Lattice QCD with Wilson fermions

Leonardo Giusti

CERN - Theory Group

Outline

- 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)

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

$$F_{\mu\nu} \equiv \partial_\mu A_\nu - \partial_\nu A_\mu + [A_\mu, A_\nu] \qquad \tilde{F}_{\mu\nu} \equiv \tfrac{1}{2} \epsilon_{\mu\nu\rho\sigma} F_{\rho\sigma} \qquad A_\mu = A^a_\mu \, \mathcal{T}^a$$

$$D = \gamma_\mu \left\{ \partial_\mu + A_\mu \right\} \qquad \psi \equiv \left\{ q_1, \ldots, q_{N_{\rm f}} \right\} \qquad M \equiv \mathrm{diag}\{ m_1, \ldots, m_{N_{\rm f}} \}$$

- For $M = 0$ the action is invariant under the global group $U(N_{\rm f})_{\rm L} \times U(N_{\rm f})_{\rm R}$

$$\psi_L \to V_L \psi_L \qquad \bar{\psi}_L \to \bar{\psi}_L V_L^\dagger \qquad \psi_{L,R} = P_\pm \psi$$

$$\psi_R \to V_R \psi_R \qquad \bar{\psi}_R \to \bar{\psi}_R V_R^\dagger \qquad P_\pm = \frac{1 \pm \gamma_5}{2}$$

- 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 $SU(3)_{\rm L} \times SU(3)_{\rm R}$

- Octet compatible with SSB pattern

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

and soft explicit symmetry breaking

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

- $m_u, m_d \ll m_s \Longrightarrow m_\pi \ll m_{\rm K}$

- A $9^{\rm th}$ pseudoscalar with $m_{\eta'} \sim \mathcal{O}(\Lambda_{\rm QCD})$

I	I_3	S	Meson	Quark Content	Mass (MeV)
1	1	0	π^+	$u\bar{d}$	140
1	-1	0	π^-	$d\bar{u}$	140
1	0	0	π^0	$(d\bar{d} - u\bar{u})/\sqrt{2}$	135
$\frac{1}{2}$	$\frac{1}{2}$	+1	$\rm K^+$	$u\bar{s}$	494
$\frac{1}{2}$	$-\frac{1}{2}$	+1	$\rm K^0$	$d\bar{s}$	498
$\frac{1}{2}$	$-\frac{1}{2}$	-1	$\rm K^-$	$s\bar{u}$	494
$\frac{1}{2}$	$\frac{1}{2}$	-1	$\overline{\rm K}^0$	$s\bar{d}$	498
0	0	0	η	$\cos\vartheta\eta_8 + \sin\vartheta\eta_0$	547
0	0	0	η'	$-\sin\vartheta\eta_0 + \cos\vartheta\eta_8$	958

$$\begin{aligned} \eta_8 &= (d\bar{d} + u\bar{u} - 2s\bar{s})/\sqrt{6} \\ \eta_0 &= (d\bar{d} + u\bar{u} + s\bar{s})/\sqrt{3} \\ \vartheta &\simeq -11^\circ \end{aligned}$$

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

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

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

where currents and densities are defined to be

$$V_\mu^a \equiv \bar\psi\gamma_\mu T^a\psi \qquad A_\mu^a \equiv \bar\psi\gamma_\mu\gamma_5 T^a\psi$$

$$S^a \equiv \bar\psi T^a\psi \qquad P^a \equiv \bar\psi\gamma_5 T^a\psi$$

- 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

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

- In the chiral limit

$$\langle \partial_\mu A^a_\mu(x) P^a(0) \rangle = 0 \qquad x \neq 0$$

and by using Lorentz invariance and power counting

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

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

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

which implies

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

Pseudoscalar mesons as Goldstone bosons of the theory

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

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

  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 $[\pi, \ldots, , K, \ldots, \eta]$

- Previous relations lead to

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

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

- When $M \neq 0$ (and for simplicity in the degenerate case $M = m\mathbb{1}$)

