

Lattice Field Theory: solving non-perturbative problems on supercomputers

Karl Jansen



- **Lattice physics program in Germany**
 - Ab-initio computations in QCD
 - Matter under extreme conditions
 - Non-QCD physics
 - Conceptual developments → problem of chiral symmetry
- **Algorithms and machines**
- **Conclusions**

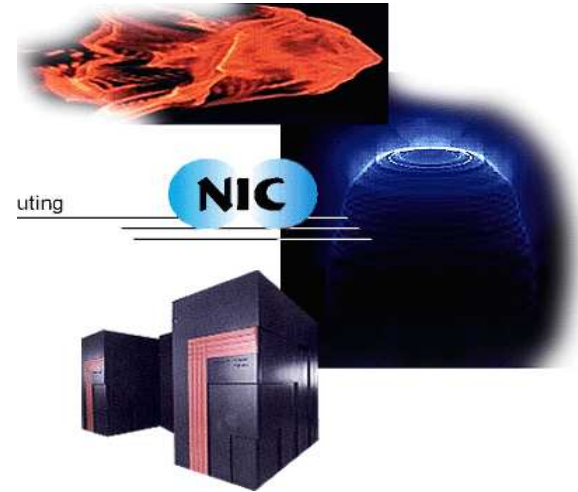
The **John von Neumann-Institute of Computing (NIC)**

cooperation between **DESY** and **research centre Jülich**

- **NIC** shall provide supercomputer resources



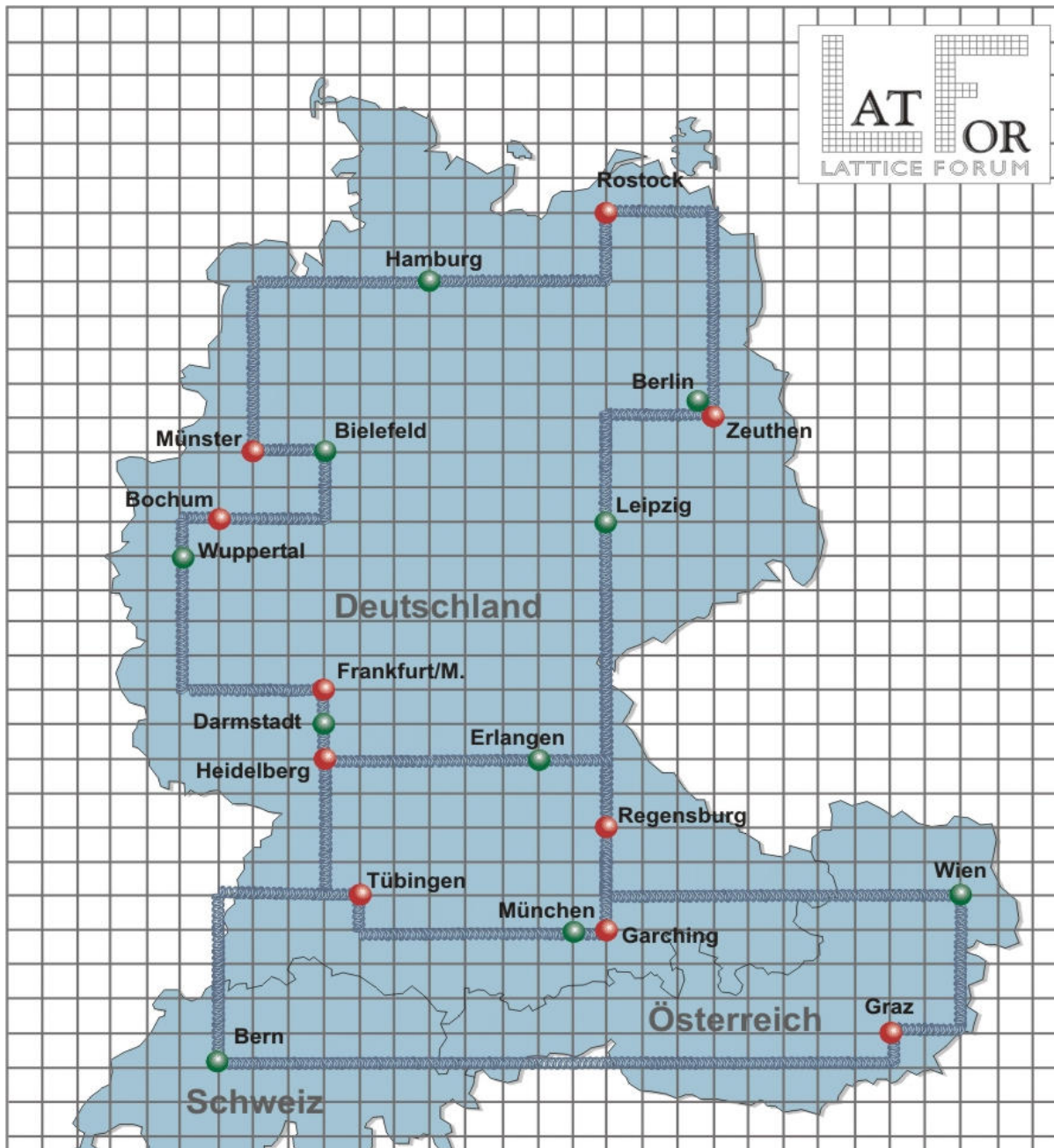
centre of Lattice gauge theory
Zeuthen



general computational science
Jülich


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

<http://www-zeuthen.desy.de/latfor>



Why Lattice Gauge Theory had to be invented

→ QuantumChromoDynamics

asymptotic freedom		confinement
distances $\ll 1\text{fm}$		distances $\gtrsim 1\text{fm}$
world of quarks and gluons		world of hadrons and glue balls
perturbative description		non-perturbative methods

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976

Lattice Gauge Theory is also important today, because

- *it serves as a precise but simple definition of quantum fields, which has its own beauty;*
- *it brings to the fore and clarifies essential aspects such as renormalization, scaling, universality, and the role of topology;*
- *it makes a fruitful connection to statistical physics;*
- *it allows numerical simulations on a computer, giving truly non-perturbative results as well as new physical intuition into the behaviour of the system;*

J. Smit, "Introduction to Quantum fields on a Lattice", 2002

Only the lattice can do this!

- *fundamental scale of QCD* Λ_{QCD}
- *Quark masses and Hadron masses*
- *Chiral condensate* $\langle \bar{q}q \rangle$
- *decay constants* f_B, f_K
- *critical temperature* T_c

what can be done in the next years → LATFOR proposal

rather critical talk about problems with present simulations

K. Jansen, Lattice2003, Tsukuba



Simulations of hypothetical worlds

- setting u-quark mass to zero → CP-violation?
- setting number of flavours very large
- large value of Higgs mass
(e.g. crossover scenario, width)
- testing extensions of the standard model
(e.g. more Higgses, ghost particles, extra dimensions)
- non-perturbative fixed points → new field theories
- simulations without certain degrees of freedom
(e.g. eliminating monopole field)

