An introduction into Lattice Gauge Theory

Karl Jansen

- **Concepts and selected results**
  - improving continuum limit
  - finite size effects
  - non-perturbative renormalization
  - chiral fermions
- **Algorithms and machines**
- **Conclusions**

not covered

- *lattice perturbation theory*
- $T > 0$ *on the lattice*
- *tests of semi-classical pictures*

quantization via Feynman's path integral in euclidean metric and its tansfer matrix $\mathbb{T}$ formulation

$$\boxed{\mathcal{Z} = \int_{\text{fields}} e^{-S_{\text{E}}} = \text{Tr}\mathbb{T}^{\text{N}}}$$

integration over *classical* fields

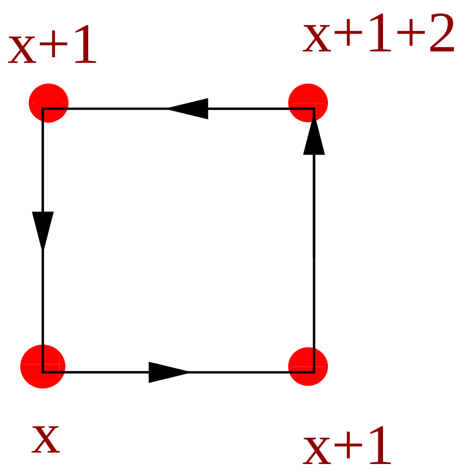
$\longrightarrow$ corresponds to partition function in statistical mechanics

plaquette gauge action

$$S_{\text{G}} = \sum_x \sum_{\substack{\mu,\nu \\ \mu<\nu}} \beta \text{Tr}\left[-\left(U_p + U_p^\dagger\right)\right], \quad \beta = \frac{N}{g_0^2}$$

$$U_p = U(x,\mu)U(x+\mu,\nu)U^{-1}(x+\nu,\mu)U^{-1}(x,\nu)$$

link variable $U(x,\mu) \in SU(N)$



fermion action in QCD

$$S = a^4 \sum_x \bar{\psi} \left[\gamma_\mu(\nabla_\mu + \nabla^*_\mu - r\nabla^*_\mu \nabla_\mu + m\right] \Psi(x)$$

gauge invariant lattice "derivatives"

$$\begin{aligned} \nabla_\mu \Psi(x) &= \tfrac{1}{a}\left[U(x,\mu)\Psi(x+\mu) - \Psi(x)\right] \\ \nabla^*_\mu \Psi(x) &= \tfrac{1}{a}\left[\Psi(x) - U^{-1}(x-\mu,\mu)\Psi(x-\mu)\right] \end{aligned}$$

rescaling the fields (usually done)

$$\Psi \to \Psi^L = \sqrt{2\kappa}\Psi$$

the lattice action becomes setting $r = 1$

$$\begin{aligned} S_{\mathrm{W}} = \ & \bar{\psi}^L(x)\{\Psi^L(x) - \kappa \sum_\mu \left[(1-\gamma_\mu)U^\dagger(x-\mu,\mu)\Psi^L(x-\mu)\right. \\ & + \quad \left.(1+\gamma_\mu)U(x,\mu)\Psi^L(x+\mu)\right]\} \end{aligned}$$

keywords: Wilson's lattice (plaquette) gauge and (2nd derivative) fermion actions

General articles

Lectures, review articles

- R. Gupta
  Introduction to Lattice QCD, hep-lat/9807028

- C. Davies
  Lattice QCD, hep-ph/0205181

- M. Lüscher
  Advanced Lattice QCD, hep-lat/9802029
  Chiral gauge theories revisited, hep-th/0102028

NIC symposium, december 2001, Jülich

- P.Hernández, L. Lellouch, K.J.,
  From enemies to friends: chiral symmetry on the lattice, hep-lat/0203029

- R. Sommer, H. Wittig
  Fundamental parameters of QCD, physics/0204015

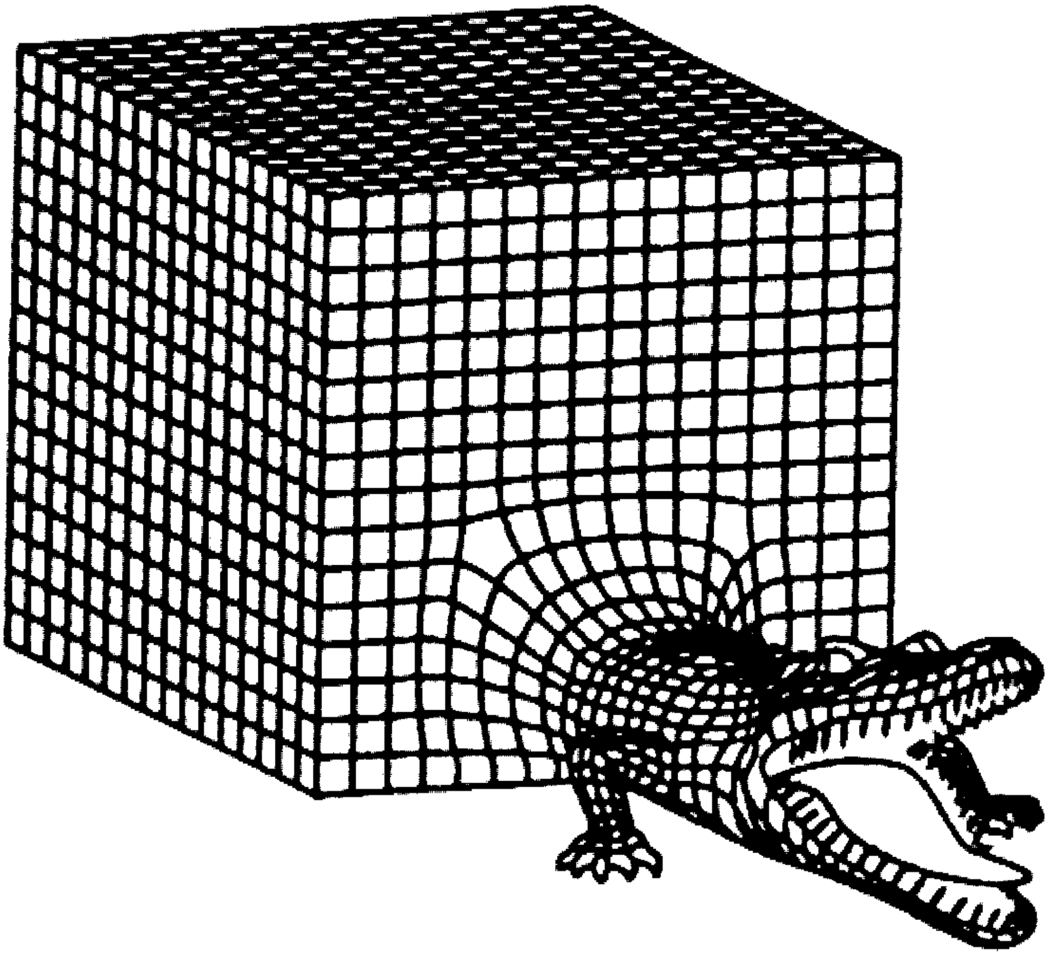
The **John von Neumann-Institute of Computing (NIC)**

coorporation between **DESY** and **research centre Jülich**

- **NIC** shall provide supercomputer resources

- **NIC** shall maintain research groups
  - *Elementary particle physics* K.J.
  - *Many particle physics* P. Grassberger

Welcome to the lattice!



$\longrightarrow$ discretization errors

$\longrightarrow$ finite volume effects

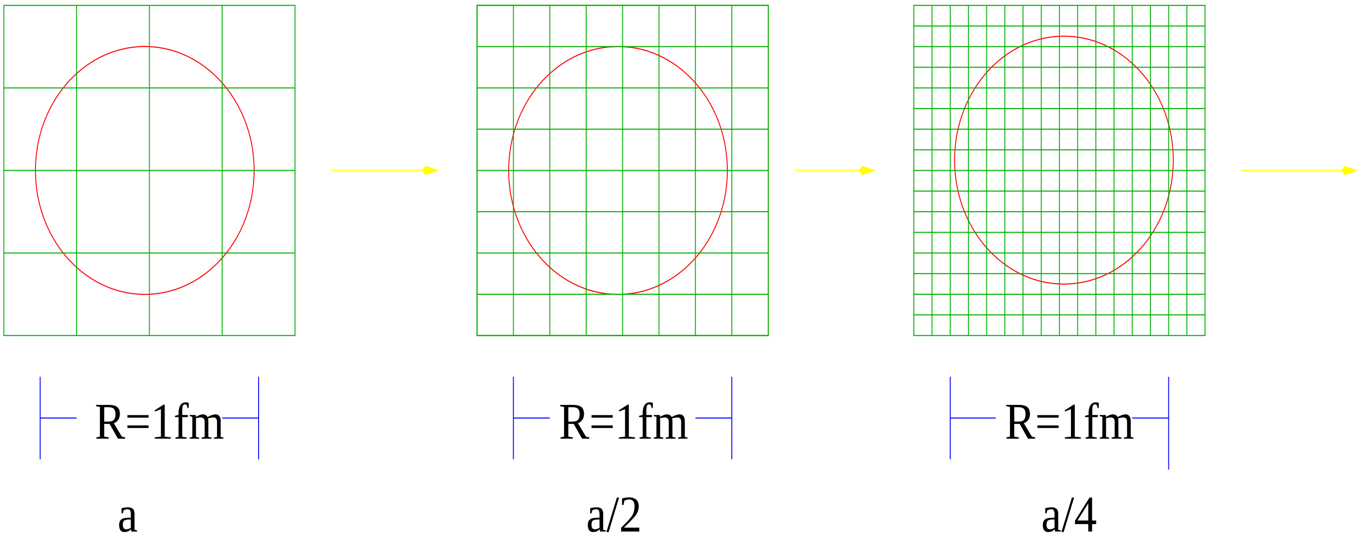
A look at the continuum limit

the general idea of the continuum limit:

we keep fixed values of physical quantities such as a particle mass $m^{\rm phys} = m^{\rm lattice}/a$

$\Rightarrow$ for $a \rightarrow 0 \Rightarrow m^{\rm lattice} \rightarrow 0$

since $m^{\rm lattice} = 1/\xi^{\rm lattice}$ in the contunuum limit
the *lattice correlation length diverges*



$\xi^{\rm lattice} \approx 2.5$ $\xi^{\rm lattice} \approx 5.0$ $\xi^{\rm lattice} \approx 10.0$

a fixed physical size of a particle (e.g. the proton) receives a finer and finer resolution as $\xi^{\rm lattice} \rightarrow \infty$

The continuum limit

fixed *physical* length $L = Na = 1\mathrm{fm}$ means

$$a = 0.1\mathrm{fm} \Rightarrow N = 10$$

$$a = 0.05\mathrm{fm} \Rightarrow N = 20$$

$$a = 0.01\mathrm{fm} \Rightarrow N = 100$$

easily running out of computertime and memory

solutions (?)

