Monte Carlo Methods in Quantum Field Theory

I. Montvay

Deutsches Elektronen-Synchrotron DESY

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Introduction

Quantum Field Theory: infinite (continuum) number of degrees of freedom.

Mathematical definition is given by "discretization": infinite volume limit and continuum limit required.

In Euclidean space time (i.e. with imaginary time) QFT is equivalent to the statistical physics of fields. The "Boltzmann-factor" is the Euclidean action.

In lattice discretization ("regularization") the quantum fields are defined on the points (elements) of the lattice.

Continuum limit: the (bare) parameters of the Euclidean action have to be tuned to a fixed point in such a way that the ratio of physical length scales to the discretization scale ("lattice spacing") tends to infinity.

If such a fixed point exists experience in statistical physics suggests "universality": many different lattice actions can be tuned to the same continuum limit.

Quantum Chrome Dynamics:

QFT of the gluon (= SU(3)-colour gauge) field and six quark fields.

In many applications only the three "light" quarks (u, d and s) are relevant.

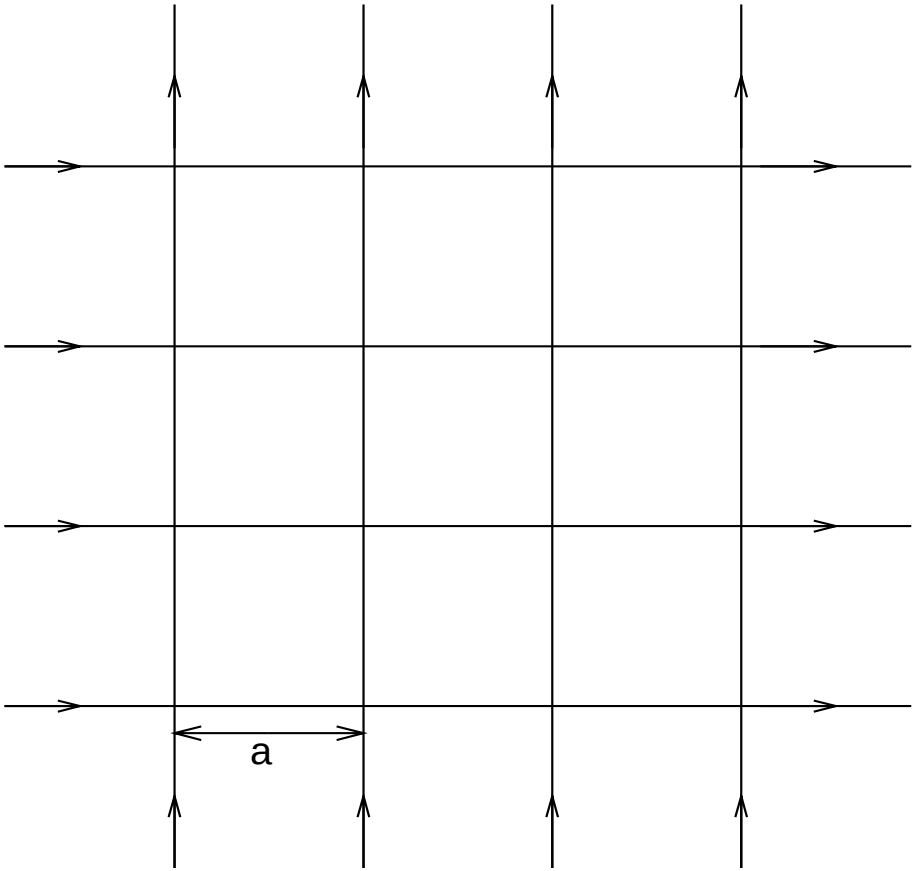
The free parameters are: the quark masses, more precisely

m_u/Λ_{QCD}, m_d/Λ_{QCD}, m_s/Λ_{QCD}, ...

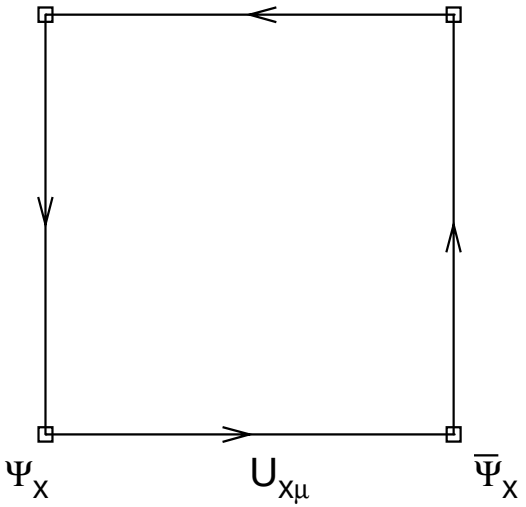
QCD is a mathematically closed highly predictive theory of strong interactions.

Lattice actions of QCD

4x4 periodic lattice



plaquette in LQCD



Plaquette action for the gluon field

Notations: I.M., G. Münster, *Quantum Fields on a Lattice*, Cambridge, 1994.

The gluon field is described by the parallel transporter of SU(3) colour on links:

$U_{x\mu} \in \mathrm{SU}(3)$ on the link $(x \longrightarrow x + \hat{\mu})$.

The gauge variables $A_{x\mu}$ are elements of the SU(3) Lie algebra.

They are defined by $U_{x\mu} = \exp(-aA_{x\mu})$ where a is the lattice spacing and

$A_{x\mu} = -igA^b_\mu(x)\frac{1}{2}\lambda_b$ (here g is the bare gauge coupling).

The field strength can be represented by

$$U_{x;\mu\nu} \equiv U^\dagger_{x,\nu} U^\dagger_{x+\hat{\nu},\mu} U_{x+\hat{\mu},\nu} U_{x,\mu} = \exp[-a^2 G_{\mu\nu}(x)]$$

where

$$G_{\mu\nu}(x) = F_{\mu\nu}(x) + \mathcal{O}(a) \ ,$$

$$F_{\mu\nu}(x) = \Delta^f_\mu A_\nu(x) - \Delta^f_\nu A_\mu(x) + [A_\mu(x), A_\nu(x)]$$

and the lattice forward derivative is defined by $\Delta^f \varphi(x) \equiv \varphi(x+\hat{\mu}) - \varphi(x)$.

Because of

$$\mathrm{Re}\,\mathrm{Tr}\, U_{x;\mu\nu} = N_c + \frac{a^4}{2}\,\mathrm{Tr}\, F_{\mu\nu}(x)^2 + \mathcal{O}(a^5)$$

the Wilson (plaquette) gauge field action for the $\mathrm{SU}(N_c)$ gauge field can be defined as $\mathcal{EXERCISE}$

$$S_{gauge} \equiv S_g = \sum_x \sum_{1\le\mu<\nu\le 4} \beta \left\{ 1 - \frac{1}{N_c}\,\mathrm{Re}\,\mathrm{Tr}\,(U_{x;\mu\nu}) \right\}$$

$$= -\frac{\beta}{4N_c} \sum_{x\mu\nu} a^4\,\mathrm{Tr}\, F_{\mu\nu}(x) F_{\mu\nu}(x) + \mathcal{O}(a^5) \qquad \left(\beta \equiv \frac{2N_c}{g^2}\right)$$

Gauge invariance:

the Wilson action is gauge invariant since the gauge transformation of the gauge (link) variables is $U'_{x\mu} = \Lambda^{-1}(x+\hat{\mu})\, U_{x\mu}\, \Lambda(x) \qquad [\Lambda(x) \in \mathrm{SU}(N_c)]$.

Expectation values:

in terms of the invariant group (Haar-) measure $dU_{x\mu}$ we have

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \prod_{x\mu} dU_{x\mu}\ \exp\{-S_{gauge}[U]\}\, \mathcal{O}[U] \equiv \int [dU]\, e^{-S_{gauge}[U]}\, \mathcal{O}[U]$$

where the partition function for the gauge field is defined as

$$Z = \int \prod_{x\mu} dU_{x\mu}\ \exp\{-S_{gauge}[U]\} \equiv \int [dU]\, e^{-S_{gauge}[U]}$$

This shows that in the Euclidean path integral formulation lattice gauge theory is equivalent to the statistical physics of gauge fields.

Lattice actions for the quark field

The Dirac equation for fermions can also be similarly discretized.

A simple choice is the Wilson action for fermions:

$$S_q^{Wilson} = \sum_x \left\{ \mu_0 \overline{\psi}_x \psi_x - \frac{1}{2} \sum_\mu \overline{\psi}_{x+\hat{\mu}} \gamma_\mu U_{x\mu} \psi_x - \frac{r}{2} \sum_\mu [\overline{\psi}_{x+\hat{\mu}} U_{x\mu} - \overline{\psi}_x] \psi_x \right\}$$

Here ψ_x, $\overline{\psi}_x$ are anticommuting Grassmann variables. $\mathcal{EXERCISE}$

The lattice spacing is set to unity: $a \equiv 1$ (which is often done in the literature), μ_0 is the bare quark mass in lattice units, the Wilson parameter is $r \neq 0$ and the summation runs over both positive and negative directions: $\sum_\mu \equiv \sum_{\mu=\pm 1}^{\pm 4}$ (by definition we have $\gamma_{-\mu} = -\gamma_\mu$).

The rôle of the Wilson term proportional to r will be discussed next.

Often used notations:

after redefining the field normalizations according to

$$(\mu_0 + 4r)^{1/2}\,\psi_x \;\Rightarrow\; \psi_x\;, \qquad (\mu_0 + 4r)^{1/2}\,\overline{\psi}_x \;\Rightarrow\; \overline{\psi}_x$$

and introducing the hopping parameter by $\kappa \equiv (2\mu_0 + 8r)^{-1}$ the Wilson action can be rewritten as

$$S_q^{Wilson} = \sum_x \left\{ (\overline{\psi}_x \psi_x) - \kappa \sum_\mu (\overline{\psi}_{x+\hat{\mu}} U_{x\mu} [r + \gamma_\mu] \psi_x) \right\} \equiv \sum_{xy} (\overline{\psi}_y Q_{yx} \psi_x)$$

where the Wilson fermion matrix is (without explicit colour- and Dirac-indices)

$$Q_{yx} = \delta_{yx} - \kappa \sum_\mu \delta_{y,x+\hat{\mu}}\, U_{x\mu}\, (r + \gamma_\mu)$$

Wilson fermion propagator: the inverse of the free fermion matrix is defined by

$$\sum_y \Delta_{zy} Q_{yx} = \delta_{zx} \ , \qquad \Delta_{yx} = \Delta_{y-x} = \frac{1}{\Omega} \sum_k e^{ik\cdot(y-x)} \tilde{\Delta}_k$$

here $\Omega = N_1 N_2 N_3 N_4$ is the number of lattice points and the values of the momenta for periodic and antiperiodic boundary conditions, respectively, are

$$ap_\mu \equiv k_\mu = \frac{2\pi}{N_\mu}\nu_\mu \ , \qquad k_\mu = \frac{2\pi}{N_\mu}\left(\nu_\mu + \frac{1}{2}\right) \qquad (\nu_\mu \in \{0, 1, 2, \ldots, N_\mu - 1\})$$

Using the notations $\hat{k}_\mu \equiv 2 \sin \frac{k_\mu}{2}$, $\bar{k}_\mu \equiv \sin k_\mu$ the solution is $\mathcal{EXERCISE}$

$$\tilde{\Delta}_k = \frac{1 - r\kappa(8 - \hat{k}^2) - 2i\kappa\gamma\cdot\bar{k}}{[1 - r\kappa(8 - \hat{k}^2)]^2 + 4\kappa^2\bar{k}^2} = (2\kappa)^{-1} \frac{\mu_0 + (r/2)\hat{k}^2 - i\gamma\cdot\bar{k}}{[\mu_0 + (r/2)\hat{k}^2]^2 + \bar{k}^2}$$

The non-zero value of r is required in order to avoid particle poles at $k_\mu = \pi$, besides the physical ones at $k_\mu = 0$, but for $r \neq 0$ chiral symmetry is broken also for zero fermion mass!!!

