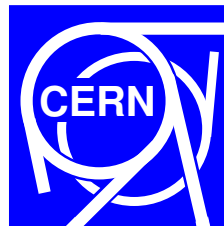


# Lattice QCD with Wilson fermions

Leonardo Giusti

CERN - Theory Group



- Spontaneous symmetry breaking in QCD
- Quark mass dependence of pion masses and decay constants
- Fermions on a lattice: the doubling problem
- Wilson fermions
- Chiral Ward identities and additive mass renormalization
- A new algorithm for full QCD simulations: SAP
- First dynamical simulations with light quarks
- Results for pion masses and decay constants

- The Euclidean QCD Lagrangian inv. under  $SU(3)$  color gauge group (formal level)

$$S_{\text{QCD}} = \int d^4x \left\{ -\frac{1}{2g^2} \text{Tr} [F_{\mu\nu} F_{\mu\nu}] + i \frac{\theta}{16\pi^2} \text{Tr} [F_{\mu\nu} \tilde{F}_{\mu\nu}] + \bar{\psi} [D + M] \psi \right\}$$

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] \quad \tilde{F}_{\mu\nu} \equiv \frac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma} \quad A_\mu = A_\mu^a T^a$$

$$D = \gamma_\mu \{ \partial_\mu + A_\mu \} \quad \psi \equiv \{ q_1, \dots, q_{N_f} \} \quad M \equiv \text{diag}\{m_1, \dots, m_{N_f}\}$$

- For  $M = 0$  the action is invariant under the global group  $U(N_f)_L \times U(N_f)_R$

$$\begin{aligned} \psi_L &\rightarrow V_L \psi_L & \bar{\psi}_L &\rightarrow \bar{\psi}_L V_L^\dagger & \psi_{L,R} &= P_\pm \psi \\ \psi_R &\rightarrow V_R \psi_R & \bar{\psi}_R &\rightarrow \bar{\psi}_R V_R^\dagger & P_\pm &= \frac{1 \pm \gamma_5}{2} \end{aligned}$$

- When the theory is quantized the chiral anomaly breaks explicitly the subgroup  $U(1)_A$
- For the purpose of this lecture we can put  $\theta = 0$
- For the rest of this lecture we will assume that heavy quarks have been integrated out and we will focus on the symmetry group  $SU(3)_L \times SU(3)_R$

# Light pseudoscalar meson spectrum

- Octet compatible with SSB pattern

$$SU(3)_L \times SU(3)_R \rightarrow SU(3)_{L+R}$$

and soft explicit symmetry breaking

$$m_u, m_d \ll m_s < \Lambda_{\text{QCD}}$$

- $m_u, m_d \ll m_s \implies m_\pi \ll m_K$

- A 9<sup>th</sup> pseudoscalar with  $m_{\eta'} \sim \mathcal{O}(\Lambda_{\text{QCD}})$

I	I <sub>3</sub>	S	Meson	Quark Content	Mass (MeV)
1	1	0	$\pi^+$	$u\bar{d}$	140
1	-1	0	$\pi^-$	$d\bar{u}$	140
1	0	0	$\pi^0$	$(d\bar{d} - u\bar{u})/\sqrt{2}$	135
$\frac{1}{2}$	$\frac{1}{2}$	+1	$K^+$	$u\bar{s}$	494
$\frac{1}{2}$	$-\frac{1}{2}$	+1	$K^0$	$d\bar{s}$	498
$\frac{1}{2}$	$-\frac{1}{2}$	-1	$K^-$	$s\bar{u}$	494
$\frac{1}{2}$	$\frac{1}{2}$	-1	$\bar{K}^0$	$s\bar{d}$	498
0	0	0	$\eta$	$\cos \vartheta \eta_8 + \sin \vartheta \eta_0$	547
0	0	0	$\eta'$	$-\sin \vartheta \eta_0 + \cos \vartheta \eta_8$	958

$$\eta_8 = (d\bar{d} + u\bar{u} - 2s\bar{s})/\sqrt{6}$$

$$\eta_0 = (d\bar{d} + u\bar{u} + s\bar{s})/\sqrt{3}$$

$$\vartheta \simeq -11^\circ$$

## Vector and Axial Ward Identities

- By grouping the generators of the  $SU(3)_L \times SU(3)_R$  group in the ones of the vector subgroup  $SU(3)_{L+R}$  plus the remaining axial generators

$$\partial_\mu \langle V_\mu^a(x) \mathcal{O} \rangle = \langle \bar{\psi}(x) [T^a, M] \psi(x) \mathcal{O} \rangle - \langle \delta_{V,x}^a \mathcal{O} \rangle$$

$$\partial_\mu \langle A_\mu^a(x) \mathcal{O} \rangle = \langle \bar{\psi}(x) \{T^a, M\} \gamma_5 \psi(x) \mathcal{O} \rangle - \langle \delta_{A,x}^a \mathcal{O} \rangle$$

where currents and densities are defined to be

$$V_\mu^a \equiv \bar{\psi} \gamma_\mu T^a \psi$$

$$A_\mu^a \equiv \bar{\psi} \gamma_\mu \gamma_5 T^a \psi$$

$$S^a \equiv \bar{\psi} T^a \psi$$

$$P^a \equiv \bar{\psi} \gamma_5 T^a \psi$$

- Ward identities encode symmetry properties of the theory, and they remain **valid even in presence of spontaneous symmetry breaking**

## Spontaneous chiral symmetry breaking in QCD

- By choosing the interpolating operator  $\mathcal{O} = P^a(0)$  the AWI reads

$$\partial_\mu \langle A_\mu^a(x) P^a(0) \rangle = \langle \bar{\psi}(x) \{T^a, M\} \gamma_5 \psi(x) P^a(0) \rangle - \frac{1}{3} \delta(x) \langle \bar{\psi} \psi \rangle$$