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

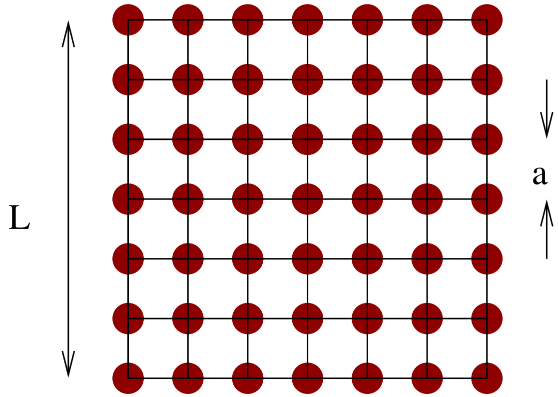
and therefore for $m \to 0$

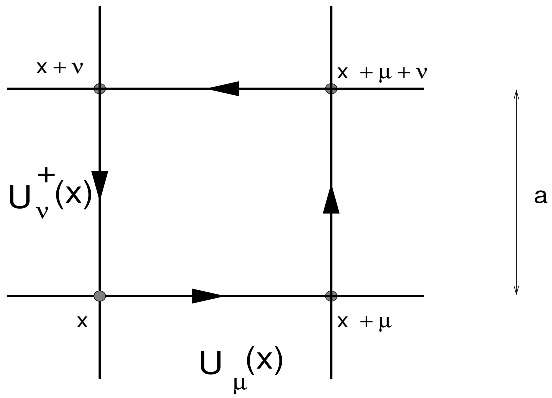
$$M_P^2 = M^2 = -2\,m \frac{\langle\bar\psi\psi\rangle}{3F^2}$$

- 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

$$\begin{aligned} M_\pi^2 &= M^2 \left\{1 + \frac{M^2}{32\pi^2 F^2}\log(M^2/\mu_\pi^2)\right\} \\ F_\pi &= F\left\{1 - \frac{M^2}{16\pi^2 F^2}\log(M^2/\mu_F^2)\right\} \end{aligned}$$





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

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

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

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

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

Lattice regularization of QCD

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

$$S_{\rm F} = \sum_{x,y} \bar\psi(x) D(x,y) \psi(x) \qquad \psi \equiv \left\{ q_1, \dots, q_{{\rm N}_f} \right\}$$

the functional integral is defined to be

$$Z = \int \delta U \delta\psi \delta\bar\psi \, \exp\left\{ -S_{\rm YM} - S_{\rm F} \right\}$$

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

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

- For vector gauge theories and positive masses, Det D is real and positive

- Correlation functions can be computed non-perturbatively via Monte Carlo techniques

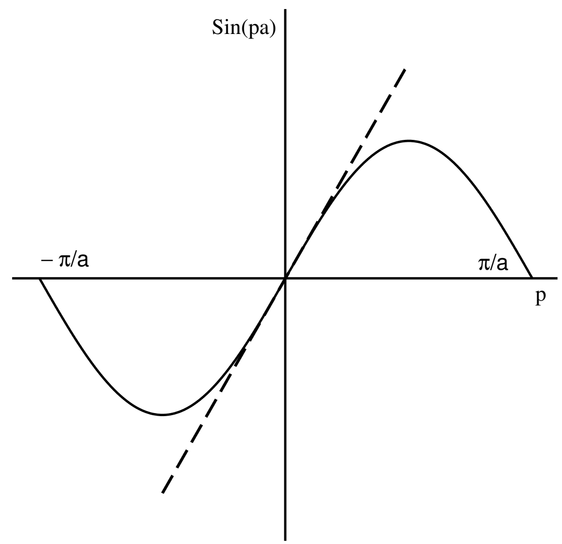
Naive discretization of the Dirac operator

- The naive gauge invariant discretization of the Dirac operator is

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

where (a is the lattice spacing)

$$\begin{aligned}\nabla_\mu \psi(x) &= \tfrac{1}{a}\Big[U_\mu(x)\psi(x+a\hat{\mu}) - \psi(x)\Big] \\ \nabla_\mu^* \psi(x) &= \tfrac{1}{a}\Big[\psi(x) - U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})\Big]\end{aligned}$$



- 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)!

Nielsen-Ninomiya theorem Nielsen Ninomiya 81

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

  1. $\tilde{D}(P)$ is an analytic periodic function of p_μ with period $2\pi/a$
  2. For $p_\mu \ll \pi/a \quad \tilde{D}(P) = i\gamma_\mu p_\mu + \mathcal{O}(ap^2)$
  3. $\tilde{D}(P)$ is invertible at all non-zero momenta (mod $2\pi/a$)
  4. D anti-commute with γ_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. $\Longrightarrow$ no chiral anomaly