Kogut-Susskind staggered lattice fermions:

the "naive" free fermion action without the Wilson term ($r = 0$) describes 16 fermion "flavours"

$$S_q^{naive} = \sum_x \left\{ \mu_0 \overline{\Psi}_x \Psi_x + \frac{1}{2} \sum_{\mu=1}^{4} \left[\overline{\Psi}_x \gamma_\mu \Psi_{x+\hat{\mu}} - \overline{\Psi}_{x+\hat{\mu}} \gamma_\mu \Psi_x \right] \right\}$$

One can perform spin diagonalization by $\Psi_x = A_x \psi_x$, $\overline{\Psi}_x = \overline{\Psi}_x A_x^\dagger$,

$A_x^\dagger \gamma_\mu A_x = \alpha_{x\mu} \, \mathbf{1}_4 = (-1)^{x_1 + \cdots + x_{\mu-1}} \, \mathbf{1}_4 \quad (\mu = 1, 2, 3, 4)$.

One out of four identical components gives the "staggered" fermion action

$$S_q^{staggered} = \sum_x \left\{ \mu_0 \overline{\psi}_x \psi_x + \frac{1}{2} \sum_{\mu=1}^{4} \alpha_{x\mu} \, \left[\overline{\psi}_x \psi_{x+\hat{\mu}} - \overline{\psi}_{x+\hat{\mu}} \psi_x \right] \right\}$$

This describes four degenerate flavours with components scattered on the points of 2^4 hypercubes. (There are no Dirac spinor indices.) $\mathcal{EXERCISE}$

At zero mass $\mu_0 = 0$ there is an exact chiral symmetry $U_{even}(1) \otimes U_{odd}(1)$.

Improved lattice actions

The freedom of choosing the lattice action in the universality class of the same limiting theory in the continuum can be used for:

- accelerating the convergence to the continuum limit,
- achieving enhanced symmetries already at non-zero lattice spacings.

The basic tools are:

renormalization group block transformations (Wilson, ..., Hasenfratz)

and the local effective theories at non-zero cut-off (Symanzik, ..., Lüscher, Weisz).

In QCD particularly interesting is the improvement of chiral symmetry at non-zero lattice spacings which implies simpler renormalization patterns for composite (e.g. current-) operators.

Improved actions with smeared links:

smoothed gauge fields for moving closer to the continuum limit.

The links $U_{x,\mu}$ in the fermion action can be replaced by *stout*-smeared links.

This has the advantage that short range *topological defects* of the gauge field and the corresponding small eigenvalues of the fermion matrix are removed.

The stout smeared links are defined as (Morningstar, Peardon):

$$U^{(1)}_{x,\mu} \equiv U_{x,\mu} \, \exp\left\{ \frac{1}{2} \left(\Omega_{x,\mu} - \Omega^\dagger_{x,\mu} \right) - \frac{1}{2N_c} \, \mathrm{Tr} \left(\Omega_{x,\mu} - \Omega^\dagger_{x,\mu} \right) \right\} \ .$$

Here $U_{x,\mu}$ denotes the original "thin" gauge links and

$$\Omega_{x,\mu} \equiv \rho \, U^\dagger_{x,\mu} \, C_{x,\mu}$$

with the sum of "staples"

$$C_{x,\mu} \equiv \sum_{\nu \neq \mu} \left(U^\dagger_{x+\hat{\mu},\nu} U_{x+\hat{\nu},\mu} U_{x,\nu} + U_{x-\hat{\nu}+\hat{\mu},\nu} U_{x-\hat{\nu},\mu} U^\dagger_{x-\hat{\nu},\nu} \right) \ .$$

Twisted-mass LQCD

Chiral rotation of the Wilson term in S_q^{Wilson} : Frezzotti, Grassi, Sint, Weisz

For two equal mass quark flavours ($N_f = 2$) the unbroken $\mathrm{SU}(2)$ subgroup of the $\mathrm{SU}(2) \otimes \mathrm{SU}(2)$ chiral symmetry can be partly rotated to axialvector directions. In addition, "automatic" $\mathcal{O}(a)$ improvement is possible.

The "twisted mass" lattice fermion action is:

$$S_q^{tm} = \sum_x \Bigg\{ \mu_q \overline{\psi}_x \psi_x - \frac{1}{2} \sum_\mu \overline{\psi}_{x+\hat{\mu}} \gamma_\mu U_{x\mu} \psi_x$$

$$+ \mu_{cr} \overline{\psi}_x e^{-i\omega\gamma_5\tau_3} \psi_x - \frac{r}{2} \sum_\mu [\overline{\psi}_{x+\hat{\mu}} U_{x\mu} - \overline{\psi}_x] e^{-i\omega\gamma_5\tau_3} \psi_x \Bigg\}$$

Here ω is the twist angle, μ_q the bare quark mass in lattice units and $\mu_{cr} = (\frac{1}{2}\kappa_{cr}^{-1} - 4r) < 0$ the critical bare quark mass where $\mu_q^{physical} = 0$.

The twist can be moved to the mass term by a chiral transformation

$$\chi_x = \exp(-\tfrac{i}{2}\omega\gamma_5\tau_3)\psi_x, \quad \overline{\chi}_x = \overline{\psi}_x \exp(-\tfrac{i}{2}\omega\gamma_5\tau_3)$$

(hence the name "twisted mass") $\mathcal{EXERCISE}$

The quark determinant in the path integral over the gauge field is

$$\det\left[(D^{cr} + \mu_q \cos\omega)^\dagger (D^{cr} + \mu_q \cos\omega) + \mu_q^2 \sin^2\omega\right]$$

where the single-flavour critical fermion matrix is

$$D^{cr}_{yx} = \mu_{cr}\delta_{yx} - \frac{1}{2}\sum_\mu \left[\delta_{y,x+\hat{\mu}}\gamma_\mu U_{x\mu} + r(\delta_{y,x+\hat{\mu}}U_{x\mu} - \delta_{yx})\right]$$

The fermion matrix $D^{cr} + \mu_q(\cos\omega + i\gamma_5\tau_3 \sin\omega)$ cannot have zero eigenvalues for non-zero quark mass if $\omega \neq 0, \pi$: there are no spurious zero modes and no exceptional gauge configurations with anomalously small eigenvalues of the fermion matrix.

Chiral $SU(2) \otimes SU(2)$ Ward-Takahashi-identities:

the conserved SU(2) subgroup is also "twisted".

Exactly conserved axialvector currents can be achieved with $\omega = \frac{1}{2}\pi$.

In this special case the conserved currents are ($j = 1, 2$):

$$A^{con}_{jx\mu} = \frac{1}{2}\left\{\left(\overline{\psi}_{x+\hat{\mu}}\gamma_\mu\gamma_5\frac{\tau_j}{2}U_{x\mu}\psi_x\right) + \left(\overline{\psi}_x\gamma_\mu\gamma_5\frac{\tau_j}{2}U^\dagger_{x\mu}\psi_{x+\hat{\mu}}\right)\right.$$

$$\left. + r\left(\overline{\psi}_{x+\hat{\mu}}\frac{\overline{\tau}_j}{2}U_{x\mu}\psi_x\right) - r\left(\overline{\psi}_x\frac{\overline{\tau}_j}{2}U^\dagger_{x\mu}\psi_{x+\hat{\mu}}\right)\right\}$$

with $\overline{\tau}_1 \equiv \tau_2$ and $\overline{\tau}_2 \equiv -\tau_1$, and

$$V^{con}_{3x\mu} = \frac{1}{2}\left\{\left(\overline{\psi}_{x+\hat{\mu}}\gamma_\mu\frac{\tau_3}{2}U_{x\mu}\psi_x\right) + \left(\overline{\psi}_x\gamma_\mu\frac{\tau_3}{2}U^\dagger_{x\mu}\psi_{x+\hat{\mu}}\right)\right.$$

$$\left. - \frac{ir}{2}\left(\overline{\psi}_{x+\hat{\mu}}\gamma_5 U_{x\mu}\psi_x\right) + \frac{ir}{2}\left(\overline{\psi}_x\gamma_5 U^\dagger_{x\mu}\psi_{x+\hat{\mu}}\right)\right\}$$

The invariance of the path integral with respect to the change of variables

$$\psi'_x = (1 + \tfrac{i}{2}\alpha_{Vrx}\tau_r + \tfrac{i}{2}\alpha_{Arx}\gamma_5\tau_r)\psi_x, \quad \overline{\psi}'_x = \overline{\psi}_x(1 - \tfrac{i}{2}\alpha_{Vrx}\tau_r + \tfrac{i}{2}\alpha_{Arx}\gamma_5\tau_r)$$

implies the WT-identities: $\mathcal{EXERCISE}$

$$\langle \mathcal{O}\ \Delta^b_\mu A^{con}_{jx\mu}\rangle + \left\langle \frac{\mathcal{O}\ \overleftarrow{\partial}}{\partial\psi_x}\ \gamma_5\frac{\tau_j}{2}\psi_x + \overline{\psi}_x\gamma_5\frac{\tau_j}{2}\ \frac{\overrightarrow{\partial}\ \mathcal{O}}{\partial\overline{\psi}_x}\right\rangle = \mu_q \langle \mathcal{O}\ \overline{\psi}_x\gamma_5\tau_j\psi_x\rangle$$

$$\langle \mathcal{O}\ \Delta^b_\mu V^{con}_{3x\mu}\rangle + \left\langle \frac{\mathcal{O}\ \overleftarrow{\partial}}{\partial\psi_x}\ \frac{\tau_3}{2}\psi_x - \overline{\psi}_x\frac{\tau_3}{2}\ \frac{\overrightarrow{\partial}\ \mathcal{O}}{\partial\overline{\psi}_x}\right\rangle = 0$$

with the backward lattice derivative defined as $\Delta^b_\mu\varphi(x) \equiv \varphi(x) - \varphi(x - \hat{\mu})$.

$\mathcal{O}(a)$ improvement (Frezzotti, Rossi): for the Wilson fermion action one can show

$$\langle\mathcal{O}\rangle^{WA}_{(m_q)} \equiv \frac{1}{2}\left[\langle\mathcal{O}\rangle_{(r,m_q)} + \langle\mathcal{O}\rangle_{(-r,m_q)}\right] \propto \langle\mathcal{O}\rangle^{cont}_{(m_q)} + \mathcal{O}(a^2)$$

This is averaging over opposite sign Wilson parameters ("Wilson average").