- In the chiral limit

$$\langle \partial_\mu A_\mu^a(x) P^a(0) \rangle = 0 \quad x \neq 0$$

and by using Lorentz invariance and power counting

$$\langle A_\mu^a(x) P^a(0) \rangle = c \frac{x_\mu}{(x^2)^2} \quad x \neq 0$$

- Integrating by parts the AWI in a ball of radius  $r$

$$\int_{|x|=r} ds_\mu(x) \langle A_\mu^a(x) P^a(0) \rangle = -\frac{3}{2} \langle \bar{\psi} \psi \rangle$$

which implies

$$\langle \partial_\mu A_\mu^a(x) P^a(0) \rangle = -\frac{3}{4\pi^2} \langle \bar{\psi} \psi \rangle \frac{x_\mu}{(x^2)^2} \quad x \neq 0$$

- If  $\langle \bar{\psi}\psi \rangle \neq 0$  the relation

$$\langle \partial_\mu A_\mu^a(x) P^a(0) \rangle = -\frac{3}{4\pi^2} \langle \bar{\psi}\psi \rangle \frac{x_\mu}{(x^2)^2} \quad x \neq 0$$

implies that the **current-density correlation function is long-ranged**

- The energy spectrum does not have a gap and the correlation function has a **particle pole at zero momentum (Goldstone theorem)**
- In the chiral limit  $\langle \bar{\psi}\psi \rangle \neq 0$  implies the presence of **8 Goldstone bosons identified with the 8 pseudoscalar light mesons  $[\pi, \dots, K, \dots, \eta]$**
- Previous relations lead to

$$\langle 0 | A_\mu^a | P^a, p_\mu \rangle = p_\mu F$$

which in turn implies that interactions among pseudoscalar mesons vanish for  $p^2 = 0$

## Quark mass dependence of the pseudoscalar mesons

- When  $M \neq 0$  (and for simplicity in the degenerate case  $M = m$ )

$$2m \int \langle P_\mu^a(x) P^a(0) \rangle = \frac{1}{3} \langle \bar{\psi} \psi \rangle$$

and therefore for  $m \rightarrow 0$

$$M_P^2 = M^2 = -2m \frac{\langle \bar{\psi} \psi \rangle}{3F^2}$$

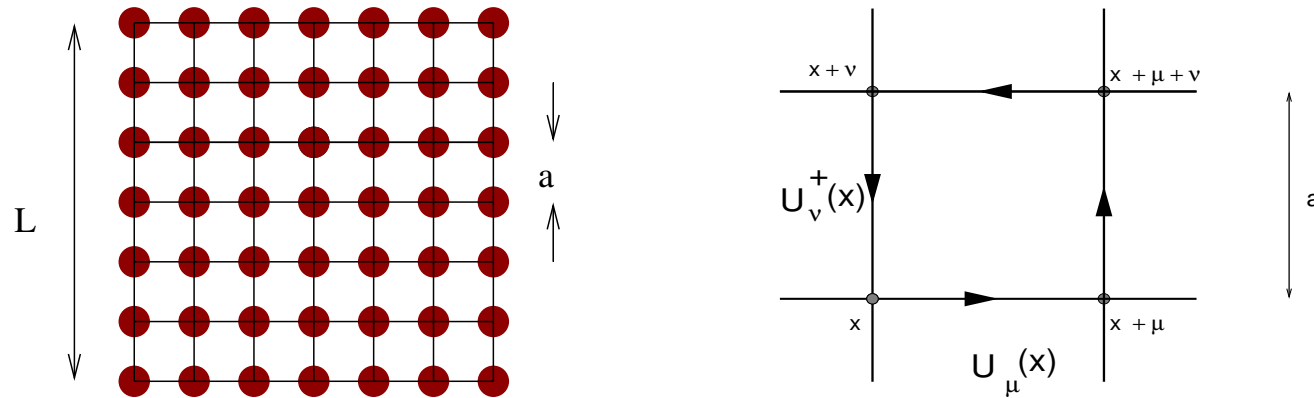
- It is possible to build an effective theory of QCD with 8 light pseudoscalar mesons as fundamental degrees of freedom
- In particular for pions, it predicts the following functional forms for masses and decay constants at NLO

$$M_\pi^2 = M^2 \left\{ 1 + \frac{M^2}{32\pi^2 F^2} \log(M^2/\mu_\pi^2) \right\}$$

$$F_\pi = F \left\{ 1 - \frac{M^2}{16\pi^2 F^2} \log(M^2/\mu_F^2) \right\}$$



# Lattice regularization of QCD



- The Wilson action for the  $SU(3)$  Yang–Mills theory is

$$S_{\text{YM}} = \frac{6}{g^2} \sum_{x, \mu < \nu} \left\{ 1 - \frac{1}{6} \text{Tr} \left[ U_{\mu\nu}(x) + U_{\mu\nu}^\dagger(x) \right] \right\}$$

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

- For small gauge fields (perturbation theory)  $U_\mu(x) \simeq 1 - aA_\mu(x)$
- Correlation functions computed non-perturbatively via **Monte Carlo** techniques

$$\langle O_1(x) O_2(0) \rangle = \int \mathcal{D}U e^{-S_{\text{YM}}(U)} O_1(U; x) O_2(U; 0)$$

- Given a generic massive Dirac operator  $D(x, y)$  and the corresponding action

$$S_F = \sum_{x,y} \bar{\psi}(x) D(x, y) \psi(x) \quad \psi \equiv \{q_1, \dots, q_{N_f}\}$$

the functional integral is defined to be

$$Z = \int \delta U \delta \psi \delta \bar{\psi} \exp \{-S_{\text{YM}} - S_F\}$$

- By integrating over the Grassman fields, a generic Euclidean corr. function is

$$\langle O_1(x_1) O_2(x_2) \rangle = \frac{1}{Z} \int \delta U e^{-S_{\text{YM}}} \text{Det} D [O_1(x_1) O_2(x_2)]_{\text{Wick}}$$

- For vector gauge theories and positive masses,  $\text{Det} D$  is real and positive
- Correlation functions can be computed non-perturbatively via **Monte Carlo** techniques