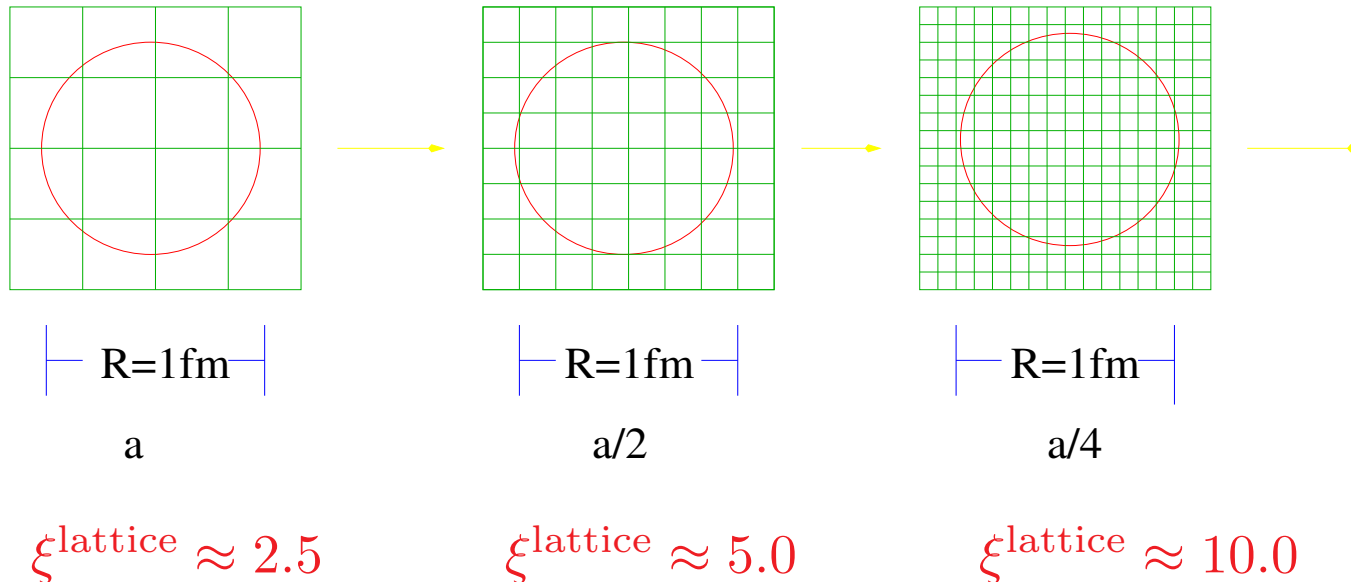
A look at the continuum limit

the general idea of the continuum limit:

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

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

since $m^{\text{lattice}} = 1/\xi^{\text{lattice}} \Rightarrow$ lattice correlation length diverges



The continuum limit

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

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

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

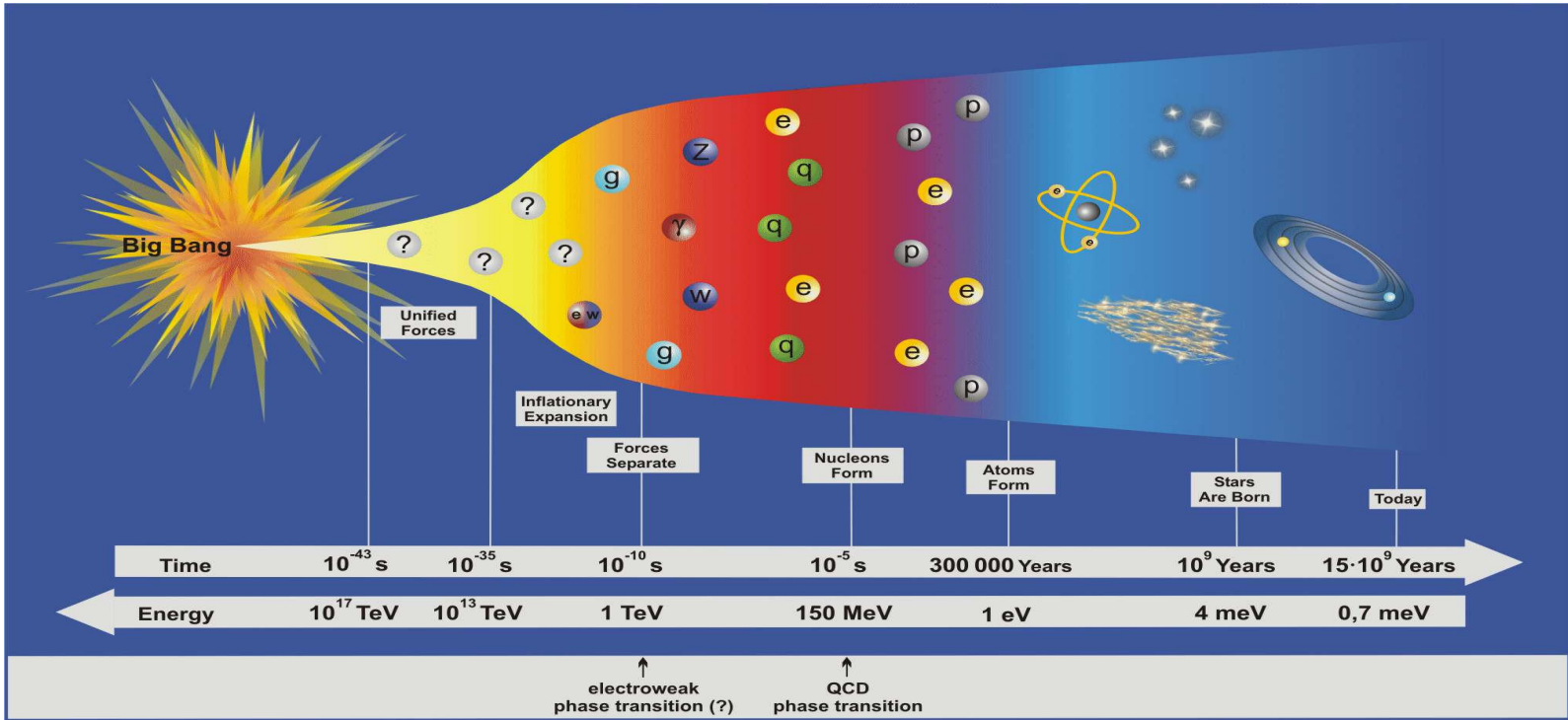
$$a = 0.01\text{fm} \Rightarrow N = 100$$

problem scales at least with $N^4 \Rightarrow$ easily run out of **computertime** and **memory**
solutions (?)

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

modern approach through theoretical advances

- \rightarrow accelerate continuum limit: **improvement programme**
- \rightarrow do not be afraid of finite size effects: **make use of them**



Example: electroweak phase transition

exciting possibility: *baryon-asymmetry* of the universe is generated in an early stage of the universe at the *electroweak phase transition* at $T_c \approx 250\text{GeV}$

Condition Sakharov;Kuzmin,Rubakov,Shaposhnikov

- rate of baryon generation \neq rate of baryon annihilation
- out of equilibrium phenomena
- strong enough *first order* phase transition