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

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

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

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

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 $a \to 0$

Axial Ward identities for Wilson fermions Bochicchio et al. 85

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

$$\partial_\mu \langle A^a_\mu(x) \mathcal{O}\rangle = \langle \bar\psi(x) \left\{T^a, M^0\right\} \gamma_5 \psi(x) \mathcal{O}\rangle + \langle X^a(x)\mathcal{O}\rangle - \langle \delta^a_x \mathcal{O}\rangle$$

- At the classical level the operator $X^a(x)$ vanishes for $a \to 0$. 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

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

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

$$Z_A \partial_\mu \langle A^a_\mu(x) \mathcal{O} \rangle = \langle \bar{\psi}(x) \left\{ T^a, M^0 - \bar{M} \right\} \gamma_5 \psi(x) \mathcal{O} \rangle + \langle \bar{X}^a(x) \mathcal{O} \rangle - \langle \delta^a_x \mathcal{O} \rangle$$

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

$$\hat{A}^a_\mu = Z_A A^a_\mu \qquad \hat{M} = \frac{M^0 - \bar{M}}{Z_P}$$

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

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

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

Some comments on Wilson fermions

- 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 effecs
- Lengthy but known procedure to remove them and remain with $\mathcal{O}(a^2)$

First-principle results from lattice simulations

- First-principle results when all systematic uncertainties quantified

- Main sources of errors:

  1. Statistical errors
  2. Finite volume: $L = 1.5 \rightarrow 5$ fm
  3. Continuum limit: $a = 0.04 \rightarrow 0.1$ fm
  4. Chiral extrapolation: $M_\pi = 200 \rightarrow 500$ 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

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

- For two degenerate flavors and positive mass, ${\rm Det} D_W$ is real and positive.

- $L \sim 2$ fm and $a \sim 0.08$ fm $\Longrightarrow$ ${\rm dim}[D_W] \sim 4 \cdot 10^6$: computing and diagonalizing the full matrix is not feasible

- By introducing pseudo-fermion fields

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

- 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

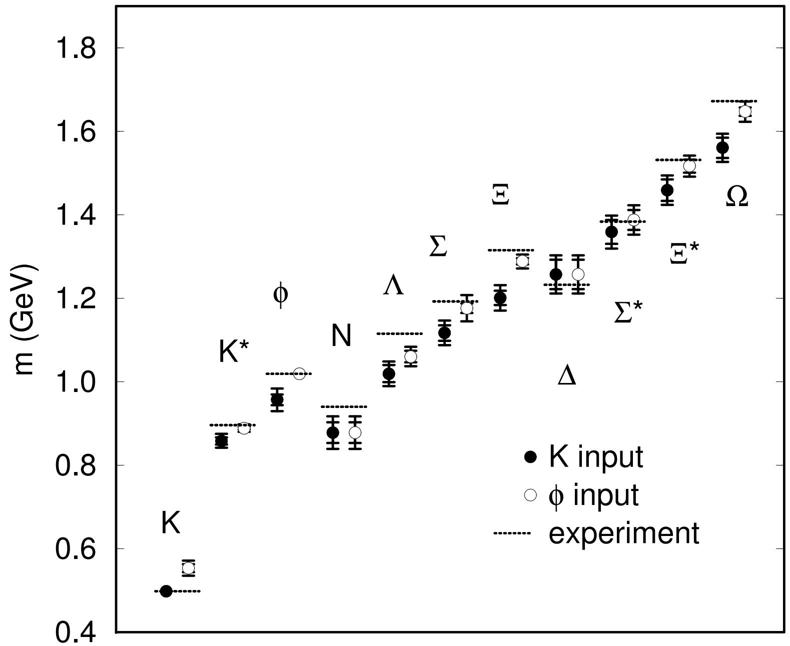
$$\langle O \rangle = \int \mathcal{D}U e^{-S_{\rm G}} \, \cancel{[\mathrm{Det}\,\mathrm{D}]^{\mathrm{N_f}}} \; O$$

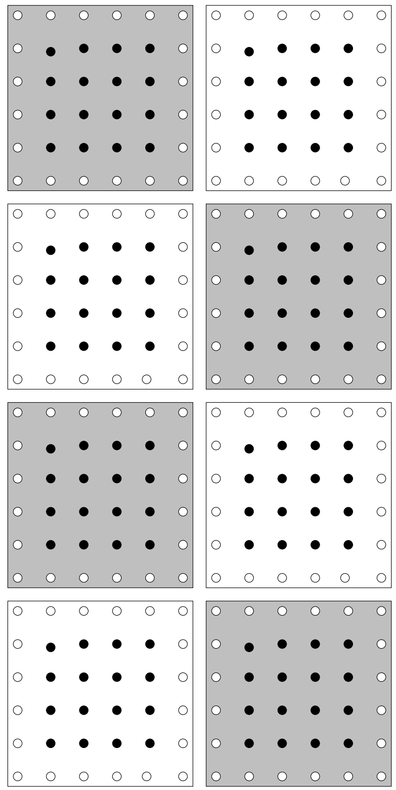
- Quenching is not a systematic approximation

