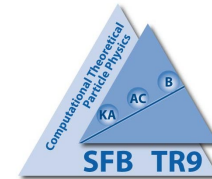
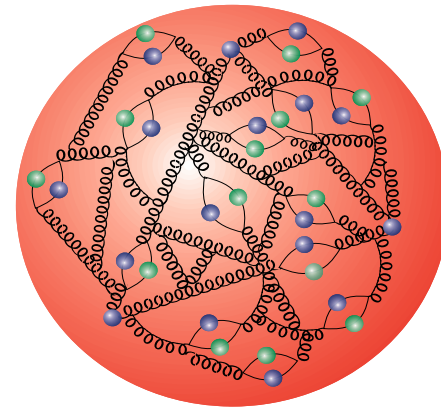


# Introduction to Lattice QCD II

Karl Jansen



- **Task: compute the proton mass**
  - need an action
  - need an algorithm
  - need an observable
  - need a supercomputer
- **Anomalous magnetic moment of Muon**



## Monte Carlo Method

$$\langle f(x) \rangle = \int dx f(x) e^{-x^2} / \int dx e^{-x^2}$$

→ solve numerically:

- generate successively Gaussian random numbers  $x_i$
- do this  $N$ -times

$$\Rightarrow \langle f(x) \rangle \approx \frac{1}{N} \sum_i f(x_i) \pm O(1/\sqrt{N})$$

- but, what if I have a distribution  $e^{-S(\phi)}$ ?  
( $\Phi$  representing generic degrees of freedom)

find a transition probability  $W(\phi, \phi')$  that brings us from a set of generic fields  $\{\phi\} \rightarrow \{\phi'\}$  and which satisfies

- $W(\phi, \phi') > 0$  **strong ergodicity** ( $W \geq 0$  is weak ergodicity)
- $\int d\phi' W(\phi, \phi') = 1$
- $W(\phi, \phi') = \int d\phi'' W(\phi, \phi'') W(\phi'', \phi')$  (**Markov chain**)
- $W(\phi, \phi')$  is measure preserving,  $d\phi' = d\phi$

under these conditions, we are guaranteed

- to converge to a unique equilibrium distribution  $P^{\text{eq}}$  namely the Boltzmann distribution  $e^{-S}$
  - that this is independent from the initial conditions
- proof: (Creutz and Freedman; Lüscher, Cargese lectures)

Markov chain condition

$$W(\phi, \phi') = \int d\phi'' W(\phi, \phi'') W(\phi'', \phi')$$

can be rephrased when taking the equilibrium distribution itself

$$P(\phi') = \int d\phi W(\phi', \phi) P(\phi)$$

to fulfill (most of) our conditions it is *sufficient not necessary* that  $W$  fulfills the **detailed balance condition**:

$$\frac{W(\phi, \phi')}{W(\phi', \phi)} = \frac{P(\phi')}{P(\phi)}$$

for example

$$\begin{aligned} \int d\phi P(\phi) W(\phi, \phi') &= \int d\phi P(\phi) \frac{P(\phi')}{P(\phi)} W(\phi', \phi) \\ &= \int d\phi P(\phi') W(\phi', \phi) = P(\phi') \end{aligned}$$

in the following discuss particular choices for  $W$  for problems of interest

## Metropolis Algorithms

$$W_{\text{Metro}}(\Phi, \Phi') = \Theta(S(\Phi(x)) - S(\Phi'(x))) \\ + \exp(-\Delta S(\Phi', \Phi)) \Theta(S(\Phi'(x)) - S(\Phi(x)))$$

$$\Delta S(\Phi'(x), \Phi(x)) = S(\Phi'(x)) - S(\Phi(x)), \Theta() \text{ Heavyside function}$$

How this works:

- i)* generate uniformly distributed  $\Phi'(x)$  in a neighbourhood of  $\Phi(x)$ 
  - discretized quantum mechanics:  $x'_i \in [x_i - \Omega, x_i + \Omega]$
  - $SU(N)$ :  $U'_{n,\mu} = RU_{n,\mu}$ , elements of  $R$  “close to”  $U_{n,\mu}$
- ii)* if  $\Delta S(\Phi'(x), \Phi(x)) \leq 0$  accept  $\Phi'(x)$
- iii)* if  $\Delta S(\Phi'(x), \Phi(x)) > 0$  accept with probability  $\exp(-\Delta S(\Phi'(x), \Phi(x)))$ 
  - steps *i)* – *iii)* are repeated  $N$ -times
  - step *iii)* can be realized by uniformly choosing random number  $r \in [0, 1]$  and accept, if  $\exp(-\Delta S) > r$

## Metropolis Algorithms

- very general algorithm, can be used for many physical systems
- shows, however, often very long autocorrelation times
- much too costly for fermionic systems (why?)

## Hybrid Monte Carlo Algorithm

expectation values in lattice field theory

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi O e^{-S}}{\int \mathcal{D}\Phi e^{-S}}$$

do not change if field independent contributions are added to the action

$$\langle O \rangle = \frac{\int \mathcal{D}\Phi \int \mathcal{D}\pi O e^{-\frac{1}{2}\pi^2 - S}}{\int \mathcal{D}\Phi \int \mathcal{D}\pi e^{-\frac{1}{2}\pi^2 - S}}$$

field configurations are generated chronologically in a fictitious (computer) time  $\tau$

take  $\pi$ 's Gaussian distributed, satisfying

$$\langle \pi(\tau) \rangle = 0, \quad \langle \pi(\tau)\pi(\tau') \rangle = \delta(\tau - \tau')$$

consider a 4-dimensional Hamiltonian

$$H = \frac{1}{2}\pi^2 + S$$

consider quantum mechanical action:  $S = \sum_n (x(n+a) - x(n))^2 + m^2 x^2(n)$

in fictitious time  $\tau$  the system develops according to

**Hamilton's equations of motion**

$$\frac{\partial}{\partial \tau} \pi(n) = -\frac{\partial}{\partial \mathbf{x}(n)} S \equiv \text{force}, \quad \frac{\partial}{\partial \tau} \mathbf{x}(n) = \pi(n)$$

$\Rightarrow$  conservation of energy

in practice, equations are integrated numerically up to time  $T = 1$

divide  $T$  into  $N$  intervals of length  $\delta\tau$  such that  $T = N\delta\tau$  : **leap-frog scheme**

$$\begin{aligned} \pi(\delta\tau/2) &= \pi(0) - \frac{\delta\tau}{2} \frac{\partial}{\partial \mathbf{x}} S \Big|_{\mathbf{x}(0)} \\ \mathbf{x}(\delta\tau) &= \mathbf{x}(0) + \pi(\delta\tau/2) \delta\tau \\ \pi(3\delta\tau/2) &= \pi(\delta\tau/2) - \delta\tau \frac{\partial}{\partial \mathbf{x}} S \Big|_{\mathbf{x}(\delta\tau)} \\ &\vdots \\ \pi(T) &= \pi(N\delta\tau/2) - \frac{\delta\tau}{2} \frac{\partial}{\partial \mathbf{x}} S \Big|_{\mathbf{x}((N-1)\delta\tau)} \end{aligned}$$



leap-frog scheme has a *finite* step-size  $\delta\tau \Rightarrow$  energy is no longer conserved

$$H(\mathbf{x}_{\text{ini}}, \pi_{\text{ini}}) \neq H(\mathbf{x}_{\text{end}}, \pi_{\text{end}})$$

introduce a **Metropolis** like **accept/reject step**

accept new field configuration  $\{\mathbf{x}_{\text{end}}, \pi_{\text{end}}\}$  with a probability

$$P_{\text{acc}} = \min(1, e^{H(\mathbf{x}_{\text{ini}}, \pi_{\text{ini}}) - H(\mathbf{x}_{\text{end}}, \pi_{\text{end}})})$$

## Hybrid Monte Carlo Algorithm

general transition matrix:

$$W(\Phi', \Phi) = \frac{1}{\mathcal{Z}_\pi} \int \mathcal{D}[\pi] e^{-\frac{1}{2}(\pi, \pi)} \left\{ P_{\text{acc}}(\pi, \Phi) \prod_x \delta(\Phi'(x), \Phi_\tau(x)) \right. \\ \left. + (1 - P_{\text{acc}}(\pi, \Phi)) \prod_x \delta(\Phi'(x), \Phi(x)) \right\}$$

- fulfills detailed balance **proof:** (Lüscher, Cargese lectures)  
⇐ needs *reversibility* of the leap-frog integrator
- preserves measure
- Ergodicity?

## The case of Lattice QCD

action for two flavors of fermions (up and down quark)

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

path integral

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

interaction of the scalar fields is very complicated: inverse fermion matrix  $[M^\dagger M]^{-1}$  couples all points on the lattice with each other

*How would a Metropolis algorithm work?*

simulate with Hybrid Monte Carlo algorithm

$$\begin{aligned} \frac{d}{d\tau} \pi &= -\frac{dS}{d\Phi^\dagger} = [M^\dagger M]^{-1} \Phi \equiv \text{force} \\ \frac{d}{d\tau} \Phi &= \pi \end{aligned}$$

update of the momenta  $\pi(x)$  is completely independent of update of  $\Phi$ -field, non-locality of the action is not a problem

to update the momenta, have to compute the vector

$$X = [M^\dagger M]^{-1} \Phi$$

⇒ solve an equation

$$[M^\dagger M] X = \Phi$$

### Exercise:

estimate the number of flops to apply the Wilson operator on a vector

assume you want to have 2000 thermalization and 5000 measurement steps on a  $48^3 \cdot 96$  lattice

assume number of iterations to solve  $[M^\dagger M] X = \Phi$  is 500

assume number of time steps in the HMC is 100

How long would the program run on your laptop?  
(assume –unrealistic– efficiency of 50%)

If you save the 5000 configurations, would this fit on your laptop disk?

## autocorrelation times

generating field configurations as a Markov process,  
 $\Rightarrow$  configurations are not independent from each other

free field theory  $S = \int d^4x \Phi(x) [\nabla_m u^* \nabla_\mu + m_0^2] \Phi(x)$  in Fourier space

$$S = \int d^4k \Phi(k) [k^2 + m_0^2] \Phi(k)$$

Langevin equation  $\leftrightarrow$  HMC algorithm

$$\frac{d}{d\tau} \Phi(k, \tau) = -[k^2 + m_0^2] \Phi(k, \tau) + \eta(k, \tau)$$

$$\langle \eta(\tau) \rangle = 0, \quad \langle \eta(\tau) \eta(\tau') \rangle = \delta(\tau - \tau')$$

then a solution may be written down

$$\Phi(k, \tau) = \int^\tau ds \exp \{ -(\tau - s) [k^2 + m_0^2] \} \eta(k, s)$$

compute correlation of fields at  $\tau = 0$  with fields at  $\tau$

consider the autocorrelation function

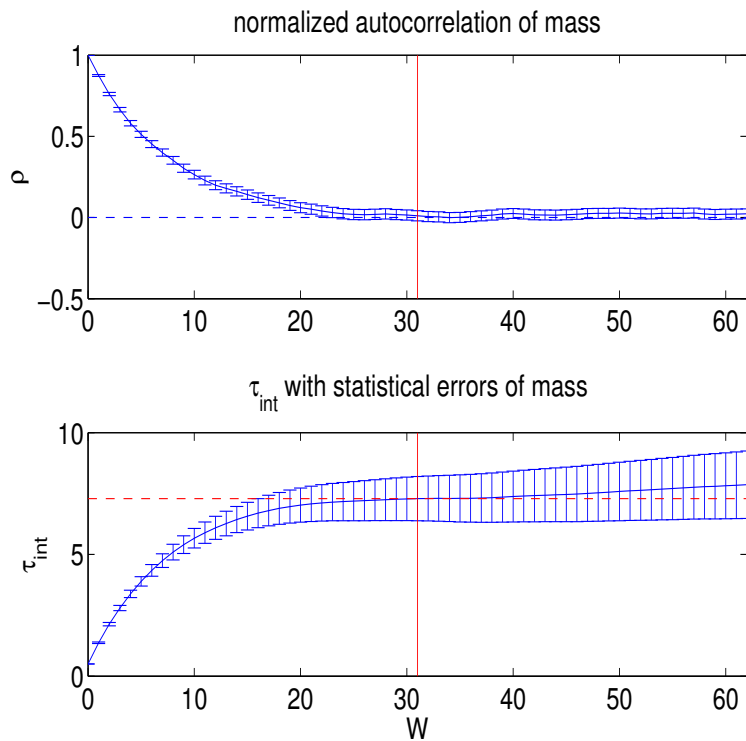
$$\begin{aligned} C(k, \tau) &= \Phi(k, 0)\Phi(k, \tau) \\ &= \int ds_1 ds_2 \exp \{ [k^2 + m_0^2]s_1 (-(\tau - s)[k^2 + m_0^2]) \\ &\quad \eta(k, s_1)\eta(k, s_2) \} \\ &\propto \frac{e^{-[k^2+m_0^2]\tau}}{k^2+m_0^2} \equiv \frac{e^{-\tau/\tau_0}}{k^2+m_0^2} \end{aligned}$$

- the autocorrelation function  $C(k, \tau)$  decays exponentially  
autocorrelation time  $\tau_0$
- decay is lowest for the zero mode  $k = 0$
- $\tau \propto 1/m_0^2 \Rightarrow$  the correlations become stronger closer to  
the critical point  $m_0 = 0 \rightarrow$  *critical slowing down*
- scaling law  $\tau_0 \propto 1/m^z$ ,  $z$  *the dynamical critical exponent*

How to deal with the autocorrelation?

measure it:

$$\Gamma(\tau) = \langle x(\tau) \cdot x(0) \rangle / \langle x(0) \rangle^2 \propto e^{-\tau/\tau_{\text{int}}}$$



Comment: *integrated auto correlation time*  $\tau_{\text{int}}$  observable dependent

## A consequence from autocorrelations: Errors

measure average position of quantum mechanical particle  $\bar{x}$  from  $N$  measurements

$$\bar{x} = \frac{1}{N} \sum_{i=1}^N x_i$$

This has a variance

$$\sigma = \frac{1}{N-1} (\bar{x^2} - \bar{x}^2)$$

and a standard deviation

$$\Delta_0 \equiv \sqrt{\sigma} \propto 1/\sqrt{N} \text{ for } N \gg 1$$

If we have an autocorrelation time  $\tau \Rightarrow$  statistics reduces to  $n = N/\tau$

$$\Rightarrow \Delta_{\text{true}} \propto 1/\sqrt{n} = \sqrt{\tau}/\sqrt{N} = \sqrt{\tau}\Delta_0$$



## Can we improve the error scaling for evaluating pathintegrals?

reminder:

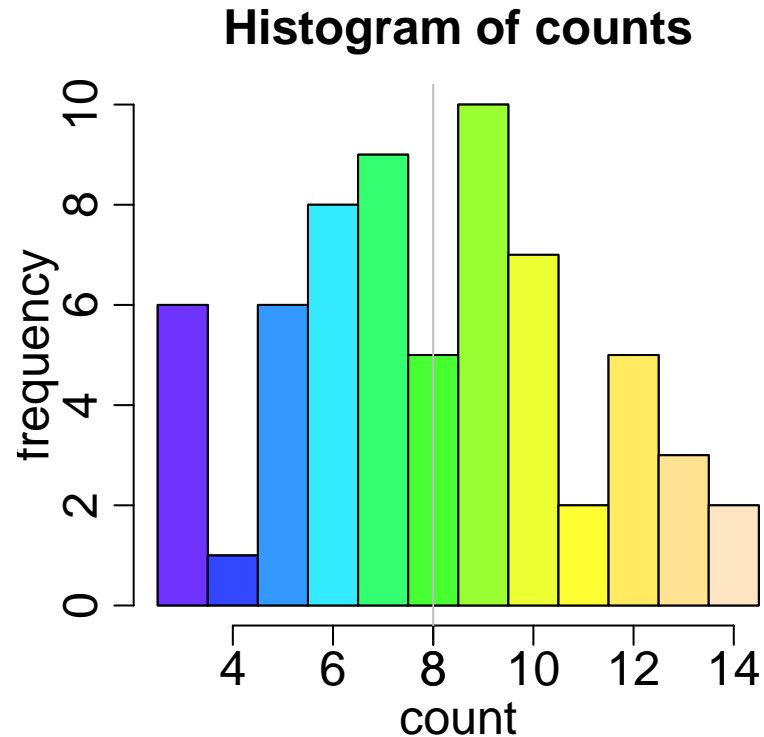
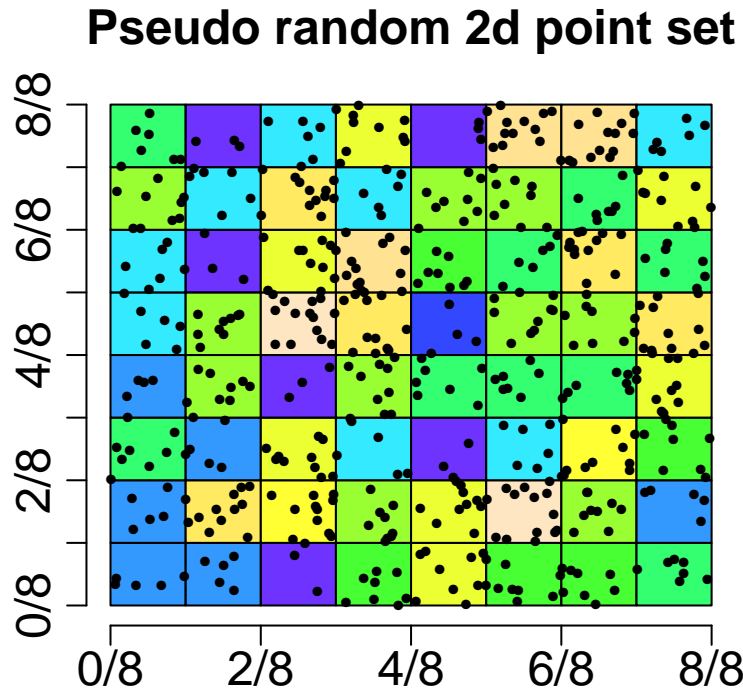
$$Z = \int \mathcal{D}x e^{-S[x]} ; \quad x = (x_1, \dots, x_d) ; \mathcal{D}x = \prod_{i=1}^d dx_i$$

$$\langle O \rangle = Z^{-1} \int \mathcal{D}x e^{-S[x]} O[x]$$

- stochastically through Markov chain Monte Carlo methods
- finite Markov chain:  $x_1, \dots, x_N \rightarrow N$  samples of  $O$ :  $O_1, \dots, O_N$
- estimate  $\overline{\langle O \rangle} = \frac{1}{N} \sum_{i=1}^N O_i$  has standard error  $\Delta \overline{\langle O \rangle} = \frac{\sigma_O}{\sqrt{N}}$

## Distribution of integration variables

**Example:** 512 two-dimensional pseudo-random points



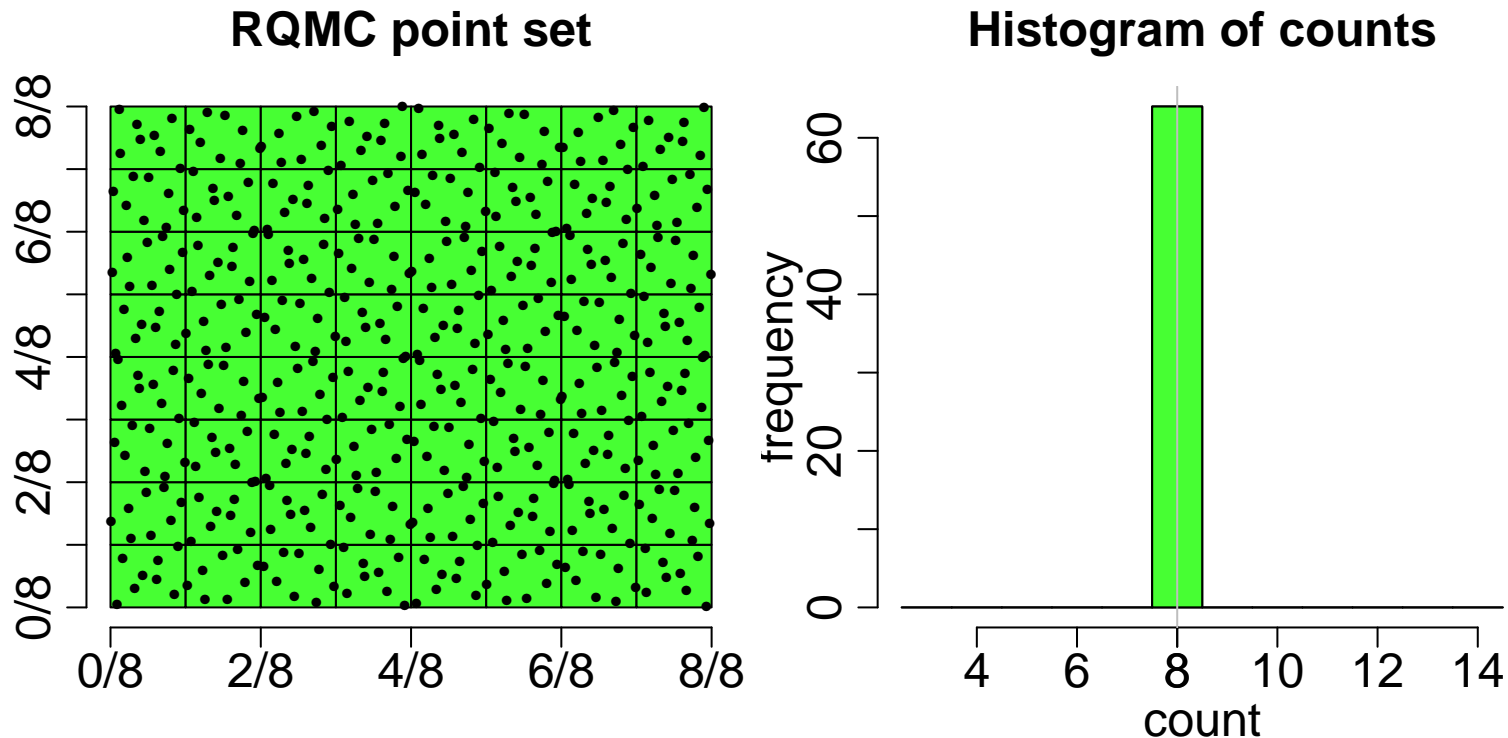
- sample 512 points grid of  $8 \times 8$  equal squares
- count number of points in each square
- count occurrence of  $1, 2, \dots$  points in a square
- $\approx$  Poisson distribution  $\rightarrow$  uneven sampling  $\rightarrow$  large stochastic error

## Improved integration: Quasi Monte Carlo

- construction of deterministic low-discrepancy point-sets
- low-discrepancy  $\rightarrow$  “more uniform”
- promises  $N^{-1}$  asymptotic error behaviour for suitable integrands
- applied successfully to financial problems

## Distribution of integration points

QMC point set (2d Sobol samples):



- each square contains same number of points → delta distribution
- even coverage → less stochastic fluctuations
- makes QMC a most promising tool
- randomisation possible (RQMC): → practical error estimation

## First investigation for quantum mechanical model in Euclidean time

(K. Jansen, H. Leovey, A. Ammon, A. Griewank, T. Hartung, M. Müller-Preußker)

$$S = a \sum_{i=1}^d \left( \frac{M_0}{2} \frac{(x_{i+1} - x_i)^2}{a^2} + \frac{\omega^2}{2} x_i^2 + \lambda x_i^4 \right) ; \quad x_{d+1} = x_1$$

- $M_0$ : particle mass
- $\omega$ : frequency
- $a$ : lattice spacing
- $d$  number of lattice sites,  $\rightarrow T = da$  time extent
- $\lambda = 0 \rightarrow$  harmonic oscillator
- $\lambda > 0 \rightarrow$  anharmonic oscillator  
(  $\mu^2 < 0 \rightarrow$  double well potential)

## Observables considered

### Cumulants

$$\langle x^2 \rangle = \langle \frac{1}{d} \sum_i x_i^2 \rangle$$

$$\langle x^4 \rangle = \langle \frac{1}{d} \sum_i x_i^4 \rangle$$

### Correlator

$$\langle x_k x_{k+t} \rangle = \langle \frac{1}{d} \sum_i x_i x_{i+t} \rangle \propto e^{-(E_1 - E_0)t}$$

### Energies

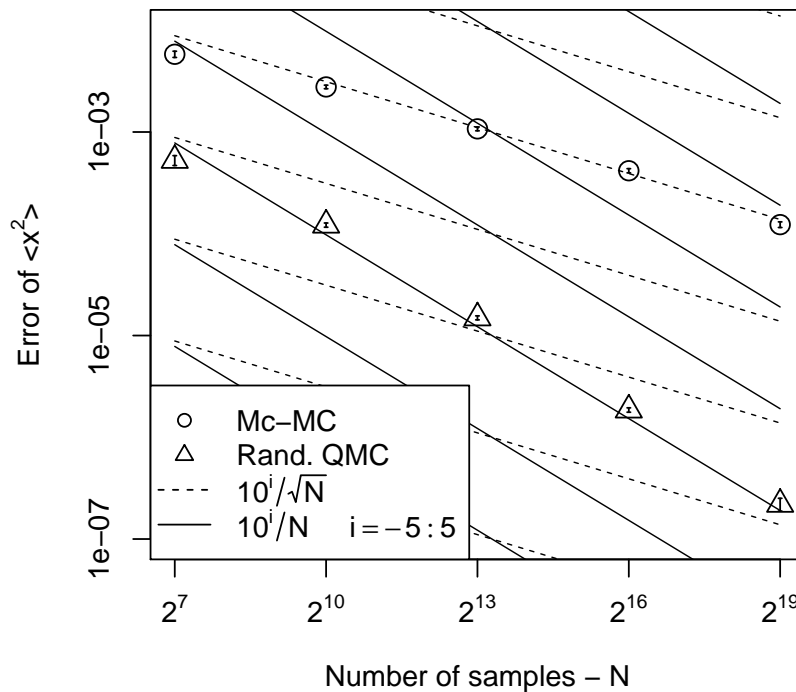
ground state energy:  $E_0 = 3\lambda \langle x^4 \rangle + \mu^2 \langle x^2 \rangle + \frac{\omega^4}{16}$

energy gap  $E_1 - E_0$

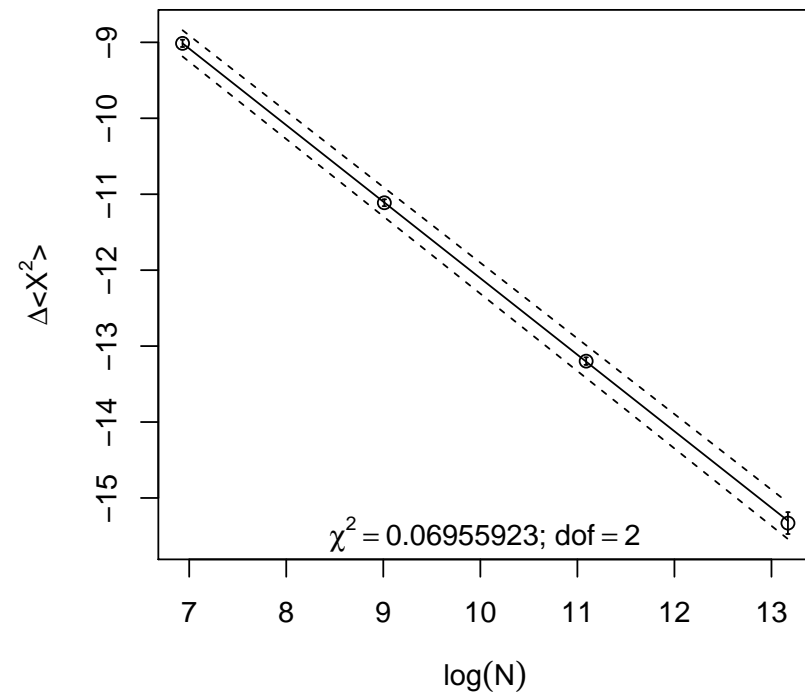
## Case of harmonic oscillator

parameters:  $\omega^2 = 2.0$  ,  $M_0 = 0.5$ ,  $a = 0.5$ ,  $d = 100$

Error of  $\langle x^2 \rangle$  for the Harmonic Oscillator



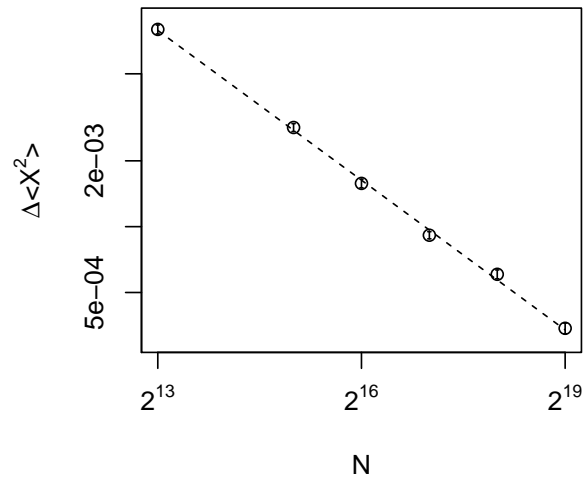
Fit QMC,  $\alpha = -1.007799 \pm 0.01490616$



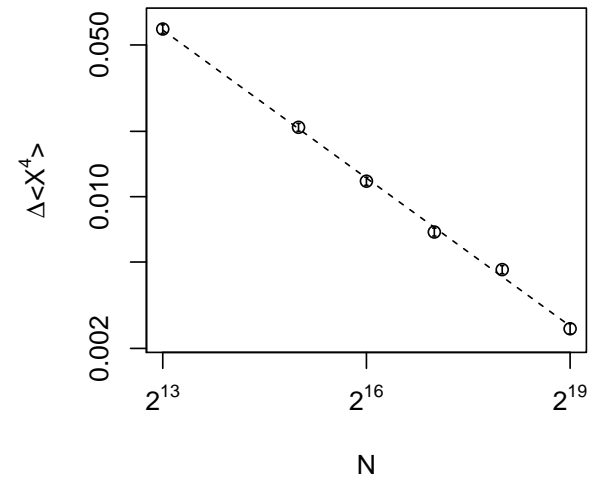
- fit  $\Delta \langle x^2 \rangle = c \cdot N^\alpha \rightarrow \alpha = -1.007799$
- perfect error scaling  $\rightarrow$  QMC at work
- trivial, but successful application to physical problem

## Case of anharmonic oscillator

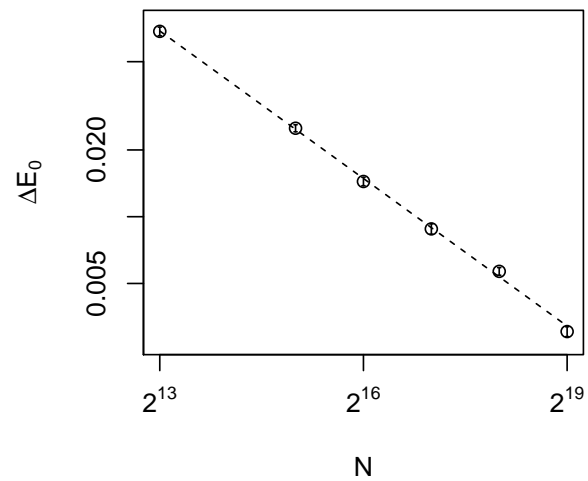
Error of  $\langle X^2 \rangle$ ,  $d = 1000$



Error of  $\langle X^4 \rangle$ ,  $d = 1000$



Error of  $E_0$ ,  $d = 1000$





## Case of anharmonic oscillator

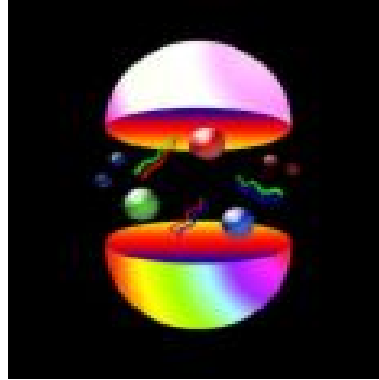
- parameters:  $M_0 = 0.5$  ,  $a = 0.015$  ,  $\omega^2 = -16$
- fit:  $\Delta O \sim c \cdot N^\alpha$