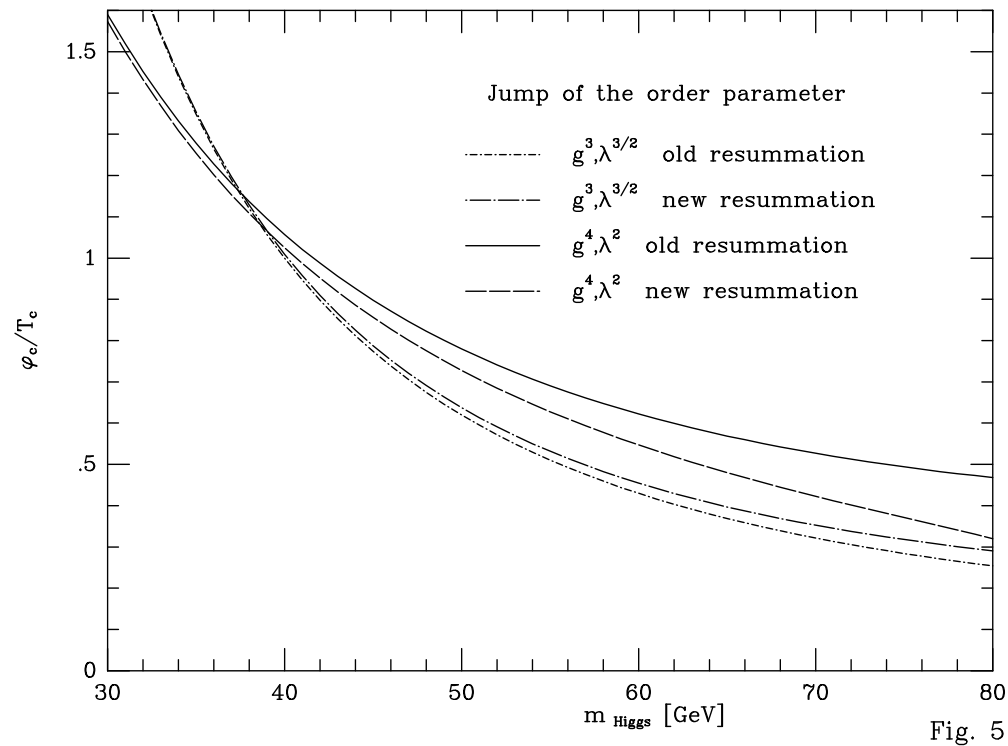
$$\frac{v_T}{T_c} > 1 \quad \text{jump of order parameter } v_T \text{ large enough}$$

v_T Higgs vacuum expectation value
 T_c critical temperature

electroweak physics \Rightarrow use perturbation theory

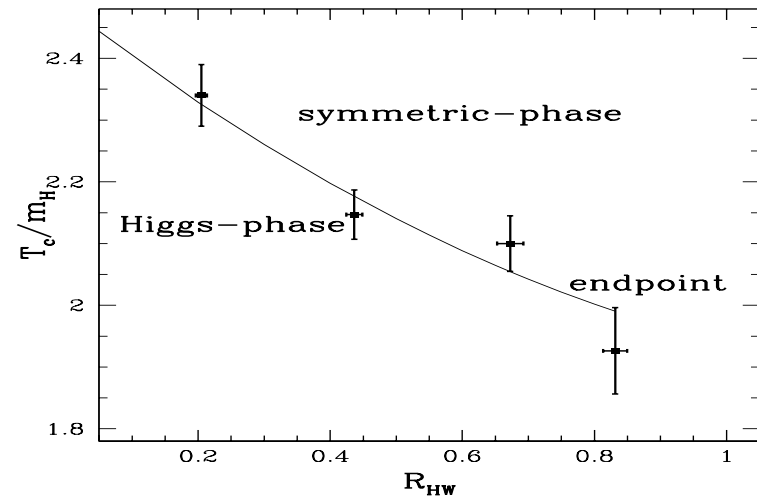
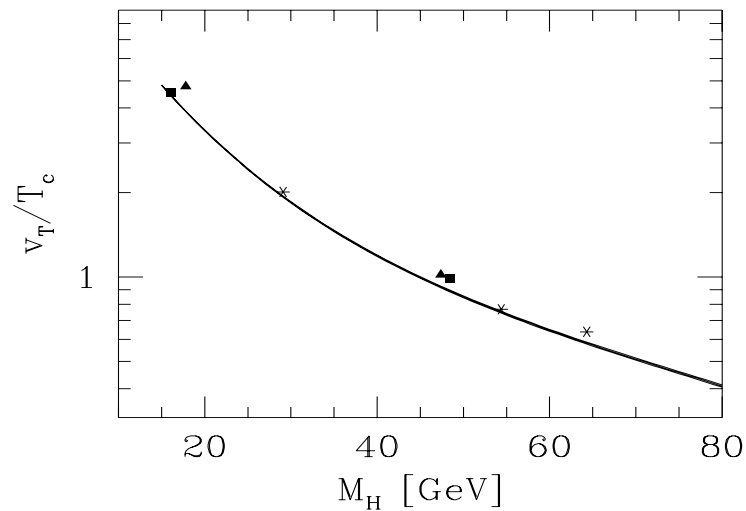
Buchmüller, Fodor, Hebecker

However: problem with perturbation theory



uncertainty in perturbation theory triggered
numerical lattice simulations of the electroweak sector
(SU(2)-Higgs model)

- 4-dimensional simulations at finite temperature
Fodor, Hein, Jansen, Jaster, Montvay
- 3-dimensional effective field theory simulations
Kajantie, Laine, Shaposhnikov, Rummukainen



The physics program of **LATFOR**



- Ab-initio computations in QCD
- Matter under extreme conditions
- Hadron and Nuclear physics
- Non-QCD physics
- Conceptual developments

Ab initio calculations in QCD

- Mass spectrum

a major goal (and major virtue) of lattice QCD

→ computation of hadron masses from first principles

← evaluate euclidean correlation functions

(for unitary theories a rotation back to Minkowski space is always possible)

operator $O(\mathbf{x}, t)$ quantum numbers (spin, charge, parity)

corresponding to the particle we are interested in

if we are only interested in zero momentum we can project $O(t) = \sum_{\mathbf{x}} O(\mathbf{x}, t)$

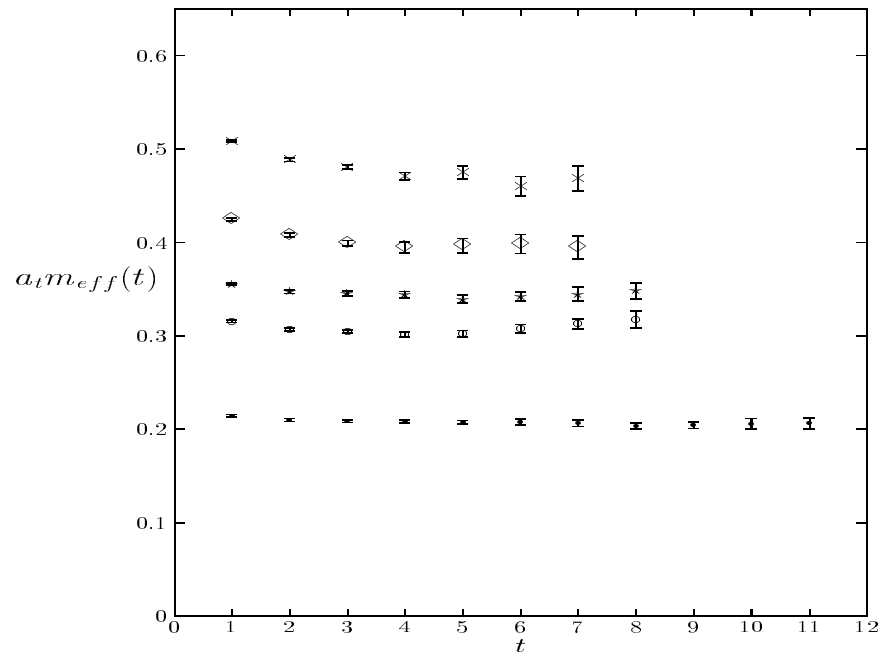
its correlation function is then (infinite lattice)