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

- For some quantities quenching is the only systematics not quantified

CP-PACS Coll 02





- Decomposition of the lattice into blocks with Dirichlet b.c. with $q \geq \pi/L > 1$ GeV

- Asymptotic freedom: quarks are weakly interacting in the blocks $\Longrightarrow$ 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

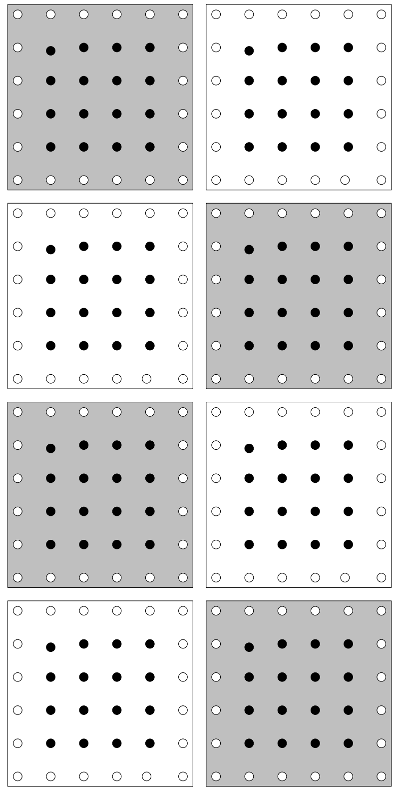
- The Wilson–Dirac operator

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

can be decomposed as

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

where



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

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

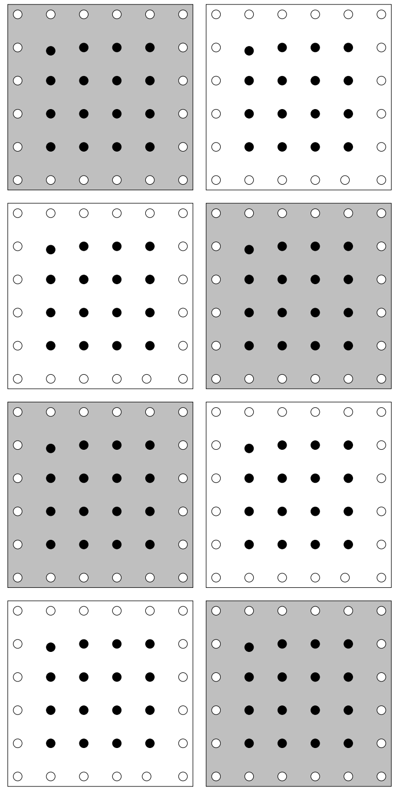
Factorization of the determinant

- The determinant of the Dirac operator written as

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

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

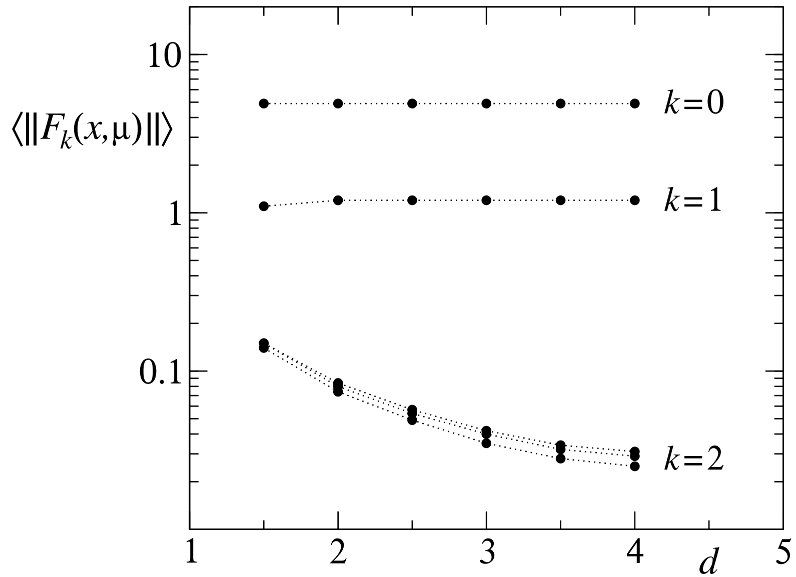
$$S_{\phi\chi} = \sum_{\mathrm{all}\ \Lambda} ||\hat{D}_\Lambda^{-1}\phi_\Lambda||^2 + ||R^{-1}\chi||^2$$