In tmLQCD changing the sign of r is equivalent to shifting the twist angle by π. In the special case of $\omega = \frac{1}{2}\pi$ this is equivalent to $\omega \to -\omega$, therefore expectation values even in ω are "automatically" $\mathcal{O}(a)$ improved, without any averaging!

Automatically $\mathcal{O}(a)$ improved physical quantities are, for instance:

- the energy eigenvalues, hence the masses
- on-shell matrix elements at zero spatial momenta
- matrix elements of operators with formal parity equal to the product of the parities of the external states

Note: in case of non-zero twist parity (as well as some vector flavour symmetries) are broken by lattice artifacts.

Domain wall fermions

The chiral symmetry of massless fermions can be realized (at non-zero lattice spacing) by introducing a fifth "extra" dimension: Kaplan, Shamir.

In the fifth direction there is a "defect": either the mass term changes sign (Kaplan) or there are the "walls" at the two ends (Shamir).

There are chiral fermion solutions which are exponantially localized in the fifth dimension near these defects.

The gauge field remains four-dimensional (independent on the fifth dimension).

In the limit of infinitely large fifth dimension the positive and negative chirality solutions (at opposite walls or at opposite sign changes on a torus) have zero overlap with each other and the chiral symmetry becomes exact.

The domain wall fermion action can be written (with $1 \le s \le N_s$) as

$$S_F = \sum_{s,s'} \overline{\Psi}_{xs} (D_F)_{xs,x's'} \Psi_{x's'}$$

where in an s-block form $\mathcal{EXERCISE}$

$$D_F = \begin{pmatrix} \sigma + D & -\sigma P_L & 0 & 0 & \dots & 0 & 0 & m_f P_R \\ -\sigma P_R & \sigma + D & -\sigma P_L & 0 & \dots & 0 & 0 & 0 \\ 0 & -\sigma P_R & \sigma + D & -\sigma P_L & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -\sigma P_R & \sigma + D & -\sigma P_L \\ m_f P_L & 0 & 0 & 0 & \dots & 0 & -\sigma P_R & \sigma + D \end{pmatrix}$$

The chiral projectors are, as usual, $P_{R,L} \equiv \frac{1}{2}(1 \pm \gamma_5)$, the quark mass in lattice units is m_f, the ratio of lattice spacings is $\sigma = a/a_s$ and the four-dimensional Wilson-Dirac matrix with negative mass ($0 > -m_0 > -2$) is ($r = 1$)

$$D_{xx'} = (4 - m_0)\delta_{xx'} \; - \; \frac{1}{2}\sum_{\mu=1}^{4}\Big[\delta_{x',x+\hat{\mu}}(1+\gamma_\mu)U_{x\mu} + \delta_{x'+\hat{\mu},x}(1-\gamma_\mu)U^\dagger_{x'\mu}\Big]$$

The hermitean fermion matrix: useful e.g. for Monte Carlo simulations.

Since with an s-reflection $(R_5)_{ss'} \equiv \delta_{N_s+1-s,s'}$ we have $D_F = R_5\gamma_5 D_F^\dagger R_5\gamma_5$, the hermitean fermion matrix can be defined as

$$\tilde{D}_F \equiv R_5\gamma_5 D_F = \tilde{D}_F^\dagger$$

The chiral symmetry is broken by a non-zero overlap of the opposite chirality wave functions. Enhanced symmetry breaking occurs if D has small eigenvalues.

Neuberger overlap fermions

Another (related) possibility to achieve chiral symmetry of the lattice fermion action is the Neuberger (overlap) fermion action.

Let us rewrite the (free) Wilson fermion action for $r = 1$ and $\mu_0 \equiv a m_0$ as

$$S_q^{Wilson} = \sum_x a^4 \, \overline{\psi}_x [m_0 + D_W] \psi_x \; , \qquad D_W \equiv \sum_{\mu=1}^{4} \left[\frac{1}{2} \gamma_\mu (\nabla_\mu + \nabla_\mu^*) - \frac{a}{2} \nabla_\mu^* \nabla_\mu \right]$$

where the lattice derivatives are $\nabla_\mu \equiv a^{-1} \Delta_\mu^f, \quad \nabla_\mu^* \equiv a^{-1} \Delta_\mu^b$.

The Neuberger lattice fermion operator with zero mass is given by

$$D_N \equiv \frac{1}{a} \left(1 - A \frac{1}{\sqrt{A^\dagger A}} \right) \; , \qquad\qquad A \equiv 1 - a D_W$$

The inverse square-root can be defined by polynomial or rational approximations.

Note that A is proportional to the Wilson operator with bare mass $-a^{-1}$.

An important feature of D_N is that $V \equiv 1 - aD_N$ is unitary: $V^\dagger V = 1$.

The spectrum of $D_N = a^{-1}(1 - V)$ is on a circle going through the origin.

Ginsparg-Wilson relation: the Neuberger operator satisfies the relation

$$\gamma_5 D_N + D_N \gamma_5 = a D_N \gamma_5 D_N$$

This is equivalent to the condition introduced by Ginsparg and Wilson (GW) $\gamma_5 D^{-1} + D^{-1}\gamma_5 = 2aR\gamma_5$. The GW-relation is the optimal approximation to chiral symmetry which can be realized by a lattice fermion operator ($a \to 0$). R is in general a local operator, for $D = D_N$ we have $R = \frac{1}{2}$. $\mathcal{EXERCISE}$

Lattice chiral symmetry: it can be shown (Lüscher) that

$$\delta\psi = \gamma_5 \left(1 - \frac{a}{2}D\right)\psi \,, \qquad \delta\overline{\psi} = \overline{\psi}\left(1 - \frac{a}{2}D\right)\gamma_5$$

is an exact chiral symmetry (for any a) if the GW-relation is satisfied.

Lattice actions satisfying the GW-relation:

- the fixed point action, which is the fixed point of some renormalization group transformation (Hasenfratz),
- Neuberger action D_N
- the effective (four-dimensional) action of the light fermion field of the domain wall fermion (Neuberger, Kikukawa)

Note: the inverse of the effective Dirac operator of the light fermion field of the domain wall fermion is equivalent to the inverse of the truncated overlap Dirac operator (except for a local contact term).

Using GW-fermions one can prove the index theorem about topological charge (Hasenfratz, Laliena, Niedermayer) and introduce the θ-parameter, etc.

How did we avoid the Nielsen-Ninomiya theorem?

Theorem: there is no (free) lattice fermion action

$$S_f = a^4 \sum_{xy} \overline{\psi}_y D(y-x) \psi_x$$

which would satisfy

- $D(x)$ is local (bounded by $e^{-\gamma|x|}$)
- its Fourier-transform is $\tilde{D}(p) = i\gamma_\mu p_\mu + \mathcal{O}(ap^2)$ for $p \ll \pi/a$
- $\tilde{D}(p)$ is invertible for $p \neq 0$ (no massless doubler poles)
- $\gamma_5 D + D\gamma_5 = 0$ (chiral symmetry)

The lattice chiral symmetry is defined differently:

it is non-ultralocal (involves neighbouring lattice sites).

The last requirement in the Nielsen-Ninomiya theorem is replaced by the Ginsparg-Wilson relation.

The question of locality:

locality can be proven if the gauge field is smooth enough ("admissible"), namely if every plaquette value is close to unity. (Hernandez, Jansen, Lüscher)

In actual simulations there are always plaquettes with small values.

The lattice spacing has to be small enough in order to avoid the "Aoki phase" with lots of small eigenvalues of D_W: the small eigenvalues make D_N non-local and the "residual mass" breaking the chiral symmetry of domain wall fermions large (Golterman, Shamir).

Monte Carlo simulations

The goal of numerical simulations is to estimate the expectation value of some functions $A[\varphi]$ of the field variables generically denoted by $[\varphi] \equiv \{\varphi_{x\alpha}\}$. This is given by path integrals as

$$\langle A \rangle = Z^{-1} \int [d\varphi] e^{-S[\varphi]} A[\varphi] \;, \qquad Z = \int [d\varphi] e^{-S[\varphi]}$$

$S[\varphi]$ is the lattice action, which is assumed to be a real function of the field variables. (For the moment we only consider bosonic path integrals.)

A typical lattice action contains a summation over the lattice sites.

Since the number of lattice points Ω is large, in the path integral only a small vicinity of the minimum of the "free energy" density will substantially contribute. $\longrightarrow$ Monte Carlo integration (see e.g. C. Morningstar, hep-lat/0702020)

Simple Monte Carlo integration:

consider a continuous real function $f(X)$ of a continuous random variable X having probability distribution $p_X(s)$ and hence the expectation value

$$\langle f(X)\rangle = \int ds\, f(s)\, p_X(s)$$

Using $p_X(s)$ to obtain N outcomes $X_1, X_2, \ldots, X_N$ then the random variables $Y_j = f(X_j)$ give

$$\lim_{N\to\infty} \frac{1}{N}\sum_{j=1}^{N} Y_j = \langle Y\rangle = \langle f(X)\rangle = \int ds\, f(s)\, p_X(s)$$

With a short notation:

$$\overline{f} \equiv \frac{1}{N}\sum_{j=1}^{N} f(X_j), \qquad \lim_{N\to\infty} \overline{f} = \langle f\rangle = \int ds\, f(s)\, p_X(s)$$

For large N, the central limit theorem tells us that the error in approximating $\langle f(X)\rangle$ is given by the variance $V[f(X)]$ as $\sqrt{V[f(X)]/N}$.

The Monte Carlo estimate of the variance is:

$$V[Y] = \left\langle (Y - \langle Y\rangle)^2 \right\rangle \approx \overline{(f-\overline{f})^2} = \overline{f^2} - \overline{f}^2$$

Generalising this to several (D) integration variables:

simple Monte Carlo integration is acomplished by

$$\int_{\mathcal{V}} d^D x\, p(\vec{x})\, f(\vec{x}) \approx \overline{f} \pm \left(\frac{\overline{f^2} - \overline{f}^2}{N} \right)^{\frac{1}{2}}$$

$$\overline{f} \equiv \frac{1}{N} \sum_{i=1}^{N} f(\vec{x}_i), \qquad \overline{f^2} \equiv \frac{1}{N} \sum_{i=1}^{N} f(\vec{x}_i)^2$$

where the points $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N$ are chosen *independently* and *randomly* with probability distribution $p(\vec{x})$ in the D-dimensional volume $\mathcal{V}$.

Importance sampling:

Simple Monte Carlo integration works best for flat functions but is problematic if the integrand is sharply peaked or rapidly oscillating.

Therefore, a good procedure is to apply *importance sampling*: find a positive function $g(x)$ with integral norm $\int dx\, g(x) = 1$ such that $h(x) \equiv f(x)/g(x)$ is as close as possible to a constant and then calculate

$$\int_a^b dx\, f(x) = \int_a^b dx\, g(x) h(x) \approx \frac{(b-a)}{N} \sum_{j=1}^{N} h(x_j)$$

where the points x_j are chosen with probability density $g(x)$ and we used simple Monte Carlo integration with a constant probability in an interval

$$\int_a^b dx\, f(x) \approx \frac{(b-a)}{N} \sum_{j=1}^{N} f(x_j)$$

It is assumed: one can find $g(x)$ and generate points with it.