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

effective masses

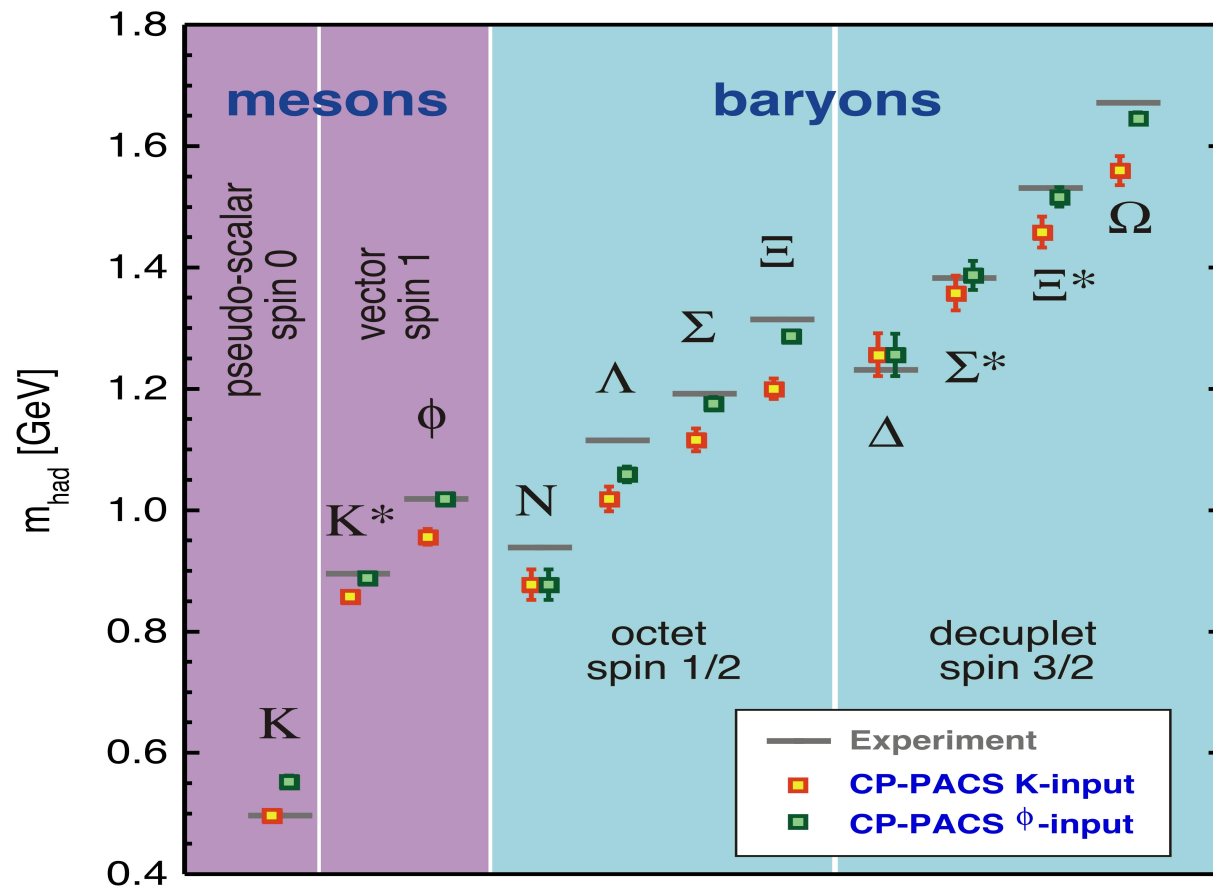
$$m_{\text{eff}}(t) = -\ln \frac{\Gamma(t+1)}{\Gamma(t)}$$

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



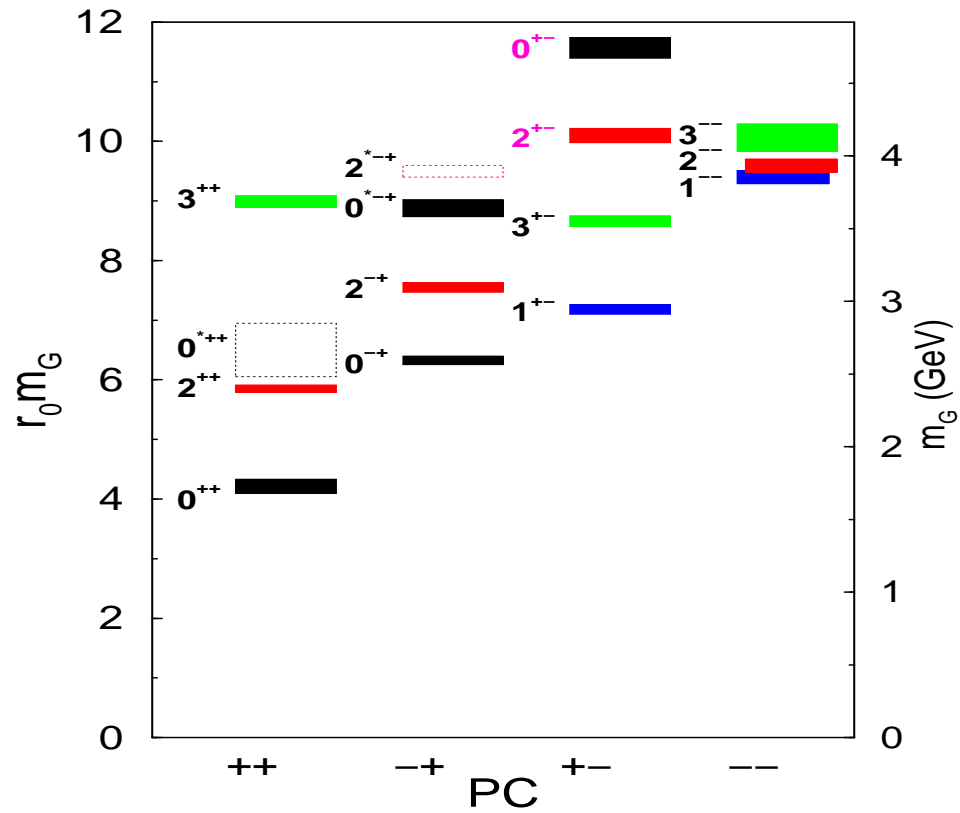
a complete hadron spectrum in the quenched approximation

→ neglect dynamical fermion effects, i.e. exchange of virtual quarks in the hadron