where ϕ_Λ defined on Λ and χ on $\partial\Omega^*$

- In molecular dynamics force naturally split

$$\frac{d}{dt}\Pi(x,\mu) = -F_{\rm G}(x,\mu) - F_{\Lambda}(x,\mu) - F_{\rm R}(x,\mu)$$

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



- Integration step-sizes chosen such that

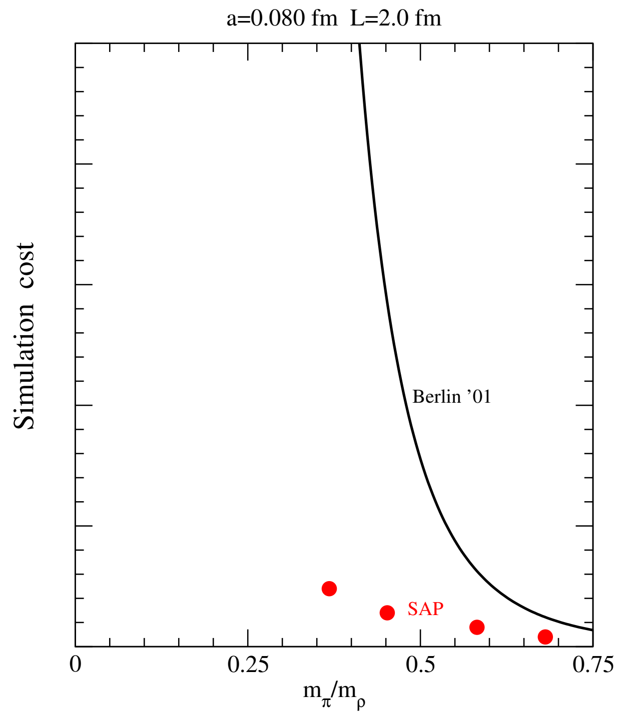
$$\epsilon_{\rm G}||F_{\rm G}|| \sim \epsilon_{\Lambda}||F_{\Lambda}|| \sim \epsilon_{\rm R}||F_{\rm R}||$$

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

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

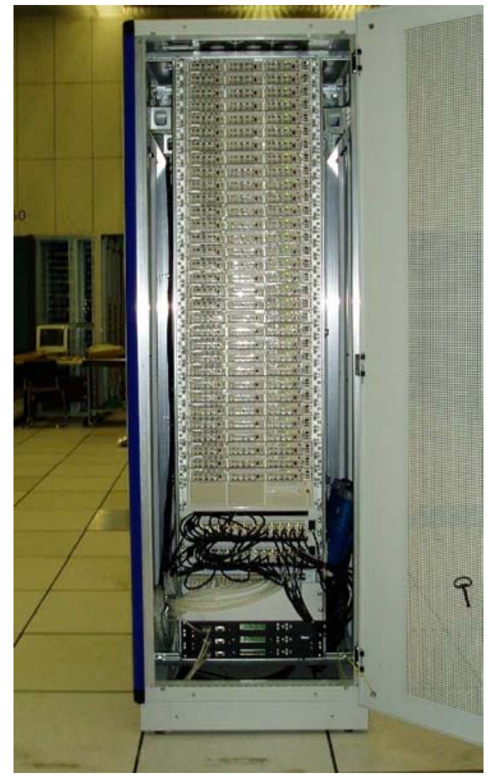
$$\mathrm{C_{ost}} \propto \mathrm{N_{conf}}\; m_q^{-1}\; L^5\; a^{-6}$$

First simulations with SAP for $N_{\mathrm{F}} = 2$ Lüscher 04; Del Debbio, L.G., Lüscher, Petronzio, Tantalo 05



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

PC cluster with 32 Nodes (64 Xeon procs)
(∼160 Gflops sustained)



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

Extraction of masses from numerical simulations

- 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 $t \to \infty$ (and for $T \to \infty$)