	$O$	$\alpha$	$\log C$	$\chi^2/\text{dof}$
$d = 100$	$X^2$	-0.763(8)	2.0(1)	7.9 / 6
	$X^4$	-0.758(8)	4.0(1)	13.2 / 6
	$E_0$	-0.737(9)	4.0(1)	8.3 / 6
$d = 1000$	$X^2$	-0.758(14)	2.0(2)	5.0 / 4
	$X^4$	-0.755(14)	4.0(2)	5.7 / 4
	$E_0$	-0.737(13)	4.0(2)	4.0 / 4

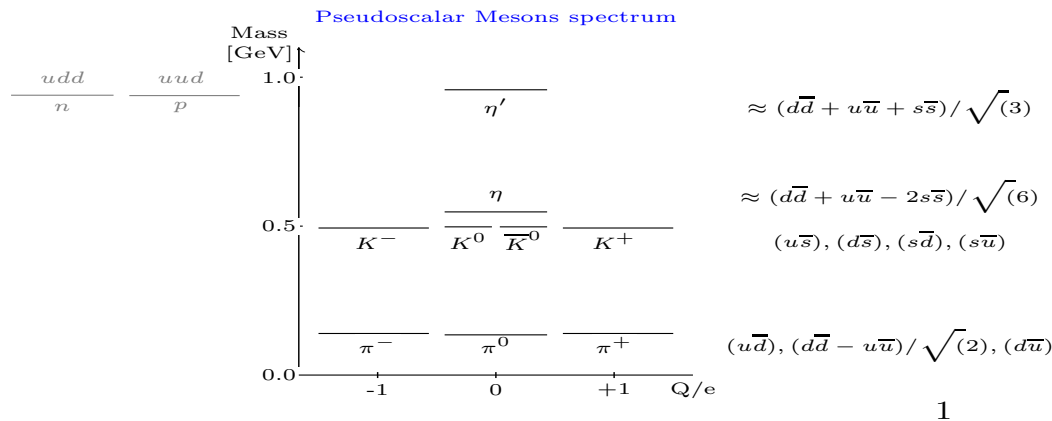
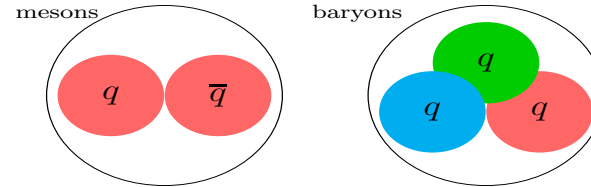
### Energy gap

- parameters:  $d = 100$ ,  $N = 2^5, 2^8, 2^{11}, 2^{14}$
- 400 Sobol' sequences each  $\rightarrow$  error estimate  $\rightarrow \alpha = -0.735(13)$

## The observable



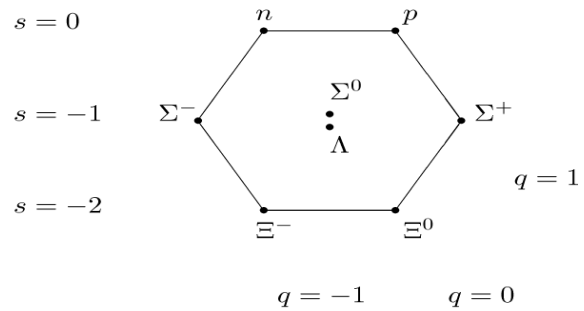
# What we learn from mesons and baryons



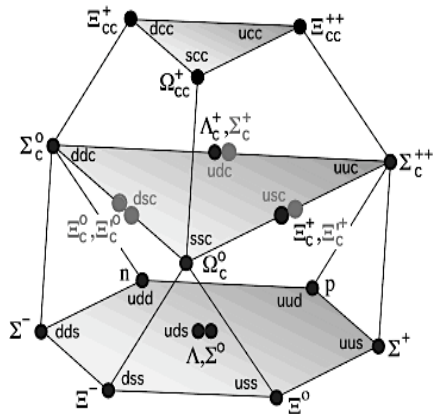
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- confinement of quarks
- spontaneous chiral symmetry breaking
- topological effects of gluon field configurations

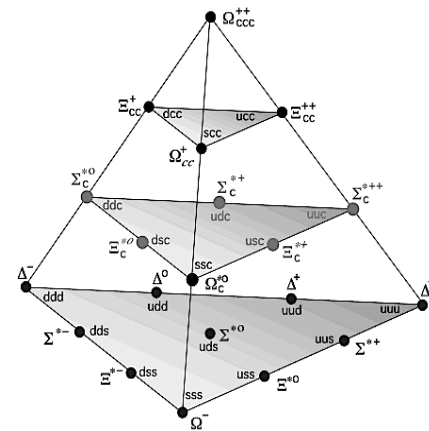
# The complicated baryon spectrum



Octet



Decuplett



32-plet

## QCD: the Mass Spectrum

goal: **non-perturbative computation of this rich bound state spectrum**

using QCD alone

→ euclidean correlation functions

Reconstruction theorem relates this to Minkowski space

operator  $O(\mathbf{x}, t)$  with quantum numbers of a given particle

correlation function decays exponentially:  $e^{-Et}$ ,  $E^2 = m^2 + \mathbf{p}^2$

⇒ mass obtained at zero momentum

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

correlation function

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

connected correlation function

$$\lim_{t \rightarrow \infty} [\langle O(0)O(t) \rangle - |\langle O(0) \rangle|^2] \propto e^{-E_1 t}$$

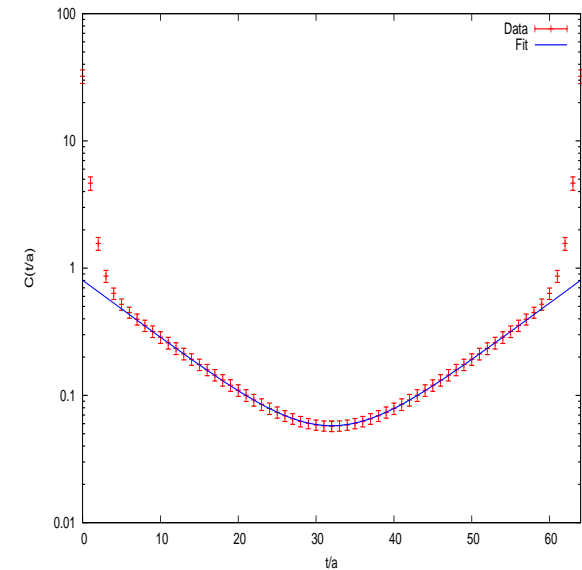
vanishing of connected correlation function at large times

→ cluster property  $\Rightarrow$  locality of the theory

periodic boundary conditions

$$\langle O(0)O(t) \rangle_c = \sum_n c_n [e^{-E_n t} + e^{-E_n(T-t)}]$$

$$1 \ll t \ll T : \langle O(0)O(t) \rangle_c \propto e^{-mt} + e^{-m(T-t)}$$



## Hadron Spectrum in QCD

hadrons are bound states in QCD

- **mesons** pion, kaon, eta, ...
- **baryons** neutron, proton, Delta, ..

for the computation of the hadon spectrum

- construct operators with the suitable quantum numbers
- compute the connected correlation function
- take the large time limit of the correlation function

## Lorentz symmetry, parity and charge conjugation

rotational symmetry  $\rightarrow$  hypercubic group: discrete rotations and reflections

classification of operators: irreducible representations  $R$

(note hypercubic group is a subgroup of  $SO(3)$ )

parity	charge conjugation
$\Psi(\mathbf{x}, t) \rightarrow \gamma_0 \Psi(-\mathbf{x}, t)$	$\Psi(\mathbf{x}, t) \rightarrow C \bar{\Psi}^T(\mathbf{x}, t)$
$\bar{\Psi}(\mathbf{x}, t) \rightarrow \bar{\Psi}(-\mathbf{x}, t) \gamma_0$	$\bar{\Psi}(\mathbf{x}, t) \rightarrow -\Psi^T(\mathbf{x}, t) C^{-1}$

$C$  charge conjugation matrix  $C = \gamma_0 \gamma_2$

$C$  satisfies

$$C \gamma_\mu C^{-1} = -\gamma_\mu^T = -\gamma_\mu^*$$



## The Proton

Nucleon: baryonic isospin-doublet,  $I = \frac{1}{2}$ :

proton (**uud**)  $I_3 = +\frac{1}{2}$  and neutron (**udd**)  $I_3 = -\frac{1}{2}$

local interpolating field of proton

$$P(x) = -\epsilon_{abc} [u_a^T(x) C \gamma_5 d_b(x)] u_c(x), \quad [ ] \text{ spin trace}$$

$u^C$  charged conjugate quark field

$$\psi^C(x) = C \bar{\psi}^T(x), \quad \bar{\psi}^C = -\psi^T(x) C^{-1}$$

leading to

$$\Gamma_P(t) = \sum_{\vec{x}} \langle 0 | P(x) \bar{P}(0) | 0 \rangle$$

## Exercise:

using the operator

$$P(x) = -\epsilon_{abc} [u_a^T(x) C \gamma_5 d_b(x)] u_c(x), \quad [ ] \text{ spin trace}$$

will we really get the proton?

→ check quantum numbers

## Contraction

- 2-point-function calculation

$$\mathcal{O}_\Gamma(x) = \bar{\psi}\Gamma\psi(0)$$

$$\langle \mathcal{O}_\Gamma(x)\mathcal{O}_\Gamma(0) \rangle =$$

$$\overbrace{\bar{\psi}(x)\Gamma\bar{\psi}(0)\psi(x)\Gamma\psi(0)} \quad (1)$$

$$= tr[\Gamma S(x, 0)\Gamma S(0, x)]$$

in terms of eigenvalues and eigenvectors:

$$tr[\Gamma S(x, 0)\Gamma S(0, x)] = \sum_{\lambda_i, \lambda_j} \frac{1}{\lambda_i \lambda_j} \sum_{\alpha\beta\gamma\delta} \left[ (\phi_j^{\dagger\alpha}(x)\Gamma_{\alpha\beta}\phi_i^\beta(x))(\phi_i^{\dagger\gamma}(0)\Gamma_{\gamma\delta}\phi_j^\delta(0)) \right]$$

Example: pion operator  $\rightarrow$  need pseudoscalar operator

$$O_{\text{PS}}(\mathbf{x}, t) = \bar{\Psi}(\mathbf{x}, t)\gamma_5\Psi(\mathbf{x}, t)$$

correlation function

$$\begin{aligned} f_{\text{PS}}(t) \equiv \langle O_{\text{PS}}(0)O_{\text{PS}}(t) \rangle &= \sum_{\mathbf{x}} [\bar{\psi}(\mathbf{x}, t)\gamma_5\Psi(\mathbf{x}, t)] [\bar{\psi}(0, 0)\gamma_5\Psi(0, 0)] \\ &= \sum_{\mathbf{x}} \text{Tr} [S_F(0, 0; \mathbf{x}, t)\gamma_5 S_F(\mathbf{x}, t; 0, 0)\gamma_5] \end{aligned}$$

used Wick's theorem and  $S_F = D^{-1}$  the fermion propagator

remark: formula simplifies using  $\gamma_5$  hermiticity of  $D_{\text{Wilson}}$

$\Rightarrow$  need to compute inverse of the fermion matrix

$$a \ll t \ll T : \quad f_{\text{PS}}(t) = \underbrace{\frac{|\langle 0|P|\text{PS}\rangle|^2}{2m_{\text{PS}}}}_{\equiv F_{\text{PS}}^2/2m_{\text{PS}}} \cdot (e^{-m_{\text{PS}}t} + e^{-m_{\text{PS}}(T-t)})$$

$F_{\text{PS}}$  pion decay constant

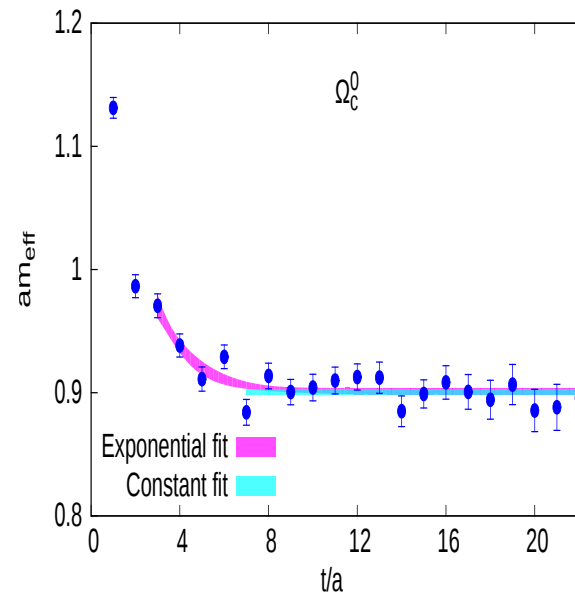
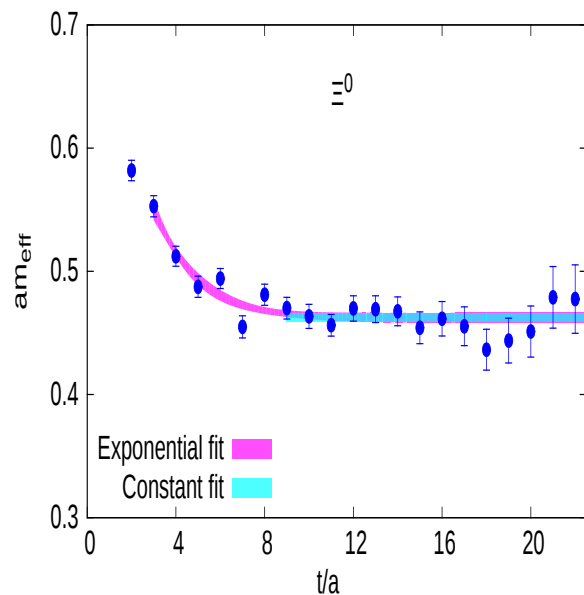
## Effective Masses and exponential fits

effective mass (neglecting boundary)

$$am_{\text{eff}}^X(t) = \log \left( \frac{C_X(t)}{C_X(t+1)} \right) = am_X + \log \left( \frac{1 + \sum_{i=1}^{\infty} c_i e^{-\Delta_i t}}{1 + \sum_{i=1}^{\infty} c_i e^{-\Delta_i (t+1)}} \right) \xrightarrow{t \rightarrow \infty} am_X$$

$\Delta_i = m_i - m_X$  mass difference of the excited state  $i$  to the ground mass  $m_X$

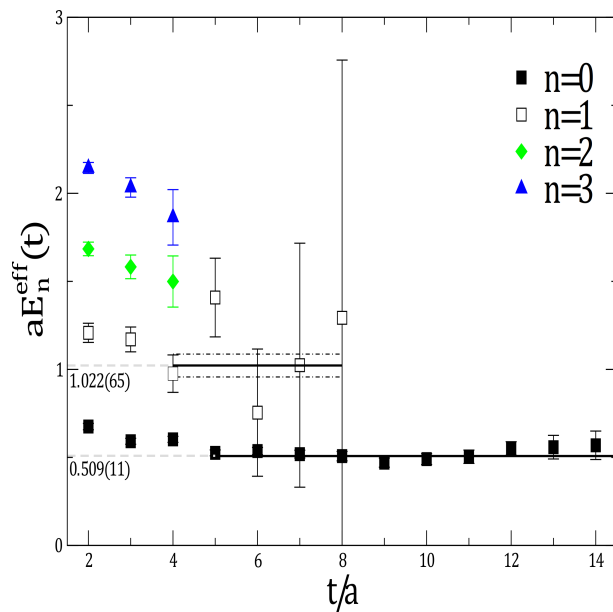
in practise:  $am_{\text{eff}}^X(t) \approx am_X + \log \left( \frac{1 + c_1 e^{-\Delta_1 t}}{1 + c_1 e^{-\Delta_1 (t+1)}} \right)$



## Identifying excited states

$$am_{\text{eff}}^X(t) = \log \left( \frac{C_X(t)}{C_X(t+1)} \right) = am_X + \log \left( \frac{1 + \sum_{i=1}^{\infty} c_i e^{-\Delta_i t}}{1 + \sum_{i=1}^{\infty} c_i e^{-\Delta_i (t+1)}} \right) \xrightarrow{t \rightarrow \infty} am_X$$