- keep $a \gg 0 \Rightarrow$ lattice artefacts
- keep $L < 1\mathrm{fm} \Rightarrow$ finite size effects

modern approach through theoretical advances

$\longrightarrow$ accelerate continuum limit: improvement programme

$\longrightarrow$ do not be afraid of finite size effects: make use of them

Acceleration to the continuum limit

(old) standard lattice action of QCD is

$$S_{\rm old} = \underbrace{S_{\rm G}}_{{\rm O}(a^2)} + \underbrace{S_{\rm wilson}}_{{\rm O}(a)}$$

$\Rightarrow$ expectation values of physical observables

$$\langle O \rangle = \langle O \rangle_{\rm cont} + {\rm O}(a)$$

employing all lattice symmetries, equations of motions

$\Rightarrow$ only one more term in ${\rm O}(a)$ possible

(improved) standard lattice action
Skeikoleslami and Wohlert

$$S_{\rm new} = S_{\rm old} + \underbrace{S_{\rm sw}}_{{\rm O}(a)}$$

$$S_{\rm sw} = a^5 \sum_x c_{\rm sw} \bar{\psi}(x) \tfrac{i}{4} \hat{F}_{\mu\nu}(x) \Psi(x)$$

with $c_{\rm sw}$ a *tunable* parameter

$\Rightarrow$ compute non-perturbatively $c_{\rm sw}$ such that ${\rm O}(a)$ cancel

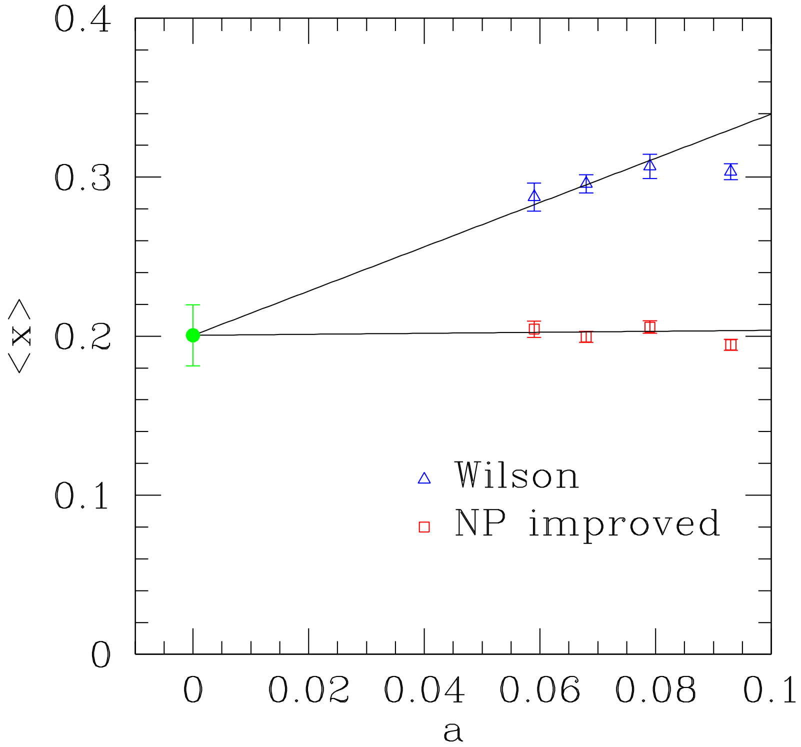
$\Rightarrow$ (nota bene: if also the operator is improved)

$$\langle O \rangle = \langle O \rangle_{\text{cont}} + \mathrm{O}(a^2)$$

succesful *Symanzik improvement programme* of the

ALPHA Collaboration

Example of physical quantity: *avererage momentum* $< x >$ *of non-singlet, twist-2 operator in a pion*



keyword: non-perturbative $O(\mathrm{a})$ *improvement*

Explosion of lattice actions

- *Symanzik improved*
- *renormalization group improved, Iwasaki, DBW2*
- *fixed point (perfect)*
- *fat link*
- *FLIC*
- *tadpole improved*
- *hypercube*

of course, each of them is the best!

$\longrightarrow$ important:

- results have to agree in the continuum limit
- provide valuable crosscheck

pure gauge theory

static potential

Green function

$$G(q_{\mathrm{N}}, t_{\mathrm{N}}; q_0, t_0) = \langle q_{\mathrm{N}} | e^{-\frac{i}{\hbar}\mathbb{H}(t_{\mathrm{N}}-t_0)} | q_0 \rangle$$

with

$\mathbb{H} = \frac{\hat{p}}{2m} + V(\hat{q})$

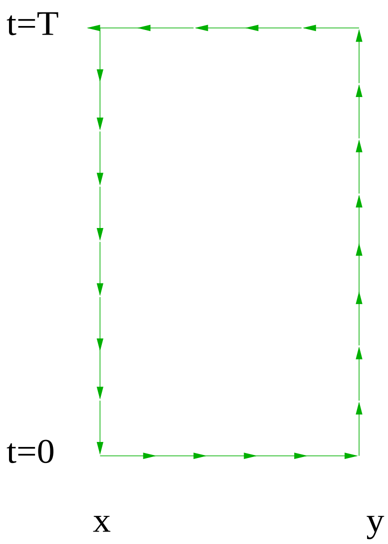
$$\Rightarrow \lim_{m\to\infty} G(q_{\mathrm{N}}, t_{\mathrm{N}}; q_0, t_0) = \underbrace{\delta(q_{\mathrm{N}} - q_0)}_{\text{static}} e^{-V(q)(t_{\mathrm{N}}-t_0)}$$

$\longrightarrow$ in the infinite mass limit we obtain the static potential

$$V(q) = -\lim_{t\to\infty}\left(\frac{1}{t}\ln\left[\lim_{m\to\infty} G(q, t; 0, 0)\right]\right)$$

note: order of limites is important

for gauge theories consider *gauge invariant* observables:
Wilson loop $W(C(R,T))$, $R = \|x-y\|$



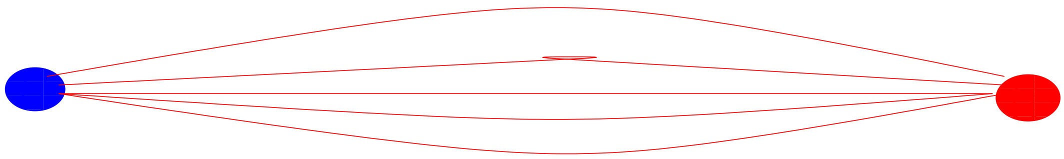
$$\boxed{V(R) = \lim_{T\to\infty}\left[-\frac{1}{T}\ln\langle W(C(R,T))\rangle\right]}$$

pieces of potential

- Coulomb piece
  $V(R) = \frac{\alpha(\mu)}{R} \leftarrow$ weak coupling perturbation theory

- linear piece $\sigma \cdot R \leftarrow$ strong coupling expansion

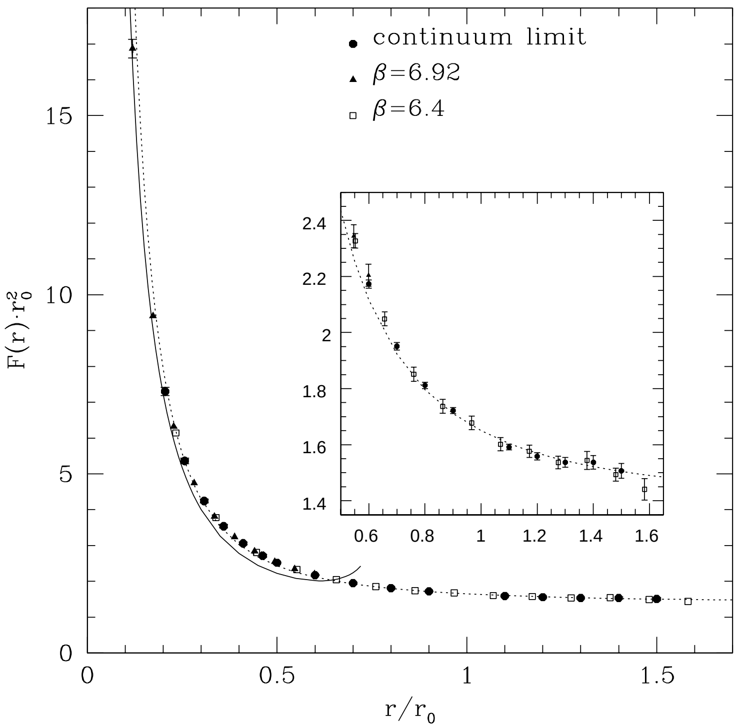
- string piece $-\frac{\pi}{12}\cdot 1/R, \quad R \gg 1 \leftarrow$ string picture



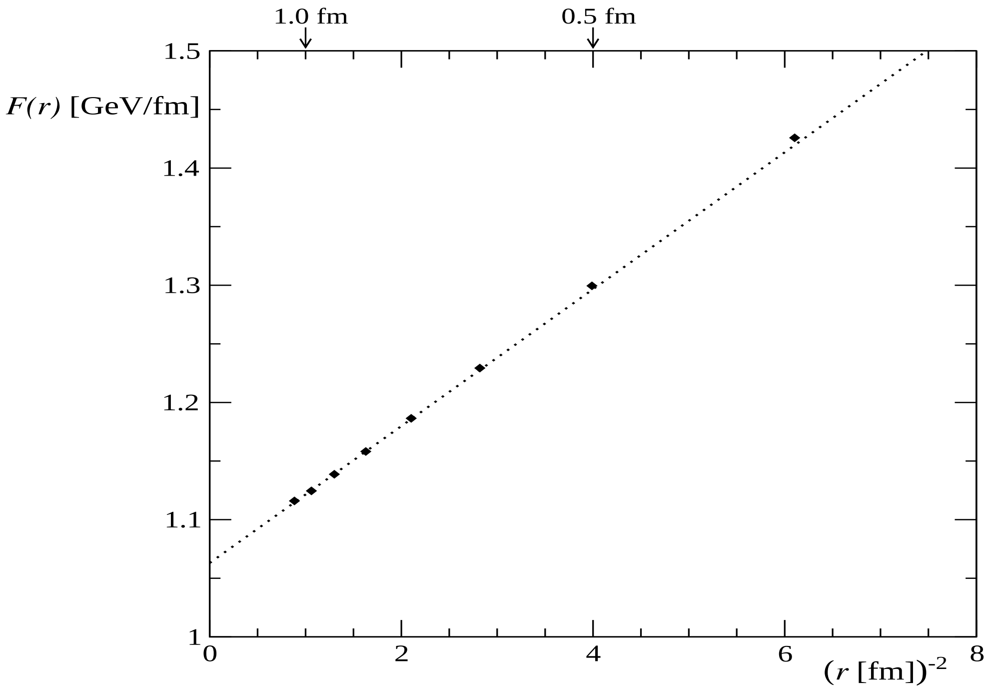
Test of the pieces

- short to intermediate ranges (Necco and Sommer)

  $r_0 \approx 0.5\text{fm}$



- long range (Lüscher and Weisz)



keyword: static potential, string picture

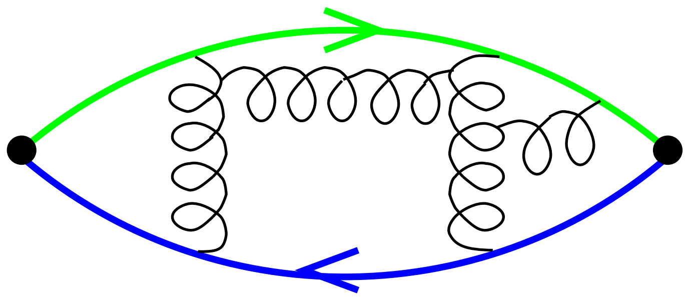
Adding fermions

simulations are mostly done within *quenched approximation*

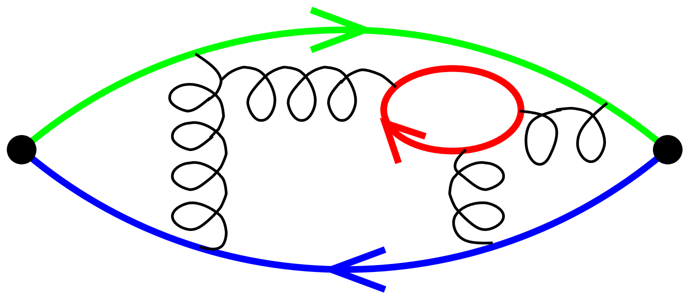
$\longrightarrow$ truncation of the theory

$\longrightarrow$ simulations much cheaper

$\longrightarrow$ often surprisingly close to experimental values
O(20%) deviation for many quantities