Monte Carlo using a Markov process:

How can one generate the desired (possibly complicated) distribution?

Rejection method for (low-dimensional) integrals: sampling with $p_X(x)$ for $x \in [b, a]$ is equivalent to choosing a random point uniformy in two dimensions in the area under the curve $p_X(x)$.

Multi-dimensional integrals can be handled by exploiting Markov processes.

Markov process ("Markov chain"): generating a sequence of states with probabilities depending only on the current state of the system.

For simplicity, for discrete states $s_1, s_2, \ldots, s_R$ the *transition probability* is p_{ij}.

The matrix $\mathbf{P}$ with elements p_{ij} is called *transition (Markov-) matrix*.

Properties of Markov chains: among others

- The product of two Markov matrices $\mathbf{P_1 P_2}$ is again a Markov matrix.
- Every eigenvalue of a Markov matrix satisfies $|\lambda| \leq 1$.
- Every Markov matrix has at least one eigenvalue $\lambda = 1$.

Fundamental limit theorem for (irreducible, aperiodic) Markov chains:

they have a unique stationary distribution satisfying $\mathbf{w}^T = \mathbf{w}^T \mathbf{P}$ which is identical to the limiting distribution $w_j = \lim_{n\to\infty} p_{ij}^{(n)}$.

Autocorrelation: points depend on previous points in the Markov chain.

The *autocorrelation function* for some observable O_i is defined by

$$\rho(t) \equiv \left(\langle O_i O_{i+t}\rangle - \langle O_i\rangle^2\right) \Big/ \left(\langle O_i^2\rangle - \langle O_i\rangle^2\right)$$

Decreasing autocorrelations decrease the Monte Carlo error.

The Monte Carlo integration in QFT by "importance sampling":

the distribution of configurations generated during the Monte Carlo integration process follows the Boltzmann factor $e^{-S[\varphi]}$ ("canonical distribution").

A configuration sequence $\{[\varphi_n],\ 1 \le n \le N\}$ is generated by a Markov process.

In this sample the expectation value is approximated by the sample average:

$$\overline{A} \equiv \frac{1}{N} \sum_{n=1}^{N} A[\varphi_n] \quad \longrightarrow \quad \langle A \rangle$$

The updating (Markov) process: a stochastic process where the transition from a configration to the next one $[\varphi] \to [\varphi']$ happens with probability $P\left([\varphi'] \leftarrow [\varphi]\right)$.

In order to generate the canonical distribution $e^{-S[\varphi]}$ a sufficient condition is

$$P\left([\varphi'] \leftarrow [\varphi]\right) e^{-S[\varphi]} = P\left([\varphi] \leftarrow [\varphi']\right) e^{-S[\varphi']}$$

This condition is called detailed balance.

Metropolis algorithm: the "ancestor" of updating processes. $\mathcal{EXERCISE}$

For a system with $\mathcal{N}$ possible configurations the transition probability for $[\varphi'] \neq [\varphi]$ is defined by

$$P([\varphi'] \leftarrow [\varphi]) = \mathcal{N}^{-1} \ \min\left\{1, \frac{e^{-S[\varphi']}}{e^{-S[\varphi]}}\right\}$$

This transition matrix is realized by the following numerical procedure:

i.) choose first a trial configuration randomly from $\mathcal{N}$ configurations and

ii.) accept it as the next configuration in any case if the Boltzmann factor is increased (the action is decreased). If the Boltzmann factor is decreased (the action is increased), then accept the change with probability equal to the ratio of the Boltzmann factors.

The accept–reject step can be implemented by comparing the ratio of the Boltzmann factors to a pseudo-random number between 0 and 1. $\mathcal{EXERCISE}$

Quarks (fermions) in numerical simulations:

The lattice action has the form $S[U,\psi,\overline{\psi}] = S_g[U] + S_q[U,\psi,\overline{\psi}]$ where S_q is quadratic in the Grassmann-variables: $S_q = \sum_{xy}(\overline{\psi}_y Q_{yx}\psi_x)$. The expectation values have the form

$$\langle F\rangle = \frac{\int [dU\, d\overline{\psi}\, d\psi] e^{-S_g-S_q} F[U,\psi,\overline{\psi}]}{\int [dU\, d\overline{\psi}\, d\psi] e^{-S_g-S_q}} \equiv Z^{-1}\int [dU\, d\overline{\psi}\, d\psi] e^{-S_g-S_q} F[U,\psi,\overline{\psi}]$$

After performing the Grassmann integration:

$$\left\langle \psi_{y_1}\overline{\psi}_{x_1}\psi_{y_2}\overline{\psi}_{x_2}\cdots\psi_{y_n}\overline{\psi}_{x_n} F[U]\right\rangle = Z^{-1}\int [dU] e^{-S_g[U]}\ \det Q[U]\ F[U]$$

$$\cdot \sum_{z_1\cdots z_n} \epsilon^{z_1 z_2\cdots z_n}_{y_1 y_2\cdots y_n}\, Q[U]^{-1}_{z_1 x_1} Q[U]^{-1}_{z_2 x_2}\cdots Q[U]^{-1}_{z_n x_n}$$

Here $Q[U]^{-1}$ is an (external) quark propagator and $\det Q[U]$ generates the virtual quark loops.

"Quenched approximation": $\det Q[U] \Rightarrow 1$ (this implies unphysical "ghosts").

Updating with dynamical fermions ("unquenching"):

The fermion determinant is non-local: it is a great challenge for computation.

Pseudofermion representation: (Petcher, Weingarten)

$$\det\left(Q^\dagger Q\right) \propto \int [d\phi\, d\phi^+] \exp\left\{ -\sum_{xy} (\phi^+_y [Q^\dagger Q]^{-1}_{yx} \phi_x) \right\}$$

Because of $Q^\dagger = \gamma_5 Q \gamma_5$ and $\det Q^\dagger = \det Q$ this describes two degenerate quark flavours. In the Hybrid Monte Carlo algorithm this is implemented using molecular dynamics equations. (Duane, Kennedy, Pendleton, Roweth)

For single quark flavours HMC is not applicable.

One can, however, use *Polynomial HMC* (PHMC) or *Rational HMC* (RHMC).

HMC updating algorithm

HMC = Hybrid Monte Carlo

S. Duane, A.D. Kennedy, B.J. Pendleton, D. Roweth, Phys. Lett. **B195** (1987) 216

The basic idea of HMC is to employ molecular dynamics equations in order to collectively move the field configuration in the whole volume.

Since discretised molecular dynamics equations are used, at the end of a *trajectory* a Metropolis *accept-reject step* is implemented.

The equations of motion are derived from a Hamiltonian (here for the colour gauge field $U_{x,\mu} \in \mathrm{SU}(3)$):

$$H[P,U] = \frac{1}{2}\sum_{x\mu j} P_{x\mu j}^2 + S_g[U]$$

The real variables $P_{x\mu j},\ j=1,\ldots,8$ (*conjugate momenta*) are Gaussian:

$$P_{x\mu j} \propto \exp\left\{-\frac{1}{2}\sum_{x\mu j} P_{x\mu j}^2\right\} \equiv P_M[P]$$

They are the expansion coefficients of the Lie algebra element

$$P_{x,\mu} \equiv \sum_j i\lambda_j P_{x\mu j}$$

The expectation values are defined by

$$\langle F\rangle = \int [d\,P][d\,U]\exp(-H[P,U])\,F[U] \Big/ \int [d\,P][d\,U]\exp(-H[P,U])$$

By a proper choice of the discretised trajectories one can achieve that the transition probability from a configuration to the next satisfies *detailed balance*. Therefore, the correct canonical distribution is reproduced.

The Hamiltonian equations of motion are:

$$\frac{d\,P_{x\mu j}}{d\,\tau} = -D_{x\mu j} S_g[U]\ , \qquad \frac{d\,U_{x\mu}}{d\,\tau} = i P_{x,\mu} U_{x,\mu}$$

where the derivative with respect to the gauge field is defined as

$$D_{x\mu j} f[U] \equiv \frac{d}{d\,\alpha}\bigg|_{\alpha=0} f\left(e^{i\alpha\lambda_j}\, U_{x,\mu}\right)$$

Proof of detailed balance:

the discretised trajectories T_H provide the following transition probability distribution at the end of the trajectory:

$$P_H\left([P',U'] \leftarrow [P,U]\right) = \delta\left([P',U'] - T_H[P,U]\right)$$

We assume that the trajectories satisfy *reversibility*:

$$P_H\left([P',U'] \leftarrow [P,U]\right) = P_H\left([-P,U] \leftarrow [-P',U']\right)$$

The Metropolis acceptance step is described by the well known probability distribution:

$$P_A\left([P',U']\leftarrow[P,U]\right)=\min\left\{1,e^{-H[P',U']+H[P,U]}\right\}$$

The total transition probability is then

$$P\left([U']\leftarrow[U]\right)=\int[dP\,dP']P_A\left([P',U']\leftarrow[P,U]\right)P_H\left([P',U']\leftarrow[P,U]\right)P_M[P]$$

Using the relation

$$e^{-H[P,U]}\min\left\{1,e^{-H[P',U']+H[P,U]}\right\}=e^{-H[P',U']}\min\left\{1,e^{-H[P,U]+H[P',U']}\right\}$$

one shows

$$e^{-H[P,U]}P_A\left([P',U']\leftarrow[P,U]\right)=e^{-H[P',U']}P_A\left([P,U]\leftarrow[P',U']\right)$$

$$=e^{-H[-P',U']}P_A\left([-P,U]\leftarrow[-P',U']\right)$$

Therefore, due to reversibility we have with $W_c[U] \propto \exp\{-S_g[U]\}$:

$$W_c[U] \int [dP\, dP'] P_A\left([P', U'] \leftarrow [P, U]\right) P_H\left([P', U'] \leftarrow [P, U]\right) P_M[P]$$

$$= W_c[U'] \int [dP\, dP'] P_A\left([-P, U] \leftarrow [-P', U']\right) P_H\left([-P, U] \leftarrow [-P', U']\right) P_M[-P']$$

Taking into account that $[dP\, dP'] = [d(-P)\, d(-P')]$, this is just the detailed balance condition.

Leapfrog trajectories: satisfy reversibility.

First we update the conjugate momente with a step size $\Delta\tau = \frac{1}{2}\delta\tau$.

This is followed by $(n-1)$ update steps with $\Delta\tau = \frac{1}{2}\delta\tau$ for the gauge variables, alternating with the momentum variables.

Finally, the gauge variables are updated with $\Delta\tau = \delta\tau$ and the momentum variables with $\Delta\tau = \frac{1}{2}\delta\tau$.

The explicit formulae for these steps are:

$$P'_{x\mu j} = P_{x\mu j} - D_{x\mu j} S_g[U]\,\Delta\tau$$

$$U'_{x,\mu} = \exp\left\{\sum_j i\lambda_j\, P_{x\mu j}\,\Delta\tau\right\} U_{x,\mu}$$

The single steps cause a discretisation error of the order $\delta\tau^3$.