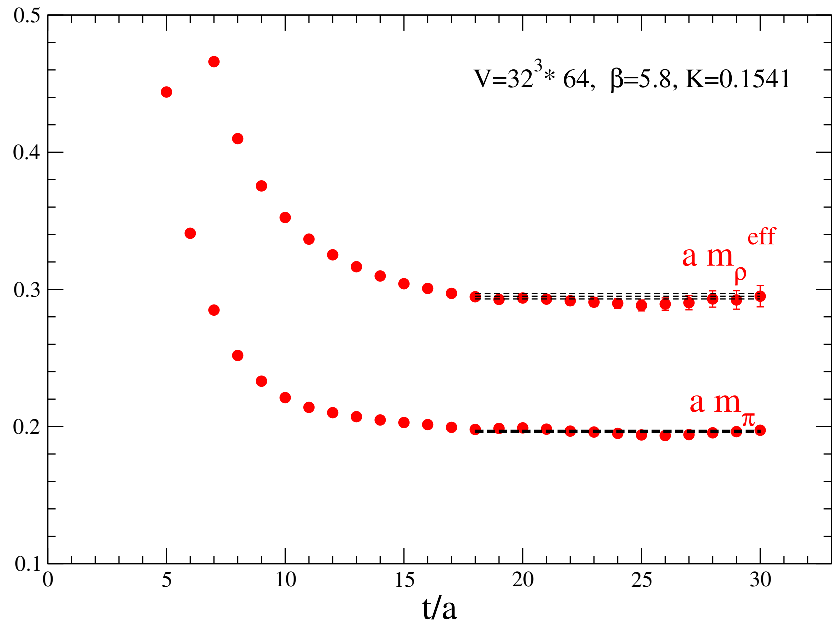
$$C_{AA}(t) \longrightarrow \frac{|\langle 0|A_0^a|\pi\rangle|^2}{M_P} e^{-\frac{M_P T}{2}} \cosh\left[M_P\left(\frac{T}{2} - t\right)\right]$$

$$\longrightarrow \frac{|\langle 0|A_0^a|\pi\rangle|^2}{2M_P} e^{-\frac{M_P t}{2}}$$

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

Correlation functions on the finer lattice

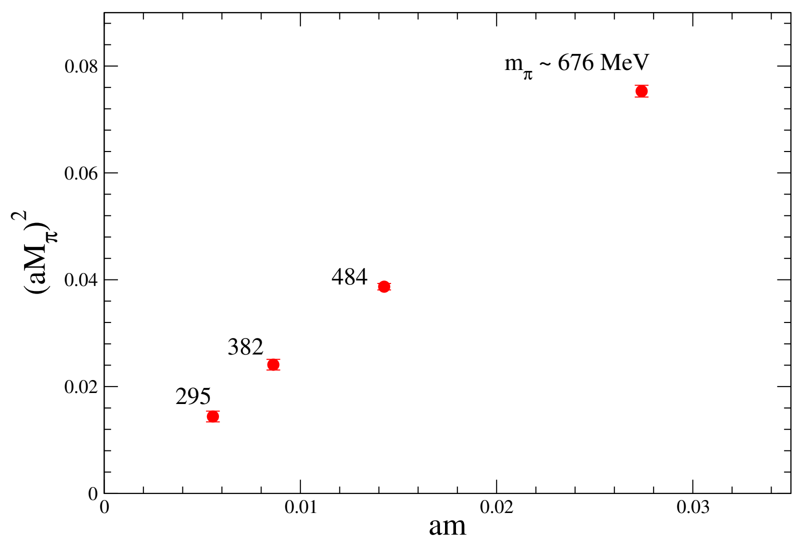
$$\sum_{\vec{x}} \langle O(x,t) O(0,0) \rangle \propto e^{-m_O(t)t}$$