(A) Quenched QCD: no internal quark loops



(B) full QCD

keyword: quenched approximation

mass spectrum

one of the major goals (and major virtues) of lattice QCD is that within this framework the hadron masses can be computed non-perturbatively from first principles

the mass spectrum is obtained by studying euclidean correlation functions (for unitary theories a rotation back to Minkowski space is always possible)

consider some operator $O(\mathbf{x}, t)$ possesing quantum numbers corresponding to the ones of a particle we are interested in

if we are only interested in zero momentum we can project

$$O(t) = \sum_{\mathbf{x}} O(\mathbf{x}, t)$$

its correlation function is then (infinite lattice)

$$\begin{aligned} \langle O(0)O(t)\rangle &= \frac{1}{\mathcal{Z}} \sum_n \langle 0|O(0)e^{-\mathbb{H}t}|n\rangle\langle n|O(0)|0\rangle \\ &= \frac{1}{\mathcal{Z}} \sum_n |\langle 0|O(0)|n\rangle|^2 e^{-(E_n - E_0)t} \end{aligned}$$

effective masses

$$m_{\text{eff}}(t) = -\ln \frac{\Gamma(t+1)}{\Gamma(t)}$$

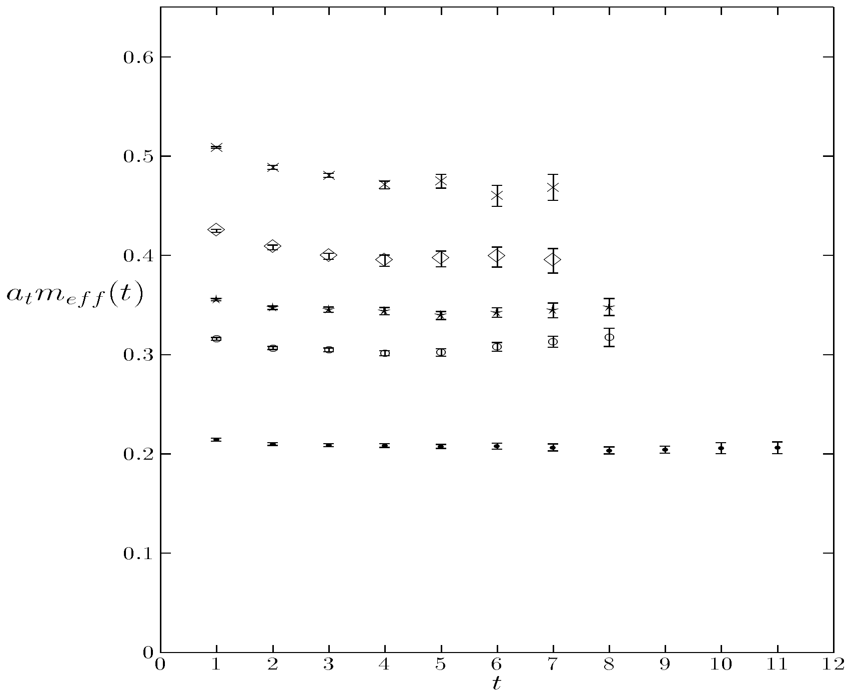
periodic boundary conditions

fit function

$$f(t) = A\cosh(m_{\text{eff}}t)$$

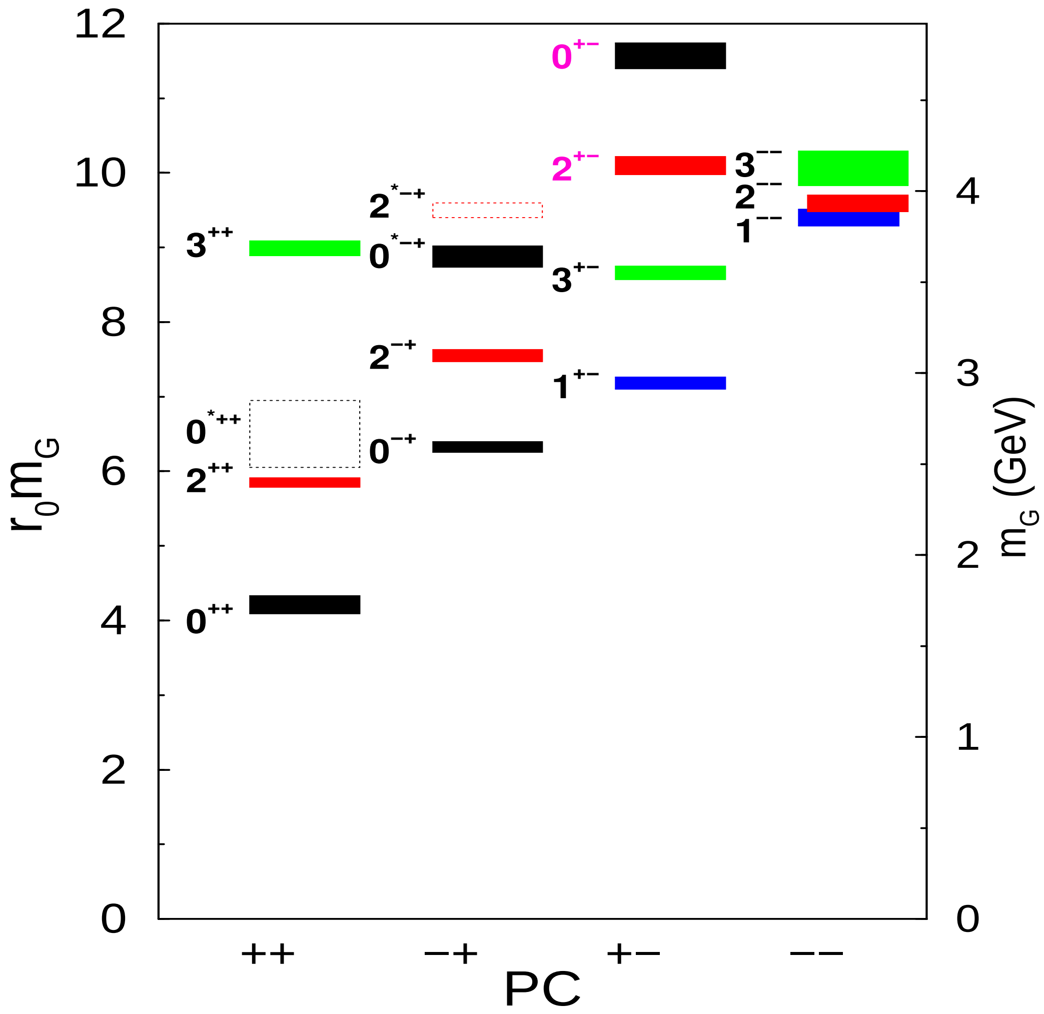
$\longrightarrow$ solve

$$\frac{f(t+1)}{f(t)} = \frac{\Gamma(t+1)}{\Gamma(t)}$$



keyword: effective masses, spectrum

a complete spectrum in pure gauge theory
$\longrightarrow$ neglect dynamical fermion effects



Bali, Teper

Non-perturbative renormalization

$\Leftarrow$ basic demand on lattice simulations

- running strong coupling constant $\alpha(\mu)$
- renormalization constants, e.g. $Z_A(g_0)$
- scale μ dependend renormalization constants, e.g. Z_P, $Z_{\mathcal{O}}$

Methods

– momentum space method
(Martinelli, Pittori, Sachrajda, Testa, Vladikas)

– finite size scaling method
(ALPHA collaboraton)

Finite size scaling for *non-perturbative renormalization*

in principle: need a box covering all energy scales

$$a \ll \underbrace{0.001\mathrm{fm}}_{\mathrm{M_W}} - \underbrace{1\mathrm{fm}}_{\mathrm{conf.scale}} \ll L$$

$\Rightarrow$ huge and unrealistic number of lattice points N^4

trick: *identify energy scale* μ *with inverse box length* L^{-1}

$$\mu = 1/L$$

evolution from scale $\mu_0 = 1/L_0$ to scale $\mu = 1/L$ desribed by step scaling function $\sigma(L/L_0)$

$\rightarrow$ split the problem: compute only small steps in the scale evolution of

$$\sigma(L/L_0) = \sigma(2L_0/L_0) \cdot \sigma(4L_0/2L_0) \cdot \ldots \cdot \sigma(2L/L)$$

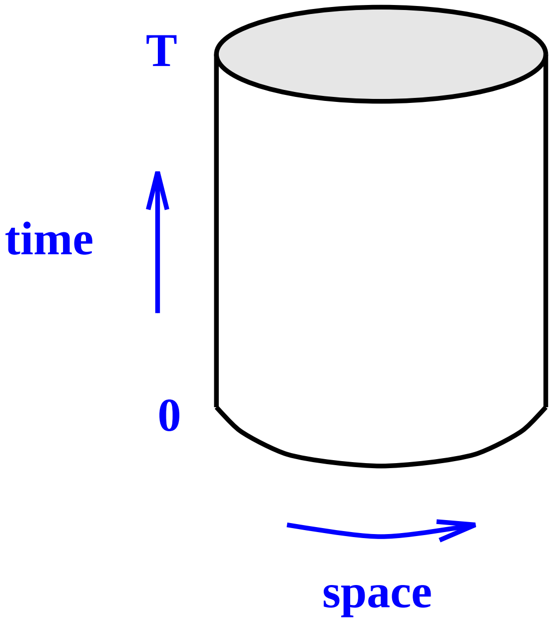
$\Rightarrow$ idea can be realized in the *Schrödinger functional renormalization scheme* that

- is a finite volume renormalization scheme
- can be implemented on the lattice

(Liu, Lüscher, Simma, Sint, Sommer, Weisz, Wolff, K.J.)

The Schrödinger functional

SU(N) Yang-Mills theory on $[0, T] \times S^1 \times S^1 \times S^1$



(LxLxL box with periodic b.c.)

Gauge potentials $A_\mu(x)$ are periodic in space, with period L, and

$$A_k(x)|_{x_0=0} = C_k(\mathbf{x}), \qquad A_k(x)|_{x_0=T} = C'_k(\mathbf{x})$$

($k = 1, 2, 3,$ $A_0(x)$ remains unconstrained, C and C' are prescribed smooth fields)

$$U_k(x) = e^{aA_k}$$

(Lüscher, Narayanan, Weisz, Wolff)

Yang-Mills action

$$S[A] = -\frac{1}{2g_0^2}\int_0^T \mathrm{dx_0}\int_0^{\mathrm{L}} \mathrm{d^3\mathbf{x}\,tr\{F_{\mu\nu}(x)F_{\mu\nu}(x)\}}$$

$$\mathcal{Z}[C',C] = \int \mathrm{D[A]\,e^{-S[A]}}$$

quantum mechanical interpretation

Hamilton operator

$$\mathcal{Z}[C',C] \quad = \quad \langle C'|\mathrm{e}^{-\mathbb{H}\mathrm{T}}\mathrm{P}|\mathrm{C}\rangle$$

projector on gauge invariant states

$\longrightarrow$ standard and straightforward lattice formulation $F_{\mu\nu}F_{\mu\nu} \rightarrow U_p$
fermions: standard formulations with Dirichlet boundary conditions (Sint)

keyword: Schrödinger Functional

Example: running strong coupling

the effective action of the background field is

$$\Gamma[B] = -\ln \mathcal{Z}(C, C')$$

choice of particular, classical, abelian background fields

$C = \frac{i}{L}\mathrm{diag}(\phi_1, \phi_2, \phi_3)$ and $C' = \frac{i}{L}\mathrm{diag}(\phi'_1, \phi'_2, \phi'_3)$

$$\begin{array}{rclrcl}
\phi_1 & = & \eta - \pi/3, & \phi'_1 & = & -\phi_1 - \frac{4\pi}{3} \\
\phi_2 & = & -\frac{1}{2}\eta, & \phi'_2 & = & -\phi_3 + \frac{2\pi}{3} \\
\phi_3 & = & -\frac{1}{2}\eta + \frac{\pi}{3}, & \phi'_3 & = & -\phi_2 + \frac{2\pi}{3}
\end{array}$$

in leading, tree level order

$$\Gamma_0[B] = \frac{3L^4}{g_0^2} \sum_\alpha \left\{ \frac{2}{a^2} \sin\left[\frac{a^2}{2L^2}(\phi'_\alpha - \phi_\alpha) \right] \right\}$$

the effective action depends explicitly on L
(and only on L if we scale all other dimensionful quantities in proportion to L)