Therefore, the action for the final configuration is expected to differ from the initial configuration by an error of order $\delta\tau^2$.

Functions of SU(3) matrices: one can show for $A \in \mathrm{SU}(3)$ that $\mathcal{EXERCISE}$

$$A^3 = \left(\frac{1}{2}\mathrm{Tr}\,A^2\right) A + \left(\frac{1}{3}\mathrm{Tr}\,A^3\right) I$$

Therefore any analytic function $f(A)$ can be written as

$$f(A) = a_2\,A^2 + a_1\,A + a_0\,I$$

For the exponential function $a_{0,1,2}$ can be calculated by recursion relations.

HMC for QCD:

The fermionic (quark) fields are replaced by bosonic pseudofermion fields.

First let us consider two equal mass quarks. By using an auxiliary complex scalar field $\phi_{qx\alpha c}$, which has the same number of components as the fermion field $\psi_{qx\alpha c}$, we have

$$\det\left(Q^+Q\right) \propto \int [d\phi\, d\phi^+] \exp\left\{ -\sum_{xy} (\phi^+_y [Q^+Q]^{-1}_{yx} \phi_x) \right\}$$

This means that the fermion determinant induces an effective action for the gauge field

$$S_{eff}[U] \equiv \sum_{xy} (\phi^+_y \{Q[U]^+ Q[U]\}^{-1}_{yx} \phi_x)$$

which has to be added to the pure gauge action: $S_g \to S_g + S_{eff}$.

PHMC updating algorithm

R. Frezzotti and K. Jansen, Phys. Lett. **B402** (1997) 328; hep-lat/9702016

I. Montvay and E. Scholz, Phys. Lett. B **623** (2005) 73; hep-lat/0506006

This is applicable for any number of quark flavours, provided that the fermion determinant is positive, which is the case for positive quark mass.

(For negative quark masses there is a sign problem!)

For N_f degenerate quarks one uses

$$|\det(Q)|^{N_f} = \left\{\det(Q^\dagger Q)\right\}^{N_f/2} = \left\{\det(\tilde{Q}^2)\right\}^{N_f/2} \simeq \frac{1}{\det P_n(\tilde{Q}^2)}$$

where the *Hermitean fermion matrix* is $\tilde{Q} \equiv \gamma_5 Q$ and the polynomial P_n satisfies $\lim_{n\to\infty} P_n(x) = x^{-N_f/2}$ in an interval $[\epsilon, \lambda]$ covering the spectrum of $Q^\dagger Q$.

The effective gauge action representing the fermions in the path integral is now

$$S_{eff}[U] = \sum_{xy} (\phi^+_y P_n(\tilde{Q}^2)_{yx} \phi_x)$$

Determinant break-up:

sometimes it is more effective to simulate several fractional quark flavours

$$\left(\det \tilde{Q}^2\right)^{N_f/2} = \left[\left(\det \tilde{Q}^2\right)^{N_f/(2n_B)}\right]^{n_B}$$

In this case we need a polynomial approximations $P_n(x) \simeq x^{-\alpha}$

with $\alpha \equiv N_f/(2n_B)$ (positive integer n_B).

The effective gauge action is then

$$S_{eff}[U] = \sum_{k=1}^{n_B} \sum_{xy} (\phi^+_{ky} P_n(\tilde{Q}^2)_{yx} \phi_{kx})$$

Multi-step stochastic correction:

Polynomial approximations with a finite n cannot be exact. One can show that for small fermion masses in lattice units the (typical) smallest eigenvalue of $\tilde{Q}^2$ behaves as $(am)^2$ and for a fixed quality of approximation within the interval $[\epsilon, \lambda]$ the degree of the polynomial is growing as $n \propto \sqrt{\epsilon} \propto (am)^{-1}$.

This would require very high degree polynomials with $n \geq 10^3$-10^4.

The way out is to perform *stochastic corrections.*

For improving the approximation a second polynomial is introduced:

$$P_1(x)P_2(x) \simeq x^{-\alpha} \ , \qquad x \in [\epsilon, \lambda]$$

The first polynomial $P_1(x)$ gives a crude approximation $P_1(x) \simeq x^{-\alpha}$.

The second polynomial $P_2(x)$ gives a good approximation according to

$$P_2(x) \simeq [x^\alpha P_1(x)]^{-1}$$

During the updating process P_1 is realized by PHMC updates whereas P_2 is taken into account stochastically by a *noisy correction step*:

one generates a Gaussian random vector with distribution

$$\frac{e^{-\eta^\dagger P_2(\tilde{Q}[U]^2)\eta}}{\int [d\eta] e^{-\eta^\dagger P_2(\tilde{Q}[U]^2)\eta}}$$

and accepts the change $[U] \to [U']$ with probability $\min\{1, A(\eta, [U'] \leftarrow [U])\}$, where

$$A(\eta, [U'] \leftarrow [U]) = \exp\left\{-\eta^\dagger P_2(\tilde{Q}[U']^2)\eta + \eta^\dagger P_2(\tilde{Q}[U]^2)\eta\right\}$$

This update procedure satisfies the detailed balance condition. $\mathcal{EXERCISE}$

The Gaussian noise vector η can be obtained from η' distributed according to the simple Gaussian distribution

$$\frac{e^{-\eta'^\dagger\eta'}}{\int[d\eta']e^{-\eta'^\dagger\eta'}}$$

by setting it equal to

$$\eta = P_2(\tilde{Q}[U]^2)^{-\frac{1}{2}}\eta'$$

In order to obtain the inverse square root on the right hand side one can proceed with a polynomial approximation

$$\bar{P}_2(x) \simeq P_2(x)^{-\frac{1}{2}} \ , \quad x \in [\bar{\epsilon}, \lambda]$$

The interval $[\bar{\epsilon}, \lambda]$ can be chosen differently, usually with $\bar{\epsilon} < \epsilon$, from the approximation interval $[\epsilon, \lambda]$ for P_2.

The polynomial approximation with P_2 can only become exact in the limit when the degree n_2 of P_2 is infinite. Instead of investigating the dependence of expectation values on n_2 by performing several simulations, one fixes n_2 to some high value and performs another correction in the expectation values by still finer polynomials. This is done by *reweighting* the configurations. This *measurement correction* is based on a further polynomial approximation P' with degree n' which satisfies

$$\lim_{n'\to\infty} P_1(x)P_2(x)P'(x) = x^{-\alpha} \ , \qquad x \in [\epsilon', \lambda]$$

The interval $[\epsilon', \lambda]$ can be chosen such that $\epsilon' = 0, \lambda = \lambda_{max}$, where λ_{max} is an absolute upper bound of the eigenvalues of $\tilde{Q}^2$.

In practice it is more effective to take $\epsilon' > 0$ and determine the eigenvalues below ϵ' and the corresponding correction factors exactly.

For the evaluation of P' one can use recursive relations, which can be stopped by observing the required precision of the result.

After reweighting the expectation value of a quantity A is given by

$$\langle A \rangle = \frac{\langle A \exp\{\eta^\dagger [1 - P'(\tilde{Q}^2)]\eta\}\rangle_{U,\eta}}{\langle \exp\{\eta^\dagger [1 - P'(\tilde{Q}^2)]\eta\}\rangle_{U,\eta}} \ ,$$

where η is a simple Gaussian noise.

Here $\langle \ldots \rangle_{U,\eta}$ denotes an expectation value on the gauge field sequence, which is obtained in the two-step process described before, and on a sequence of independent η's of arbitrary length.

tmLQCD is easier: the quark determinant of a degenerate quark doublet becomes $\det(\tilde{Q}^2+\mu_s^2)$ where $\mu_s \equiv \mu_q \sin\omega$ with μ_q the quark mass in lattice units and ω the twist angle.

The polynomials $P_{1,n_1}(x)$ and $P_{2,n_2}(x)$ now satisfy

$$\lim_{n_2\to\infty} P_{1,n_1}(x)\,P_{2,n_2}(x) = (x+\mu_s^2)^{-N_f/2}\ , \quad x\in[\epsilon,\lambda]$$

In case of $\omega \simeq \frac{\pi}{2}$ the polynomial approximations have lower orders and the updating is faster due to the absence of exceptional configurations with very small eigenvalues originating from topological defects at the cutoff scale.

We need Tflops: an example (for the near future) is

$\Omega = 50^3\cdot 100 = 1.25\cdot 10^7$ and $am_q = 0.005$,

for instance, $a = 0.1\,\mathrm{fm},\ m_q = 10\,\mathrm{MeV},\ L = 5\,\mathrm{fm},\ m_\pi \simeq 200\,\mathrm{MeV}$.

Error estimates

In numerical simulations the updating process creates a configuration sample $[\varphi_n]$, $(n = 1, 2, \ldots, N)$.

The task is to determine the expectation value of different quantities.

The simplest kind of quantities are defined by a function of the field variables $A[\varphi]$. An estimator of their expectation values is given by the sample average

$$\overline{A} \equiv \frac{1}{N} \sum_{n=1}^{N} A[\varphi_n] \ .$$

wich gives for $N \to \infty$ the true expectationtation value $\overline{A} \to \langle A \rangle$.

These quantities can be called primary quantities.

The secondary quantities are functions of the primary quantities.

For instance, the correlation of two primary quantities $A[\varphi], B[\varphi]$, which is defined as

$$(AB) \equiv \langle AB \rangle - \langle A \rangle \langle B \rangle$$

In the ideal case, when the configurations contained in a sample are all statistically independent, the sample average $\overline{A}$ is normally distributed around the mean value $\overline{\overline{A}}$, with variance

$$\sigma^2_{\overline{A}} = \frac{\overline{A^2} - \overline{A}^2}{N-1} = \frac{\overline{(A - \overline{A})^2}}{N-1}$$

This is the consequence of the central limit theorem.

In this case the error on the sample average of a primary quantity would be $\overline{\overline{A}} = \overline{A} \pm \sigma_{\overline{A}}$.

The above error estimate in is usually too optimistic, because the subsequent configurations have lots of similarities, they are by no means independent. This correlation in the sequence of generated configurations is called *autocorrelation*. For a primary quantity A the autocorrelation is defined as

$$(A_n A_{n+\tau}) \equiv \langle A_n A_{n+\tau}\rangle - \langle A_n\rangle\langle A_{n+\tau}\rangle$$

$$= \langle A_n A_{n+\tau}\rangle - \langle A\rangle^2 = \langle (A_n - \overline{A})(A_{n+\tau} - \overline{A})\rangle$$

In terms of the autocorrelation the true variance of $\overline{A}$ is $\mathcal{EXERCISE}$

$$\sigma^2_{\overline{A}} = \left\langle \left[\frac{1}{N}\sum_{n=1}^{N} (A_n - \langle A\rangle)\right]^2 \right\rangle = \sum_{\tau=-N}^{N} \frac{N-|\tau|}{N^2}(A_n A_{n+\tau})$$

$$\stackrel{N\to\infty}{\longrightarrow} (AA)\frac{2\tau_{int,A}}{N} \simeq (\overline{A^2} - \overline{A}^2)\frac{2\tau_{int,A}}{N} \ ,$$

where the *integrated autocorrelation time* $\tau_{int,A}$ is defined as

$$\tau_{int,A} \equiv \frac{1}{2} \sum_{\tau=-\infty}^{+\infty} \frac{(A_n A_{n+\tau})}{(AA)} \; .$$

One can see that due to the autocorrelation the effective number of independent measurements is $N/(2\tau_{int,A})$.