$\Delta_i = m_i - m_X$  mass difference of the excited state  $i$  to the ground mass  $m_X$



- large errors for excited states
- generalized eigenvalue approach
- need of large operator basis

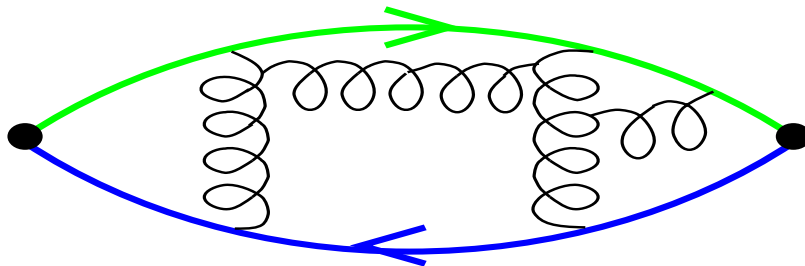
## Quenched approximation



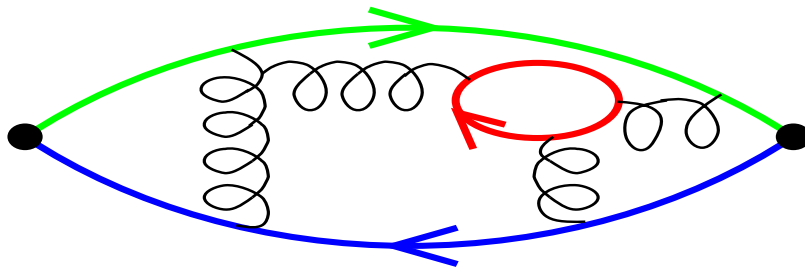
# The Quenched Approximation

→ neglect steady generation of quarks and antiquarks in physical quantum processes

⇒ *truncation*, works surprisingly well however



(A) Quenched QCD: no internal quark loops



(B) full QCD



# A short history of proton mass computation

(take example of Japanese group)

**1986** (Itoh, Iwasaki, Oyanagi and Yoshie)

quenched approximation,  $12^3 \cdot 24$  lattice

$a \approx 0.15\text{fm}$ , 30 configurations

Machine: HITAC S810/20  $\rightarrow$  630 Mflops

$\Rightarrow$  only meson masses, conclusion:

time extent of  $T = 24$  too small to extract baryon ground state

**1988** (plenary talk by Iwasaki at Lattice symposium at FermiLab)

quenched approximation,  $16^3 \cdot 48$  lattice

$a \approx 0.11\text{fm}$ , 15 configurations

particle	lattice	experiment
Kaon	470(45)	494
Nucleon	866(108)	938
$\Omega$	1697(89)	1672

## The story goes on ...

**1992** (Talk Yoshie at Lattice '92 in Amsterdam):

quenched approximation,  $24^3 \cdot 54$  lattice

two lattice spacings:  $a \approx 0.11\text{fm}$ ,  $a \approx 0.10\text{fm}$ ,  $O(200)$  configurations

Machine: QCDPAX 14 Gflops

⇒ worries about excited state effects

⇒ worries about finite size effects

**1995** (paper by QCDPAX collaboration)

		stat.	sys.(fit-range)		sys.(fit-func.)		
$\beta = 6.00$	$m_N = 1.076$	$\pm 0.060$	+0.047	-0.020	+0.0	-0.017	GeV
$\beta = 6.00$	$m_\Delta = 1.407$	$\pm 0.086$	+0.096	-0.026	+0.038	-0.015	GeV

*“Even when the systematic errors are included, the baryon masses at  $\beta = 6.0$  do not agree with experiment. Our data are consistent with the GF11<sup>1</sup> data at finite lattice spacing, within statistical errors. In order to take the continuum limit of our results, we need data for a wider range of  $\beta$  with statistical and systematic errors much reduced.”*

---

<sup>1</sup>GF11 has been a 5.6Gflops machine developed by IBM research.

## where the quenched story ends

**2003** (Paper by CP-PACS collaboration):

quenched approximation from  $32^3 \cdot 56$  to  $64^3 \cdot 112$  lattice

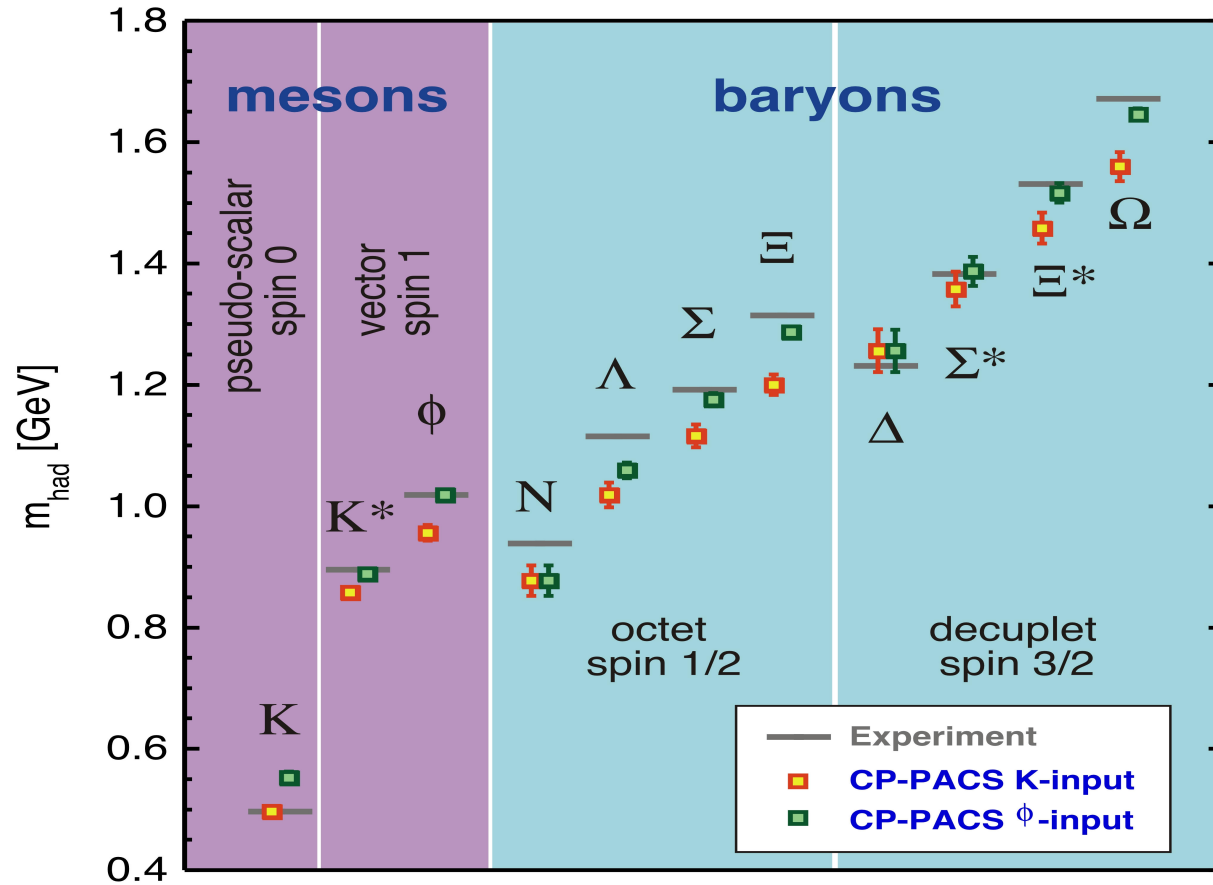
two lattice spacings:  $a \approx 0.05\text{fm}$  –  $a \approx 0.10\text{fm}$ ,  $O(150)$  –  $O(800)$  configurations

Machine: CP-PACS, massively parallel, 2048 processing nodes,  
completed september 1996

→ reached 614Gflops

- control of systematic errors
  - finite size effects
  - lattice spacing
  - chiral extrapolation
  - excited states





quenched

quenched

CP-PACS collaboration

Solution of QCD?

→ a number of systematic errors

## Another example: glueballs

*prediction* of QCD: the existence of states made out of gluons alone, **the glueballs**

- hard to detect experimentally
- difficult to compute, of purely non-perturbative nature

⇒ challenge for lattice QCD

transformation laws for gauge links

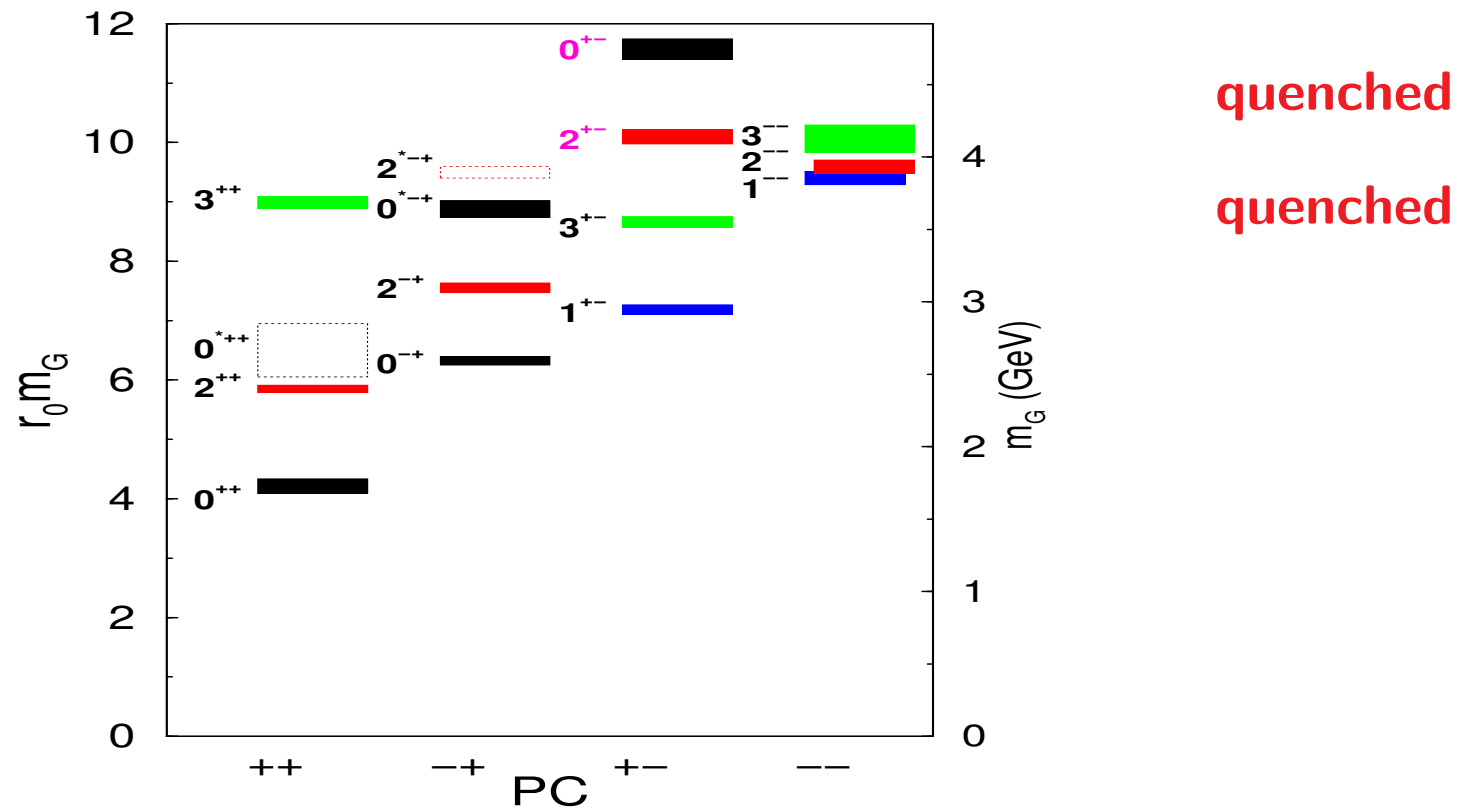
parity	charge conjugation
$U(\mathbf{x}, t, 4) \rightarrow U(-\mathbf{x}, t, 4)$	$U(\mathbf{x}, t, 4) \rightarrow U^*(\mathbf{x}, t, 4)$
$U(\mathbf{x}, t, i) \rightarrow U(-\mathbf{x}, t, -i)$	$U(\mathbf{x}, t, i) \rightarrow U^*(\mathbf{x}, t, i)$

example: combination of  $1 \times 1$  Wilson loops  $W(C)_{xy}$

$$O(\mathbf{x}, t) = W_{(\mathbf{x}, t), 12} + W_{(\mathbf{x}, t), 13} + W_{(\mathbf{x}, t), 23}$$

invariant under hypercubic group, parity and charge conjugation  $\rightarrow 0^{++}$

glueball spectrum  $\rightarrow$  unique prediction from lattice QCD



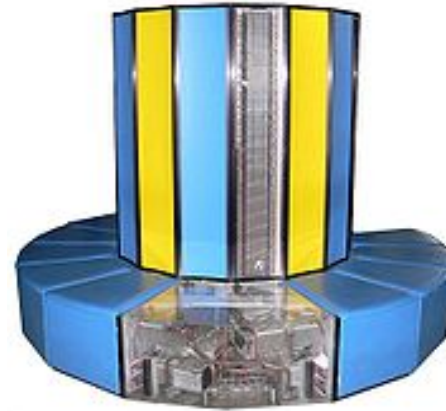
# start of dynamical (mass-degenerate up and down) quark simulations

**1998** (Paper by UKQCD collaboration):

lattices: from  $8^3 \cdot 24$  to  $16^3 \cdot 24$

$a \approx 0.10\text{fm}$ ,  $m_\pi/m_\rho > 0.7$

Machine: CRAY T3E  $\approx 1\text{Tflop}$



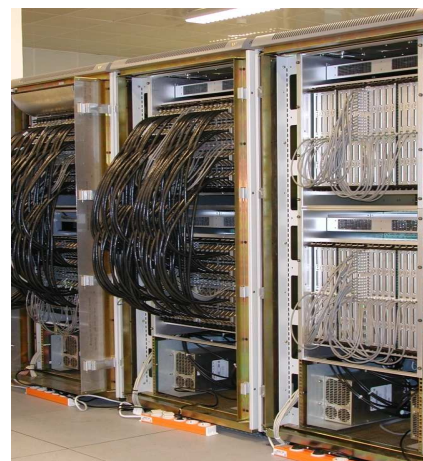
**1999** (Paper by SESAM collaboration):

lattice:  $16^3 \cdot 32$  lattice

$a \approx 0.10\text{fm}$ ,  $m_\pi/m_\rho > 0.7$

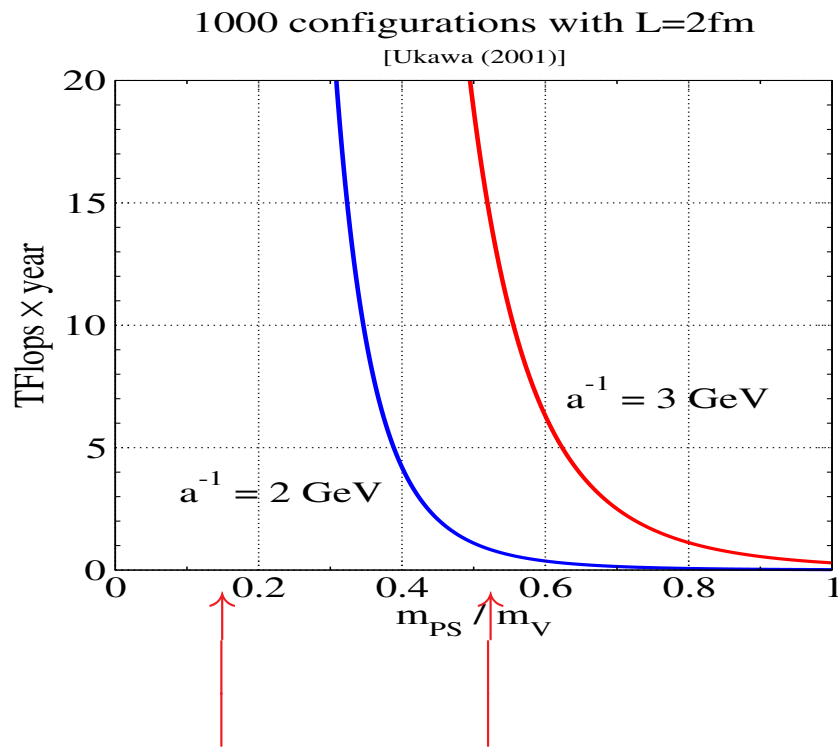
Machine: APE100  $\approx 100\text{Gflop}$