$\Rightarrow$ definition of a renormalized coupling constant computed at a scale $\mu = L^{-1}$

$$\boxed{\left.\frac{\partial \Gamma[B]}{\partial \eta}\right|_{\eta=0} = \frac{k}{\bar{g}^2(L)}}$$

in general, we can compute the derivative of the effective action as an expectation value

$$\frac{\partial\Gamma}{\partial\eta} = -\frac{\partial}{\partial\eta}\ln\int\mathcal{D}U e^{-S} = \langle\frac{\partial S}{\partial\eta}\rangle$$

- definition is equally applicable on the lattice

- results in a local (plaquette like) observable

- well suitable for numerical calculations

At this point: *choose lattice formulation for non-perturbative computations*

$\Rightarrow$ quantities depend on lattice spacing a

step scaling function at non-vanishing lattice spacing

$$\Sigma(a/L, \bar{g}^2(L, a))$$

knowing the coupling at a scale $\mu = L^{-1}$ we can compute the scaling function as the coupling at scale $\mu = (2L)^{-1}$

$$\Sigma(a/L, \bar{g}^2(L, a)) \equiv \bar{g}^2(2L, a)$$

$\Rightarrow$ in the case of the running coupling,
step scaling function is the coupling
at scale $\mu = (2L)^{-1}$ itself

compute $\Sigma(a/L, \bar{g}^2(L, a))$ for different a/L

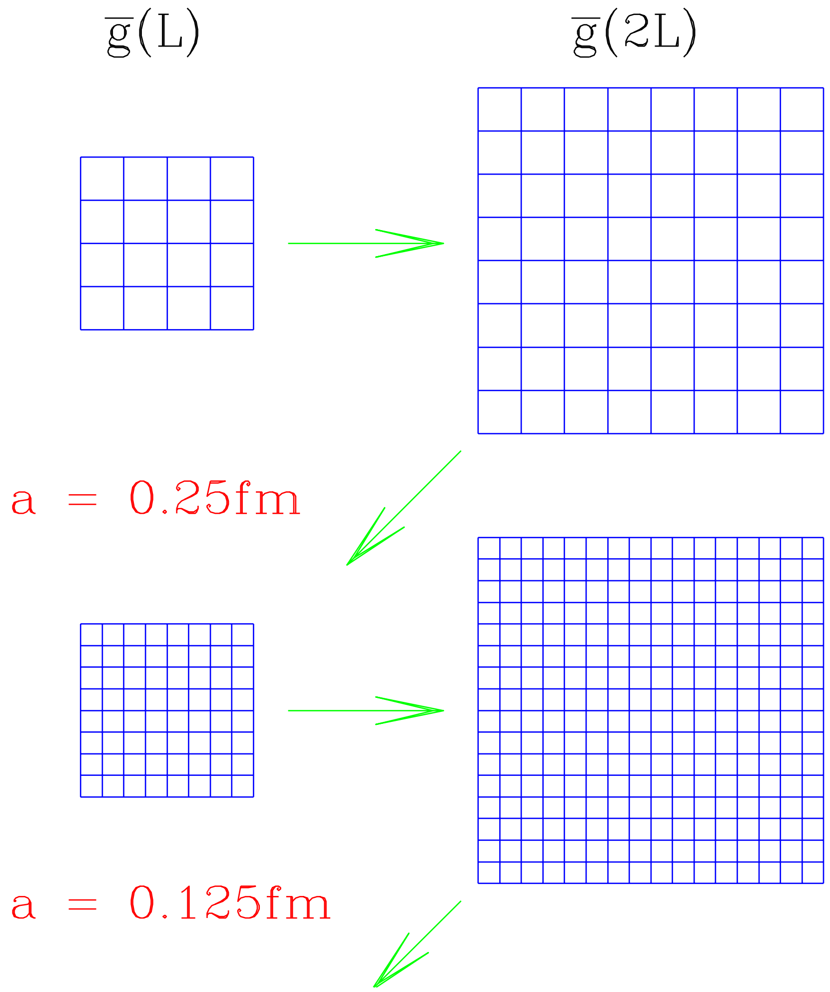
$\Rightarrow$ *if we keep* $\bar{g}^2(L, a)$ *fixed and take the limit* $a/L \to 0$

we can evaluate the continuum step scaling function

$$\boxed{\sigma(s, \bar{g}^2(L)) = \lim_{a/L\to 0} \Sigma(2, a/L, \bar{g}(L, a))}$$

keywords: step scaling function

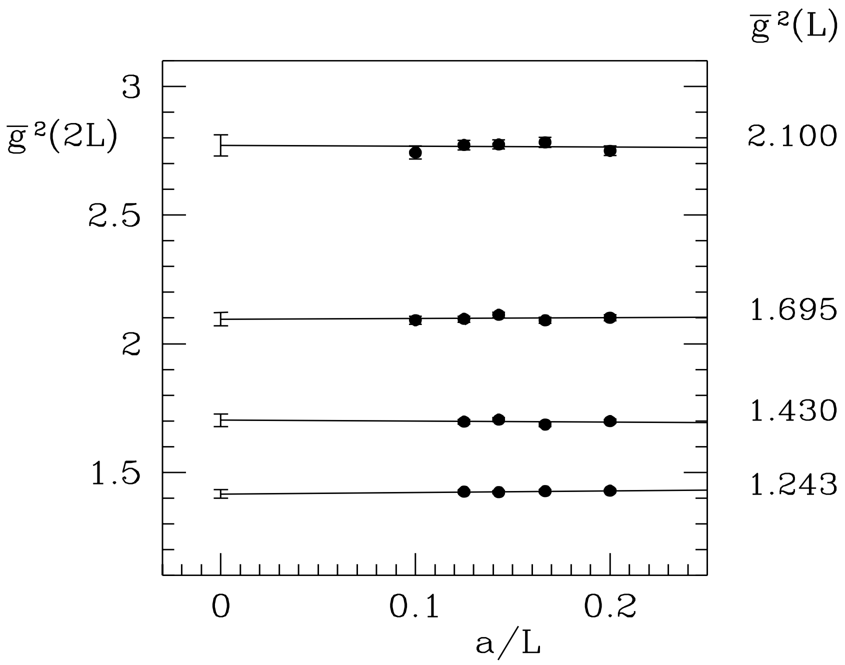
continuum limit is reached through a matching procedure



$$a \to a/2 \Leftarrow \beta \to \beta'$$

while keeping $\bar{g}^2(L)$ fixed

examples for the continuum limit of the step scaling function



- the step scaling function has a well defined continuum limit

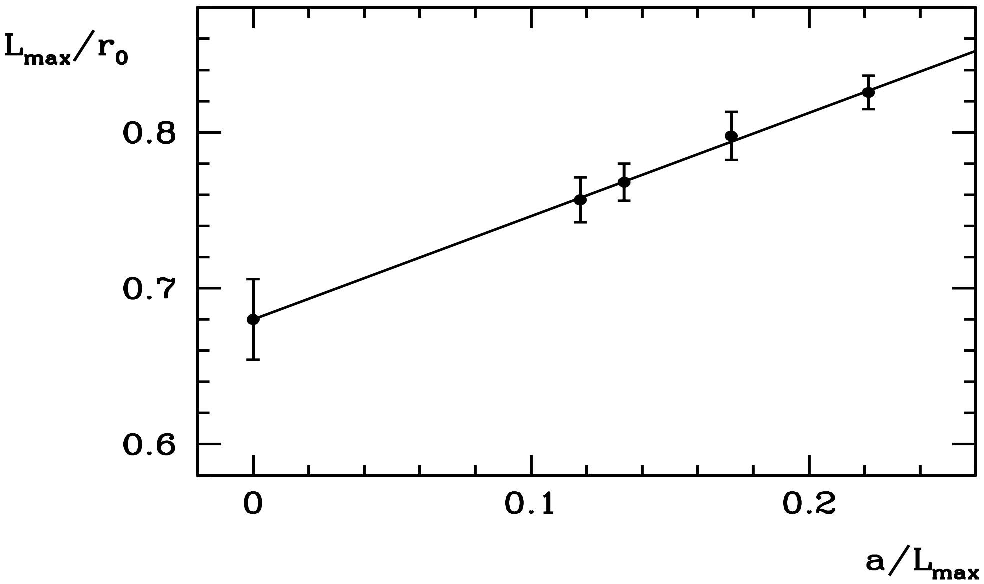
- after the continuum extrapolation all reference to the lattice formulation is lost

- we are then using a particular (Schrödinger functional) renormalization scheme *in the continuum*

- can make contact with other schemes in the perturbative region our largest value of the running coupling is $\bar{g}^2(L) = 3.48$

it is reached at the smallest scale $\mu^{-1} \equiv L_{\rm max}$

to express $L_{\rm max}$ in physical units we have to



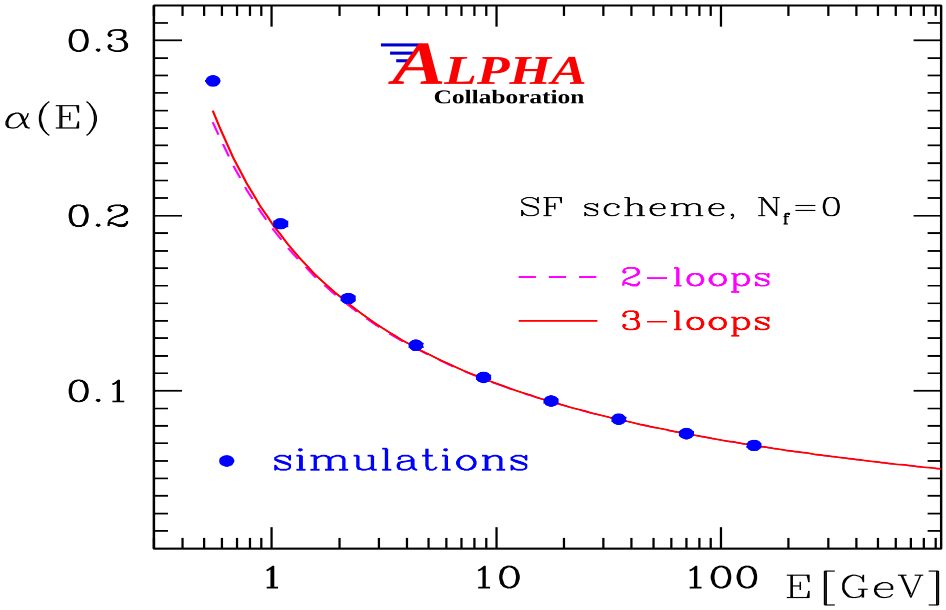
- choose a value of L/a
- tune g_0 such that $\bar{g}^2(L) = 3.48$
- compute $r_0/a \Rightarrow \frac{L_{\rm max}}{a}/\frac{r_0}{a} = L_{\rm max}/r_0$
  $r^2 F(r)|_{r=r_0=0.5{\rm fm}} = 1.65$
- repeat the game for different L/a and extrapolate to the continuum limit

at small enough values of the coupling

$\longrightarrow$ define the renormalization group invariant

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

knowing the Λ parameter, the coupling can be evolved within any preferred scheme (like $\overline{\mathrm{MS}}$) to any desired scale