## Naive discretization of the Dirac operator

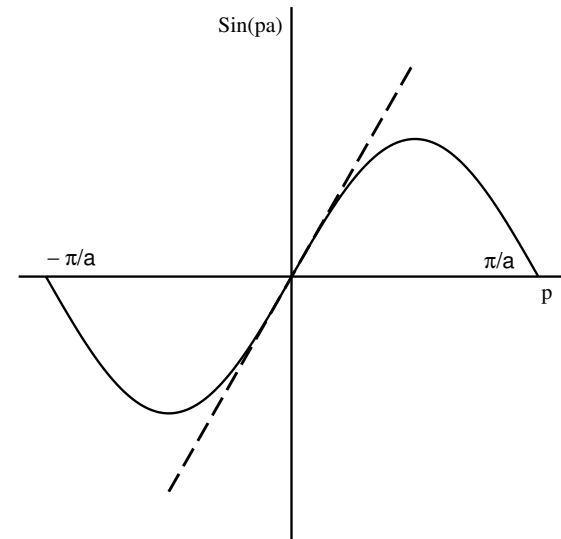
- The naive gauge invariant discretization of the Dirac operator is

$$D = \frac{1}{2} \gamma_\mu \{ \nabla_\mu^* + \nabla_\mu \} + m$$

where ( $a$  is the lattice spacing)

$$\nabla_\mu \psi(x) = \frac{1}{a} \left[ U_\mu(x) \psi(x + a\hat{\mu}) - \psi(x) \right]$$

$$\nabla_\mu^* \psi(x) = \frac{1}{a} \left[ \psi(x) - U_\mu^\dagger(x - a\hat{\mu}) \psi(x - a\hat{\mu}) \right]$$



- In the free case and in the Fourier basis ( $\bar{p}_\mu = \sin(p_\mu a)/a$ )

$$\tilde{D}^{-1}(p) = \frac{-i\gamma_\mu \bar{p}_\mu + m}{\bar{p}^2 + m^2}$$

there are 15 extra poles (doublers)!

● The following properties cannot hold simultaneously for free fermions on the lattice:

1.  $\tilde{D}(P)$  is an analytic periodic function of  $p_\mu$  with period  $2\pi/a$
2. For  $p_\mu \ll \pi/a$   $\tilde{D}(P) = i\gamma_\mu p_\mu + \mathcal{O}(ap^2)$
3.  $\tilde{D}(P)$  is invertible at all non-zero momenta (mod  $2\pi/a$ )
4.  $D$  anti-commute with  $\gamma_5$  (for  $m = 0$ )

● (1) is needed for locality, (2) and (3) ensures the correct continuum limit

● Chiral symmetry in the continuous form (4) must be broken on the lattice

● Physics essence: if action invariant under standard chiral sym.  $\implies$  no chiral anomaly

- Wilson's proposal is to add an **irrelevant operator** to the action

$$D_W = \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - a \nabla_\mu^* \nabla_\mu \} + m^0$$

which breaks chiral symmetry explicitly ( $SU(3)_{L+R}$  vector symmetry preserved!)

- The Wilson term  $a \nabla_\mu^* \nabla_\mu$  removes the doubler poles. In the free case

$$\tilde{D}^{-1}(p) = \frac{-i\gamma_\mu \bar{p}_\mu + m^0(p)}{\bar{p}^2 + m^0(p)^2} \quad m^0(p) \equiv m^0 + \frac{a}{2} \hat{p}^2$$

where  $\hat{p}_\mu = \frac{2}{a} \sin\left(\frac{p_\mu a}{2}\right)$

- At the classical level **Wilson term is irrelevant**, it gives vanishing contributions for  $a \rightarrow 0$

- By performing a non-singlet axial rotation in the functional integral

$$\partial_\mu \langle A_\mu^a(x) \mathcal{O} \rangle = \langle \bar{\psi}(x) \{ T^a, M^0 \} \gamma_5 \psi(x) \mathcal{O} \rangle + \langle X^a(x) \mathcal{O} \rangle - \langle \delta_x^a \mathcal{O} \rangle$$

- At the classical level the operator  $X^a(x)$  vanishes for  $a \rightarrow 0$ . In the quantum theory the  $1/a$  ultraviolet divergences make the insertion of this operator non-vanishing

$$\frac{1}{a} \mathcal{O}(a) \simeq \mathcal{O}(1)$$

- The operator  $X^a(x)$  can be made finite by subtracting all operators of lower dimensions with proper coefficients

$$\bar{X}^a = X^a + \bar{\psi} \left\{ T^a, \bar{M} \right\} \gamma_5 \psi + (Z_A - 1) \partial_\mu A_\mu^a$$

- By inserting  $\bar{X}^a$  in the AWI

$$Z_A \partial_\mu \langle A_\mu^a(x) \mathcal{O} \rangle = \langle \bar{\psi}(x) \{ T^a, M^0 - \bar{M} \} \gamma_5 \psi(x) \mathcal{O} \rangle + \langle \bar{X}^a(x) \mathcal{O} \rangle - \langle \delta_x^a \mathcal{O} \rangle$$

- If we define the renormalized pseudoscalar density to be  $\hat{P}^a = Z_P P^a$ , since it cannot mix with  $\partial_\mu A_\mu^a$

$$\hat{A}_\mu^a = Z_A A_\mu^a \quad \hat{M} = \frac{M^0 - \bar{M}}{Z_P}$$

are finite and correspond to the proper definition of axial currents and quark masses, i.e. the ones that satisfy the AWI in the continuum limit

- For degenerate quarks the “on-shell” non-perturbative definition of the quark mass is

$$\hat{m} = \frac{1}{2} \frac{Z_A \partial_\mu \langle A_\mu^a(x) P^a(0) \rangle}{\langle P^a(x) P^a(0) \rangle}$$

and if there is SSB the Goldstone bosons become massless when  $\hat{m} = 0$

- No conceptual problems for defining non-perturbatively a theory with a global chiral-symmetry
- Operators in different chiral representations get mixed: renormalization procedure complicated, but extra mixings fixed by WIs
- Additive quark-mass renormalization
- Spectrum and matrix elements have  $O(a)$  discretization effects
- Lengthy but known procedure to remove them and remain with  $O(a^2)$