- period of algorithm development
  - improved higher order integrators
  - multiboson algorithm
  - PHMC algorithm



# Costs of dynamical fermions simulations, the “Berlin Wall”

see panel discussion in Lattice2001, Berlin, 2001



physical  
point

contact to  
 $\chi\text{PT}$  (?)

$$\text{formula } C \propto \left( \frac{m_\pi}{m_\rho} \right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$$

$$z_\pi = 6, \quad z_L = 5, \quad z_a = 7$$

*“both a  $10^8$  increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place.”*

(Wilson, 1989)

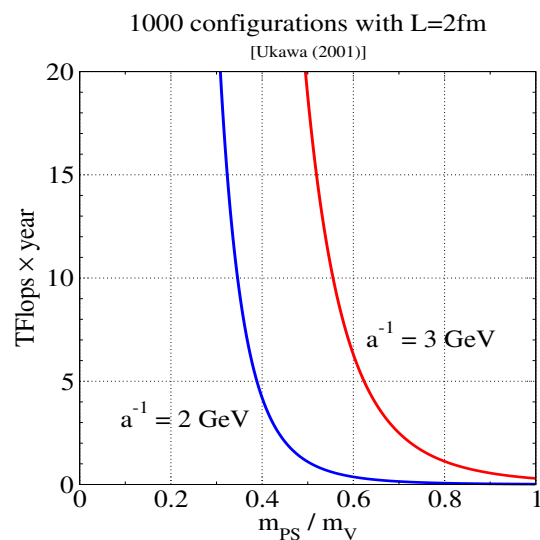
$\Rightarrow$  need of **Exaflops Computers**



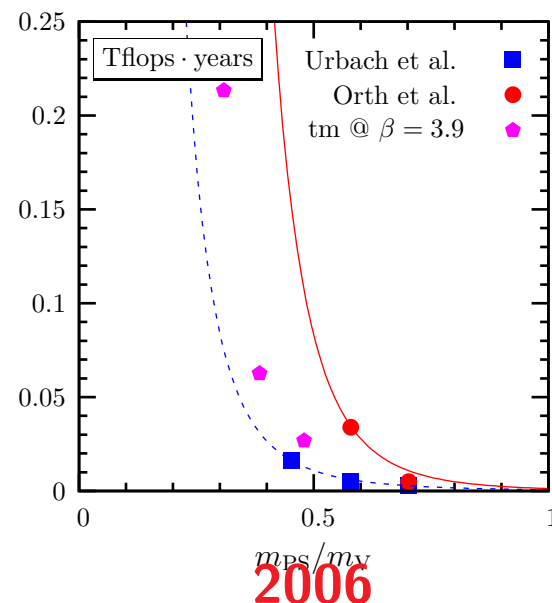
## A generic improvement for Wilson type fermions

New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)  
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps



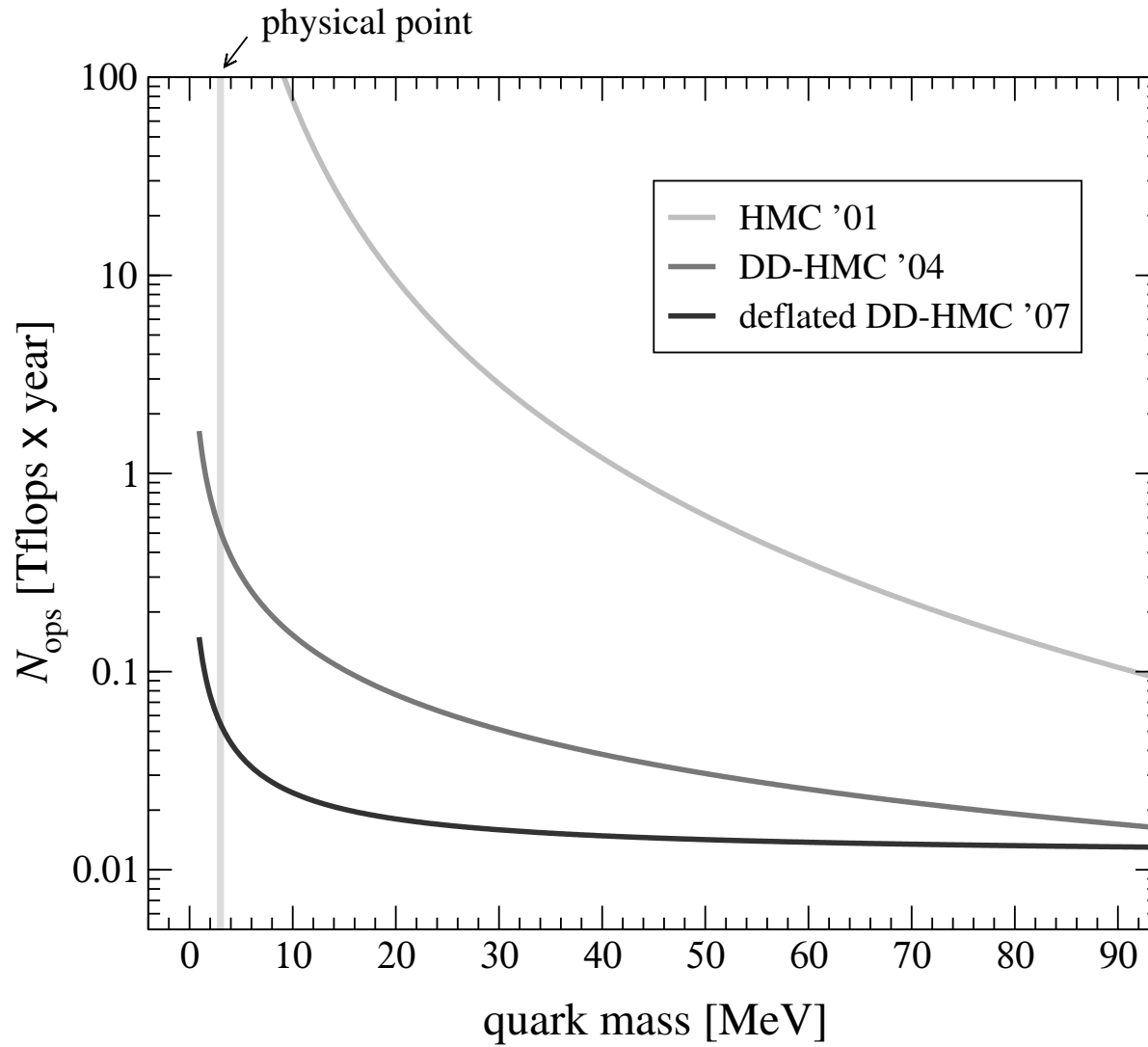
2001



2006

- comparable to staggered
- reach small pseudo scalar masses  $\approx 300\text{MeV}$

# Recent picture



## Supercomputer

ca. 1700, Leibniz Rechenmaschine

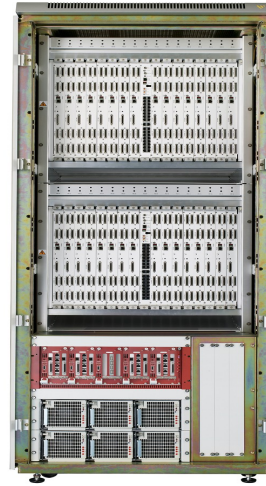


*Denn es ist eines ausgezeichneten Mannes nicht würdig, wertvolle Stunden wie ein Sklave im Keller der einfachen Rechnungen zu verbringen. Diese Aufgaben könnten ohne Besorgnis abgegeben werden, wenn wir Maschinen hätten.*

*Because it is unworthy for an excellent man to spent valuable hours as a slave in the cellar of simple calculations. These tasks can be given away without any worry, if we would have machines.*

## German Supercomputer Infrastructure

- apeNEXT in Zeuthen **3 Teraflops**  
and Bielefeld **5 Teraflops**  
→ dedicated to LGT



- NIC 72 racks of BG/P System  
at FZ-Jülich **1 Petaflops**

- 2208 Nehalem processor  
Cluster computer:  
**208 Teraflops**



- Altix System at LRZ Munic
- SGI Altix ICE 8200 at HLRN (Berlin, Hannover)  
**31 Teraflops**  
→ will be upgraded to a **3 Petaflops system**



# State of the art

- BG/Q

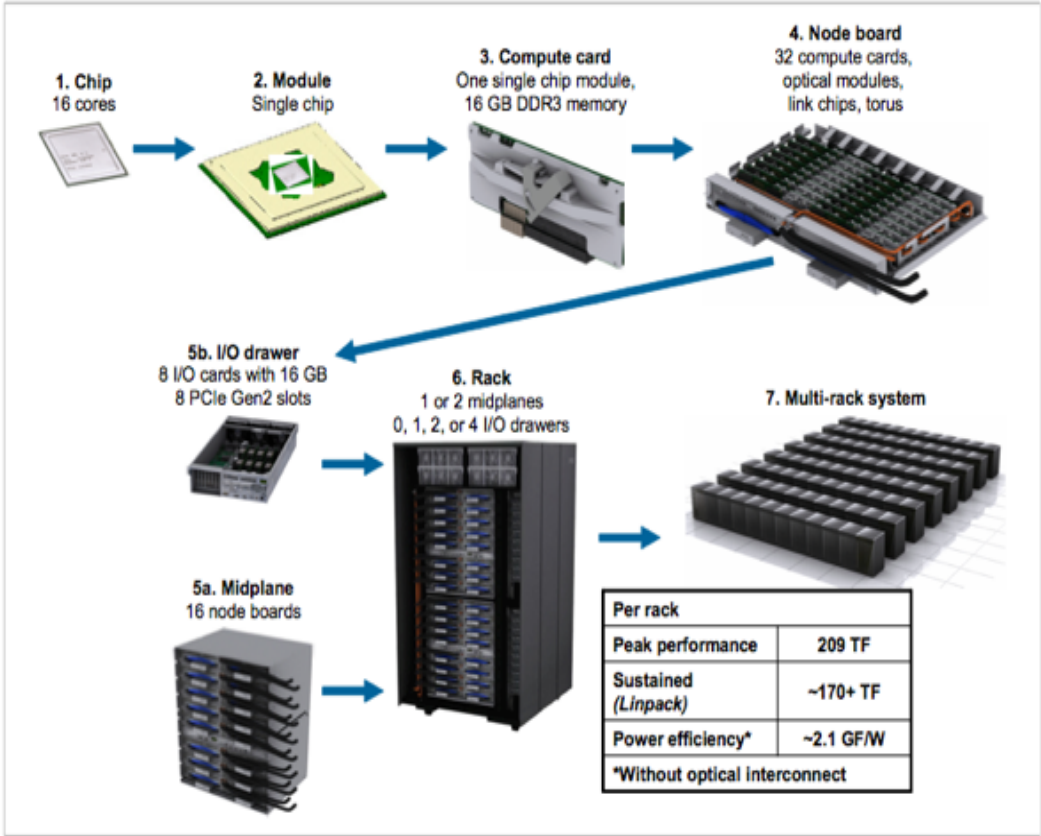
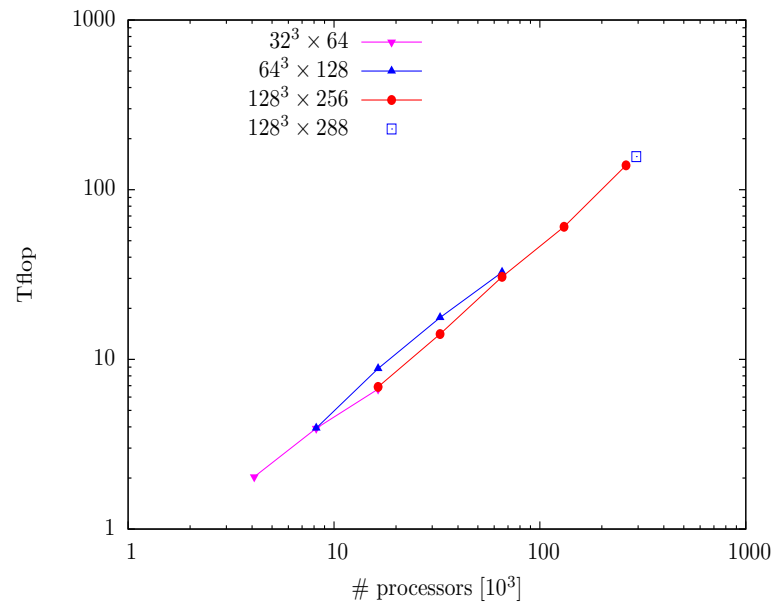


Figure 1-2 Blue Gene/Q hardware overview

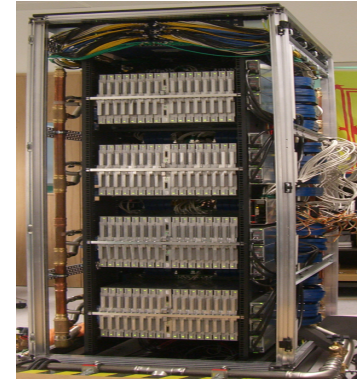
## Strong Scaling

- Test on 72 racks BG/P installation at supercomputer center Jülich (Gerhold, Herdioza, Urbach, K.J.)
- using tmHMC code (Urbach, K.J.)



## Low budget machines

- QPACE 4+4 Racks in Jülich und Wuppertal  
1900 PowerXCell 8i nodes **190 TFlops (peak)**  
based on cell processor  
3-d torus network  
low power consumption **1.5W/Gflop**



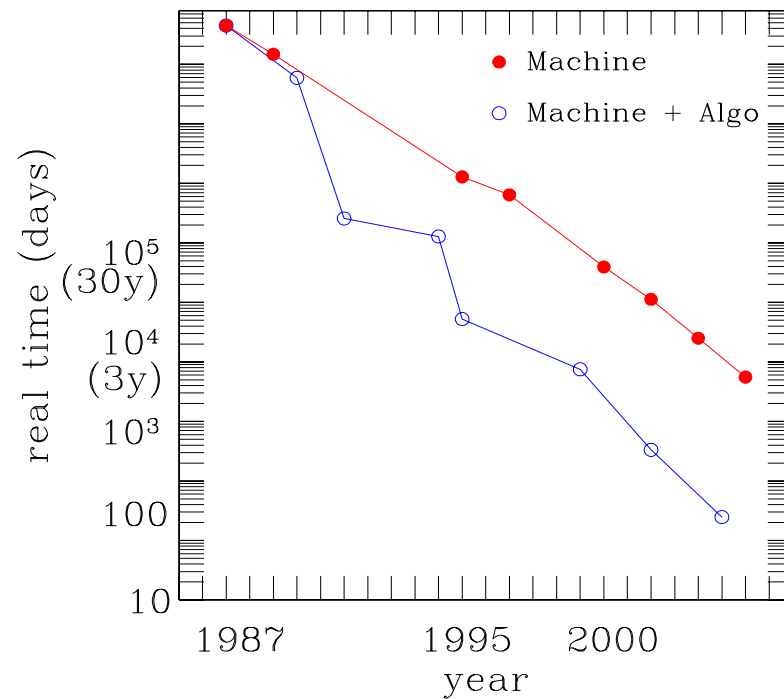
- **Videocards (NVIDIA Tesla)**  
**CUDA** programming language (**C extension**)
- Judge GPU cluster at research center Jülich with 206 nodes



- GPU: 2 NVIDIA Tesla M2050 (Fermi) 1.15 GHz (448 cores)
- GPU: 2 NVIDIA Tesla M2070 (Fermi) 1.15 GHz (448 cores)
- 240 Tflops peak performance
- trend: hybrid architectures with accelerators
- challenge for 2020: **Exaflop Computing**