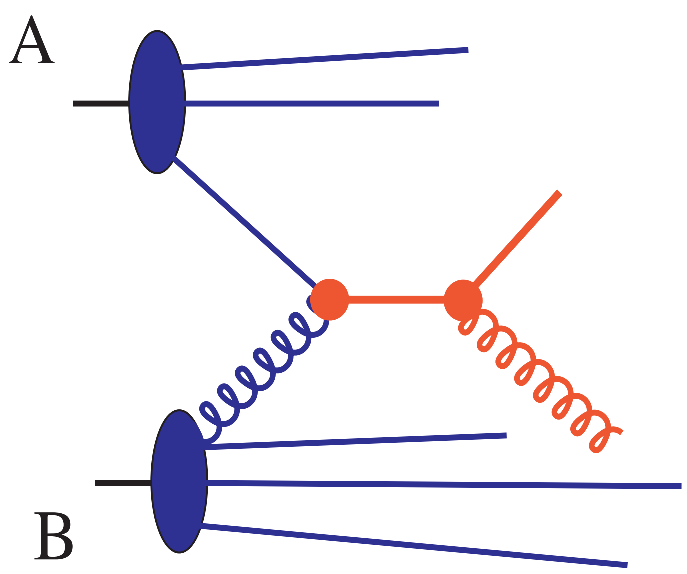
scale set by physical quantity: r_0, M_{Hadron}, $\cdots$

keywords: running strong coupling constant

Parton distribution functions

Consider the process

$$\text{hadron } A + \text{hadron } B \to \text{jet} + X$$



A parton a carries a fraction x_A of the hadron momentum

probability to find it

$$f_a(x_A)dx_A$$

we call

$$f_a(x_A) \quad (f_b(x_B))$$

the **"parton (gluon) distribution functions"**

Moments $\leftrightarrow$ local operators

Instead of studying the parton distribution functions themselves, we consider *scale dependent* moments

$$M_a^{(n)}(\mu) = \int_0^1 dx x^{n-1} f_a(x,\mu)$$

$$n = 1, 2, \cdots$$

the reason is that the moments can be related to expectation values of *local operators* $\mathcal{O}_a^n$

$$M_a^{(n)}(\mu) = \langle \mathcal{O}_a^n \rangle$$

where

$$\{p^{\mu_1} \cdots p^{\mu_n}\}_{\mathrm{TS}} \langle \mathcal{O}_a^n \rangle =$$

$$\langle p | \bar{\psi}_a(x) \{\gamma^{\mu_1} i D^{\mu_2} \cdots i D^{\mu_n}\}_{\mathrm{TS}} \psi_a(x) | p \rangle$$

- $\langle p|$ state vector of a hadron with momentum p
- D^μ covariant derivative (gauge invariance)
- TS means to take traceless symmetric part

Examples of Moments

unpolarized quark distributions:

$$\langle x^n \rangle \sim \langle \, | \overline{\psi} \, \gamma_{\{\mu} D_{\mu_1} \cdots D_{\mu_n\}} \, \psi \, | \, \rangle$$

spin-dependent structure function g_1:

$$\langle (\Delta x)^n \rangle \sim \langle \, | \overline{\psi} \, \gamma_5 \gamma_{\{\mu} D_{\mu_1} \cdots D_{\mu_n\}} \, \psi \, | \, \rangle$$

spin-dependent structure function g_2:

$$\langle x^n \rangle_{g_2} \sim \langle \, | \overline{\psi} \, \gamma_5 \gamma_{[\mu} D_{\{\mu_1} D_{\mu_2]} \cdots D_{\mu_n\}} \, \psi \, | \, \rangle$$

transversity structure function h_1:

$$\langle (\delta x)^n \rangle \sim \langle \, | \overline{\psi} \, \gamma_5 \sigma_{\mu\{\mu_1} D_{\mu_2} \cdots D_{\mu_n\}} \, \psi \, | \, \rangle$$

unpolarized gluon distribution

$$\langle x^n \rangle_g \sim \langle \, h \, | \sum_\rho \mathrm{Tr} \, (F_\mu{}^\rho D_{\mu_2} \cdots D_{\mu_n} F_{\rho\mu_1}) \, | \, h \, \rangle$$

latter have been so far quite hard to compute on the lattice

QCDSF collaboration, Rome-Zeuthen collaboration, LHPC collaboration

all these moments can be extracted from experimental data the local operators are to be renormalized

Example: renormalized average momentum (pion) at scale μ_0

$$\langle x\rangle(\mu_0) = \langle\pi|\mathcal{O}^{\mathrm{ren}}(\mu_0)|\pi\rangle \equiv \langle\pi|\mathcal{O}^{\mathrm{bare}}/Z(\mu_0)|\pi\rangle$$

renormalized average momentum at a different scale

$$\langle x\rangle(\mu) = \langle x\rangle(\mu_0)\cdot\sigma_Z(\mu/\mu_0)$$

with

$$\sigma_Z(\mu/\mu_0) = \frac{Z(\mu_0)}{Z(\mu)}$$

Schödinger functional renormalization scheme
$\longrightarrow$ renormalization condition

$$\langle SF|\mathcal{O}^R(\mu = 1/L)|SF\rangle = \langle SF|\mathcal{O}^{\mathrm{tree}}|SF\rangle$$

with $|SF\rangle$ a Schödinger functional state, i.e. a classical quark at the (time) boundary with an external momentum $\mathbf{p}$

in perturbation theory

$$Z(1/\mu) = 1 - \bar{g}^2(\mu)\left[\gamma^{(0)}\ln(\mu) + B_0\right]$$

with $\gamma^{(0)}$ the anomalous dimension B_0 the constant part

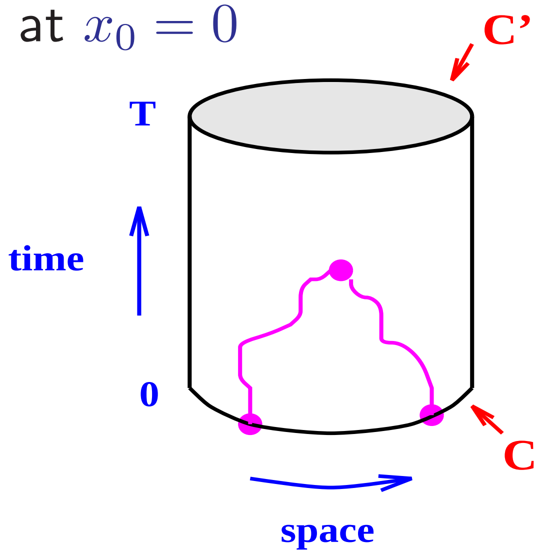
Z can be computed in practise by calculating fermion correlation functions in the Schrödinger functional set up

consider a correlation function f_O of our operator $\mathcal{O}$ at a distance x_0/L fixed (e.g. $x_0/L = 1/2$)

$$f_Z(x_0) = \sum_{\mathbf{y},\mathbf{z}} \mathrm{e}^{\mathrm{i}\mathbf{p}(\mathbf{y}-\mathbf{z})} \langle \bar{\psi}(\mathrm{x})\gamma_{[1} \overleftrightarrow{\mathrm{D}}_{2]} \tfrac{1}{4}\tau^3 \psi(\mathrm{x}) \bar{\zeta}(\mathbf{y}) \Gamma \tfrac{1}{4}\tau^3 \zeta(\mathbf{z})\rangle$$

with some choice of the momentum $\mathbf{p}$ and $\Gamma = \gamma_2$

ζ, $\bar{\zeta}$ are boundary quark fields at $x_0 = 0$



the desired value of Z is then obtained by normalizing with $f_Z^{\mathrm{tree}}(x_0)$

$$\boxed{Z(L) = \left.\frac{f_Z(x_0)}{f_Z^{\mathrm{tree}}(x_0)}\right|_{x_0/L=\mathrm{fixed}}}$$

(we neglect another normalization from the boundary fields) physical scales in the problem

– lattice extent L

– lattice momentum $p = k2\pi/L, \; k = 0, \cdots, L/a - 1$

– time x_0 distance from the boundary at $T = 0$

– quark mass $\underline{m = 0} \leftarrow$ Schrödinger functional boundary conditions

then the normalization constant is a function of *dimensionless quantities*

$$Z = Z(pL, x_0/L, a/L)$$

if we only want to change the scale, identified as $\mu^{-1} = L$, we have to keep

$$\boxed{pL, \; x_0/L \text{ fixed}}$$

while tuning $a/L \to 0$ to reach the continuum limit:

- $pL = 2\pi$ (lowest momentum)
- $x_0/L = 1/2$

Excursion to the lattice

non-perturbative information from numerical simulations

$\rightarrow$ make $Z(\mu)$ dependend on the lattice spacing

$$Z(\mu) = Z(\mu, a)$$

the lattice step scaling function is then (step size s)

$$\Sigma_Z(a) = \frac{Z(sL,a)}{Z(L,a)}$$

s usually taken to be 2

aim: continuum limit ($\exists$ for Σ_Z!)

$$\sigma_Z = \lim_{a\to 0} \Sigma_Z(a)|_{\mu^{-1}=L \text{ fixed}}$$

how do we fix the scale?

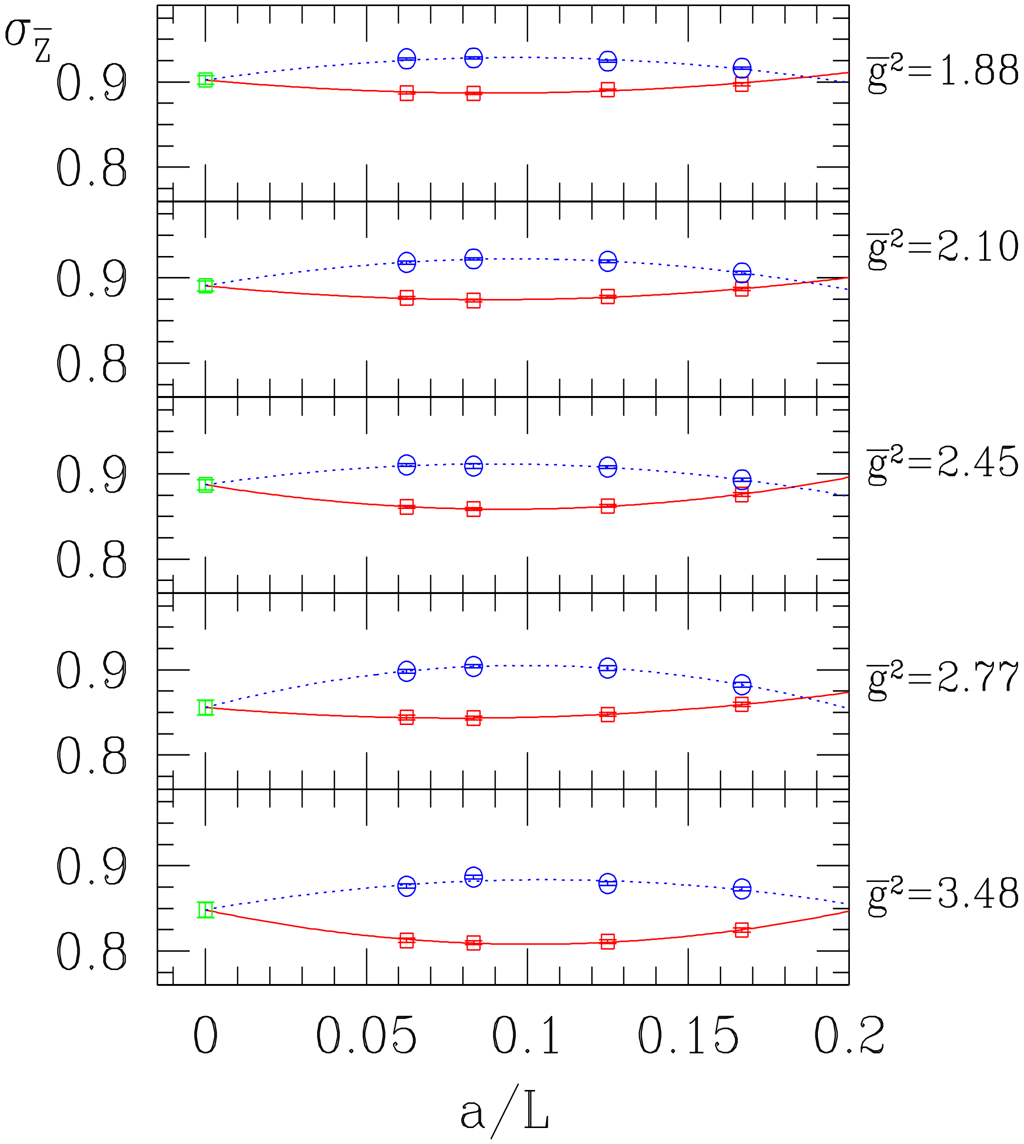
$\rightarrow$ through the coupling constant $g = \bar{g}(\mu = 1/L)$
(computation of running coupling necessary prerequisite)

computation of $\Sigma_Z(a)$ with 2 different lattice discretizations:

— Wilson formulation

— Non-perturbatively improved formulation

Combined fit $\sigma_{\bar{Z}}$



having the running matrix element $\langle x \rangle_{\mathrm{SF}}(\mu)$

$\Rightarrow$ for small enough coupling $\bar{g}$, define the
renormalization group invariant matrix element

$$O_{\mathrm{INV}}^{\mathrm{ren}} = O_{\mathrm{SF}}^{\mathrm{ren}}(\mu) \cdot f^{\mathrm{SF}}(\bar{g}^2(\mu))$$

$$f^{\mathrm{SF}}(\bar{g}^2(\mu)) = (\bar{g}^2(\mu))^{-\gamma_0/2b_0} \exp\left\{ - \int_0^{\bar{g}(\mu)} dg \left[\frac{\gamma(g)}{\beta(g)} - \frac{\gamma_0}{b_0 g} \right] \right\}$$

$\gamma(g)$: anomalous dimension function
$\beta(g)$: β-function
knowing O^{ren} we can get "easily" the matrixelement
in a desired scheme

$$\langle x \rangle^{\mathrm{SF}} = O_{\mathrm{INV}}^{\mathrm{ren}} / f^{\mathrm{SF}}(\bar{g}^2(\mu))$$

$$\langle x \rangle^{\overline{\mathrm{MS}}} = O_{\mathrm{INV}}^{\mathrm{ren}} / f^{\overline{\mathrm{MS}}}(\bar{g}^2(\mu))$$

$$\langle x \rangle^{\mathrm{myprefered}} = O_{\mathrm{INV}}^{\mathrm{ren}} / f^{\mathrm{myprefered}}(\bar{g}^2(\mu))$$

$\Rightarrow$ make contact with analytical computations in perturbation theory!

Moments of Parton distribution functions

(Guagnelli, Palombi, Petronzio, Shindler, K.J.)

example: lowest moment of twist-2, non-singlet operator in pion

- discretization errors:
  sizable lattice artefacts

  $\langle x\rangle(a=0.093)=0.30 \rightarrow \langle x\rangle(a=0)=0.20$

- renormalization:
  non-perturbative renormalization $\rightarrow$ 10-15% e ffect

- final numbers:
  putting it all together

$$\langle x\rangle^{\text{experiment}}(\mu=2.4\text{GeV}) = 0.23(2)$$

$$\langle x\rangle^{\text{quenched}}_{\overline{\text{MS}}}(\mu=2.4\text{GeV}) = 0.30(3)$$

- *renormalization group invariant matrix element*

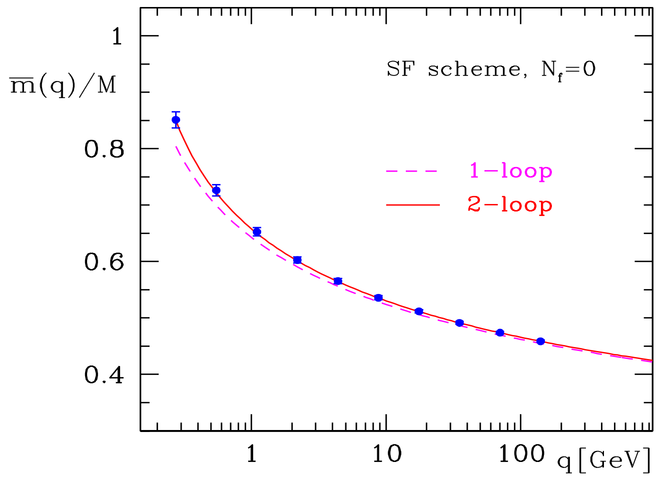
$$\boxed{O^{\text{ren}}_{\text{INV}} = O^{\text{ren}}_{\text{SF}}(\mu_0)\mathfrak{S}^{\text{UV}}_{\text{INV}}(\mu_0) = 0.20\cdot 1.11}$$

$\uparrow$

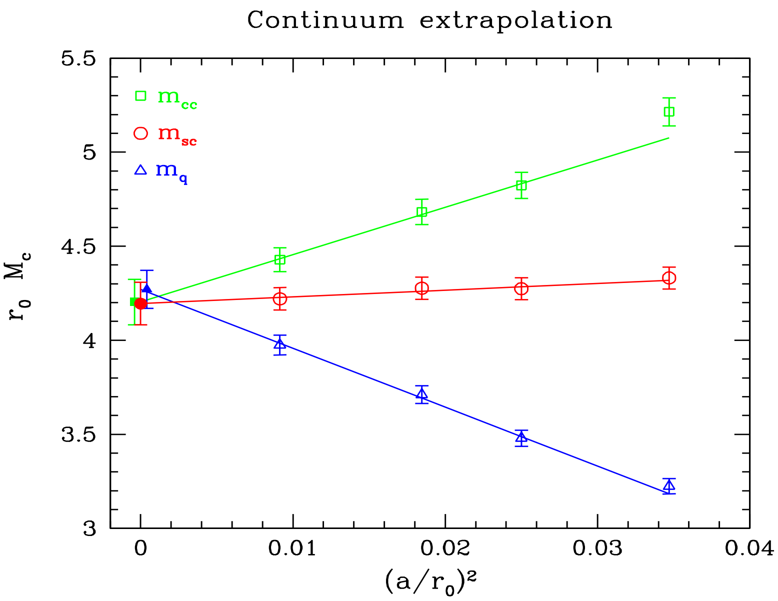
μ_0 dependence cancelled

Other examples

strange quark mass (ALPHA collaboration)



charm quark mass (Rolf, Sint)



static approximaton, etc.

Chiral symmetry on the lattice

one of our main problems with the lattice is the question of *chiral symmetry*

the problem is
how to have right massless spectrum on the lattice
and preserve continuum chiral symmetry

$\Leftarrow$ impossible due to Nielsen-Ninomiya theorem
(while keeping also locality)

for Wilson fermions $\longrightarrow$ demonstration in perturbation theory (although in all orders) that *in the continuum limit* chiral symmetry is restored

non-perturbatively: . . . to be proven

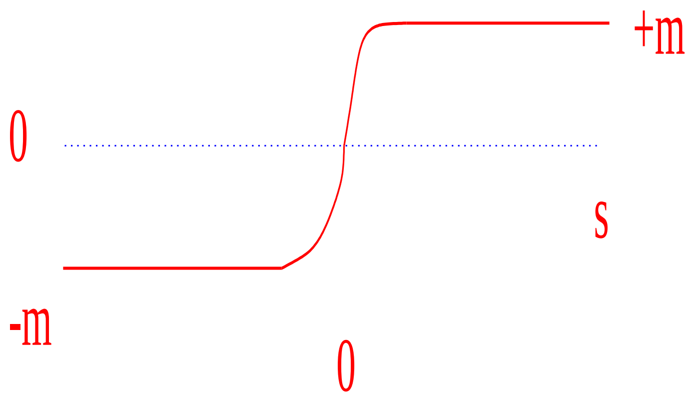
let me take you to outer space in extra dimensions (Kaplan)

we leave the lattice for a moment and are back in the continuum

we consider a 5-dimensional theory
(free fermions for the moment)
with a *mass defect* in one extra dimension s

$$D_5 = \partial_\mu \gamma_\mu + m_0 + \gamma_5 \partial_s + m(s)$$

$$m(s) = \begin{cases} -m; & s \rightarrow -\infty \\ +m; & s \rightarrow +\infty \end{cases}$$



let us try to solve the massless Dirac equation

$$D_5(m_0 = 0)\psi = 0$$

this can be solved by the ansatz

$$\begin{aligned}
\psi_\pm &= e^{ipx}\Phi_\pm(s)u_\pm \\
\Phi_\pm(s) &= \exp\left\{\pm\int_0^s m(s')ds'\right\} \\
\gamma_5 u_\pm &= \pm u_\pm
\end{aligned}$$

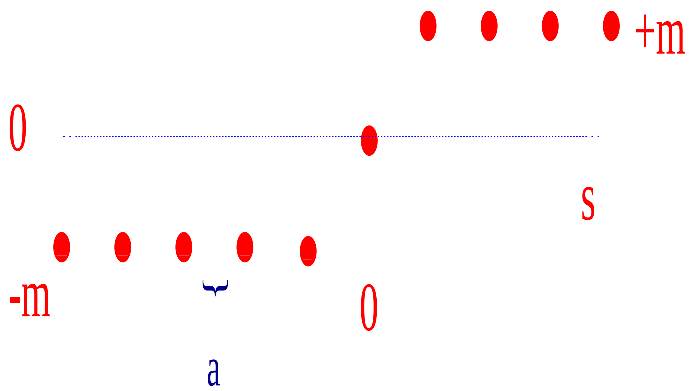
only Φ_- *normalizable* $\Rightarrow$ only one solution

- massless fermion travelling along the domain wall
- it has a definite chirality
- bound to the domain wall with exponential fall-off with a rate $|m|$ when going to $|s| \gg 1$

on a (still infinite) lattice $\longrightarrow$

$$m(s) = \begin{cases} -m; & s \leq a \\ 0; & s = 0 \\ +m; & s \geq a \end{cases}$$

derivatives $\longrightarrow$ finite lattice differences



imposing a similar ansatz as in the continuum

$$\psi_\pm = e^{ipx}\Phi_\pm(s)u_\pm$$

we find a normalizable solution

$$\Phi_-(s) = e^{-\mu_0|s|}, \;\; \sinh\mu_0 = m$$

however, there is now a second normalizable solution

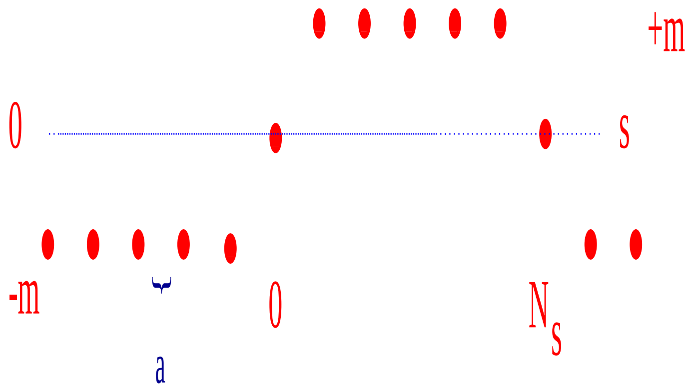
$$\Phi_+(s) = (-1)^s\Phi_-(s)$$

$\longrightarrow$ doubler in the extra dimension solution $\Rightarrow$ add Wilson term in extra dimension

$$D_5 = \partial_\mu \gamma_\mu + m_0 + \gamma_5 \partial_s + m(s) - \nabla^*_\mu \nabla_\mu - \nabla^*_s \nabla_s$$

this kills all the doublers and we are left with a single chiral fermion on the lattice

on a finite lattice the extra dimension has an extent N_s and we have to impose some boundary conditions