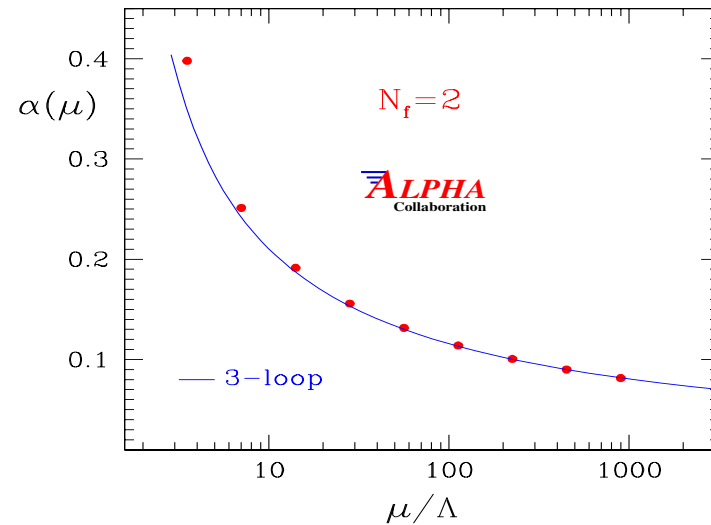
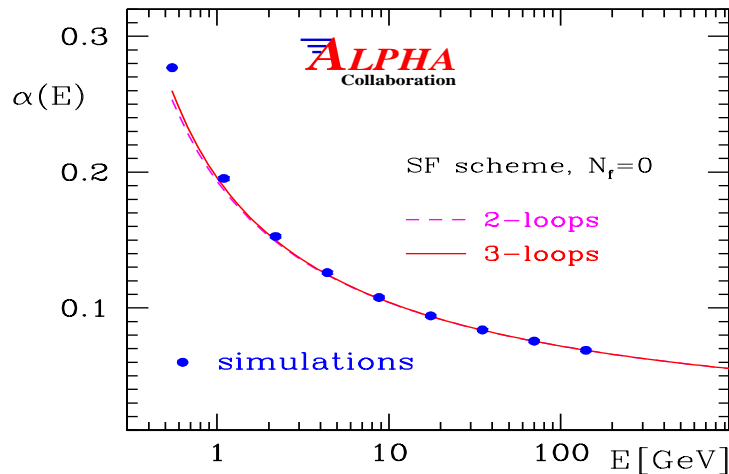
CP-PACS collaboration

glueball spectrum \rightarrow unique prediction from lattice QCD



Ab initio calculations in QCD

- Fundamental parameters \rightarrow fundamental scale Λ_{QCD}
 - running strong coupling constant



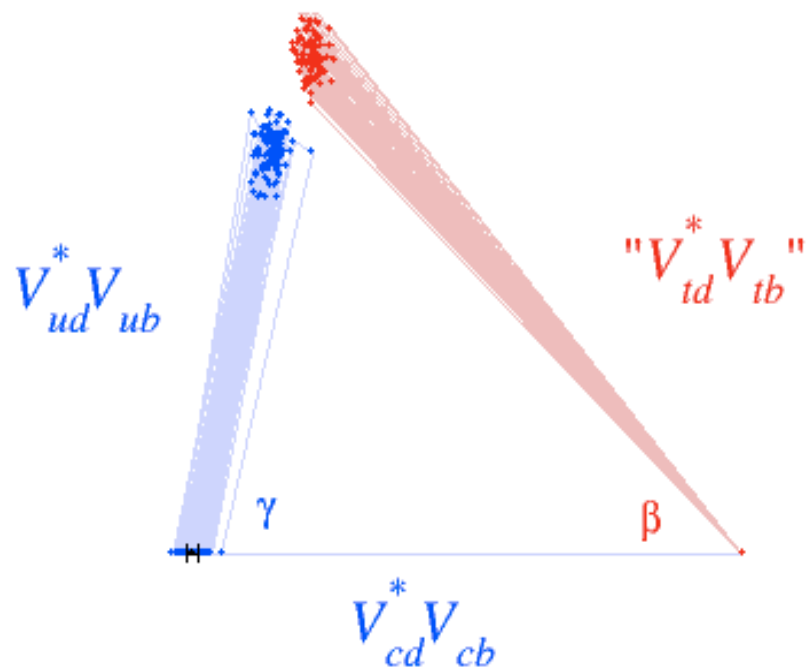
calculation finished
 $\Lambda_{\text{QCD}} = 238(19)\text{MeV}$

Scale Λ not yet known
larger lattices needed \rightarrow **apeNEXT**

Unitarity triangle

- parameters of the CKM matrix
- promising place to look for new physics

Standard UT fit is now entirely in the hands of Lattice QCD
(up to, perhaps, $\|V_{ub}\|$) M. Beneke, Lattice 2001, Berlin



A. Kronfeld, Lattice 2003, Tsukuba

- assume lattice calculations are precise to the 2-3% level

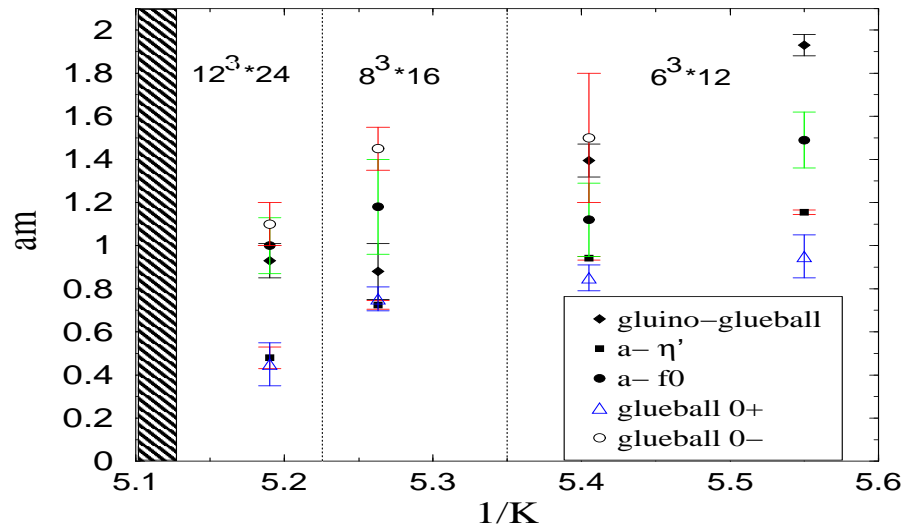
- what are effects of new physics in experiment?

Non-QCD physics

- **Electroweak phase transition**
 - include fermions, Higgs-duplett models, supersymmetric extensions
- **Quantum gravity and matrix models**
 - pure definition and getting ideas
- **Supersymmetry**
 - phase diagram, supersymmetry breaking mechanism

Non-QCD physics

- supersymmetry restoration?