## Computer and algorithm development over the years

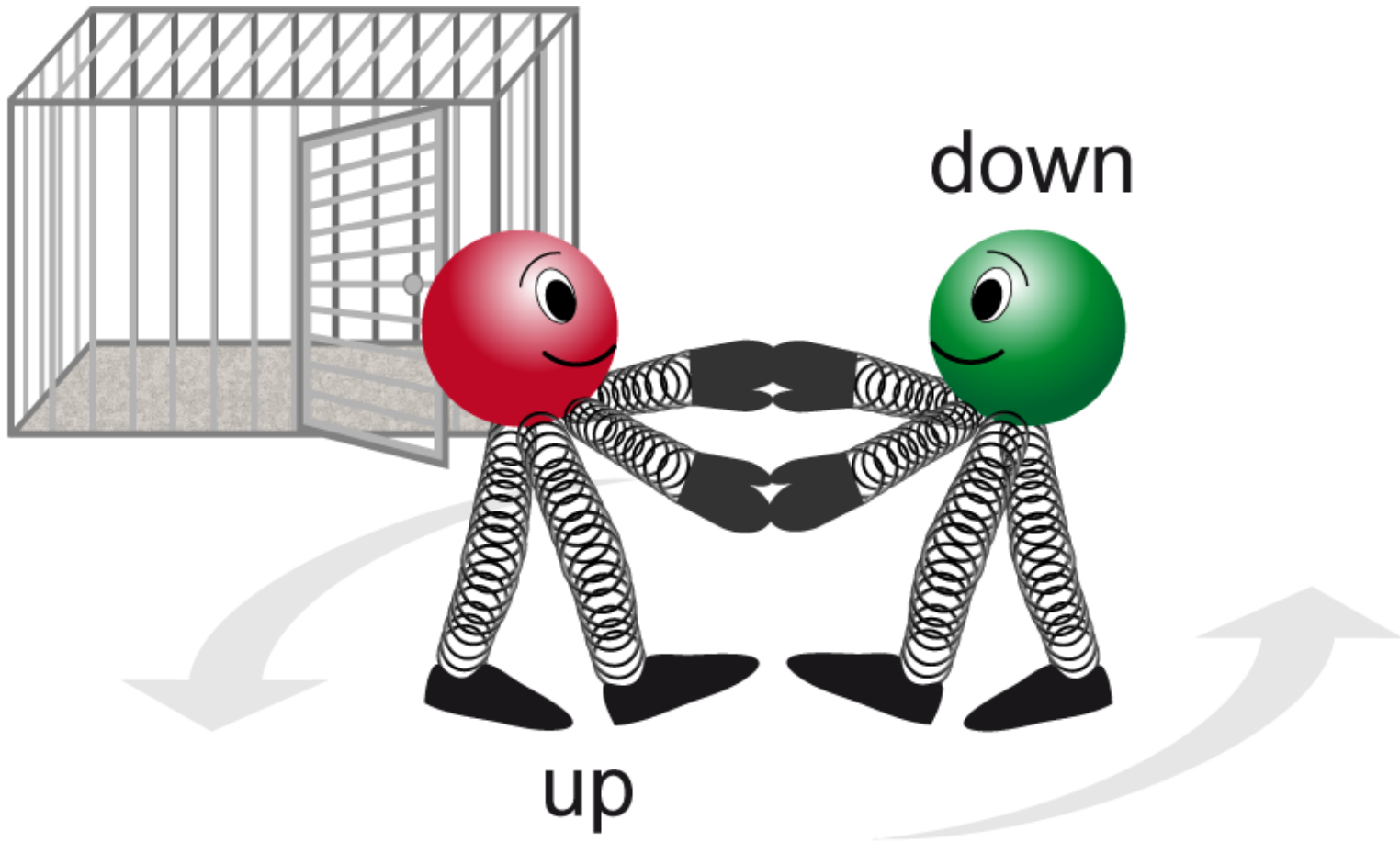
time estimates for simulating  $32^3 \cdot 64$  lattice, 5000 configurations



→ O(few months) nowadays with a typical collaboration supercomputer contingent



$N_f = 2$  dynamical flavours



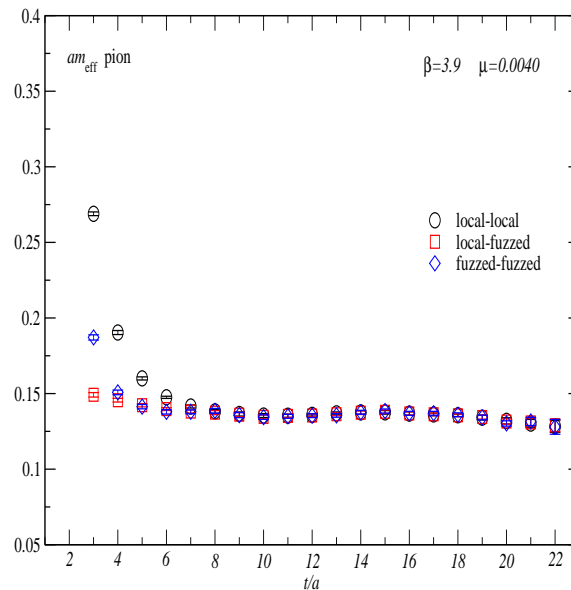
## Examples of present Collaborations (using Wilson fermions)

- CLS collaboration  
Wilson gauge and clover improved Wilson fermions
- ALPHA  
Wilson gauge and clover improved Wilson fermions  
Schrödinger functional
- QCDSF  
tadpole improved Symanzik gauge and clover improved Wilson fermions
- ETMC  
tree-level Symanzik improved gauge and  
maximally twisted mass Wilson fermions
- RBC  
domain wall fermions
- BMW  
improved gauge and  
non-perturbatively improved, 6 stout smeared Wilson fermions



## Extraction of Masses

- Quark propagator: stochastic, fuzzed sources
- Change the location of the time-slice source: reduce autocorrelations



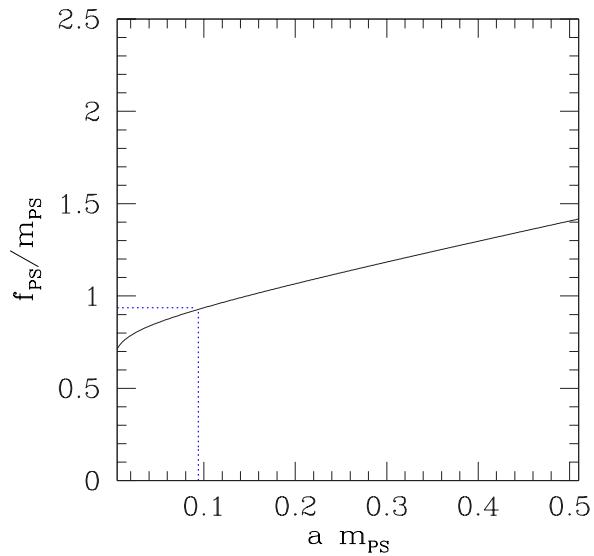
- effective mass of  $\pi^{\pm}$
- isolate ground state : small statistical errors

⇒ get a number, but what does it mean? How to get physical units?

## Setting the scale

$$m_{\text{PS}}^{\text{latt}} = a m_{\text{PS}}^{\text{phys}} \quad , \quad f_{\text{PS}}^{\text{latt}} = a f_{\text{PS}}^{\text{phys}}$$

$$\frac{f_{\text{PS}}^{\text{phys}}}{m_{\text{PS}}^{\text{phys}}} = \frac{f_{\text{PS}}^{\text{latt}}}{m_{\text{PS}}^{\text{latt}}} + \mathcal{O}(a^2)$$



→ setting  $\frac{f_{\text{PS}}^{\text{latt}}}{m_{\text{PS}}^{\text{latt}}} = 130.7/139.6$

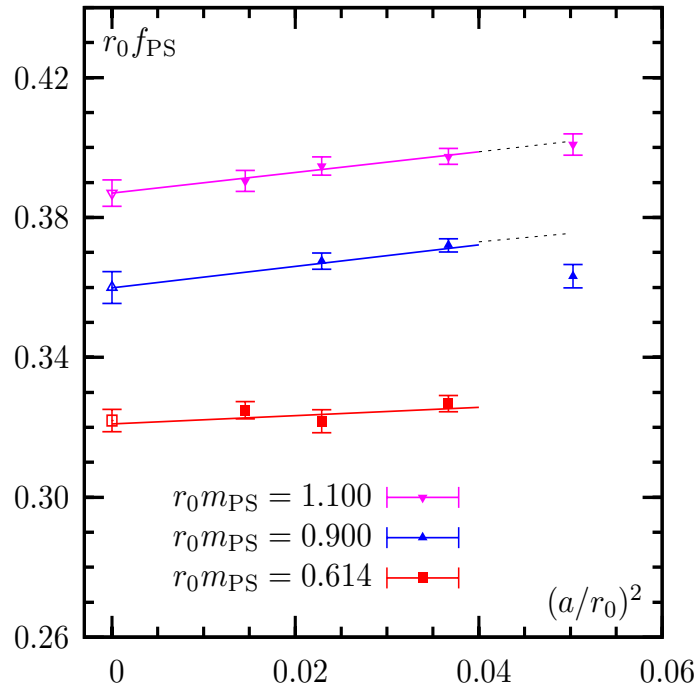
→ obtain  $m_{\text{PS}}^{\text{latt}} = a 139.6 [\text{Mev}]$

→ value for lattice spacing  $a$

available configurations (free on ILDG)

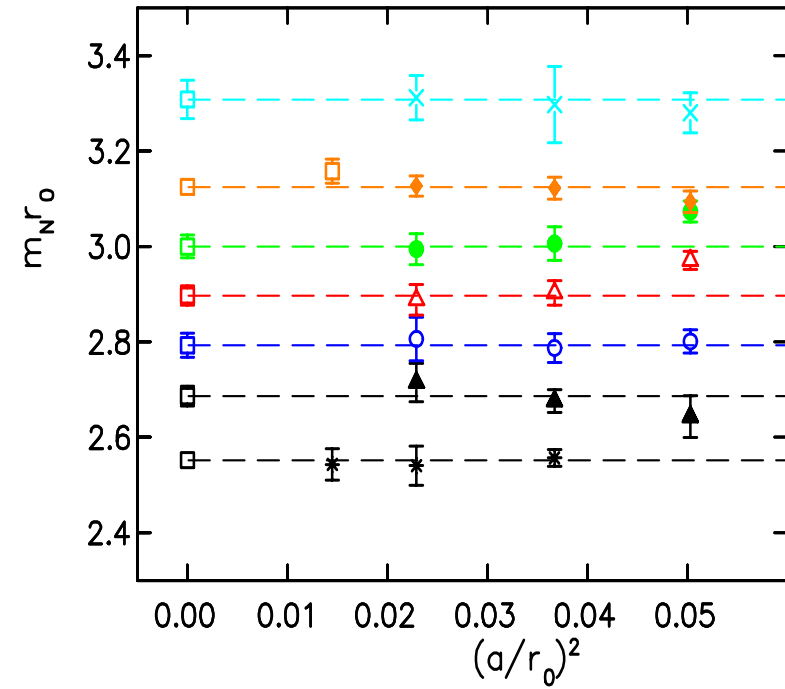
$\beta$	$a$ [fm]	$L^3 \cdot T$	$L$ [fm]	$a\mu$	$N_{\text{traj}} (\tau = 0.5)$	$m_{\text{PS}}$ [MeV]
4.20	$\sim 0.050$	$48^3 \cdot 96$	2.4	0.0020	5200	$\sim 300$
		$32^3 \cdot 64$	2.1	0.0060	5600	$\sim 420$
4.05	$\sim 0.066$	$32^3 \cdot 64$	2.2	0.0030	5200	$\sim 300$
				0.0060	5600	$\sim 420$
				0.0080	5300	$\sim 480$
				0.0120	5000	$\sim 600$
3.9	$\sim 0.086$	$32^3 \cdot 64$	2.8	0.0030	4500	$\sim 270$
				0.0040	5000	$\sim 300$
		$24^3 \cdot 48$	2.1	0.0064	5600	$\sim 380$
				0.0085	5000	$\sim 440$
				0.0100	5000	$\sim 480$
				0.0150	5400	$\sim 590$
3.8	$\sim 0.100$	$24^3 \cdot 48$	2.4	0.0060	$4700 \times 2$	$\sim 360$
				0.0080	$3000 \times 2$	$\sim 410$
				0.0110	$2800 \times 2$	$\sim 480$
				0.0165	$2600 \times 2$	$\sim 580$

## Continuum limit scaling



$f_{\text{PS}}$

observe small  $O(a^2)$  effects



$M_N$

## Chiral perturbation theory

$$r_0 f_{\text{PS}} = r_0 f_0 \left[ 1 - 2\xi \log \left( \frac{\chi_\mu}{\Lambda_4^2} \right) + \dots \right]$$

$$(r_0 m_{\text{PS}})^2 = \chi_\mu r_0^2 \left[ 1 + \xi \log \left( \frac{\chi_\mu}{\Lambda_3^2} \right) + \dots \right]$$

where

$$\xi \equiv 2B_0 \mu_q / (4\pi f_0)^2, \quad \chi_\mu \equiv 2B_0 \mu_R, \quad \mu_R \equiv \mu_q / Z_P$$

## Chiral perturbation theory

→ add finite volume and lattice spacing dependence:

$$r_0 f_{\text{PS}} = r_0 f_0 \left[ 1 - 2\xi \log \left( \frac{\chi_\mu}{\Lambda_4^2} \right) + D_{f_{\text{PS}}} a^2 / r_0^2 + T_f^{\text{NNLO}} \right] K_f^{\text{CDH}}(L)$$

$$(r_0 m_{\text{PS}})^2 = \chi_\mu r_0^2 \left[ 1 + \xi \log \left( \frac{\chi_\mu}{\Lambda_3^2} \right) + D_{m_{\text{PS}}} a^2 / r_0^2 + T_m^{\text{NNLO}} \right] K_m^{\text{CDH}}(L)^2$$

$$r_0/a(a\mu_q) = r_0/a + D_{r_0}(a\mu_q)^2$$

where

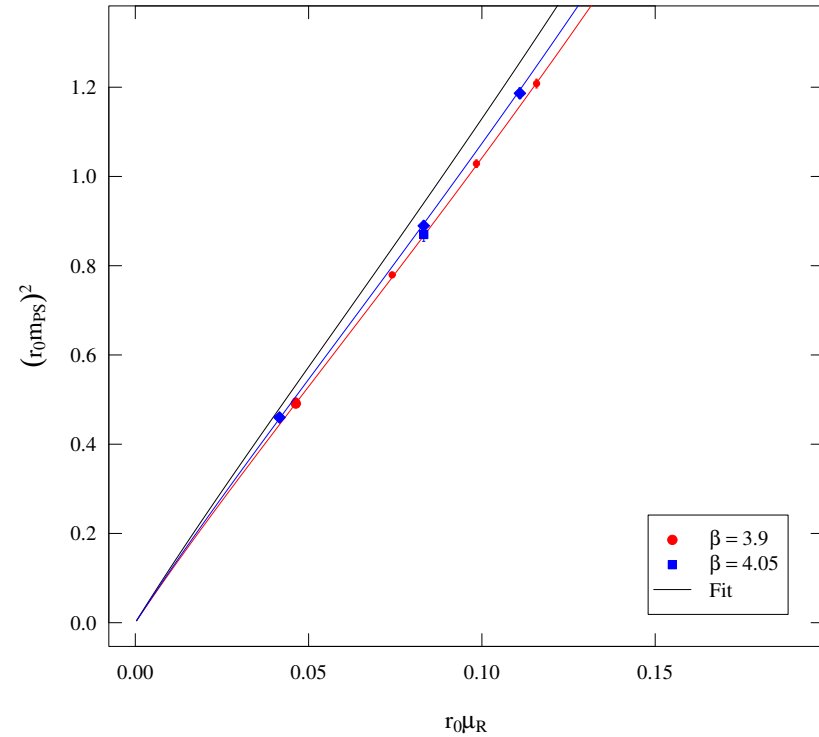
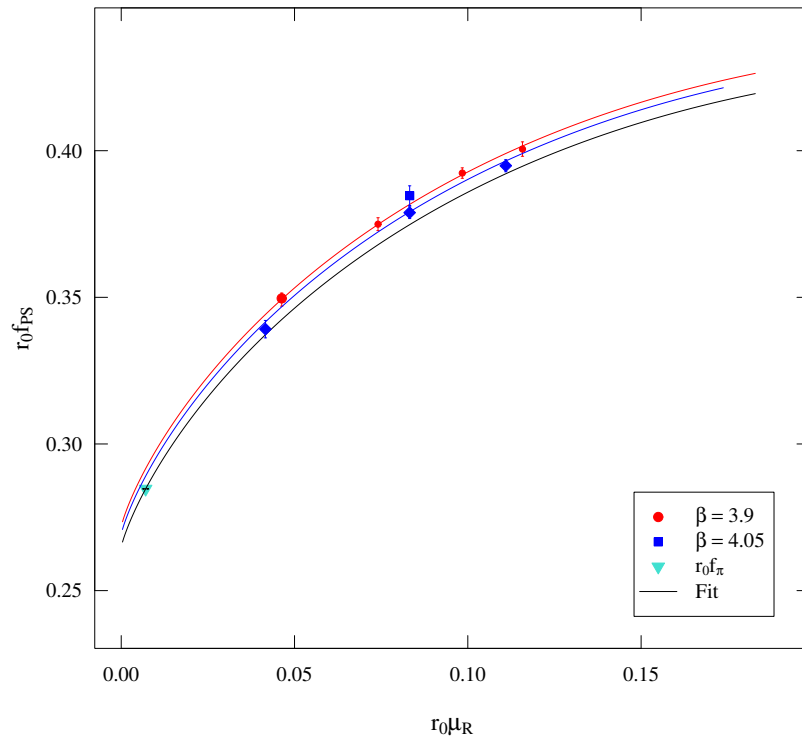
$$\xi \equiv 2B_0\mu_q/(4\pi f_0)^2, \quad \chi_\mu \equiv 2B_0\mu_R, \quad \mu_R \equiv \mu_q/Z_P$$

