 + m_v^2)^k}$$

$$= -a^{8k} \sum_{x_1 \dots x_{2k}} \langle P_{12}(x_1) P_{23}(x_2) \dots P_{2k1}(x_{2k}) \rangle$$

It follows that the mode number is a renormalization-group invariant

$$\nu_{\rm R}(\Lambda_{\rm R},m_{\rm R})=\nu(\Lambda,m)$$

and its continuum limit is universal for any value of  $\Lambda$  and m

# Numerical computation (I) [LG, Lüscher 09]

- Lattice details:
  - $* N_f = 2$  degenerate quarks
  - \* Action: O(a)-improved Wilson
  - $\ast \, a = 0.0784 \ \mathrm{fm}$
  - \*  $V=2L\times L^3,\,L=1.9,2.5~{\rm fm}$
  - $* m_{\rm R}^{\overline{
    m MS}}(2\,{
    m GeV}) = 0.013, 0.026, 0.046~{
    m GeV}$
  - $* \Lambda_{R}^{\overline{MS}}(2 \, \text{GeV}) = 0.07, 0.085, 0.1, 0.115 \text{ GeV}$



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   ChPT suggests a fraction of a percent
- In the effective theory at NLO

$$\nu^{\rm nlo}(\Lambda,m) = \frac{2\Lambda\Sigma V}{\pi} \left\{ 1 - \frac{m\Sigma}{(4\pi)^2 F^4} \left[ 3\ln\left(\frac{\Lambda\Sigma}{F^2\Lambda_6^2}\right) + \ln(2) + \frac{\pi}{2}\frac{m}{\Lambda} + O\left(\frac{m^2}{\Lambda^2}\right) \right] \right\}$$

corrections of  $\mathcal{O}(10\%)$  for  $\Lambda = 0.05-0.1$  GeV and  $m \leq 0.02$  GeV. No chiral logs  $\propto m \ln(m)$ 



An effective condensate can be defined as

$$\overline{\Sigma}_{\mathrm{R}} = \frac{\pi}{2V} \frac{\partial}{\partial \Lambda_{\mathrm{R}}} \, \nu_{\mathrm{R}}(\Lambda_{\mathrm{R}}, m_{\mathrm{R}})$$

prefactor so that  $\overline{\Sigma}_{\rm R}$  coincides with  $\Sigma$  at LO

A linear extrapolation to the chiral limit yields

$$\left[\Sigma_{\rm R}^{\overline{\rm MS}}(2\,{\rm GeV})\right]^{1/3} = 0.276(3)(4)(5)\;{\rm GeV}$$



 $\blacksquare$  A clear and consistent picture is emerging. For  $m_R \leq 0.05~{\rm GeV}$  the GMOR formula accounts for the bulk of the pion mass. But discretization errors not quantified yet

# Why is the symmetry spontaneously broken?

Dynamical process not yet known. Studies of low modes can provide important clues

- The Banks–Casher mechanism is:
  - \* insensitive to lattice details (universality)
  - \* largely insensitive to dynamical quark effects
  - \* present also in quenched QCD

It is tempting to read the relation in the other direction, i.e. chiral symmetry is broken because the low-modes of the Dirac operator condense

 $\frac{\Sigma}{\pi} = \lim_{\lambda \to 0} \lim_{m \to 0} \lim_{V \to \infty} \rho(\lambda, m)$ 



Eigenvalues of  $D_m^{\dagger} D_m$ 

# Outline

Introduction to (lattice) QCD:

\* Asymptotic freedom and dimensional transmutation

\* Quantum chromodynamics on a lattice

Spontaneous symmetry breaking:

- \* Banks–Casher relation
- \* Renormalization of the spectral density
- \* Exploratory numerical study

● Witten–Veneziano solution to the  $U(1)_A$  problem:

- \* Definition of the topological susceptibility
- \* Non-perturbative computation