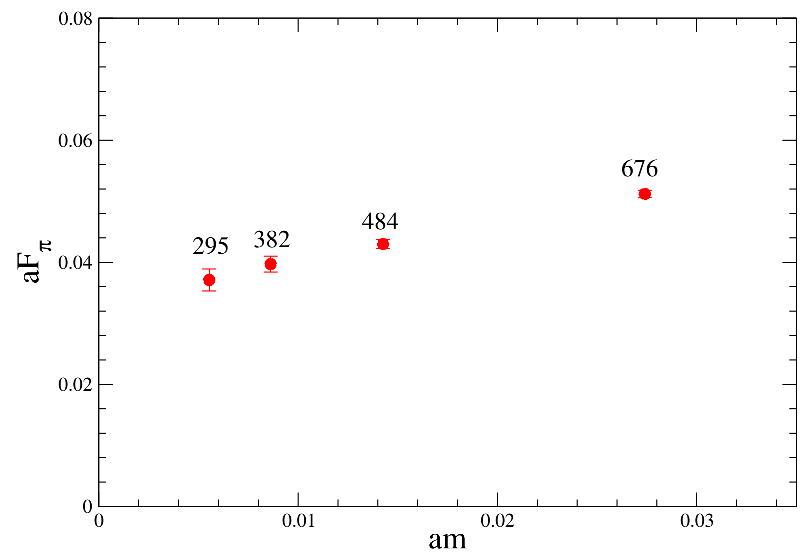


- Algorithm stable over the relevant parameter ranges:
  1. Quark mass: $m \sim m_s/6$ ✓
  2. Lattice spacing: $a \sim 0.065$ fm ✓
  3. Volume: $L \sim 2$ fm ✓

First results for pion mass and decay constant

Volume	a[fm]	am	am_π	aF_π
		0.0274(3)	0.274(2)	0.0648(8)
$24^3 \times 32$	$\sim$ 0.080	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_π

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

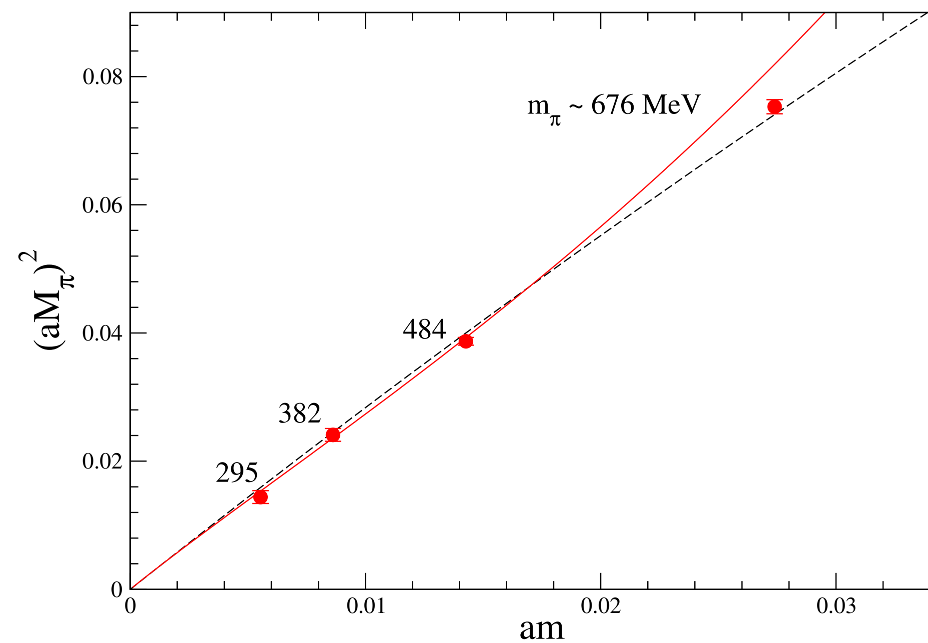
- Data below $M_\pi \sim 500$ MeV are compatible (within errors) with NLO ChPT

- 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_π

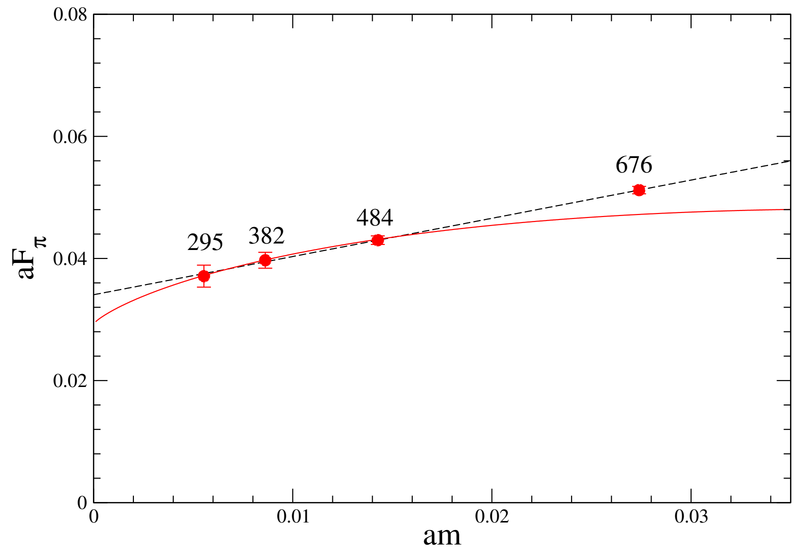
- NLO SU(2) ChPT gives [J. Gasser, H. Leutwyler '84]