- $D_{f,m}$  parametrize lattice artefacts
- $K_{f,m}^{\text{CDH}}(L)$  Finite size corrections Colangelo *et al.*, 2005
- $T_{f,m}^{\text{NNLO}}$  NNLO correction



## Chiral perturbation theory

- Fit B: NLO continuum  $\chi^{\text{PT}}$ ,  $T_{m,f}^{\text{NNLO}} \equiv 0$ ,  $D_{m_{\text{PS}}, f_{\text{PS}}}$  fitted



two values of the lattice spacing  $\rightarrow D_m = -1.07(97)$ ,  $D_f = 0.71(57)$

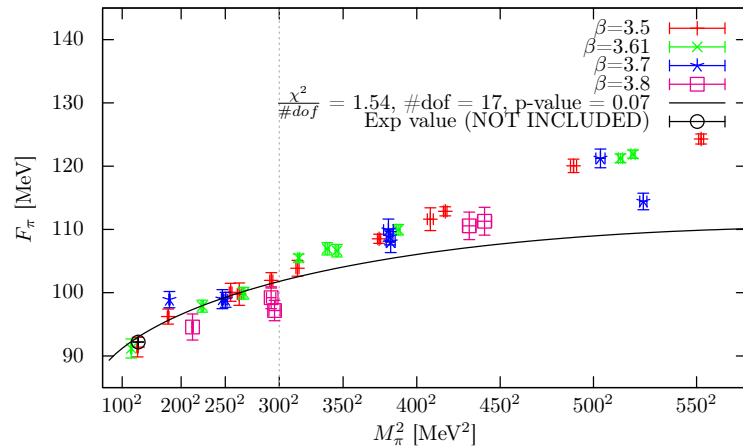
## Chiral perturbation theory: results

quantity	value
$m_{u,d}$ [MeV]	3.37(23)
$\bar{\ell}_3$	3.49(19)
$\bar{\ell}_4$	4.57(15)
$f_0$ [MeV]	121.75(46)
$B_0$ [GeV]	2774(190)
$r_0$ [fm]	0.433(14)
$\langle r^2 \rangle_s$	0.729(35)
$\Sigma^{1/3}$ [MeV]	273.9(6.0)
$f_\pi/f_0$	1.0734(40)

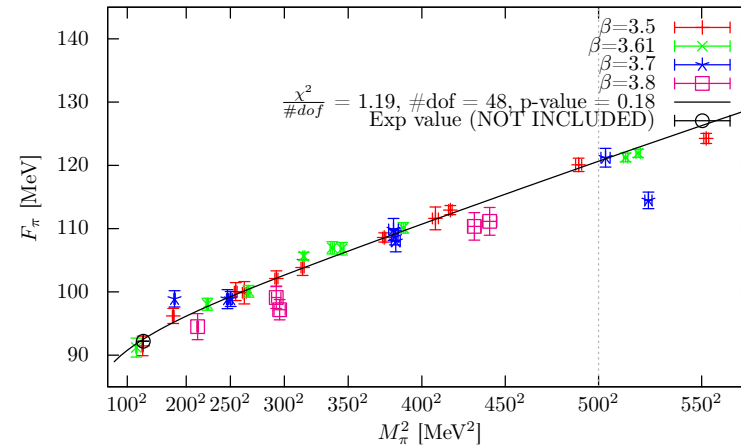
- averaged over many fit results, weighted with confidence levels
- $B_0, \Sigma, m_{u,d}$  renormalised in  $\overline{\text{MS}}$  scheme at scale  $\mu = 2 \text{ GeV}$
- LECs can be used to compute further quantities: scattering lengths

# A more rigorous approach to chiral perturbation theory

**BMW collaboration** → pion masses down to 120MeV



NLO, fit for  $M_\pi < 300\text{MeV}$



NNLO, fit for  $M_\pi < 500\text{MeV}$

- NLO: only applicable for  $M_\pi \leq 300\text{MeV}$
- NNLO: wider applicability  $M_\pi \lesssim 300\text{MeV}$  but need very precise data for stable fit

⇒ better work directly at physical point

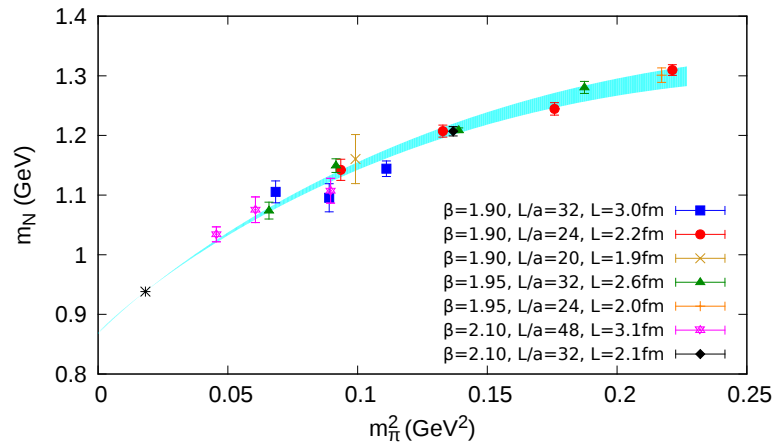
## What about chiral extrapolations for the nucleon mass?

simplest,  $O(p^3)$  formula  $m_N = m_N^{(0)} - 4c_1 m_\pi^2 - \frac{3g_A^2}{32\pi f_\pi^2} m_\pi^3$

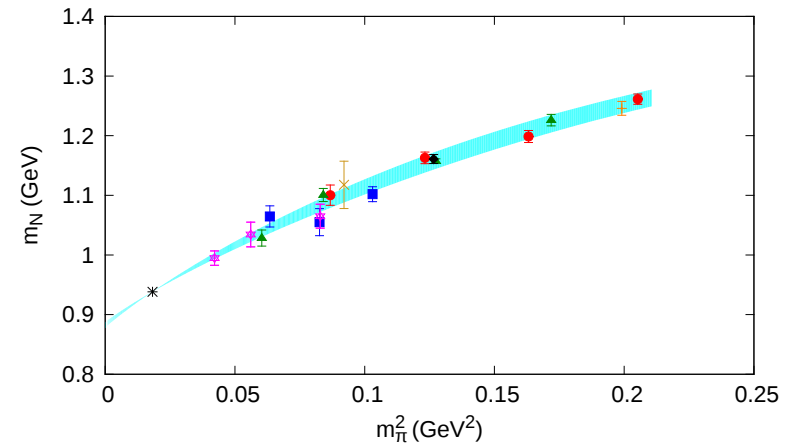
next order,  $O(p^4)$

$$m_N = m_N^0 - 4c_1 m_\pi^2 - \frac{3g_A^2}{32\pi f_\pi^2} m_\pi^3 - 4E_1(\lambda) m_\pi^4 - \frac{3(g_A^2 + 3c_A^2)}{64\pi^2 f_\pi^2 m_N^0} m_\pi^4 - \frac{(3g_A^2 + 10c_A^2)}{32\pi^2 f_\pi^2 m_N^0} m_\pi^4 \log$$

$$- \frac{c_A^2}{3\pi^2 f_\pi^2} \left(1 + \frac{\Delta}{2m_N^0}\right) \left[\frac{\Delta}{4} m_\pi^2 + \left(\Delta^3 - \frac{3}{2} m_\pi^2 \Delta\right) \log\left(\frac{m_\pi}{2\Delta}\right) + (\Delta^2 - m_\pi^2) R(m_\pi)\right]$$



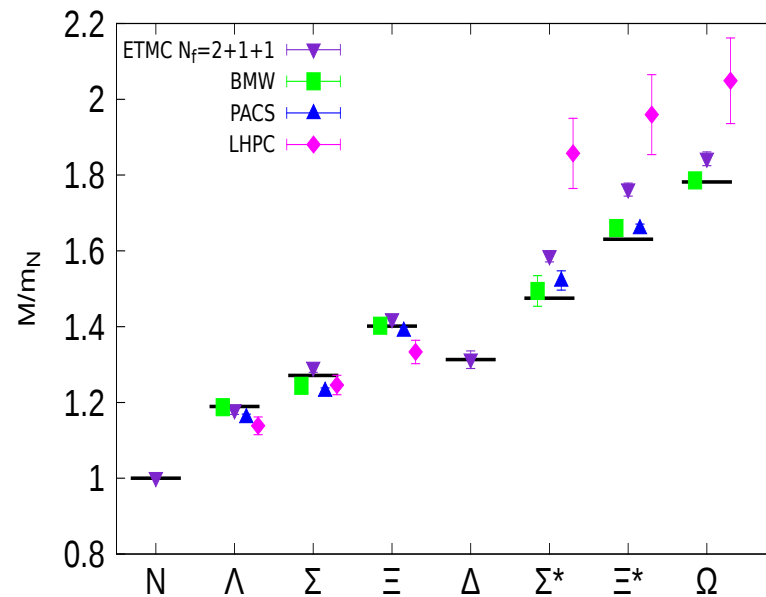
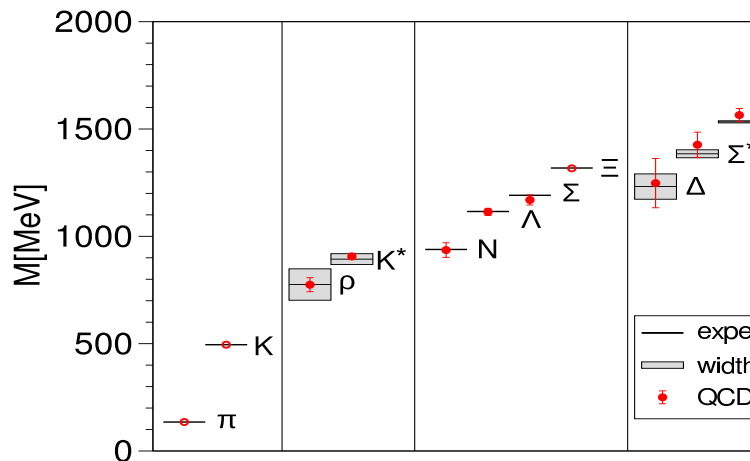
$O(p^3)$  fit



$O(p^4)$  fit

# The lattice QCD benchmark calculation: the spectrum

spectrum for  $N_f = 2 + 1$  and  $2 + 1 + 1$  flavours



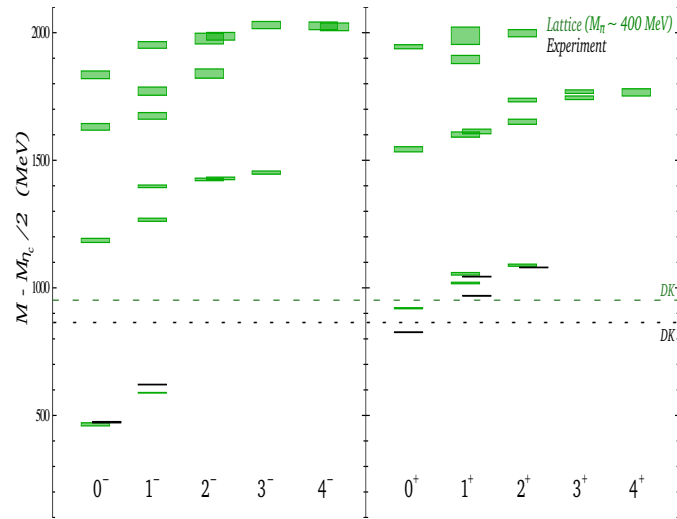
first spectrum calculation **BMW**

repeated by other collaborations

(ETMC: C. Alexandrou, M. Constantinou, V. Drach, G. Koutsou, K.J.)

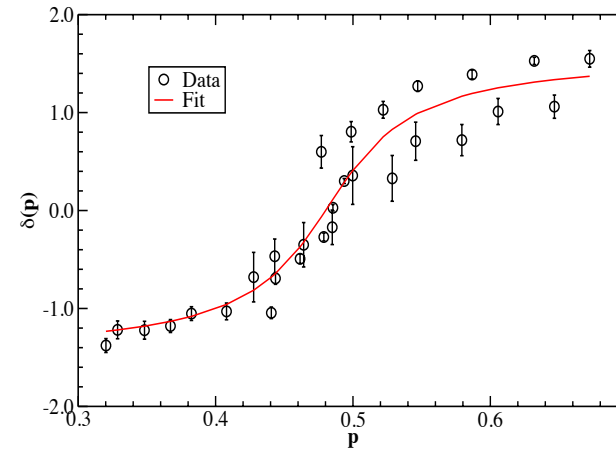
- spectrum for  $N_f = 2$ ,  $N_f = 2 + 1$  and  $N_f = 2 + 1 + 1$  flavours  
 → no flavour effects for light baryon spectrum

## We can go further



### charmed spectrum

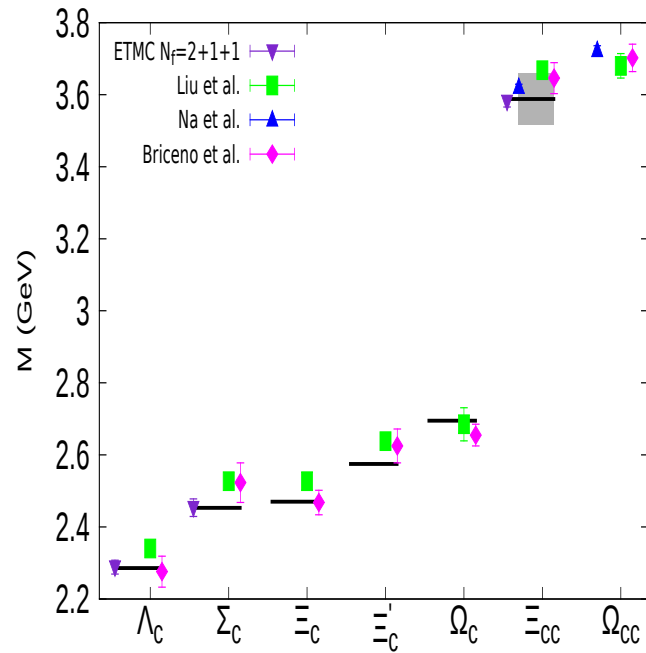
(G. Moir, M. Peardon, S. Ryan  
C. Thomas, L. Liu)



### Phase shifts (model calculation)

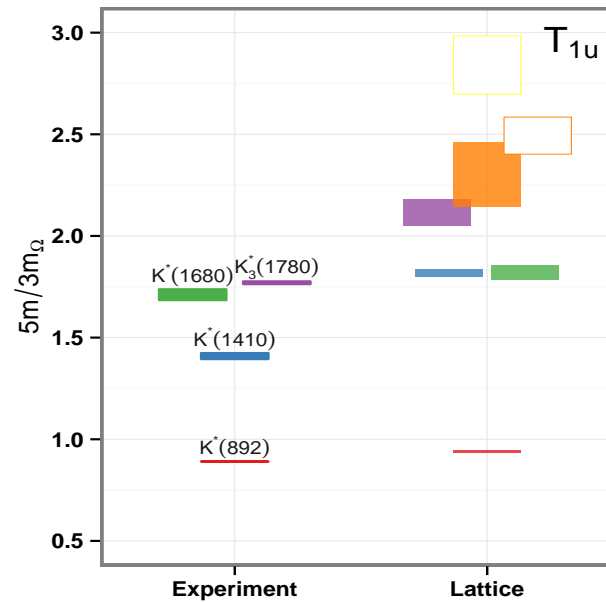
(P. Giudice, D. McManus, M. Peardon)

## We can go further



**charmed spectrum**

(C. Alexandrou, V. Drach,  
K. Hadjiyiannakou, C. Kallidonis, K.J.)