Octet compatible with SSB pattern  $SU(3)_{L} \times SU(3)_{R} \rightarrow SU(3)_{L+R}$ and soft explicit symmetry breaking  $m_u, m_d \ll m_s < \Lambda$  $m_u, m_d \ll m_s \Longrightarrow m_\pi \ll m_K$ A 9<sup>th</sup> pseudoscalar with  $m_{\eta'} \sim \mathcal{O}(\Lambda)$ 

| T                        | Т              | C          | Maga                        | n Quark                                     | Maga   |
|--------------------------|----------------|------------|-----------------------------|---|--------|
| I                        | 13             | 3          | IVIES0                      | n Quark                                     | IVIA55 |
|                          |                |            |                             | Content                                     | (GeV)  |
| 1                        | 1              | 0          | $\pi^+$                     | $uar{d}$                                    | 0.140  |
| 1                        | -1             | 0          | $\pi^{-}$                   | $dar{u}$                                    | 0.140  |
| 1                        | 0              | 0          | $\pi^0$                     | $(d\bar{d}-u\bar{u})/\sqrt{2}$              | 0.135  |
| $\frac{1}{2}$            | $\frac{1}{2}$  | +1         | K <sup>+</sup>              | $uar{s}$                                    | 0.494  |
| $\frac{1}{2}$            | $-\frac{1}{2}$ | +1         | $\mathrm{K}^{\mathrm{0}}$   | $dar{s}$                                    | 0.498  |
| $\frac{\overline{1}}{2}$ | $-\frac{1}{2}$ | -1         | $\mathrm{K}^-$              | $sar{u}$                                    | 0.494  |
| $\frac{\overline{1}}{2}$ | $\frac{1}{2}$  | -1         | $\overline{\mathrm{K}}^{0}$ | $sar{d}$                                    | 0.498  |
| 0                        | 0              | 0          | $\eta$                      | $\cos\vartheta\eta_8 - \sin\vartheta\eta_0$ | 0.548  |
|                          |                |            |                             |   |        |
| 0                        | 0              | 0          | $\eta'$                     | $\sin\vartheta\eta_8 + \cos\vartheta\eta_0$ | 0.958  |
|                          | r              | <b>]</b> 8 | =                           | $(d\bar{d}+u\bar{u}-2s\bar{s})/\sqrt{6}$    |        |
|                          | r              | 70         | =                           | $(d\bar{d} + u\bar{u} + s\bar{s})/\sqrt{3}$ |        |
|                          | ı              | 9          | $\sim$                      | $-10^{\circ}$                               |        |

An axial Ward identity of the chiral group is

$$\int d^4x \, \langle Q(x)Q(0) \rangle = m_1 m_2 \int d^4x \, \langle P_{11}(x)P_{22}(0) \rangle \,, \quad Q(x) = -\frac{1}{32\pi^2} \, \epsilon_{\mu\nu\rho\sigma} \, \mathrm{Tr} \Big[ F_{\mu\nu}(x)F_{\rho\sigma}(x) \Big] \,.$$

**9** In the limit  $N_c \to \infty$ 

$$\chi_{\infty} = \lim_{N_c \to \infty} \int d^4 x \left\langle Q(x)Q(0) \right\rangle \neq 0 \qquad \Longrightarrow \qquad \lim_{N_c \to \infty} \lim_{m_i \to 0} \frac{F^2 M_{\eta'}^2}{2N_f} = \chi_{\infty}$$

**•** Note that for  $N_c \to \infty$ :

 $* U(1)_A$  is restored

 $* \eta'$  becomes a Nambu–Goldstone boson  $\Longrightarrow M_{\eta'} = 0$ 

\* At first order in  $1/N_c$ ,  $M_{\eta'}^2 = \mathcal{O}(N_f/N_c)$ 

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An unambiguous definition of the topological susceptibility is required. Naive definition would diverge as

$$\chi = \int d^4x \left\langle Q(x)Q(0) \right\rangle \propto \frac{1}{a^4}$$

0

#### The Witten–Veneziano mechanism with Ginsparg–Wilson fermions

#### With Ginsparg–Wilson fermions the lattice Ward identity is

[Neuberger 97; Hasenfratz, Laliena, Niedermayer 98; Lüscher 98; LG, Rossi, Testa, Veneziano 01]

$$\sum_{x} a^{4} \langle Q(x)Q(0) \rangle = m_{1}m_{2} \sum_{x} a^{4} \langle P_{11}(x)P_{22}(0) \rangle , \quad Q(x) = -\frac{1}{2a^{3}} \operatorname{Tr} \Big[ \gamma_{5} D(x,x) \Big]$$