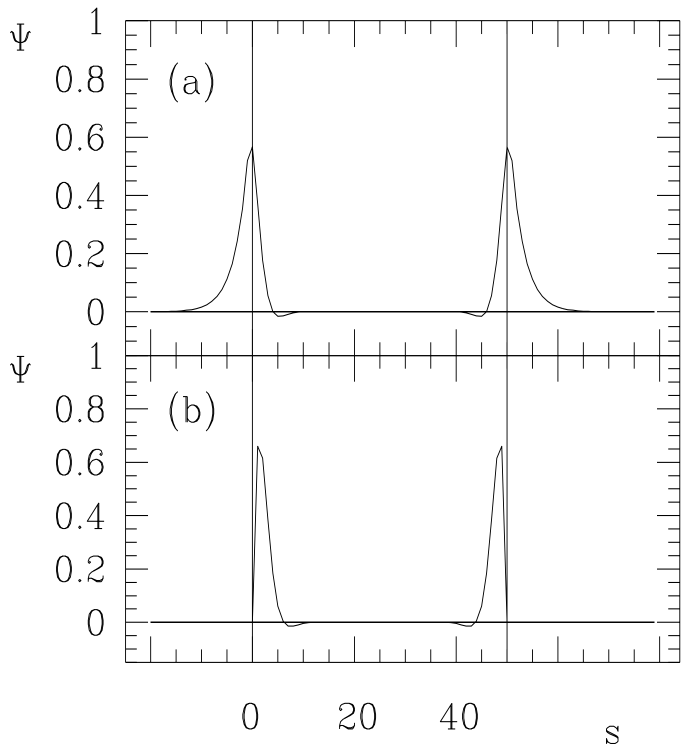


$\Rightarrow$ induce a second domain wall

$\Rightarrow$ two solutions living on their own domain wall with opposite chirality

we can also choose open boundary conditions in the extra dimension (Furmann, Shamir)
$\Rightarrow$ chiral zero modes appear as surface modes
(reminiscent of Shockley modes in solid state physics

numerically solving the Dirac equation



(a) periodic boundary conditions

(b) open boundary conditions ($\approx$ Schrödinger functional)

keyword: domain wall fermions

gauging the 5-dimensional Dirac operator:
gauge only the 4-dimensional part

$$D_5 = D_\mu \gamma_\mu + m_0 + \gamma_5 \partial_s + m(s) - D_\mu^* D_\mu - \nabla_s^* \nabla_s$$

$\Rightarrow$ our 5-dimensional lattice action becomes

$$S_{DW} = \sum_{x,y,s,s'} \bar{\psi} \left(D_{x,y} \delta_{s,s'} + D_{s,s'} \delta_{x,y} \right) \Psi$$

$$D_{x,y} = \frac{1}{2} \sum_\mu (1+\gamma_\mu) U(x,\mu) \delta_{x+\mu,y} + (1-\gamma_\mu) U^\dagger(y,\mu) \delta_{x-\mu,y}$$
$$+ (m_0 - 4)\delta_{x,y}$$

$$D_{s,s'} = \begin{cases} P_+ \delta_{2,s'} - m P_- \delta_{N_s,s'} - \delta_{1,s'}, & s = 1 \\ P_+ \delta_{s+1,s'} + P_- \delta_{s-1,s'} - \delta_{s,s'}, & 2 \le s \le N_s - 1 \\ P_- \delta_{N_s-1,s'} - m P_+ \delta_{1,s'} - \delta_{N_s,s'}, & s = N_s \end{cases}$$

projectors $P_\pm = (1 \pm \gamma_5)/2$

- m is the domain wall mass $\longrightarrow$ determines the rate of exponential decay in the extra dimension

- m_0 is the quark mass $\longrightarrow$ has to be tuned to zero to give exactly chiral fermions

- gauge fields make the walls talk to each other
  $\longrightarrow$ obtain Dirac fermions
  $\Rightarrow$ suitable formulation of lattice QCD

domain wall fermions employing the action S_{DW} are used in todays simulations (RBC, CPPACS collaborations)

$\longrightarrow$ improved chiral properties, reducing lattice artefacts

deeper understanding of properties of domain wall fermions

if the limit $N_s \rightarrow \infty$ is taken, the 5-dimensional Dirac operator is reduced to a 4-dimensional operator, the *overlap operator* (Neuberger) $(a_s \rightarrow 0)$

$$\boxed{D_{\mathrm{ov}} = \left[1 - A(A^\dagger A)^{-1/2}\right]}$$

with $A = 1 + s - D_{\mathrm{w}}$

D_{w} is the standard Wilson-Dirac operator

$$D_{\mathrm{w}} = \frac{1}{2}\left\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu\right\}$$

$0 < s < 1$ is a tunable parameter

keyword: overlap operator

chiral properties of D_{ov}

$$\gamma_5 D_{\mathrm{ov}} + D_{\mathrm{ov}}\gamma_5 = 2aD_{\mathrm{ov}}\gamma_5 D_{\mathrm{ov}}$$

D_{ov} is a (practical !) example of an operator that satisfies the celebrated **Ginsparg-Wilson relation**
(other example: fixed point/perfect lattice Dirac operator)

$$\boxed{\gamma_5 D + D\gamma_5 = 2aD\gamma_5 D}$$

$$\Rightarrow D^{-1}\gamma_5 + \gamma_5 D^{-1} = 2a\gamma_5$$

D^{-1} anti-commutes with γ_5 at all non-zero distances

$\longrightarrow$ only mild (i.e. local) violation of chiral symmetry

Ginsparg and Wilson arrived at this expression already in the early days of lattice gauge theories from a completely different path
$\Leftarrow$ block spinning from the continuum

keyword: Ginsparg-Wilson relation

Moreover: Ginsparg-Wilson relation implies an *exact lattice chiral symmetry* (Lüscher):

for any operator D which satisfies the Ginsparg-Wilson relation, the action

$$S = \bar{\psi} D \psi$$

is invariant under the transformations

$$\boxed{\begin{aligned} \delta\psi &= \gamma_5(1 - \tfrac{1}{2}aD)\psi \\ \delta\bar{\psi} &= \bar{\psi}(1 - \tfrac{1}{2}aD)\gamma_5 \end{aligned}}$$

$\Rightarrow$ have a notion of chiral symmetry on the lattice

$$\gamma_5 \rightarrow \gamma_5(1 - \tfrac{1}{2}aD)$$

the *lattice* operator D enjoys many properties of the *continuum* operator:
$Z_A = Z_V = 1$, anomaly, index theorem, ...

keyword: lattice chiral symmetry

in addition:

despite the term $1/\sqrt{A^\dagger A}$
($\Rightarrow$ all lattice points are coupled among each other)

the operator $D_{\rm ov}$ is local, $\|D_{\rm ov}\Phi\| \propto e^{-\gamma/a}$
(Hernandèz, Lüscher, K.J.)

- if plaquette is bounded: $\|1 - U_P\| < 1/30$
  (analytical proof)

- locality also demosntrated numerically when bound not satisfied

$\Rightarrow$ have

- *chiral symmetric*

- *local*

lattice QCD $\rightarrow$ non-perturbative definition of QCD ($a \rightarrow 0$)

practical application:
spontaneous chiral symmetry breaking in QCD

one of the major assumptions in QCD is that chiral symmetry is spontaneously broken by the formation of a scalar condensate $\langle\bar{\psi}\psi\rangle$

spontaneous breaking of chiral symmetry

$\Rightarrow$ appearance of Goldstone particles (pions) (Goldstone theorem)

$\Rightarrow$ many low energy relation (PCAC relation) in QCD

$\Rightarrow$ application of chiral perturbation theory

the lattice is a unique enviroment to test this basic assumption and an operator satisfying the Ginsparg-Wilson relation provides the neccessary tool to perform this test in practise simulations with overlap fermions $\gg$ more expensive than standard fermions $\Rightarrow$ use quenched approximation

results for scalar condensate $\Sigma(m,V)$ as function of quark mass m and volume V in quenched chiral perturbation theory has been worked out
(Damgaard, Osborn, Toublan, Verbaaschoot)

$$\Sigma(m,V) = \Sigma\ z\ [I_\nu(z)K_\nu(z) + I_{\nu+1}(z)K_{\nu-1}(z)] + \Sigma\frac{\nu}{z}$$

$z = m\Sigma V$, ν denotes the topological charge sector
Σ *infinite volume, chiral limit* scalar condensate

for $m \to 0$ approximate formulae are obtained

$$\Sigma_{\nu=0}(a) = m\ \Sigma^2\ V\ \left(\mathrm{const} - \ln m\Sigma V + \mathrm{O}(m\Sigma V)^2\right)$$

$$\mathrm{const} = 1/2 - \gamma + \ln 2$$

$$\Sigma_{\nu=\pm1}(a) = \frac{1}{mV} + \frac{1}{2}m\Sigma^2 V\left(1 + \mathrm{O}(m\Sigma V)^2\right)$$

at finite lattice spacing a there is a quadratic divergence $\propto 1/a^2$

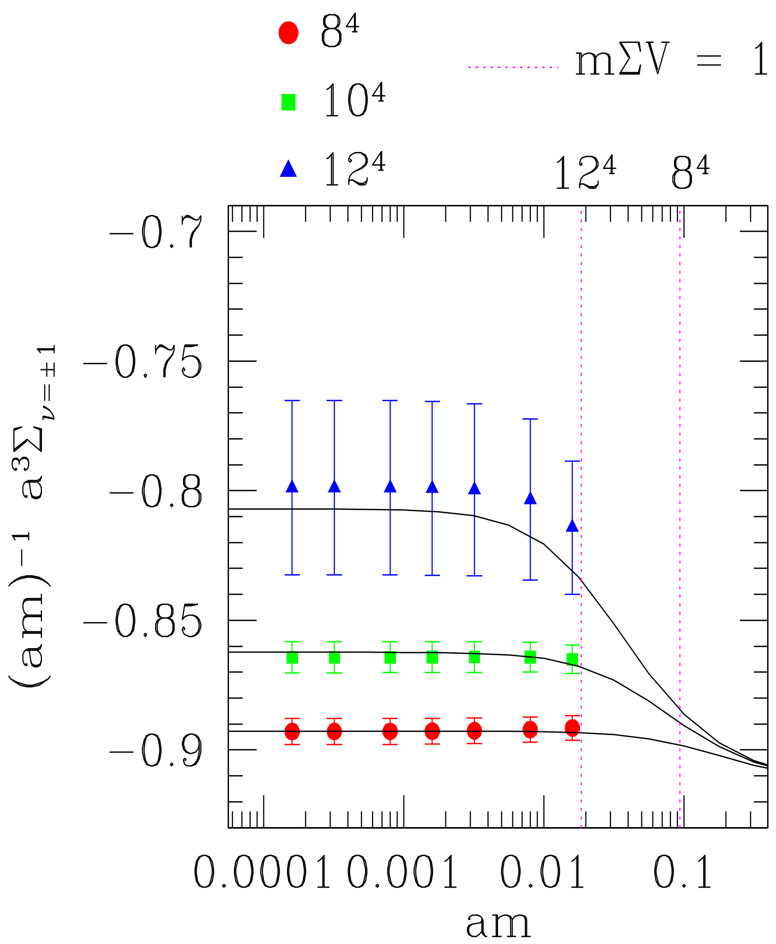
this divergence has to be subtracted (i.e. fitted)

Fit to the condensate

data points at 7 masses on 3 volumes
attempt a fit according to

$$\Sigma_{\nu=\pm 1} = \Sigma\, z\, [I_\nu(z)K_\nu(z) + I_{\nu+1}(z)K_{\nu-1}(z)] + C/a^2$$

$\longrightarrow$ only two free parameters Σ and C



(Hernandéz, Lellouch, K.J.)

$\Rightarrow$ *find strong evidence for spontaneous chiral symmetry breaking in QCD!*

Numerics (1st quenched approximation)

expensive part: fermions
physical observables:

$$\langle \bar{\psi}(x)\psi(y)\rangle \propto D^{-1}b$$

D^{-1} fermion (quark) propagator

b is external source vector

$\Rightarrow$ need to solve

$DX = b$ with D a complex matrix that is

- high-dimensional $O(10^6)$
- sparse (diagonal and a few subdiagonals)

vast knowledge for solving systems of linear equations
Saad *Iterative methods for sparse linaer systems*

- Minimal Residual, GMRES,
  Conjugate Gradient, BiCGstab, ...