- First-principle results when all systematic uncertainties quantified
- Main sources of errors:
  1. Statistical errors
  2. Finite volume:  $L = 1.5 \rightarrow 5 \text{ fm}$
  3. Continuum limit:  $a = 0.04 \rightarrow 0.1 \text{ fm}$
  4. Chiral extrapolation:  $M_\pi = 200 \rightarrow 500 \text{ MeV}$
- On the lattice they can be estimated and (eventually) removed without extra free parameters or dynamical assumptions (QFT,V, Alg., CPU)

- A generic Euclidean correlation function can be written as

$$\langle O_1(x_1) O_2(x_2) \rangle = \frac{1}{Z} \int \delta U e^{-S_{\text{YM}}} \text{Det} D_W [O_1(x_1) O_2(x_2)]_{\text{Wick}}$$

- For two degenerate flavors and positive mass,  $\text{Det} D_W$  is real and positive.
- $L \sim 2 \text{ fm}$  and  $a \sim 0.08 \text{ fm} \Rightarrow \text{dim}[D_W] \sim 4 \cdot 10^6$ : computing and diagonalizing the full matrix is not feasible
- By introducing pseudo-fermion fields

$$\langle O_1(x_1) O_2(x_2) \rangle = \frac{1}{Z} \int \delta U \delta \phi \delta \phi^\dagger e^{-S_{\text{YM}} - \sum \phi^\dagger D_W^{-1} \phi} [O_1(x_1) O_2(x_2)]_{\text{Wick}}$$

- The determinant contribution can be taken into account by computing  $\phi^\dagger D_W^{-1} \phi$  several times for each acceptance-rejection step

## Quenched approximation

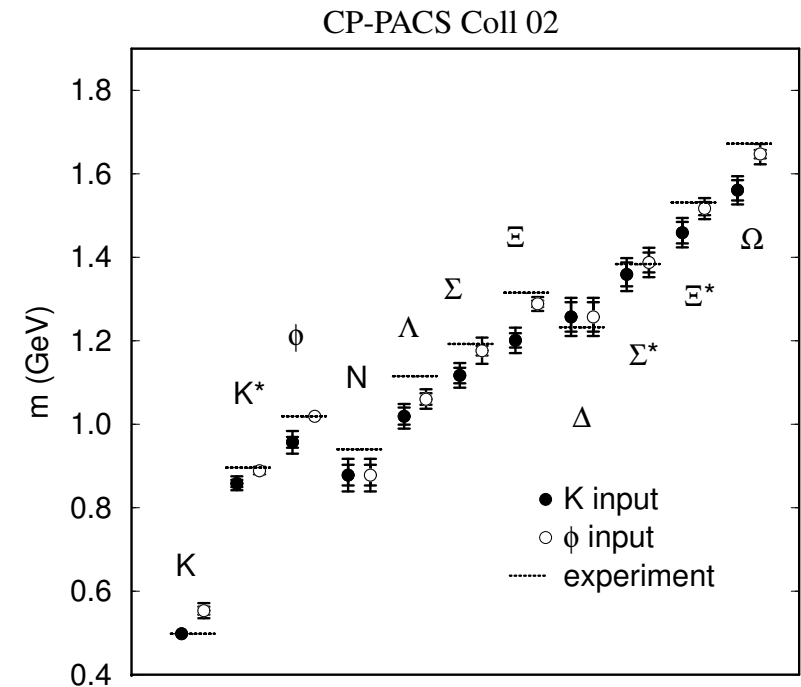
- Fermion determinant replaced by its average value

$$\langle O \rangle = \int \mathcal{D}U e^{-S_G} [\text{Det} \cancel{D}]^{N_f} O$$

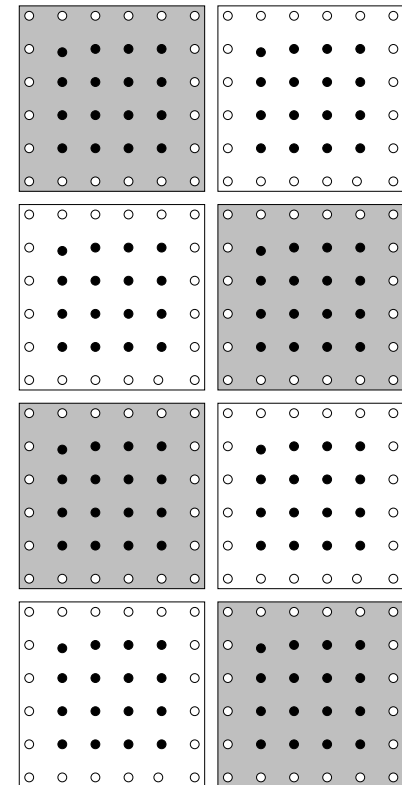
- Quenching is not a systematic approximation

- Quenched light hadron spectrum:  $\sim 10\%$  discrepancy with experiment

- For some quantities quenching is the only systematics **not quantified**



- Decomposition of the lattice into blocks with Dirichlet b.c.  
with  $q \geq \pi/L > 1 \text{ GeV}$
- Asymptotic freedom: quarks are weakly interacting in the blocks  
 $\implies$  QCD easy (*cheaper*) to simulate
- Block interactions are weak and are taken into account exactly



$$S(x, y) \sim \frac{1}{|x - y|^3}$$

# Block decomposition of the Dirac operator

## ● The Wilson–Dirac operator

$$D_W = \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^* \nabla_\mu \} + m_0$$