• In the limit  $N_c \to \infty$ 

$$\chi_{\infty} = \lim_{N_c \to \infty} \sum_{x} a^4 \left\langle Q(x)Q(0) \right\rangle \neq 0 \qquad \Longrightarrow \qquad \lim_{N_c \to \infty} \lim_{m_i \to 0} \frac{F^2 M_{\eta'}^2}{2N_f} = \chi_{\infty}$$

Need to demonstrate that the topological susceptibility suggested by GW fermions

$$\chi = \sum_{x} a^4 \left\langle Q(x)Q(0) \right\rangle$$

is ultraviolet finite and unambiguously defined

A chain of Ward identities holds

$$\begin{split} N_f &= 2 \quad \chi = m_1 m_2 \sum_{x_1} a^4 \langle P_{11}(x_1) P_{22}(0) \rangle \\ & \cdots & & \cdots \\ \dots & & \ddots \\ N_f &= 5 \quad \chi = m_1 \dots m_5 \sum_{x_1 \dots x_4} a^{16} \langle P_{31}(x_1) S_{12}(x_2) S_{23}(x_3) P_{54}(x_4) S_{45}(0) \rangle \end{split}$$

It follows that the topological susceptibility is finite, it is renormalization-group invariant and its continuum limit is universal for any value of m

**\square** A definition of  $\chi$  even if the regularization breaks chiral symmetry

**\square** The limit  $N_c \to \infty$  is given by

$$\lim_{N_c \to \infty} \chi = \lim_{N_c \to \infty} \chi^{\mathrm{YN}}$$

and finiteness in Yang–Mills theory is proven analogously by introducing pseudofermions

A Monte Carlo computation of

$$\chi^{\rm YM} = \frac{1}{V} \left\langle (n_+ - n_-)^2 \right\rangle^{\rm YM}$$

is challenging for several reasons

 $\square L \sim 2 \text{ fm and } a \sim 0.08 \text{ fm} \Longrightarrow \dim[D] \sim 4.5 \cdot 10^6$ 

**•** In finite V null probability for  $n_+ \neq 0$  and  $n_- \neq 0$ 

Simultaneous minimization of Ritz functionals for

$$D^{\pm} = P_{\pm}DP_{\pm} \qquad P_{\pm} = \frac{1 \pm \gamma_5}{2}$$

to find the gap in one of the sectors and to count the zero modes in the other

No contamination from quasi-zero modes



 $\ensuremath{{\,{\rm o}}}$  Combined fit of the form [ $\chi^2_{\rm dof}=0.73$ ]

$$r_0^4 \chi^{\text{YM}}(a,s) = r_0^4 \chi^{\text{YM}} + c_1(s) \frac{a^2}{r_0^2}$$

gives

$$r_0^4 \chi^{\rm YM} = 0.059 \pm 0.003$$



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 $\checkmark$  By setting the scale  $F_{\rm K} = 0.113(1)~{\rm GeV}$ 

 $\chi^{\rm YM} = (0.191 \pm 0.005 \; {\rm GeV})^4$ 



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to be compared with

$$\frac{F^2}{2N_f} (M_\eta^2 + M_{\eta'}^2 - 2M_K^2) \underset{\text{exp}}{\approx} (0.175 \text{ GeV})^4$$



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The (leading) QCD anomalous contribution to  $M^2_{\eta'}$  supports the Witten–Veneziano explanation for its large experimental value



Vacuum energy and charge distribution are

$$e^{-F(\theta)} = \langle e^{i\theta Q} \rangle , \quad P_Q = \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{-i\theta Q} e^{-F(\theta)}$$

Their behaviour is a distinctive feature of the configurations that dominate the path integral

**\square** Large  $N_c$  expansion predicts

$$\frac{\langle Q^{2n} \rangle^{\rm con}}{\langle Q^2 \rangle} \propto \frac{1}{N_c^{2n-2}}$$