Hamburg-Münster collaboration

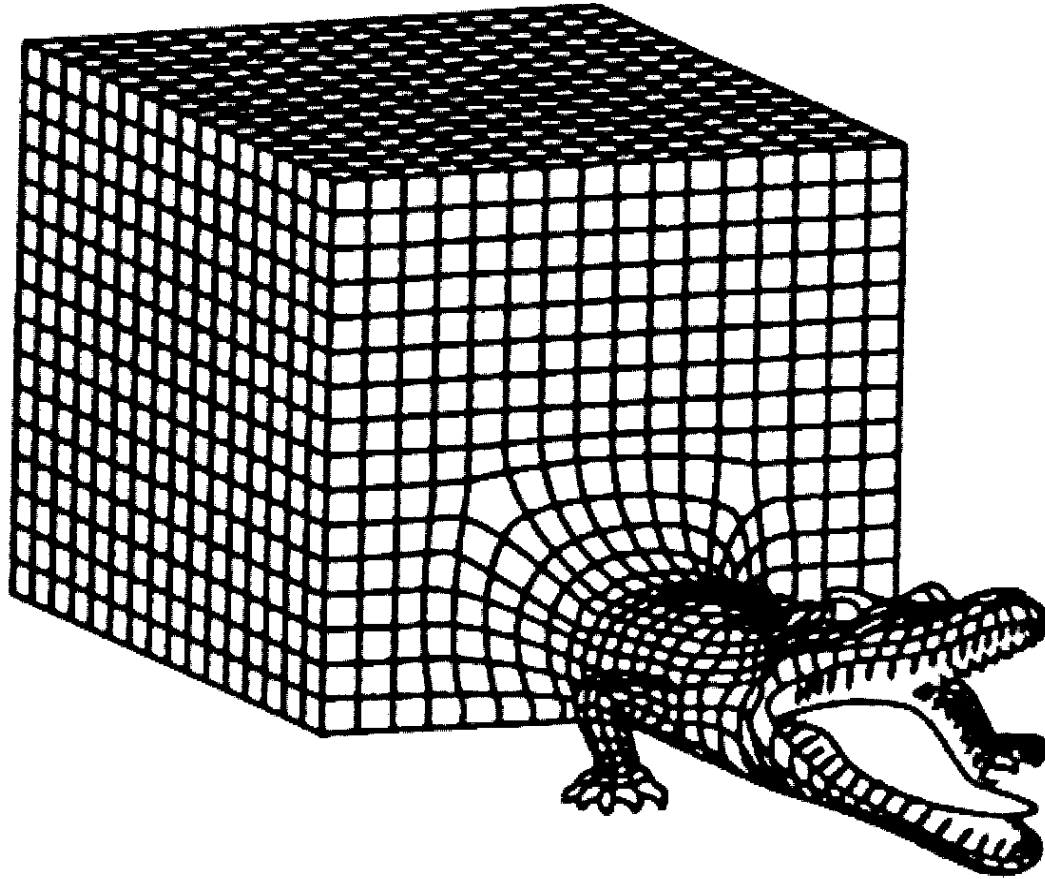
$$1/K - 1/K_c = m_{\text{quark}}$$

shaded area $m_{\text{quark}} \approx 0$

expect: gluino mass vanishes, all other masses become degenerate

- need dynamical simulations from the very beginning
- profile similar as lattice QCD simulations
- lattice breaks supersymmetry explicitly
- conceptual developments to formulate supersymmetry on the lattice D. Kaplan

There are dangerous lattice animals



- discretization errors
- finite volume effects
- chiral limit

Acceleration to the continuum limit

(old) standard lattice action of QCD is

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

⇒ expectation values of physical observables

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

employing all lattice symmetries, equations of motions

⇒ only one more term in $\mathcal{O}(a)$ possible → improved lattice action

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

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

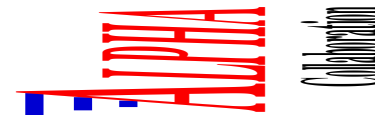
with c_{sw} a *tunable* parameter

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

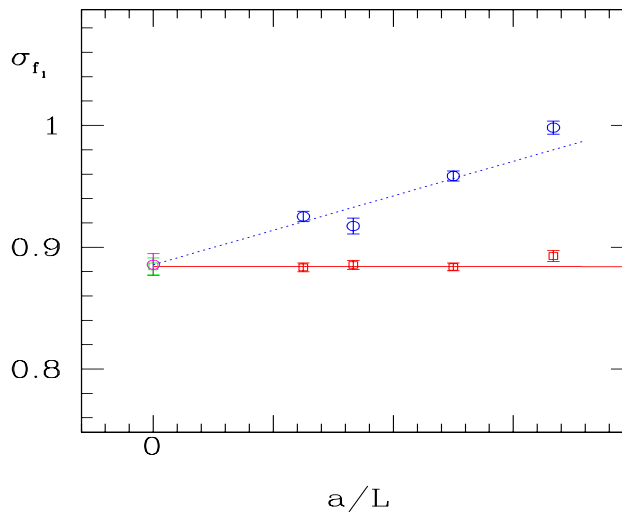
⇒ (nota bene: if also the operator is improved)

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

successful *Symanzik improvement programme* of the
Example of physical quantity derived from the action



⇒ no operator improvement necessary



Quantum chromodynamics

massless QCD has chiral symmetry

$$\psi \rightarrow e^{i\theta\gamma_5}\psi, \quad \bar{\psi} \rightarrow \bar{\psi}e^{i\theta\gamma_5}$$

or, equivalently, $\gamma_5 D_{\text{cont}} + D_{\text{cont}}\gamma_5 = 0$, D_{cont} Dirac operator

assuming that chiral symmetry is spontaneously broken and

$$\langle \bar{\psi}\psi \rangle \neq 0$$

a number of consequences follow, e.g.

- Goldstone modes = pions (having very small mass)
- low energy relations (PCAC) relying on symmetry arguments alone

description possible by chiral perturbation theory for low energy phenomena in QCD

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*

← impossible due to **Nielsen-Ninomiya theorem** (Nielsen and Ninomiya)
(while keeping also locality)

for Wilson fermions → **demonstration in perturbation theory** (although in all orders)
that *in the continuum limit* chiral symmetry is restored
(Bochiccio, Maiani, Rossi, Testa)

non-perturbatively: ... to be proven

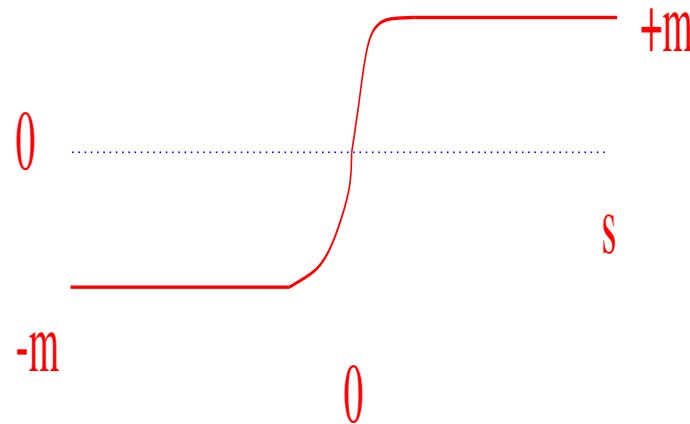
let us go to outer space in extra dimensions (following D. Kaplan)

also, let us start with *continuum field theory*

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

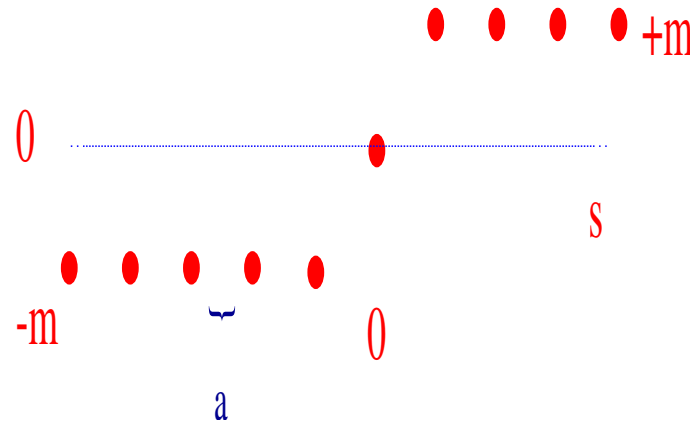
$$\begin{aligned}\psi_{\pm} &= e^{ipx} \Phi_{\pm}(s) u_{\pm} \\ \Phi_{\pm}(s) &= \exp \left\{ \pm \int_0^s m(s') ds' \right\} \\ \gamma_5 u_{\pm} &= \pm u_{\pm}\end{aligned}$$