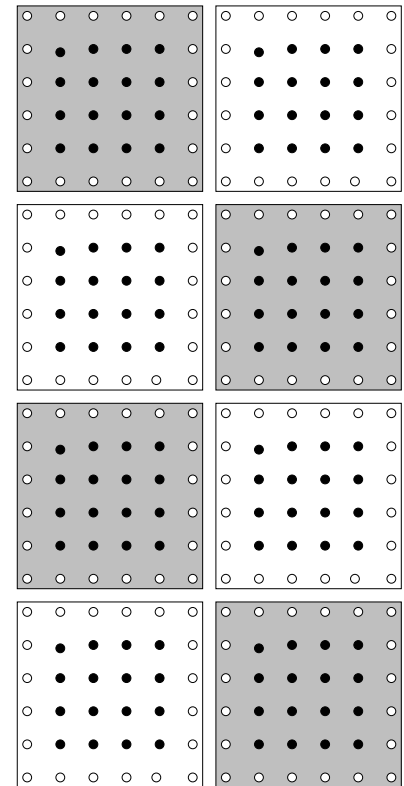
can be decomposed as

$$D_W = D_{\Omega^*} + D_{\Omega} + D_{\partial\Omega^*} + D_{\partial\Omega}$$

where

$$D_{\Omega^*} = \sum_{\text{white } \Lambda} D_{\Lambda}$$

$$D_{\Omega} = \sum_{\text{black } \Lambda} D_{\Lambda}$$



$\Omega^*$ ,  $\Omega$  are white and black blocks,  $\partial\Omega$ ,  $\partial\Omega^*$  are exterior boundaries

## Factorization of the determinant

- The determinant of the Dirac operator written as

$$\det D_W = \prod_{\text{all } \Lambda} \det \hat{D}_\Lambda \det R$$

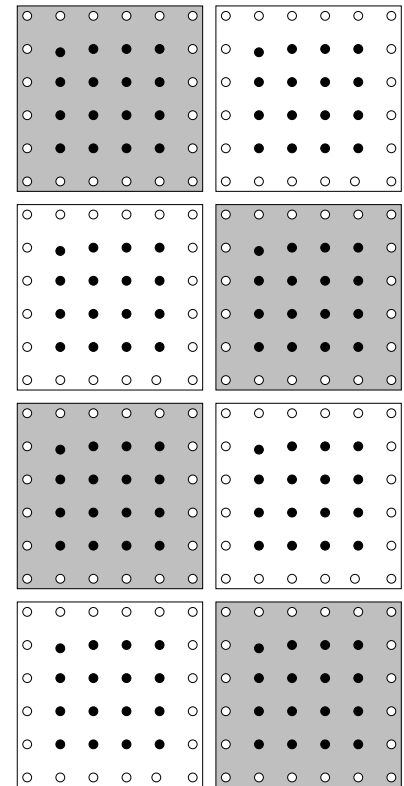
with the block interaction

$$R = 1 - P_{\partial\Omega^*} D_\Omega^{-1} D_{\partial\Omega} D_{\Omega^*}^{-1} D_{\partial\Omega^*}$$

- For two flavors can be written as integral over scalar fields

$$S_{\phi\chi} = \sum_{\text{all } \Lambda} \|\hat{D}_\Lambda^{-1} \phi_\Lambda\|^2 + \|R^{-1} \chi\|^2$$

where  $\phi_\Lambda$  defined on  $\Lambda$  and  $\chi$  on  $\partial\Omega^*$



- In molecular dynamics force naturally split

$$\frac{d}{dt}\Pi(x, \mu) = -F_G(x, \mu) - F_\Lambda(x, \mu) - F_R(x, \mu)$$

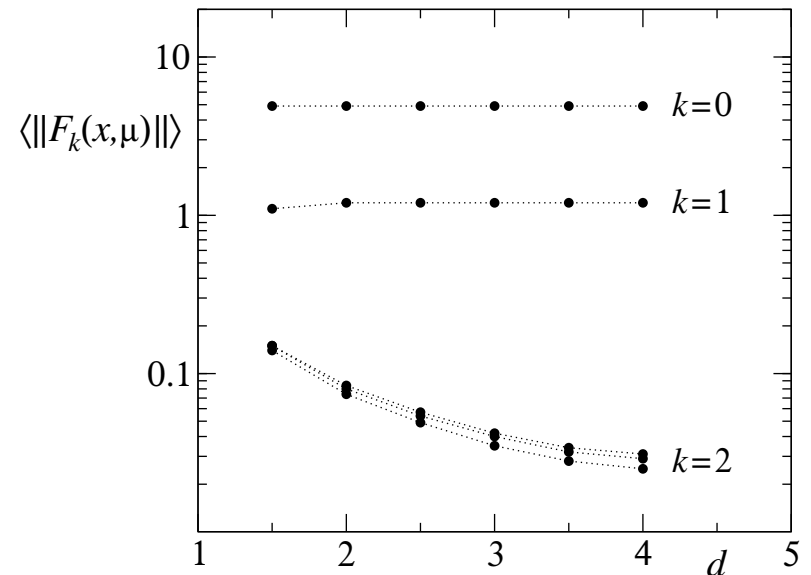
$$\frac{d}{dt}U(x, \mu) = \Pi(x, \mu)U(x, \mu)$$

- Integration step-sizes chosen such that

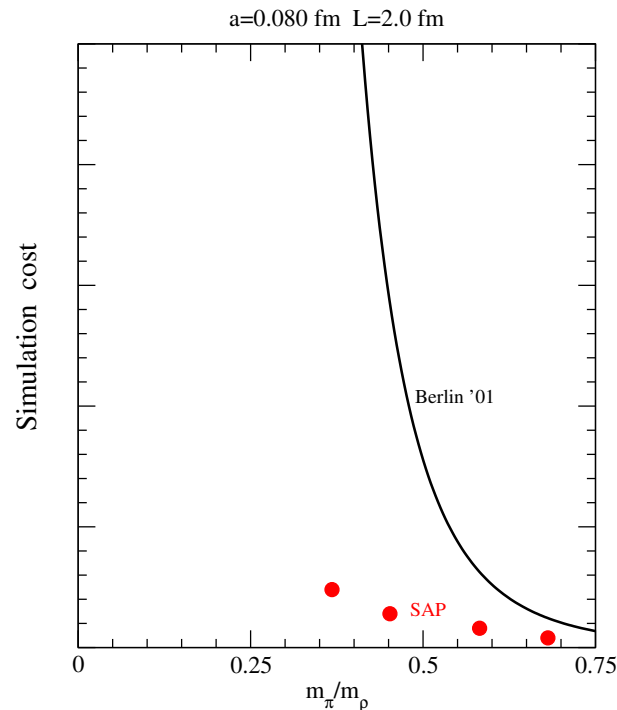
$$\epsilon_G ||F_G|| \sim \epsilon_\Lambda ||F_\Lambda|| \sim \epsilon_R ||F_R||$$

i.e. the most expensive force computed less often!