$\longrightarrow$ self correcting iterative schemes

$\longrightarrow$ number of iterations $\propto$ condition number of the matrix

$\longrightarrow$ typical iteration numbers $100 - 1000$

keyword: "matrix inversion"

example: quenched $16^3 \cdot 32$ lattice:
≈ 100Mflop for one fermion matrix times vector multiplication

need

- 12 (dirac and color components) solutions
- $\mathsf{O}(200)$ iterations of solver
- typically $\mathsf{O}(1000)$ configurations

$\longrightarrow \approx 200$ Teraflops for one physical result
having a 50 Gflops (sustained) machine
$\Rightarrow$ about 10 hours for one physical result

realistic lattices today: $32^3 \cdot 64$ or $48^3 \cdot 96$
$\longrightarrow$ factor 10 to 100

later:

- *dynamical fermions*
- *overlap fermions*

are $\mathsf{O}(100)$ more expensive $\cdots$

Additional complication with overlap operator

The square root

- Chebyshev approximation

$$P_{n,\epsilon}(A^\dagger A) \approx 1/\sqrt{A^\dagger A}$$

  where $P_{n,\epsilon}$ is a polynomial of degree n, providing an exponentially fast converging approximation to $1/\sqrt{x}$ for $x \in [\epsilon, 1]$

- MinMax polynomials
- rational approximation
- domain wall fermion approach

remarks:

- several improvements have been found
- still simulations are much more expensive than standard fermions
  (polynomial has to be evaluated in each iteration of linear solver)

Expense of the simulations

we demand a precise approximation for $1/\sqrt{A^\dagger A}$:

$$\|\Phi - P_{n,\epsilon}(A^\dagger A)A^\dagger A P_{n,\epsilon}(A^\dagger A)\Phi\|/\|\Phi\| < 10^{-8}$$

Φ is a gaussian random vector

and a correspondingly precise stopping criterion
for the inverter

$$\|(D_{\mathrm{N}}X - b)\|/\|V\| < 10^{-8}$$

b is the source and X the solution vector

L	n	n_{ev}	n_{invert}
8	190	170	80
10	250	325	200
12	325	700	300

The values for
n: degree of polynomial
n_{ev}: number of iterations for the lowest eigenvalue of D_{N}
n_{invert}: number of iterations in the inverter

Numerics (2nd dynamical fermions)

for two flavors of fermions (e.g. the up and the down quark) the fermion action becomes

$$S = a^4 \sum_x \bar{\psi} M^\dagger M \psi$$

and the path integral (fermion part)

$$\mathcal{Z} = \prod_x d\bar{\psi}(x) d\Psi(x) e^{-S} \propto \prod_x d\Phi^\dagger(x) d\Phi(x) e^{-\Phi^\dagger \left[M^\dagger M\right]^{-1} \Phi}$$

the inverse matrix $\left[M^\dagger M\right]^{-1}$ couples all points on the lattice with each other
(still, the action is field theoretically local, of course)

this pathintegral is simulated by the
Hybrid Monte Carlo algorithm

introduce Hamiltonian

$$H = \frac{1}{2}\pi^2 + S_G + \Phi^\dagger \left[M^\dagger M\right]^{-1} \Phi$$

(momenta π conjugate to gauge fields U)

and a fictitious Monte Carlo time τ

generate new configuration by integrating the field equations

$$\begin{aligned} \frac{\delta}{\delta\tau}\pi &= -\frac{\delta S}{\delta U} \propto \left[M^\dagger M\right]^{-1}\Phi + \frac{\delta S_G}{\delta U} \\ \frac{\delta}{\delta\tau}U &= \pi \end{aligned}$$

accept/reject new configuration with probability

$$e^{\Delta H}, \quad \Delta H = H_{\mathrm{new}} - H_{\mathrm{old}}$$

remarks

- integration via leap-frog integrator $\Rightarrow$
  - discretized integration step size $\delta\tau > 0$
  - $N = \mathrm{O}(10 - 100)$ integration steps such that $N\delta\tau \approx 1$ (experience)
  - each integration step $\longrightarrow$ solve linear system of equations $\Rightarrow$ dynamical fermion simulation are much more expensive than quenched simulations

- since, the update of the momenta $\pi(x)$ is completely independent of the update of U -field,
  the non-locality of the action is not a problem
  algorithm is very well suited for parallelization

keyword: Hybrid Monte Carlo

Hybrid Monte Carlo algorithm in a nutshell

- generate bosonic fields $\Phi = M\chi$, χ Gaussian fields
- generate Gaussian distributed momenta $\pi_{x,\mu}$
- integrate the equations of motion

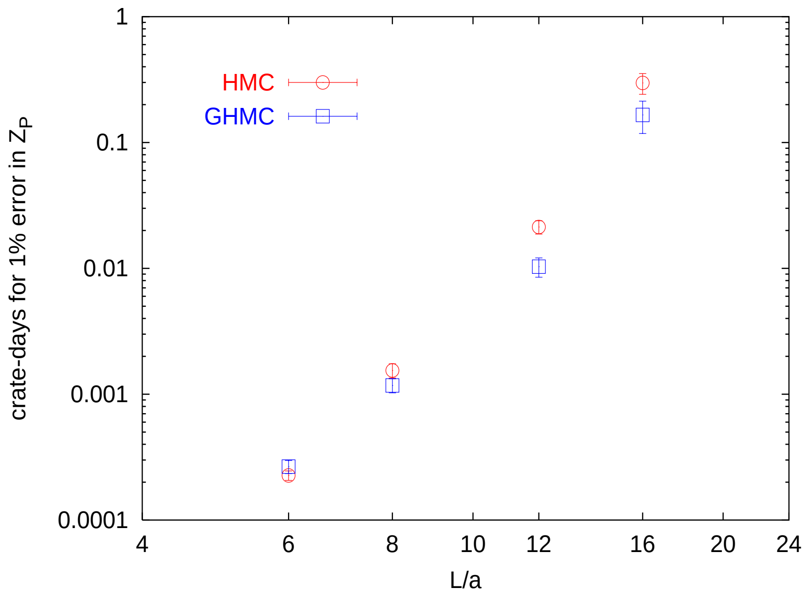
$$
\begin{aligned}
\dot{\pi}_{x,\mu} &= -D_{x,\mu}\left[S_{\mathrm{G}} + S_{\mathrm{F}}\right] \\
&\quad (\mathrm{matrix inversion!}) \\
\dot{U}_{x,\mu} &= iU_{x,\mu}\pi_{x,\mu}
\end{aligned}
$$

- accept the new gauge configuration $\{U\}$ with probability $\exp\{H(U,\pi)_{\mathrm{ini}} - H(U,\pi)_{\mathrm{final}}\}$

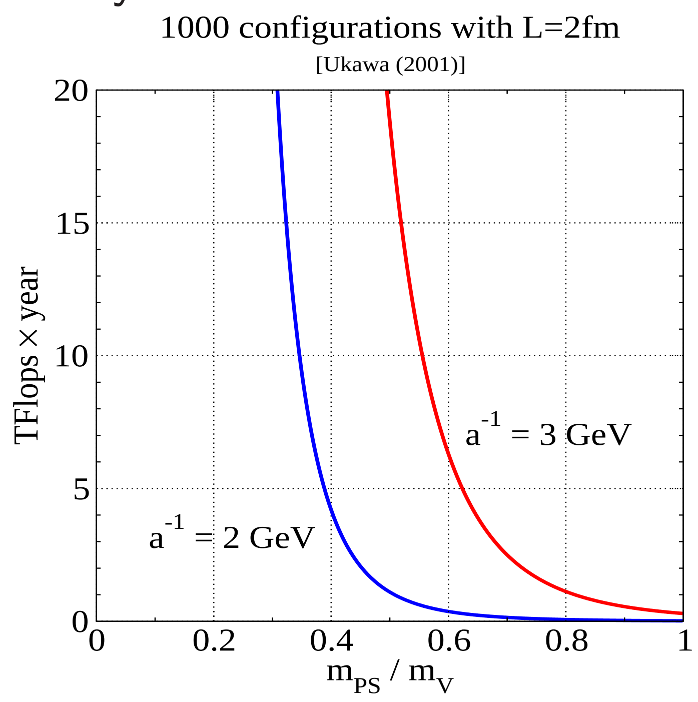
Costs of dynamical fermions simulations

see panel discussion in Lattice2001, Berlin, 2001

Schrödingerfunctional boundary conditions

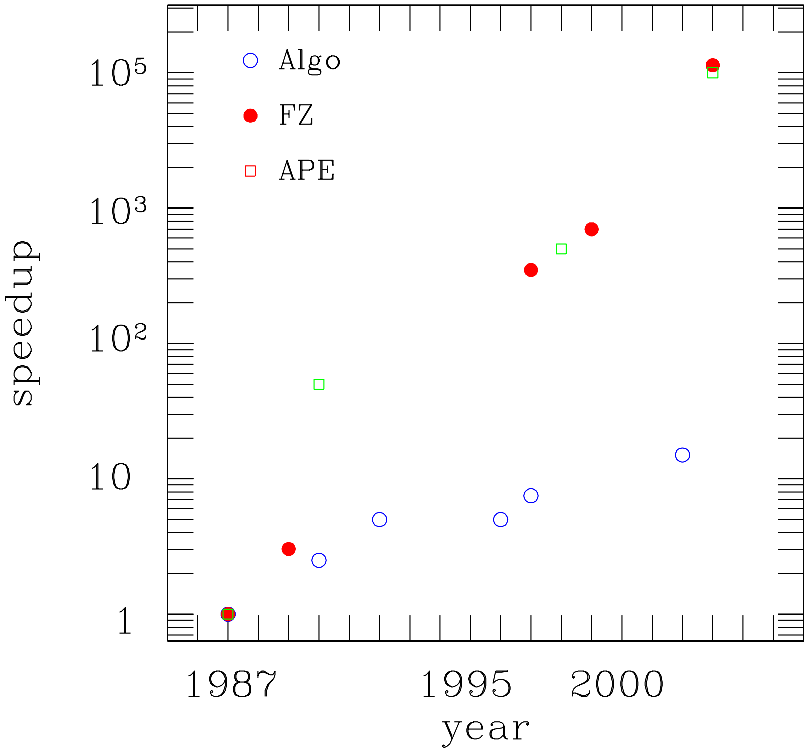


full dynamical



$\longrightarrow$ contact to chiral perturbation theory essential

Algorithm and Machine Development



○ : algorithm development: factor 20

● : FZ CRAY at Research centre Jülich

□ : "Array Processor Experiment" (APE)

– machine development most important

– APE and CRAY equal performance
(following both Moore's law)

– cost(CRAY) $\approx 10\times$ cost(APE)

$\Rightarrow$ worthwhile to build machines
APE (*Europe*), QCDOC (*USA*), PC-Cluster

Physics milestones

Europe wide evaluation of physics milestones in 2003
ECFA Report, ECFA/00/200, F. Jegerlehner et.al.

- Hadron spectrum
- Flavour-singlet mesons
- Exotic states
- α_s, quark masses and hadronic matrix elements

Special situation in Germany

- common initiative of lattice physicists
  Universities and NIC/DESY

$\Rightarrow$ needs of O(20) Teraflops
$\Rightarrow$ find out the right platform
$\Rightarrow$ coordinate activities (software/data exchange)

- activity in the US: Scidac

Conclusion

★ modern lattice computations

$\longrightarrow$ do not only want to have bigger computers

$\longrightarrow$ work hard on algorithmic improvements

$\longrightarrow$ incorporate theoretical progress:

- get rid of effects of finite physical boxlength L
  $\Leftarrow$ they use the finite extend of the box
  Finite Size Scaling technique

- continuum limit $a \longrightarrow 0$
  $\longleftarrow$ only acceleration of approach to the continuum limit

- have developed *exact chiral symmetry on the lattice:*
  important theoretical (numerical?) concept

on the machine side:

- race between apeNEXT and QCDOC

- exciting question: *role of PC-clusters*

transition period to realistic simulations with dynamical fermions $\Rightarrow$ *facing the truth*