In practice one can numerically determine the autocorrelation with a truncation in the sum over time differences.

The continuum limit of lattice quantum field theories is defined near *critical points*, that is near second order phase transitions in the bare parameter space. This causes a difficulty because the autocorrelation (usually) diverges near critical points.

Error estimates for secondary quantities: one can use the *jackknife analysis*

Consider a sample of measurements of a primary quantity A. The measured values are $A_1, A_2, \ldots, A_{N_s}$, and the sample average is

$$\overline{A} \equiv \frac{1}{N_s} \sum_{s=1}^{N_s} A_s$$

The best estimate of a secondary quantity is $\overline{y} = y(\overline{A})$ (not $\overline{y(A)}$). A stable error estimator for $\overline{y}$ can be derived from the jackknife averages obtained by omitting a single measurement from the sample in all possible ways:

$$A_{(J)s} \equiv \frac{1}{N_s - 1} \sum_{r \neq s} A_r$$

The corresponding values of the secondary quantity are the *jackknife estimators* $y_{(J)s} \equiv y(A_{(J)s})$, with an average

$$\overline{y_{(J)}} \equiv \frac{1}{N_s} \sum_{s=1}^{N_s} y_{(J)s}$$

The variance of the jackknife estimators can be obtained as

$$\sigma^2_{(J)\overline{y}} \equiv \frac{N_s - 1}{N_s} \sum_{s=1}^{N_s} \left(y_{(J)s} - \overline{y_{(J)}} \right)^2$$

For primary quantities this is equivalent to the simple variance. $\mathcal{EXERCISE}$

For secondary quantities the jackknife variance estimator gives as an error estimate $\overline{\overline{y}} = \overline{y} \pm \sigma_{(J)\overline{y}}$.

Fitting simulation data

The simplest way to determine the masses is to fit some of the correlators by an exponential function in time intervals for distant time-slices.

In case of small enough statistical errors one can also obtain good fits with a sum of two (or more) exponentials.

The best results can be achieved, however, by taking a set of some operators in a given channel and calculate the *correlator matrix* among them.

The correlator matrix can be approximated by the sum of contributions of eigenstates of the Hamiltonian (i. e. of the transfer matrix). In general, a real symmetric $D \times D$ correlator matrix $C(t_2, t_1)$ between time-slices t_1 and $t_2 > t_1$ is defined by the matrix elements of D operators $\mathcal{O}_a, \mathcal{O}_b, \ldots, \mathcal{O}_d$.

If the energy eigenstates are $|n\rangle,\ n = 1, 2, \ldots, M$ then in a shorthand notation

$$C(t_2, t_1) = \begin{pmatrix} C(t_2,t_1)_{aa} & C(t_2,t_1)_{ab} & \ldots & C(t_2,t_1)_{ad} \\ C(t_2,t_1)_{ab} & C(t_2,t_1)_{bb} & \ldots & C(t_2,t_1)_{bd} \\ \vdots & \vdots & \ldots & \vdots \\ C(t_2,t_1)_{ad} & C(t_2,t_1)_{bd} & \ldots & C(t_2,t_1)_{dd} \end{pmatrix}$$

where the matrix elements can be written as, for instance,

$$C(t_2,t_1)_{ab} = (a|1)_{t_2}(b|1)_{t_1} + (a|2)_{t_2}(b|2)_{t_1} + \ldots + (a|M)_{t_2}(b|M)_{t_1}$$

with

$$(c|k)_t \equiv \langle 0|\mathcal{O}_c(t)|k\rangle = \langle k|\mathcal{O}_c(t)|0\rangle\ ,$$

for $c = a, b, \ldots, d$ and $k = 1, 2, \ldots, M$.

Assuming that we consider bosonic (fermionic) operators, we have periodic (anti-periodic) time dependence with the time extension of the lattice L_4.
This implies

$$(a|k)_{t_2}(b|k)_{t_1} = (a|k)\,(b|k)\,\{\exp[-tE_k] \pm \exp[-(L_4-t)E_k]\} \ .$$

where the positive and negative sign stands for periodicity and anti-periodicity, respectively. Here $t \equiv t_2 - t_1$, E_k is the energy (e.g. mass) corresponding to the state $|k\rangle$ and $(a|k) \equiv (a|k)_0$, $(b|k) \equiv (b|k)_0$.

Fitting the correlator matrix by the expression given above one can obtain the energies we are looking for.

If correlators can be determined to a very good precision, one can perform least-square fits by minimising the correlated chi-squared. In order to obtain a good starting point for the minimisation, one can first minimise the *uncorrelated chi-squared* defined by

$$\chi^2_n = \sum_{i=1}^{N_C} \left(\frac{f_i(p) - \overline{X}_i}{\delta X_i} \right)^2$$

where the index i runs over the independent matrix elements to be fitted, $\overline{X}_i$ and δX_i are the mean value and error of the matrix element i, respectively, and $f_i(p)$ is the fitting function of N_P parameters $(p_1, p_2, \ldots, p_{N_P})$.

The best fit obtained in this way can be taken as a starting point to minimise the *correlated chi-squared*

$$\chi^2_c = \sum_{i,j=1}^{N_C} \left(f_i(p) - \overline{X}_i\right) M_{ij} \left(f_j(p) - \overline{X}_j\right) \ ,$$

where $M_{ij} = NC^{-1}_{ij}$, with the number N of input data and the correlator matrix

$$C_{ij} = \frac{1}{N-1} \sum_{n=1}^{N} \left(X_{i,n} - \overline{X}_i\right) \left(X_{j,n} - \overline{X}_j\right) \ .$$

Recent developments in numerical simulations of QCD

The smallness of the u-, d- and s-quark masses implies:

the numerical simulation (with dynamical quarks) is a great challenge for computations.

International collaborations in LQCD:

- USA: MILC, RBC, ... Collaboration
- Japan: CP-PACS, JLQCD, ... Collaboration
- Europe: UKQCD, Alpha, QCDSF, ETM, BMW ... Collaboration

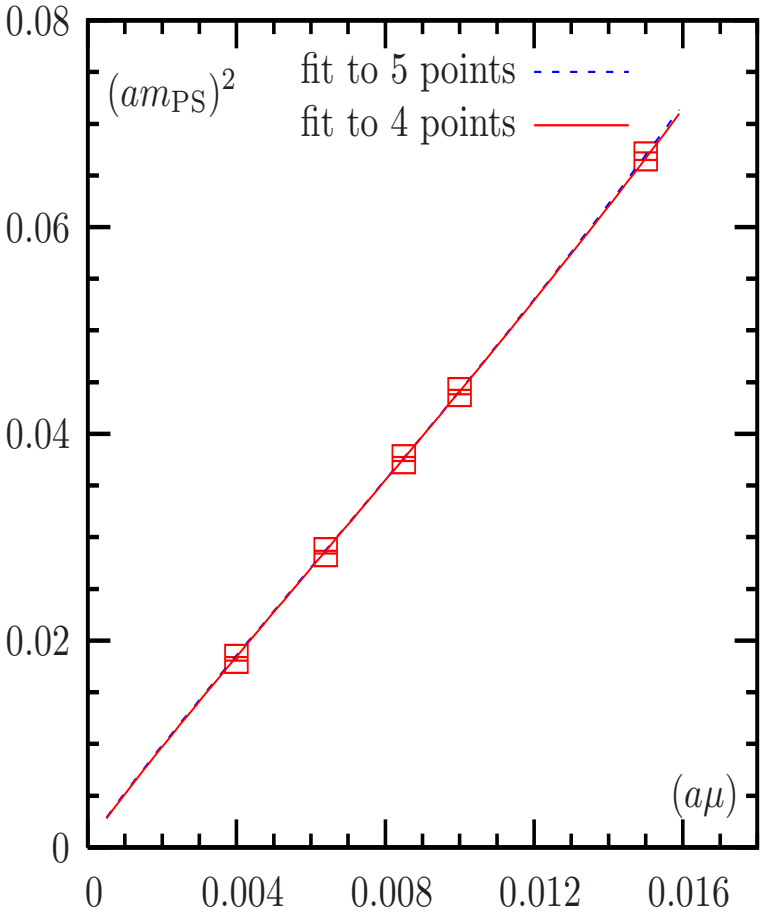
European Twisted Mass Collaboration:

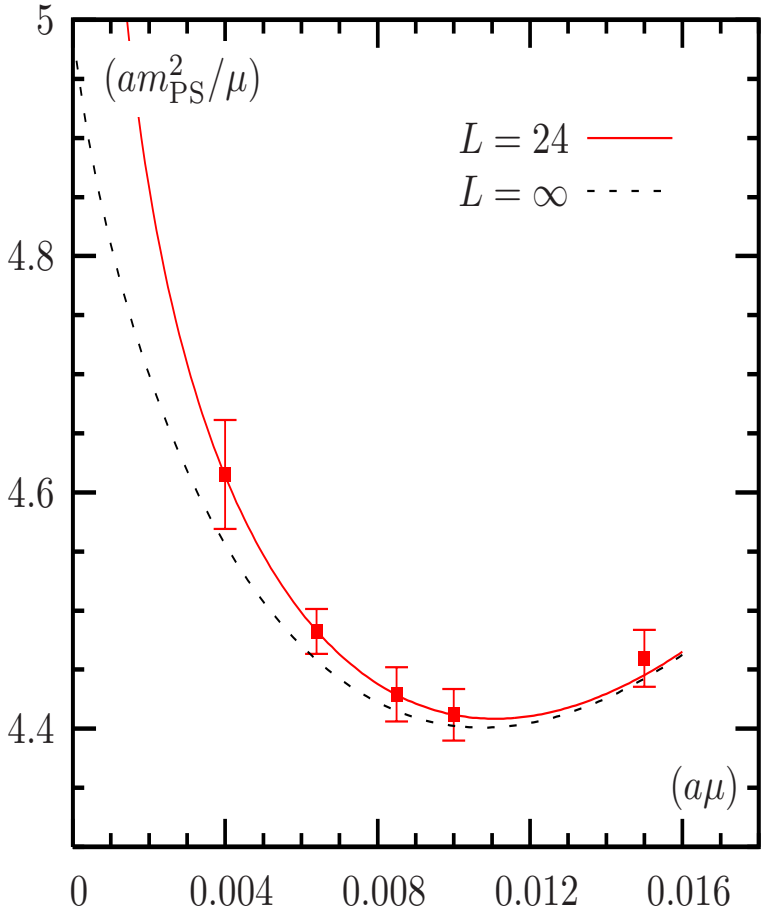
about 30 physicists from

- Cyprus: University of Cyprus
- France: Université de Paris Orsay
- Germany: DESY, Universität Münster, TU München
- Italy: Università di Roma I,II,III, INFN, ECT*
- Spain: Universidad València
- Switzerland: ETH Zürich
- United Kingdom: University of Liverpool

see e.g. Results from ETMC in the light-quark sector. P. Dimopoulos et al.