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 \rightarrow

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



imposing a similar ansatz as in the continuum

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

we find a normalizable solution

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

but, there is now a second normalizable solution

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

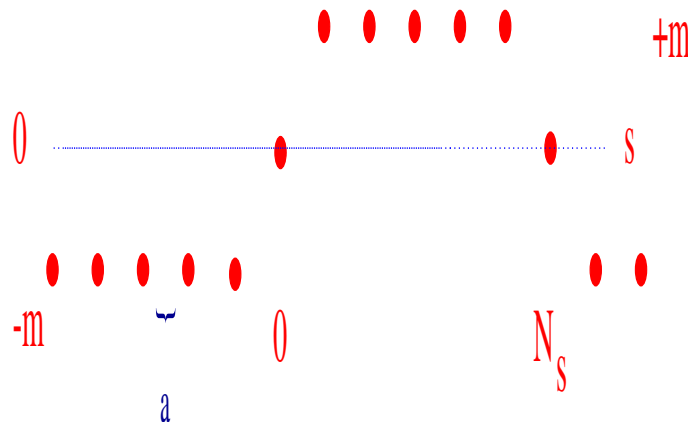
\rightarrow doubler in the extra dimension

solution \Rightarrow add Wilson term also 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

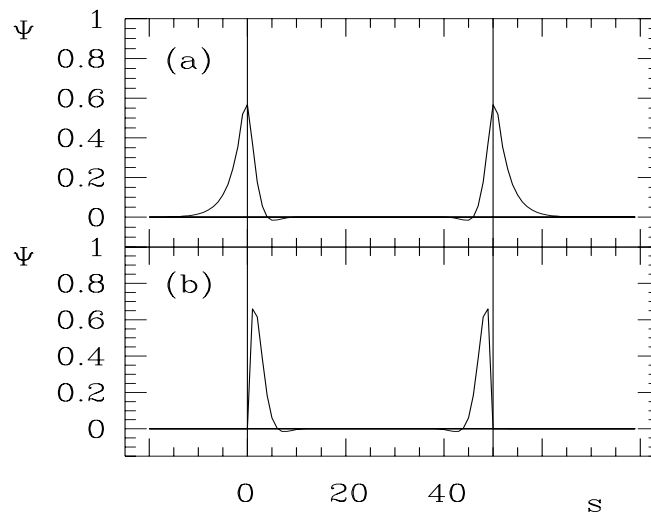
on a finite lattice the extra dimension has an extent N_s and we have to impose some boundary conditions



\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)
⇒ 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)

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

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

\Rightarrow our 5-dimensional lattice action becomes

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

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

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

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

- m is the domain wall mass \rightarrow determines the rate of exponential decay in the extra dimension
- m_0 is the quark mass \rightarrow has to be tuned to zero to give exactly chiral fermions

if we define (Neuberger, Kikukawa, Noguchi)

$$K_{\pm} \equiv \frac{1}{2} \pm \frac{1}{2} \gamma_5 \frac{a_s \mathcal{M}}{2 + a_s \mathcal{M}} \quad \mathcal{M} = D_W - m_0$$

then the domain wall operator can be written as an effective **4-dimensional** operator

$$aD_{N_s} = 1 + \gamma_5 \frac{K_+^{N_s} - K_-^{N_s}}{K_+^{N_s} + K_-^{N_s}}$$

infinite **N_s limit** \Rightarrow 4-dimensional operator

$$aD \equiv \lim_{N_s \rightarrow \infty} aD_{N_s} = 1 + \gamma_5 \text{sign}(K_+ - K_-) \quad ,$$

which is written as

$$aD = 1 - \frac{A}{\sqrt{A^\dagger A}} \quad , \quad A = -\frac{a_s \mathcal{M}}{2 + a_s \mathcal{M}} \quad .$$

anti-commutation relation for D

$$\gamma_5 D + D \gamma_5 = 2aD \gamma_5 D$$

Ginsparg-Wilson relation

$$\gamma_5 D + D \gamma_5 = 2a D \gamma_5 D$$

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

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

→ 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
⇐ block spinning from the continuum

alternative solution of GW relation: overlap operator D_{ov} (Neuberger)

$$D_{\text{ov}} = [1 - A(A^\dagger A)^{-1/2}]$$

with $A = 1 + s - D_{\text{w}}$ s a tunable parameter, $0 < s < 1$

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

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

\Rightarrow have a notion of chiral symmetry on the lattice

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

the *lattice* operator D enjoys many properties of the *continuum* operator:

$Z_A = Z_V = 1$, anomaly, index theorem, ...

in addition:

despite the term $1/\sqrt{A^\dagger A}$

(\Rightarrow all lattice points are coupled among each other)

the operator D_{ov} is local, $\|D_{\text{ov}}\Phi\| \propto e^{-\gamma/a}$

(Hernandèz, Lüscher, K.J.)

- if plaquette is bounded: $\|1 - U_P\| < 1/30$
(analytical proof)
- locality also demonstrated numerically when bound not satisfied

\Rightarrow

- *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

- ⇒ appearance of **Goldstone particles** (pions)
(Goldstone theorem)
- ⇒ many low energy relation (**PCAC relation**) in QCD
- ⇒ application of chiral perturbation theory

the lattice is a unique environment to test this basic assumption and an operator satisfying the Ginsparg-Wilson relation provides the necessary 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 $m \rightarrow 0$ approximate formulae are obtained

$$\Sigma_{\nu=0}(a) = m \Sigma^2 V (1/2 - \gamma + \ln 2 - \ln m\Sigma V + O(m\Sigma V)^2)$$

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

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

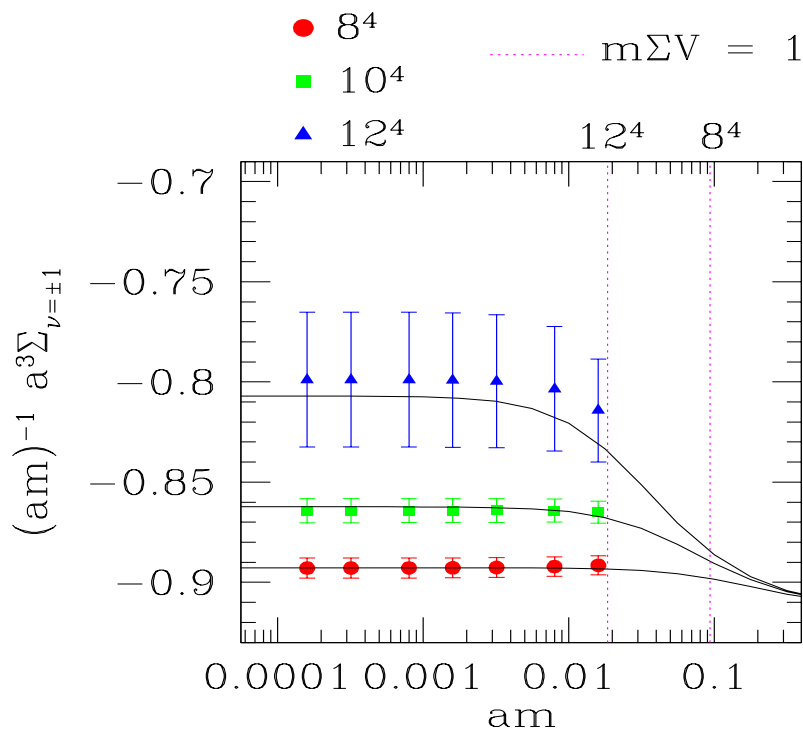
this divergence has to be subtracted (i.e. fitted)