- Do not give up first-principles: teach Physics to exact algorithms for being smarter (*faster*)!

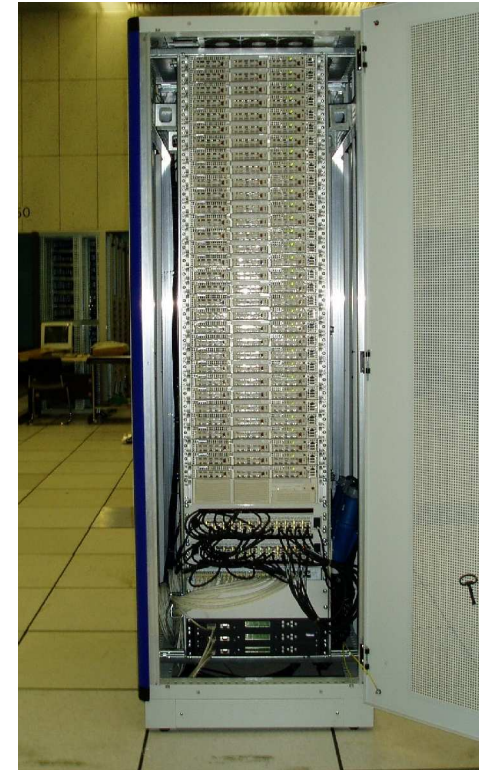


$$C_{\text{ost}} \propto N_{\text{conf}} m_q^{-1} L^5 a^{-6}$$



Volume	a[fm]	$\sim m_\pi/m_s$	$N_{\text{conf}}$
$24^3 \times 32$	$\sim 0.080$	0.93	64
		0.48	109
		0.30	100
		0.17	100
$32^3 \times 64$	$\sim 0.065$	0.72	100
		0.38	100
		0.27	100
		0.20	100

PC cluster with 32 Nodes (64 Xeon procs)  
( $\sim 160$  Gflops sustained)



- Full statistics for small lattice:  
 $\sim 60$  days @ 32 nodes
- All confs archived @ CERN
- First goal: verifying QCD SSB and make contact w. ChPT



- We computed two-point correlation functions of bilinears

$$C_{AA}(t) = \sum_{\vec{x}} \langle A_0^a(x) A_0^a(0) \rangle$$

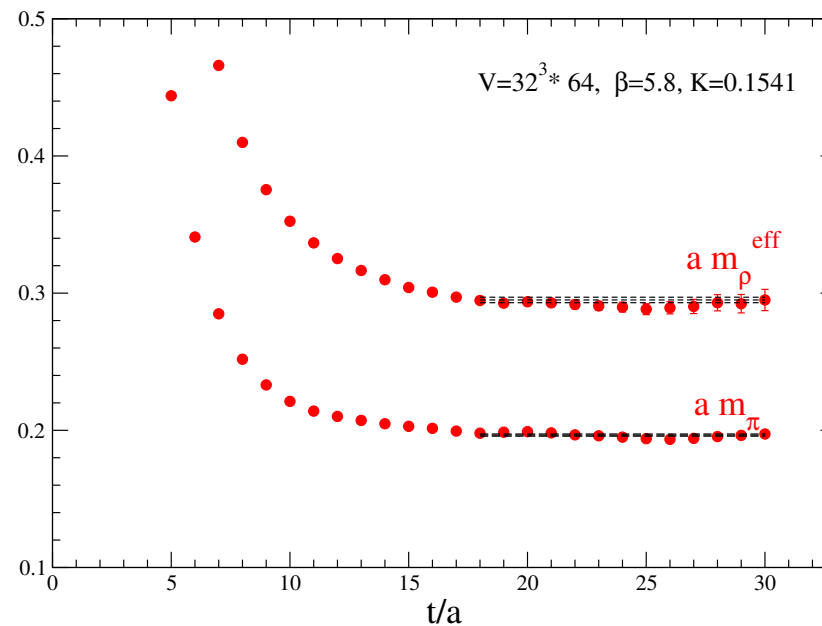
which for large times  $t \rightarrow \infty$  (and for  $T \rightarrow \infty$ )

$$\begin{aligned} C_{AA}(t) &\longrightarrow \frac{|\langle 0 | A_0^a | \pi \rangle|^2}{M_P} e^{-\frac{M_P T}{2}} \cosh \left[ M_P \left( \frac{T}{2} - t \right) \right] \\ &\longrightarrow \frac{|\langle 0 | A_0^a | \pi \rangle|^2}{2M_P} e^{-\frac{M_P t}{2}} \end{aligned}$$

- Euclidean correlation functions of **bare operators** at **finite volume** and **finite cut-off** computed **non-perturbatively** with SAP