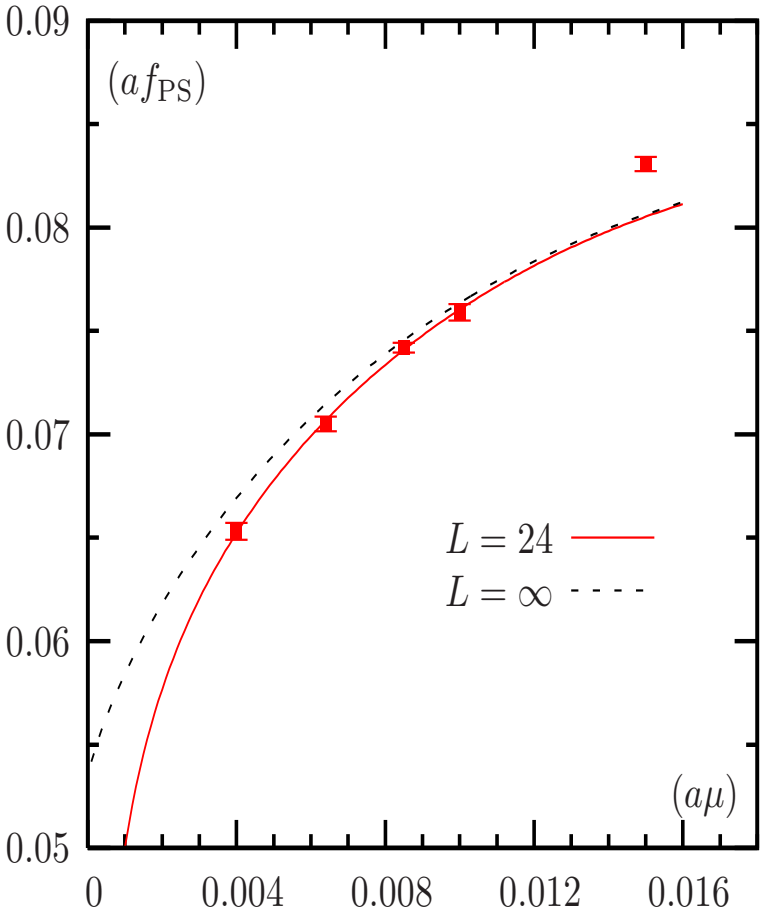
PoS CD09 (2009) 006

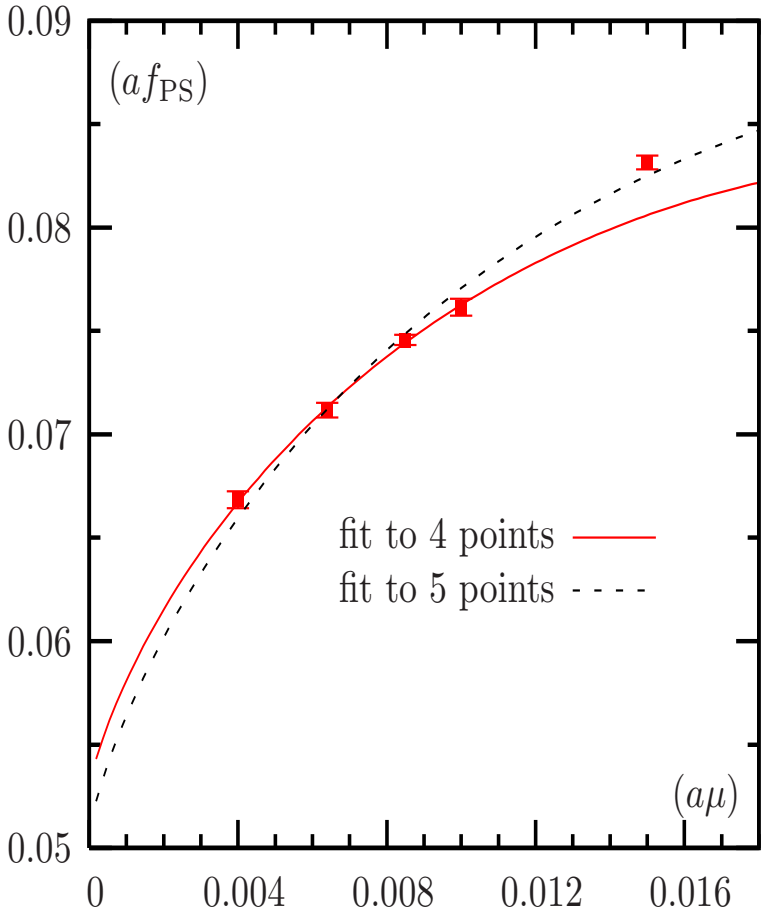




Left: $(am_\pi)^2$ as a function of the twisted mass $a\mu$.

Right: $(am_\pi)^2/(a\mu)$ versus $a\mu$. The finite volume ChPT-fit is shown, together with the infinite volume limit (dashed line): $\bar{l}_3 = 3.65(12)$.





ChPT fits to af_π versus $a\mu$. Left: the point with largest $a\mu$ left out (the dashed line is the infinite volume limit);

Right: compared to finite volume fit to every point.

The fit gives: $a = 0.087(1)\,\mathrm{fm}$, $(a^{-1} = 2264(26)\,\mathrm{MeV})$, $\bar{l}_4 = 4.52(06)$.

The physical consequence of the smallness of three quark masses is the existence of eight light pseudo-Goldstone bosons: π, K, η.

In the low-energy pseudo-Goldstone boson sector there is an $\mathrm{SU}(3) \otimes \mathrm{SU}(3)$ chiral flavour symmetry and the dynamics can be described by Chiral Perturbation Theory (ChPT).

In an expansion in powers of momenta and light quark masses several low energy constants – the Gasser-Leutwyler constants – appear which parameterize the strength of interactions in the low energy chiral Lagrangian.

An eminent task for Monte Carlo simulations in Lattice-QCD is to describe the pseudo-Goldstone boson sector.

The Gasser-Leutwyler constants are free parameters which can be constrained by analyzing experimental data.
In the framework of lattice regularization they can be determined from first principles by numerical simulations.

In numerical simulations, besides the possibility of changing momenta, one can also change the masses of the quarks.
ChPT can be extended by changing the valence quark masses in quark propagators independently from the sea quark masses in virtual quark loops.
In this way one arrives at Partially Quenched Chiral Perturbation Theory (PQChPT, Bernard, Golterman).

Ratio tests of PQChPT for m_π^2 and f_π

Taking ratios at fixed gauge coupling (β) is advantageous because the Z-factors of mutiplicative renormalization cancel (for instance, in m_q and f_π).

Also: some types of lattice artifacts may cancel.

ChPT for Wilson-type lattice actions: taking into account lattice artifacts in the Chiral Lagrangian one can reach the continuum limit faster.

Effective continuum theory (Symanzik):

cutoff effects (of the lattice regularized theory) can be described by $\mathcal{O}(a, a^2, \ldots)$ terms in a local effective Lagrangian.

This idea can be applied to low energy LQCD (Lee, Sharpe, Singleton, Rupak, Shores):

In case of the Wilson quark action the leading $\mathcal{O}(a)$ effects have a simple chiral transformation property, identical to those of the quark masses.

At leading order of ChPT an additional $\mathcal{O}(a)$ parameter appears:

$$\chi \equiv \frac{2B_0 m_q}{f_0^2} \,, \qquad \rho \equiv \frac{2W_0 a}{f_0^2} \qquad \left(\eta \equiv \frac{\rho}{\chi}\right)$$

At next to leading order (NLO):

the Gasser-Leutwyler constants $L_1, \ldots, L_8$ are doubled by the (bare parameter dependent) coefficients $W_1, \ldots, W_8$ describing $\mathcal{O}(a)$ effects.

(Extension to $\mathcal{O}(a^2)$ is possible.)

Variables to be used in ratio tests of PQChPT:

$$\xi \equiv \frac{m_{qV}}{m_{qS}} = \frac{\chi_V}{\chi_S} \,, \qquad \eta_S \equiv \frac{\rho_S}{\chi_S} \,, \qquad \sigma_i \equiv \frac{m_{qS}^{(i)}}{m_{qS}^{(R)}} = \frac{\chi_S}{\chi_R}$$

For the pion decay constants the appropriate ratios are:

$$Rf_{VV} \equiv \frac{f_{VV}}{f_{SS}} \,, \qquad Rf_{VS} \equiv \frac{f_{VS}}{f_{SS}} \,, \qquad RRf \equiv \frac{f_{VS}^2}{f_{VV} f_{SS}}$$

and for the pion mass-squares (dividing by the leading order behaviour)

$$Rn_{VV} \equiv \frac{m_{VV}^2}{\xi m_{SS}^2} \,, \qquad Rn_{VS} \equiv \frac{2m_{VS}^2}{(\xi+1) m_{SS}^2} \,, \qquad RRn \equiv \frac{4\xi m_{VS}^4}{(\xi+1)^2 m_{VV}^2 m_{SS}^2}$$

For the sea quark mass dependence

$$Rf_{SS} \equiv \frac{f_{SS}}{f_{RR}} \,, \qquad Rn_{SS} \equiv \frac{m_{SS}^2}{\sigma m_{RR}^2}$$

are appropriate.

Examples of the NLO formulas: for N_s degenerate sea quarks

$$Rf_{VV} = 1 + 4(\xi - 1)\chi_S L_{S5} + \frac{N_s \chi_S}{32\pi^2}(1+\eta_S)\log(1+\eta_S)$$

$$-\frac{N_s \chi_S}{64\pi^2}(1+\xi+2\eta_S)\log\frac{1+\xi+2\eta_S}{2}\ ,$$

$$RRf = 1 + \frac{\chi_S}{32 N_s \pi^2}(\xi - 1) - \frac{\chi_S}{32 N_s \pi^2}(1+\eta_S)\log\frac{\xi+\eta_S}{1+\eta_S}\ ,$$

$$Rf_{SS} = 1 + 4(\sigma - 1)\chi_R(N_s L_{R4} + L_{R5}) + 4(\eta_S\sigma - \eta_R)\chi_R(N_s W_{R4} + W_{R5})$$

$$-\frac{N_s \chi_R}{32\pi^2}\sigma(1+\eta_S)\log[\sigma(1+\eta_S)] + \frac{N_s \chi_R}{32\pi^2}(1+\eta_R)\log(1+\eta_R)$$

and similarly for $Rn\ldots$.

L_{Sk} denote Gasser-Leutwyler constants renormalized at the scale $f_0\sqrt{\chi_S}$.

They are related to $\bar{L}_k$ defined at the scale f_0 and L'_k defined at the generic scale μ according to

$$L_{Sk} = \bar{L}_k - c_k \log(\chi_S) = L'_k - c_k \log(\frac{f_0^2}{\mu^2}\chi_S)$$

with some (known) constants c_k.

The corresponding relations for the coefficients W_{Sk} are:

$$W_{Sk} = \bar{W}_k - d_k \log(\chi_S) = W'_k - d_k \log(\frac{f_0^2}{\mu^2}\chi_S)$$

NNLO corrections (Sharpe, van de Water): in the valence quark mass dependence the "counterterm insertion" contributions have the form

$$D_X\ \chi_S^2(\xi-1) + Q_X\ \chi_S^2(\xi-1)^2$$

which can also be taken into account in the fits.