Various conjectures. For example, dilute-gas instanton model gives ['t Hooft 74; Callan et al. 76; ...]

$$F^{\text{Inst}}(\theta) = -VA\{\cos(\theta) - 1\}$$
$$\frac{\langle Q^{2n} \rangle^{\text{con}}}{\langle Q^2 \rangle} = 1$$





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Their behaviour is a distinctive feature of the configurations that dominate the path integral

#### A lattice computation gives

$$\frac{\langle Q^4 \rangle^{\rm con}}{\langle Q^2 \rangle} = 0.30 \pm 0.11$$

Witten–Veneziano mechanism: the anomaly gives a mass to the  $\eta'$  boson thanks to the non-perturbative quantum fluctuations of the topological charge





- Lattice QCD is a phenomenal theoretical femtoscope to explore strong dynamics. Its lenses are made of quantum field theory, numerical techniques and computers
- It allows us to look at quantities not accessible to experiments that may unveil the the underlying mechanisms of non-perturbative strong dynamics
- A large variety of physics applications: QCD, flavour physics, beyond Standard Model physics, etc.
- Thanks to the recent extraordinary conceptual, technical and algorithmic advances the chiral regime of the theory is becoming accessible
- Today two particularly interesting applications:
  - \* Banks–Casher relation
  - \* Witten–Veneziano mechanism

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- It allows us to look at quantities not accessible to experiments that may unveil the the underlying mechanisms of non-perturbative strong dynamics
- A large variety of physics applications: QCD, flavour physics, beyond Standard Model physics, etc.

- Condensation of low-modes of the Dirac operator most direct piece of theoretical evidence for SSB
- The rate of condensation explains the bulk of the pion mass up to 0.5 GeV



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- Quantum fluctuations of the topological charge in Yang–Mills theory generate a non-zero value of  $\chi^{\rm YM}$
- Its value supports the Witten–Veneziano explanation for the large mass of the  $\eta'$



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- The femtoscope, however, is still rather crude. There is continuous conceptual and technical progress to empower it
- LQCD will lead us to a precise quantitative understanding of QCD in the low-energy regime, and to validate the theory to be the one of the strong interactions in Nature

- Chiral regime is becoming accessible to lattice QCD simulations
- The pion mass squared is found to be a nearly linear function of quark mass up to (0.5 GeV)<sup>2</sup>.
   At smallest masses non-linear correction is 1 3%
- Non-Abelian chiral symmetry spontaneously broken as expected
- Compatible with the fact that the bulk of the mass is given by the leading term in standard ChPT
- Relations dictated by SSB can be verified quantitatively. GMOR is maybe the simplest to start with
- An example of the potentiality. From a fit to the curve

 $0.47 \leq \Lambda_3 \leq 0.86$  GeV to be compared with



 $0.2 \leq \Lambda_3 \leq 2 \text{ GeV}$  [Gasser, Leutwyler 84]

An effective condensate can be defined as

$$\overline{\Sigma}_{\rm R} = \frac{\pi}{2V} \frac{\partial}{\partial \Lambda_{\rm R}} \, \nu_{\rm R}(\Lambda_{\rm R}, m_{\rm R})$$

prefactor so that  $\overline{\Sigma}_{\rm R}$  coincides with  $\Sigma$  at LO

A linear extrapolation to the chiral limit yields

$$\left[\Sigma_{\rm R}^{\overline{\rm MS}}(2\,{\rm GeV})\right]^{1/3} = 0.276(3)(4)(5)\;{\rm GeV}$$



The ETM collaboration from an overall fit of the pion mass and decay constant

$$\left[\Sigma_{\rm R}^{\overline{\rm MS}}(2\,{\rm GeV})\right]_{\rm GMOR}^{1/3} = 0.270(7)\,\text{GeV} \qquad \text{[ETM Coll. 09]}$$

• A clear and consistent picture is emerging. For  $m_R \leq 0.05$  GeV the GMOR formula accounts for the bulk of the pion mass. But discretization errors not quantified yet