## Correlation functions on the finer lattice

$$\sum_{\vec{x}} \langle O(x, t) O(0, 0) \rangle \propto e^{-m_O(t)t}$$

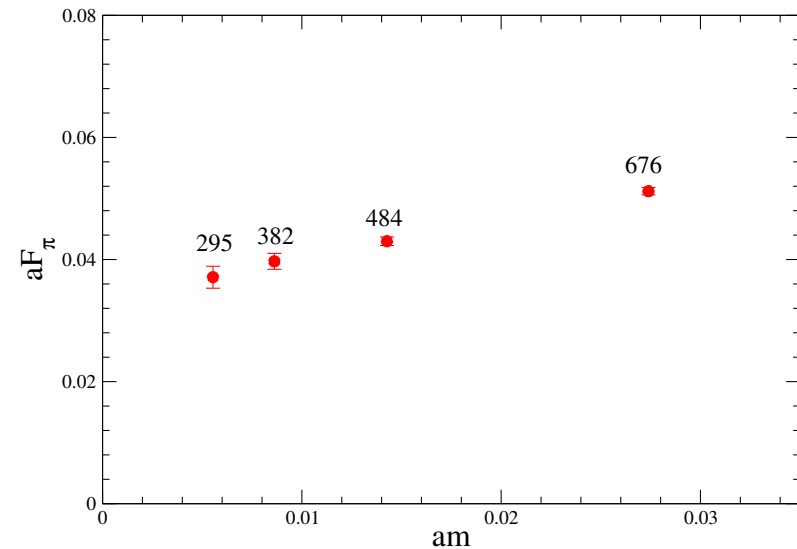
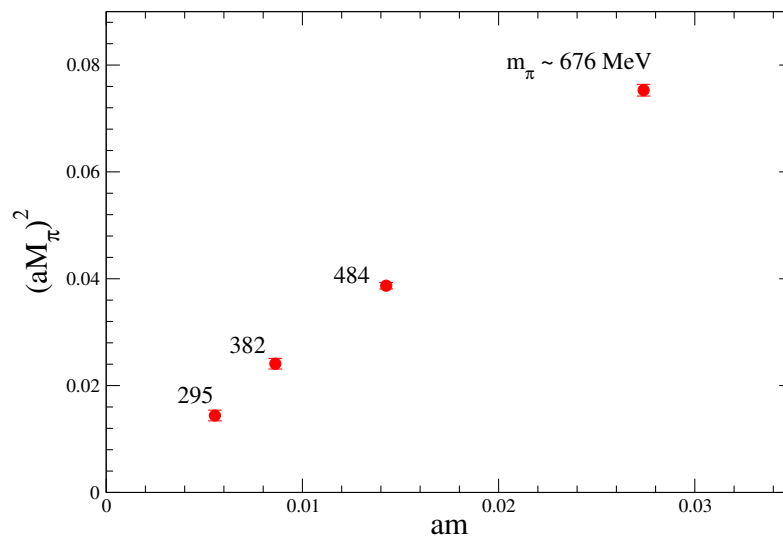


● Algorithm stable over the relevant parameter ranges:

1. Quark mass:  $m \sim m_s/6$  ✓
2. Lattice spacing:  $a \sim 0.065$  fm ✓
3. Volume:  $L \sim 2$  fm ✓

# First results for pion mass and decay constant

Volume	$a[\text{fm}]$	$am$	$am_\pi$	$aF_\pi$
$24^3 \times 32$	$\sim 0.080$	0.0274(3)	0.274(2)	0.0648(8)
		0.0143(2)	0.197(2)	0.0544(9)
		0.0086(2)	0.155(3)	0.0500(17)
		0.0055(2)	0.121(4)	0.0461(23)



## Chiral behavior of $M_\pi$

- At the NLO in SU(2) ChPT [J. Gasser, H. Leutwyler '84]

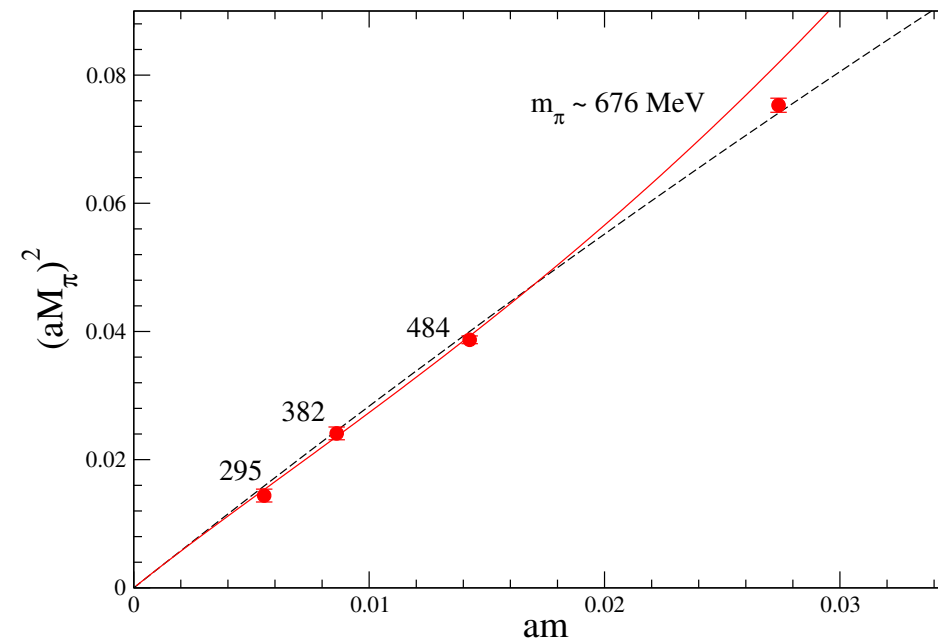
$$M_\pi^2 = M^2 \left\{ 1 + \frac{M^2}{32\pi^2 F^2} \log(M^2/\mu_\pi^2) \right\}$$

with  $M^2 = 2B\hat{m}$

- Data below  $M_\pi \sim 500$  MeV are **compatible (within errors) with NLO ChPT**
- Smaller lattice spacing confirms the picture
- For comparison: from Nature

$$M_\pi^2/M^2 \sim \text{const} \sim 0.956(8)$$

in the range  $M = 200 - 500$  MeV



## Chiral behavior of $F_\pi$

- NLO SU(2) ChPT gives [J. Gasser, H. Leutwyler '84]