Computation of chiral condensate using overlap fermions

data points at 7 masses on 3 volumes

attempt a fit according to

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

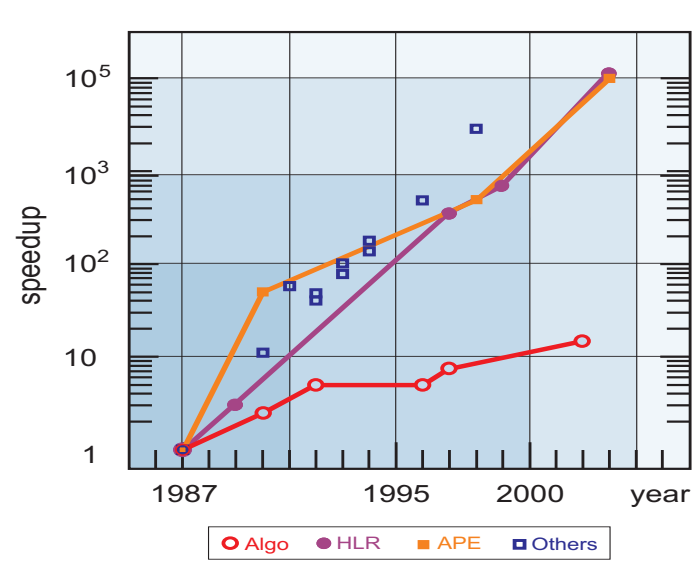


→ only two free parameters
 Σ and C

(Hernández, Lellouch, K.J.)

⇒ find strong evidence for spontaneous chiral symmetry breaking in QCD!

Algorithm and machine development (not incorporating conceptual improvements)



Japan

Computational Physics on Parallel Array Computer System → CPPACS

collaboration of lattice physicists from Tsukuba

+ industrial partner Hitachi



614 Gflops peak speed

128 Gbytes memory

2048 Processing units

future development → ? ← Earth simulator

USA

QCD on digital Signal Processor System → QCDSPP



600 Gflops peak speed

50 Gbytes memory

12 288 Processing units

future development → QCDOC (QCD On Chip)

collaboration of lattice physicists from Columbia University, RIKEN, BNL and UKQCD + industrial partner IBM

10 Tflops peak speed

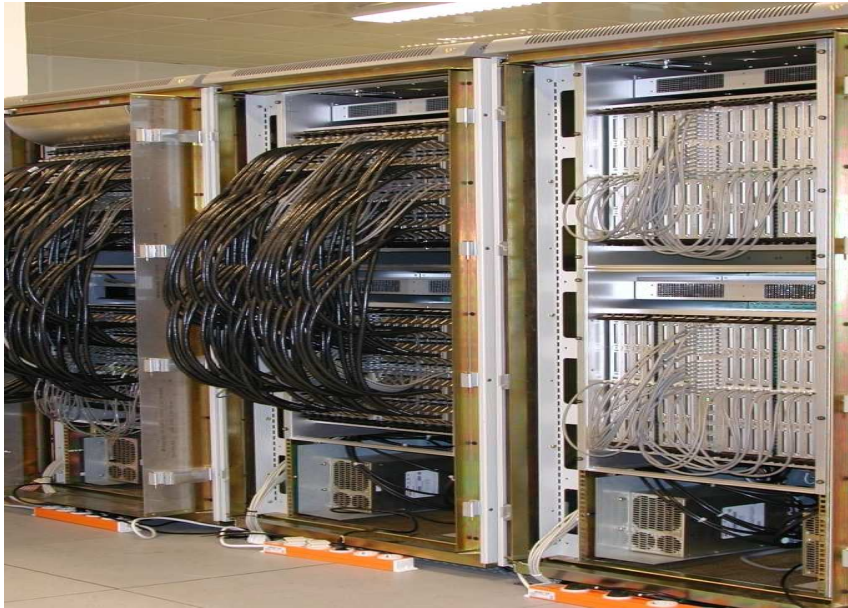
40Gbytes on chip + $O(1)$ Tbytes external memory

$O(10\ 000)$ Processing units

1 Dollar/Mflops sustained performance

Europe

Array Processor Experiment → APE



APEmille installation in Zeuthen

550 Gflops peak speed

32 Gbytes memory

1024 Processing units

future development → apeNEXT

collaboration of lattice physicists from INFN, DESY and University of Paris Sud

10 Tflops peak speed

1-4 Tbytes memory

O(6 000) Processing units

1Euro /Mflops sustained performance

LATFOR evaluationgroup

M. Hasenbusch, T. Lippert, D. Pleiter, H. Stüben, P. Wegner, T. Wettig, H. Wittig, K.J.

- definition and implementation of lattice QCD benchmark suite
- test of benchmarks on different platforms
 - apeNEXT (simulator)
 - QCDOC (simulator)
 - several PC-cluster systems (MPI)
 - commercial supercomputers
CRAY T3E-900, Hitachi SR8000-F1, IBM p690-Turbo
- consumer's report
 - Price/performance ratio
aim: 1 Euro/Mflop
 - memory, I/O
 - userfriendliness
 - electricity, footprint, cooling
 - existing Know-How

Evaluation

M. Hasenbusch, K. Jansen, T. Lippert, D. Pleiter, H. Stüben,
P. Wegner, T. Wettig and H. Wittig

single node performance

	apeNEXT	QCDOC	PC-Cluster	IBM
Peak	1600	1000	3400	5200
M	944	470	849	–
M_{eo}	944	465	930	600 – 900
M_{ssor}	368	–	545	–
(ψ, ϕ)	656	450	530	272 – 306
$\ \psi\ ^2$	592	384	510	215 – 246
zaxpy	464	450	358	210 – 301
daxpy	–	190	183	139 – 197
$U^*\phi$	1264	780	307	240 – 247
U^*V	1040	800	763	347 – 442
Clover	1136	790	800	527

Top 12 list for lattice QCD benchmark (Wilson-Dirac operator)
 if a **25 Teraflops system** would be installed end **2003**/beginning **2004**

Rank	Platform	Sustained	Peak
1	apeNEXT	12.5	25
1	QCDOC	12.5	25
3	Earth simulator (Japan)	12	40
4	ASCI Q - AlphaServer SC ES45 (Hewlett-Packard, LANL,USA)	7.4	20
5	CR Linux Cluster (Linux Networx, LLNL,USA)	2.7	11
5	AlphaServer SC ES45 (Hewlett-Packard, Pittsburg)	2.7	6
7	ASCI White (IBM, LLNL, USA)	2.5	13
8	xSeries Cluster (IBM, LLNL, USA)	2.3	9.2
8	AlphaServer SC ES45 (Hewlett-Packard, CEA, France)	2.3	5.1
10	SP Power3 (IBM, NERSC, USA)	2	10
11	PRIMEPOWER HPC2500 (Fujitsu, Japan)	1.4	12.0
12	AlphaServer SC ES45 (Hewlett-Packard, NASA)	1.3	2.8

M. Hasenbusch

- take single node performance → upper bound
- where no direct benchmark possible, take scaling of standard benchmark
- cost of other machines an order of magnitude larger than apeNEXT/QCDOC

Conclusion

- ★ modern lattice computations
- do not only want to have bigger computers
- work hard on algorithmic improvements
- incorporate theoretical progress:
 - get rid of effects of finite physical boxlength L
 - ← they use the finite extend of the box *Finite Size Scaling technique*
 - continuum limit $a \rightarrow 0$
 - ← 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*