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

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

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

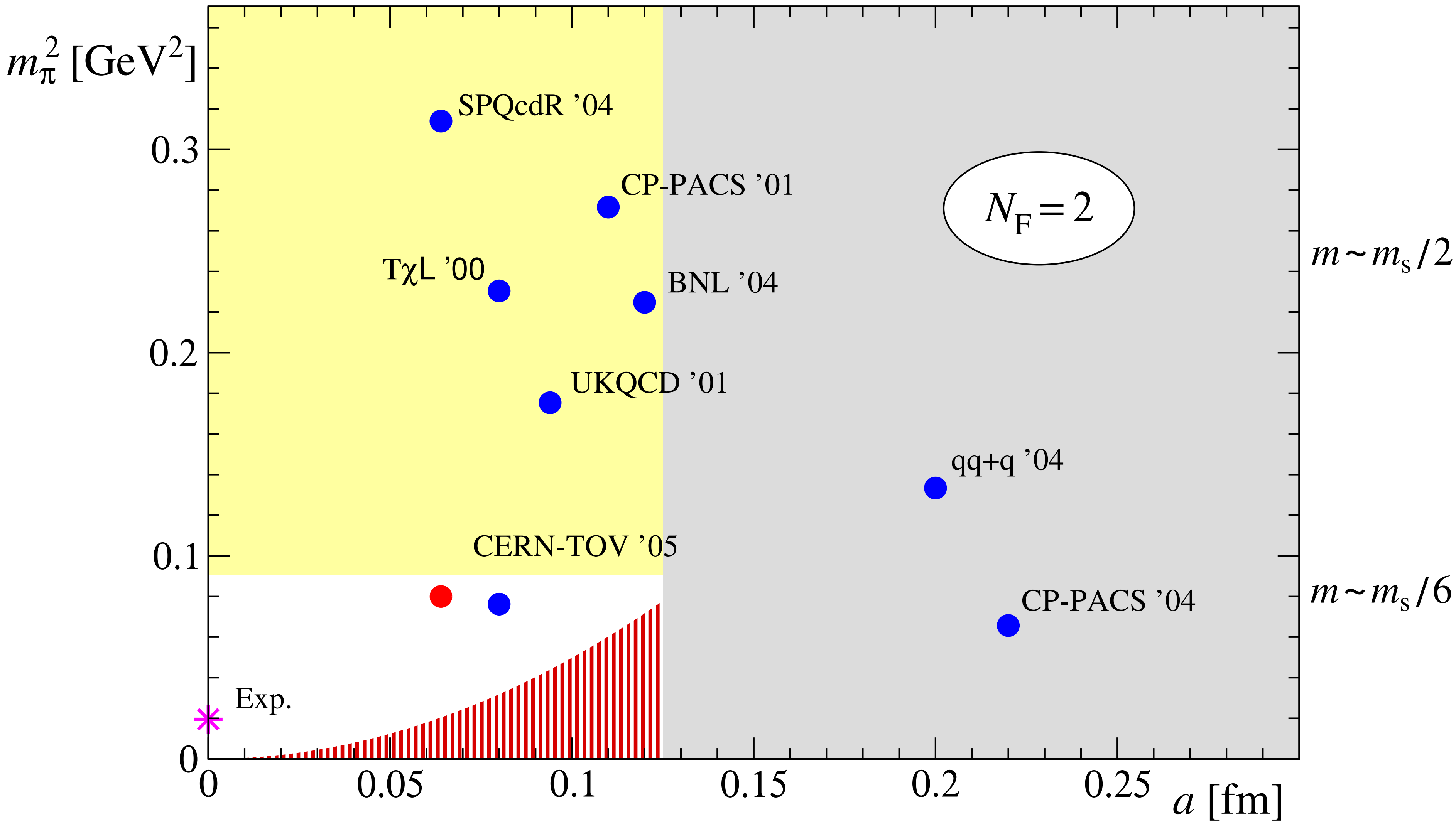
with Z_A from 1-loop PT



- Full analysis at small lattice spacing in progress

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

Where we are...Lüscher 04; Del Debbio, L.G., Lüscher, Petronzio, Tantalo 05



Summary

- 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