Recent numerical simulations (qq+q Collaboration, DESY-Münster):

16^4 and $16^3 \cdot 32$ lattices, $N_s = 2$ light quark flavours.

Gauge coupling: $\beta = 5.1$;

hopping parameter: $\kappa_0 = 0.176$, $\kappa_1 = 0.1765$, $\kappa_2 = 0.177$.

Configuration sample: between 750 and 1800 per point.

Lattice spacing determined from r_0/a: $a = 0.189(5)\,\mathrm{fm} \simeq (1.04\,\mathrm{GeV})^{-1}$

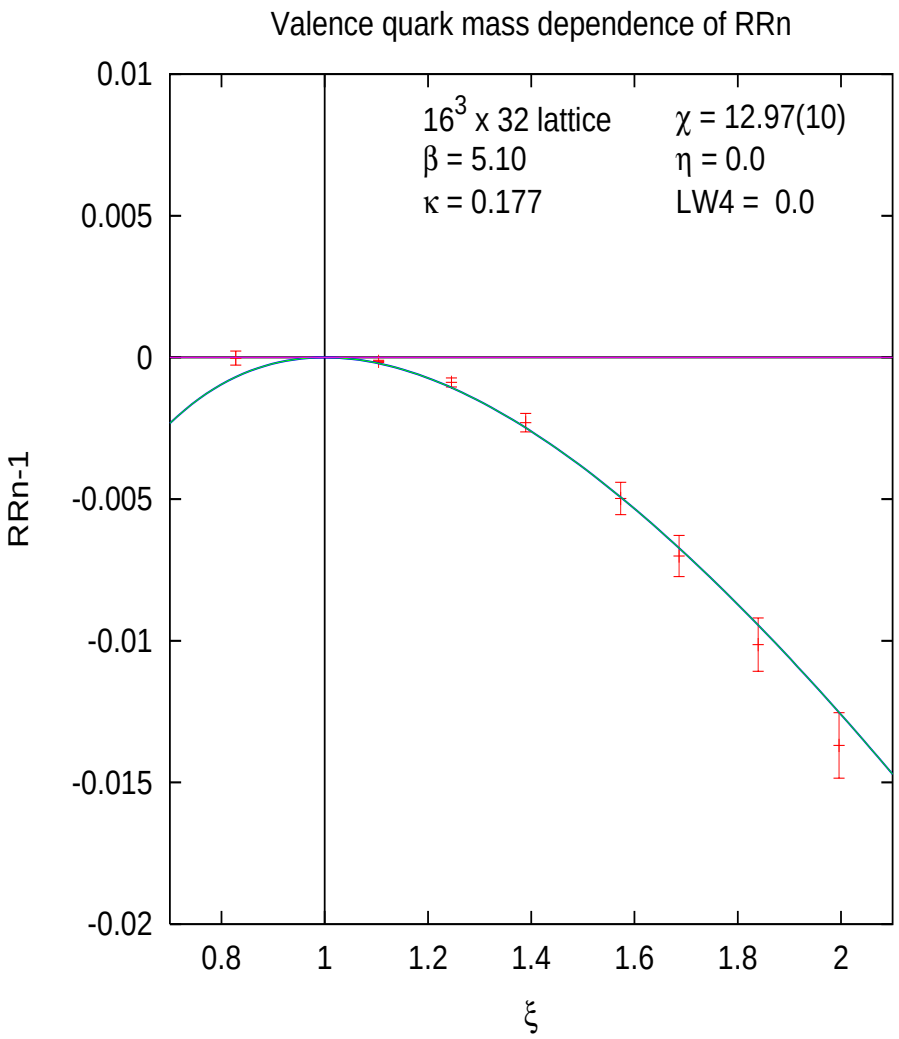
giving lattice extensions $L \simeq 3\,\mathrm{fm}$.

Pion masses: $am_\pi = 0.6747(14),\ 0.6211(22),\ 0.4354(68),\ 0.3676(23)$

which correspond to $m_\pi \simeq 702,\ 646,\ 452,\ 415\,\mathrm{MeV}$.

Sea quark masses: approximately $60\,\mathrm{MeV}$ to $25\,\mathrm{MeV}$.

Valence quark masses: $\frac{1}{2}m_{sea} \leq m_{valence} \leq 2m_{sea}$.



$16^3 \cdot 32$ lattice at ($\beta = 5.1$, $\kappa = 0.177$): one parameter fit of $(RRn - 1) = \chi_S(1 - \xi + \log \xi)/(32\pi^2)$ ("pure chiral log").

First estimates of L-G constants:

renormalized at scale $f_0\sqrt{\chi_R}$ with

$\chi_R = 33.5(2.4)$

$$L_{R5} = 3.00(19) \cdot 10^{-3} \ ,$$

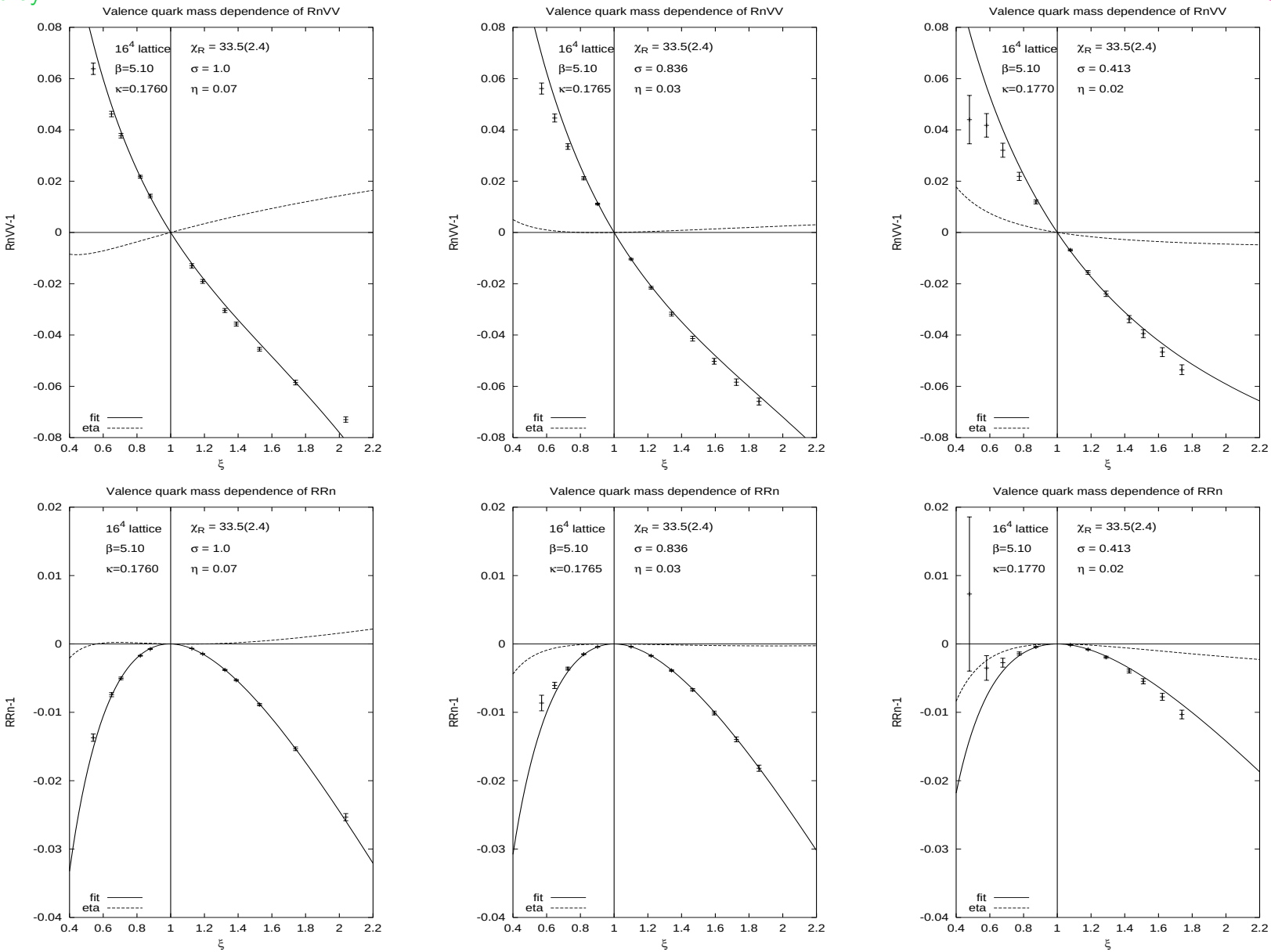
$$(2L_{R8} - L_{R5}) = -6.25(52) \cdot 10^{-4}$$

From the sea quark mass dependence:

$$(2L_{R4} + L_{R5}) = 4.34(28) \cdot 10^{-3} \ ,$$

$$(4L_{R6} + 2L_{R8} - 2L_{R4} - L_{R5}) = -9.1(6.4) \cdot 10^{-5} \ ,$$

$$\frac{\Lambda_3}{f_0} = 6.51(57) \ , \quad \frac{\Lambda_4}{f_0} = 22.9(1.5)$$



PQChPT fits of $(Rn_{VV} - 1)$ and $(RRn - 1)$ for three different sea quark mass values.

Budapest-Marseille-Wuppertal (BMW) Collaboration

Z. Fodor et al. arXiv:1011.2403 [hep-lat], arXiv:1011.2711 [hep-lat]

Lattice QCD at the physical point:

quark masses down to $120\,\mathrm{MeV}$, lattice volume up to $6\,\mathrm{fm}$.

Improved lattice action:

HEX-smeared clover (Wilson-) fermions, Symanzik-improved gauge action.

Results for light quark masses: values for $\overline{MS}(2\,\mathrm{GeV})$

$m_{u,d} = 3.47(10)\,\mathrm{MeV}$

$m_s = 95(3)\,\mathrm{MeV}$.

Outlook

Custom-designed supercomputers for lattice QCD (2004...):

QCDOC, apeNEXT, ..

QPACE: QCD Parallel Computing on the Cell,

Jülich-Wuppertal(-Regensburg): designed in 2009, based on IMB PowerXCell8i.

9 cores/CPU, network: Field-Programable-Gate-Arrays (FPGS),

1 TByte/rack, 4 racks.

Green500 list: QPACE has lead in 2009-2010

with 773 Mflops/W (57.5 kW $\longrightarrow$ 44 Tflops).

QPACE is used, for instance, by the BMW-Collaboration: (H. Baier et al., PoS **LAT2009** (2009) 001. [arXiv:0911.2174 [hep-lat]].)

GPU's: up to 1 TFlops (double precision) in peak (NVIDIA, AMD).

Massively parallel architecture (512 cores, thousands of registers).

Programming environement (NVIDIA): CUDA.

First LQCD codes are available, also used in LHC experiments (ATLAS, Alice: offline track reconstruction, trigger).

TOP500 list: Tianhe-1A (2.6 PFlops).

General purpose supercomputers: BlueGeneP, Nehalem based Supercomputer,..

Well suited for LQCD simulations, costumer friendly programming environemt.

The goal is to perform dynamical quark simulations with light quarks in large volumes.