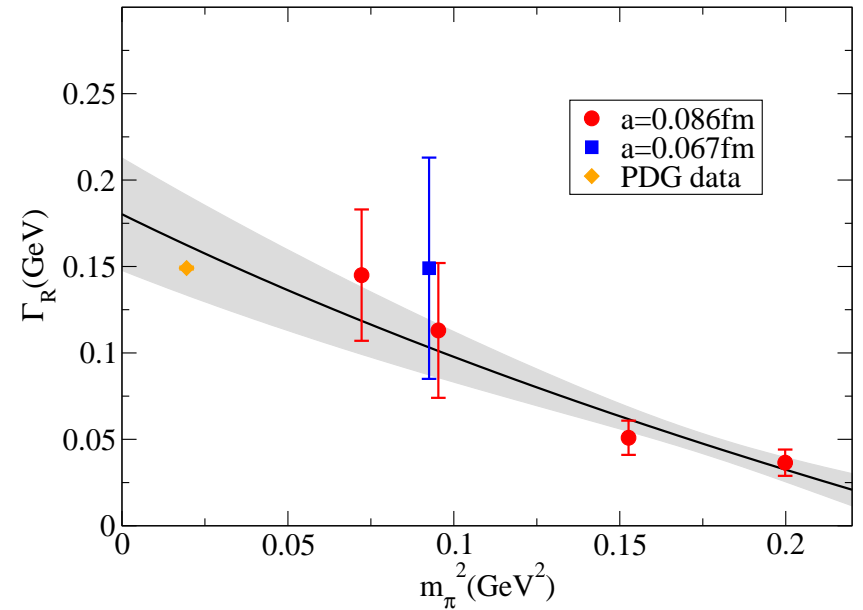
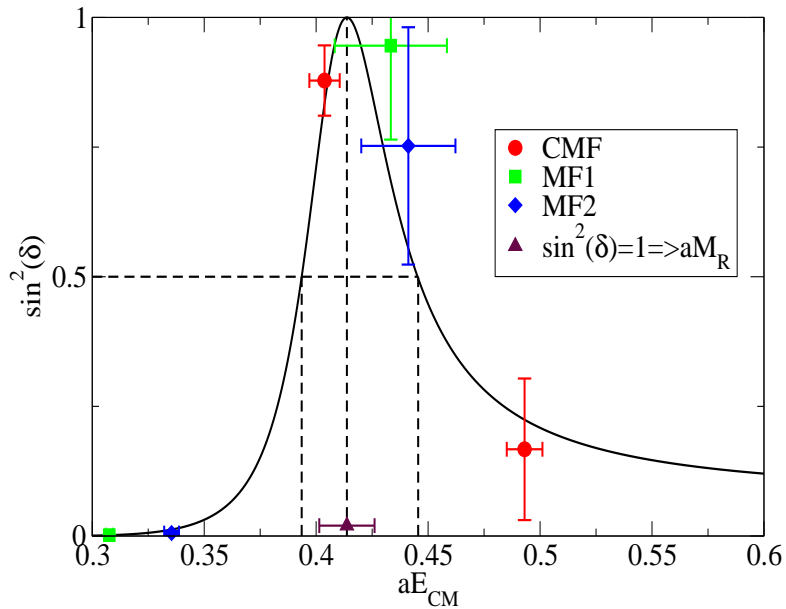
**excited K meson spectrum**

(J. Bulava, B. Fahy, J. Foley, Y. Jhang  
K. Juge, D. Lenkner, C. Morningstar, H. Wong)

# The $\rho$ -meson resonance: dynamical quarks at work

(X. Feng, D. Renner, K.J., 2011)

- usage of three Lorentz frames



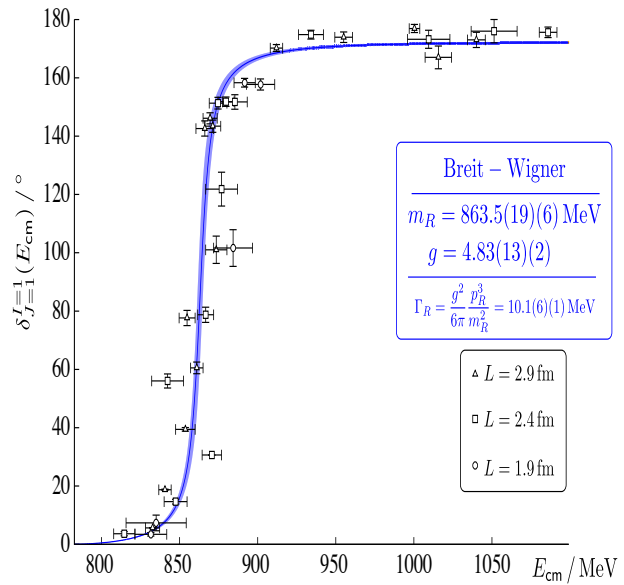
$$m_{\pi^+} = 330 \text{ MeV}, a = 0.079 \text{ fm}, L/a = 32$$

$$m_\rho = 1033(31) \text{ MeV}, \Gamma_\rho = 123(43) \text{ MeV}$$

$$\text{fitting } z = (M_\rho + i\frac{1}{2}\Gamma_\rho)^2$$



## We can go further

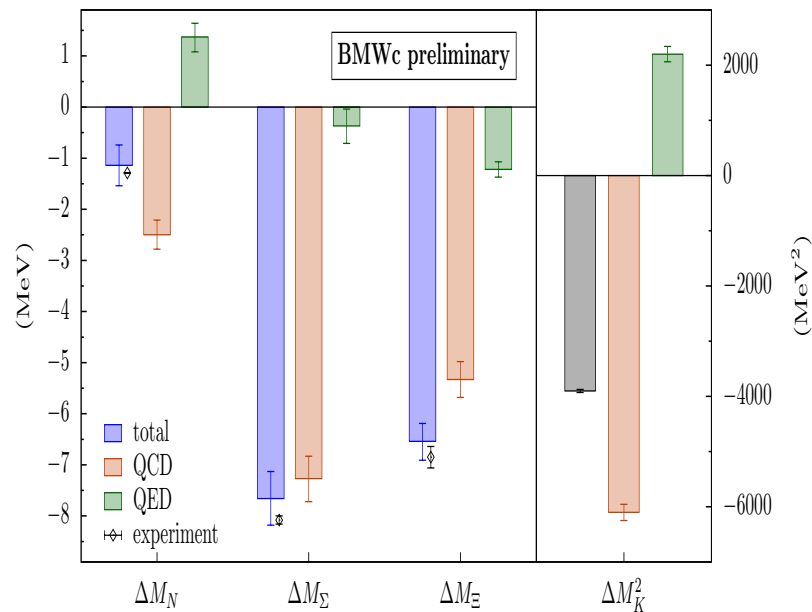


## QCD phase shift

(J. Dudek, R. Edwards, C. Thomas, 2013)

# Even isospin and electromagnetic mass splitting

(BMW collaboration)



## baryon spectrum with mass splitting

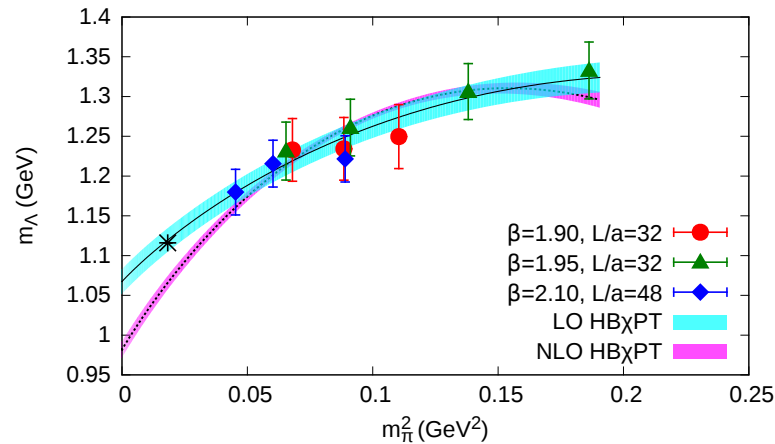
- nucleon: isospin and electromagnetic effects with opposite signs
- nevertheless physical splitting reproduced

## NLO for other masses

$$\begin{aligned}
m_{\Lambda}^{\text{NLO}}(m_{\pi}) &= m_{\Lambda}^{(0)} - 4c_{\Lambda}^{(1)} m_{\pi}^2 - \frac{g_{\Lambda\Sigma}^2}{(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, \Delta_{\Lambda\Sigma}, \lambda) - \frac{4g_{\Lambda\Sigma^*}^2}{(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, \Delta_{\Lambda\Sigma^*}, \lambda) \\
m_{\Sigma}^{\text{NLO}}(m_{\pi}) &= m_{\Sigma}^{(0)} - 4c_{\Sigma}^{(1)} m_{\pi}^2 - \frac{2g_{\Sigma\Sigma}^2}{16\pi f_{\pi}^2} m_{\pi}^3 - \frac{g_{\Lambda\Sigma}^2}{3(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, -\Delta_{\Lambda\Sigma}, \lambda) - \frac{4g_{\Sigma^*\Sigma}^2}{3(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, \Delta_{\Sigma\Sigma^*}, \lambda) \\
m_{\Xi}^{\text{NLO}}(m_{\pi}) &= m_{\Xi}^{(0)} - 4c_{\Xi}^{(1)} m_{\pi}^2 - \frac{3g_{\Xi\Xi}^2}{16\pi f_{\pi}^2} m_{\pi}^3 - \frac{2g_{\Xi^*\Xi}^2}{(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, \Delta_{\Xi\Xi^*}, \lambda) \\
m_{\Delta}^{\text{NLO}}(m_{\pi}) &= m_{\Delta}^{(0)} - 4c_{\Delta}^{(1)} m_{\pi}^2 - \frac{25}{27} \frac{g_{\Delta\Delta}^2}{16\pi f_{\pi}^2} m_{\pi}^3 - \frac{2g_{\Delta N}^2}{3(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, -\Delta_{N\Delta}, \lambda) \\
m_{\Sigma^*}^{\text{NLO}}(m_{\pi}) &= m_{\Sigma^*}^{(0)} - 4c_{\Sigma^*}^{(1)} m_{\pi}^2 - \frac{10}{9} \frac{g_{\Sigma^*\Sigma^*}^2}{16\pi f_{\pi}^2} m_{\pi}^3 - \frac{2}{3(4\pi f_{\pi})^2} \left[ g_{\Sigma^*\Sigma}^2 \mathcal{F}(m_{\pi}, -\Delta_{\Sigma\Sigma^*}, \lambda) + g_{\Lambda\Sigma^*}^2 \mathcal{F}(m_{\pi}, \Delta_{\Lambda\Sigma^*}, \lambda) \right] \\
m_{\Xi^*}^{\text{NLO}}(m_{\pi}) &= m_{\Xi^*}^{(0)} - 4c_{\Xi^*}^{(1)} m_{\pi}^2 - \frac{5}{3} \frac{g_{\Xi^*\Xi^*}^2}{16\pi f_{\pi}^2} m_{\pi}^3 - \frac{g_{\Xi^*\Xi}^2}{(4\pi f_{\pi})^2} \mathcal{F}(m_{\pi}, -\Delta_{\Xi\Xi^*}, \lambda) \\
m_{\Omega}^{\text{NLO}}(m_{\pi}) &= m_{\Omega}^{(0)} - 4c_{\Omega}^{(1)} m_{\pi}^2
\end{aligned}$$

$$\mathcal{F}(m, \Delta, \lambda) = (m^2 - \Delta^2) \sqrt{\Delta^2 - m^2 + i\epsilon} \log \left( \frac{\Delta - \sqrt{\Delta^2 - m^2 + i\epsilon}}{\Delta + \sqrt{\Delta^2 - m^2 + i\epsilon}} \right) - \frac{3}{2} \Delta m^2 \log \left( \frac{m^2}{\lambda^2} \right) - \Delta^3 \log \left( \frac{4\Delta^2}{m^2} \right)$$

## Effect of applying LO and NLO chiral perturbation theory



Baryon	$\mathcal{O}(p^3)$	NLO
$N$	64.9(1.5)	45.3(4.3)
$\Lambda$	46.0(1.8)	74.5(1.8)
$\Sigma^+$	55.6(2.1)	65.3(2.2)
$\Sigma^0$	54.7(1.7)	64.5(1.8)
$\Sigma^-$	58.3(1.9)	68.3(1.9)
$\Delta$	79.9(3.0)	100.3(3.1)
$\Sigma^*$	45.1(2.8)	68.6(2.7)
$\Xi^*$	20.8(2.2)	38.2(2.2)

### nucleon $\sigma$ -terms

- chiral extrapolation dominating systematic error

⇒ need physical point simulations

## Simulation at physical pion mass

- Lattice spacing:  $a = 0.1\text{fm}$
- Pion mass:  $m_\pi = 140\text{MeV}$
- Suppression of finite size effects:  $L \cdot m_\pi > 5$
- Requirement
  - $L \approx 5\text{fm} \rightarrow 48^3 \cdot 96$  lattice ( ← present standard)
  - for  $a = 0.05\text{fm} \rightarrow 96^3 \cdot 192$  lattice
  - grows of simulation cost  $\propto a^{-6}$

## Examples of present Collaborations (using Wilson fermions)

- BMW  
E.g., low lying baryon spectrum,  $B_K$ ,  
quark masses, QCD thermodynamics, several lattice spacings
- PACS-CS  
E.g., charmed baryons, charm physics
- MILC collaboration  
E.g.: kaon semileptonic formfactor
- ETMC  
Meson masses and decay constants, nucleon structure,  
hadronic contributions to electroweak observables
- RBC  
domain wall fermions

## Summary

- wanted to show basic step for proton mass computation
- 25 years effort
  - conceptual developments:  $O(a)$ -improved actions
  - algorithm developments
  - machine developments
- mission of hadron spectrum benchmark calculation completed
- ready for more complicated observables
  - (see other lectures at this school)

## 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  
*Simulation strategies*, hep-lat/xxxxxxx  
*Chiral gauge theories revisited*, hep-th/0102028
- A.D. Kennedy  
*Algorithms for Dynamical Fermions*, hep-lat/0607038



## Books about Lattice Field Theory

- **C. Gattringer and C. Lang**  
*Quantum Chromodynamics on the Lattice*  
Lecture Notes in Physics 788, Springer, 2010
- **T. DeGrand and C. DeTar**  
*Lattice methods for Quantum Chromodynamics*  
World Scientific, 2006
- **H.J. Rothe**  
*Lattice gauge theories: An Introduction*  
World Sci.Lect.Notes Phys.74, 2005
- **J. Smit** *Introduction to quantum fields on a lattice: A robust mate*  
Cambridge Lect.Notes Phys.15, 2002
- **I. Montvay and G. Münster**  
*Quantum fields on a lattice*  
Cambridge, UK: Univ. Pr., 1994
- **Yussuf Saad**  
*Iterative Methods for sparse linear systems*  
Siam Press, 2003