$$F_\pi = F \left\{ 1 - \frac{M^2}{16\pi^2 F^2} \log(M^2/\mu_F^2) \right\}$$

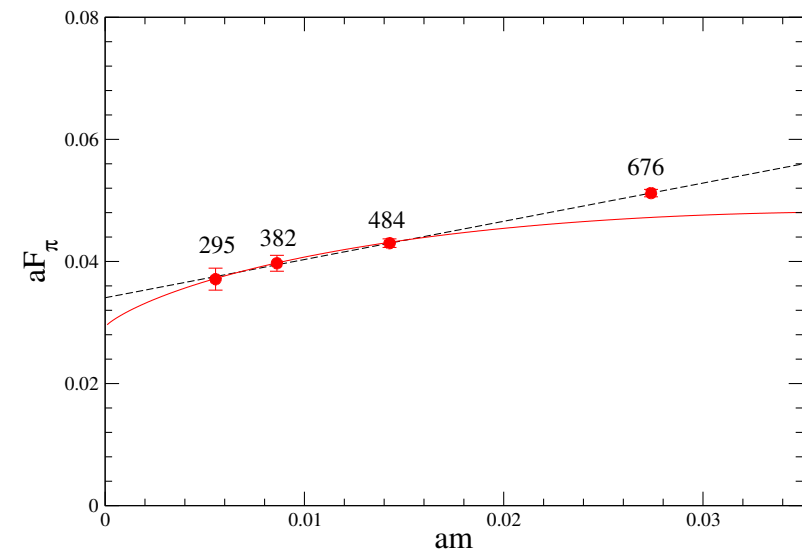
- Fitting points below  $M_\pi \sim 500$  MeV (Preliminary!)

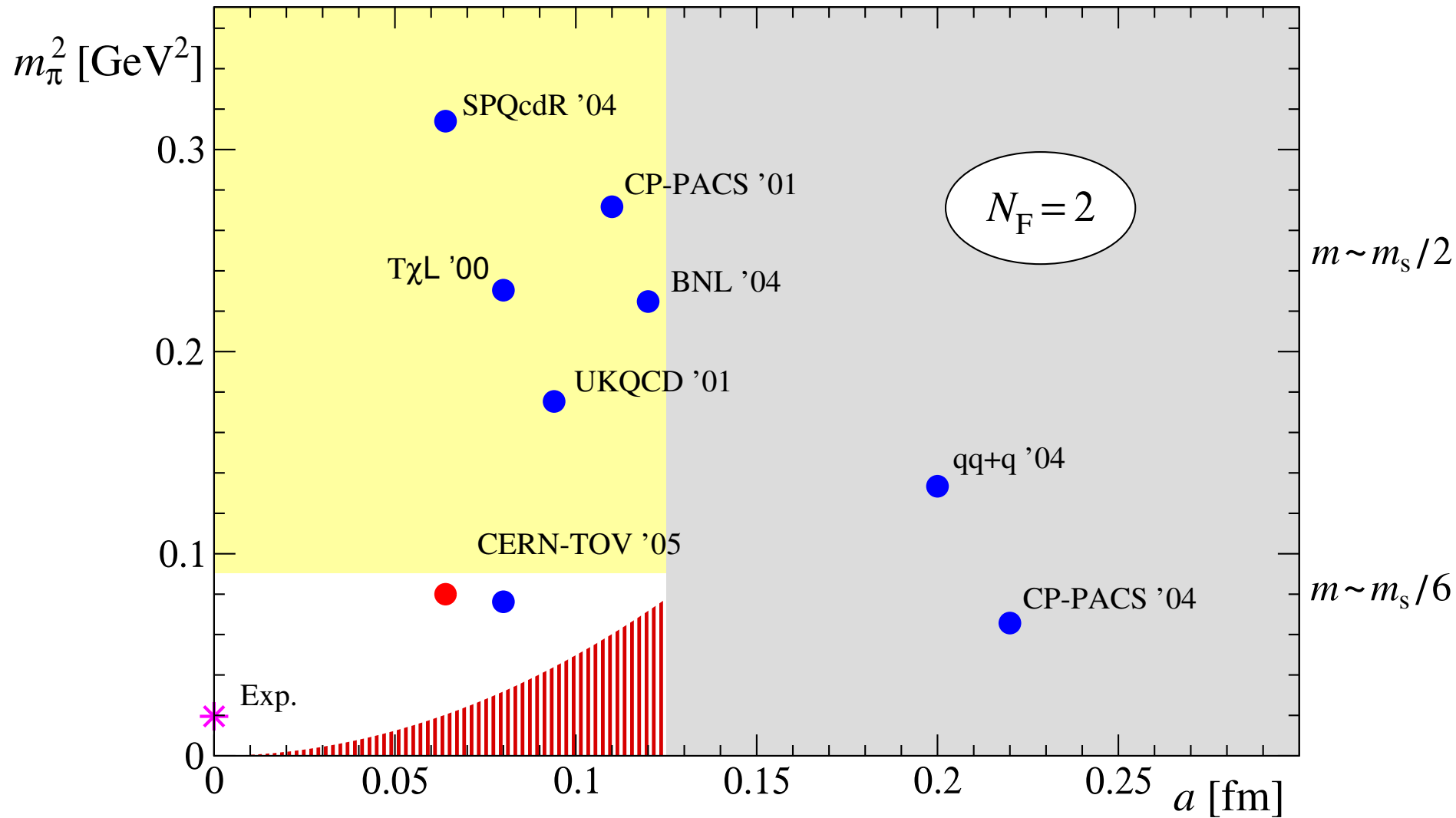
$$F_\pi \sim 80(7)\text{MeV}$$

with  $Z_A$  from 1-loop PT

- Full analysis at small lattice spacing in progress

- Also in this case data are **compatible**  
(within errors) with NLO ChPT





- Wilson fermions are theoretically well founded
- No conceptual problems for defining non-perturbatively a (global) chiral-symmetric theory with a regularization which breaks chiral symmetry
- The continuum limit has to be taken after a proper renormalization procedure
- QCD spontaneous symmetry breaking can be studied with systematics under control
- First results with SAP: a breakthrough in full QCD simulations
- First goal: SSB observed in QCD and contact with ChPT established