

What is this Lattice Stuff?

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Path Integrals (Minkowski Space)

In Quantum Mechanics the probability amplitude for a particle to move from y to x in d dimensions within time t is

$$\langle x | e^{-iHt} | y \rangle$$

and $H = H_0 + V(x)$ and potential $V(x)$. For a free particle $H_0 = p^2/2m$

$$\begin{aligned} \langle x | e^{-iH_0 t} | y \rangle &= \int dp \langle x | p \rangle \exp \left\{ -i \frac{p^2}{2m} t \right\} \langle p | y \rangle \\ &= \int \frac{dp}{2\pi} e^{ip(x-y)} \exp \left\{ -i \frac{p^2}{2m} t \right\} \\ &= \left(\frac{m}{2\pi i t} \right)^{1/2} \exp \left\{ i \frac{m}{2t} (x-y)^2 \right\} \end{aligned}$$

The time evolution operator (transfer matrix) for small ϵ can be approximated by

$$U_\epsilon = \exp(-iH\epsilon) \approx W_\epsilon = \exp(-iV\frac{\epsilon}{2}) \exp(-iH_0\epsilon) \exp(-iV\frac{\epsilon}{2})$$

Insert $N - 1$ complete set of position eigenstates:

$$\begin{aligned}
 \langle x|e^{-iHt}|y\rangle &= \lim_{N \rightarrow \infty} \int dx_1 \dots dx_{N-1} \langle x|W_\epsilon|x_1\rangle \dots \langle x_{N-1}|W_\epsilon|y\rangle \\
 &= \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} \int dx_1 \dots dx_{N-1} \times \\
 &\quad \exp\left(i\frac{m}{2\epsilon} [(x-y)^2 + \dots + (x_{N-1}-y)^2]\right. \\
 &\quad \left.- i\epsilon \left[\frac{1}{2}V(x) + V(x_1) + \dots + V(x_{N-1}) + \frac{1}{2}V(y)\right]\right)
 \end{aligned}$$

This last term can be rewritten for small ϵ

$$S = \int_0^t dt' \left[\frac{m}{2} \dot{x}^2 - V(x) \right]$$

The amplitude (path integral)

$$\langle x|e^{-iHt}|y\rangle = \int \mathcal{D}x e^{iS}$$

with measure

$$\mathcal{D}x = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i\epsilon}\right)^{1/2} dx_1 \dots dx_{N-1}$$

Amplitude widely oscillating from “ i ”. Not well defined but used formally.

Path Integrals in Euclidean Space

In “imaginary” time $t = -i\tau$, $\tau > 0$ we have

$$\langle x | e^{-H\tau} | y \rangle = \int \mathcal{D}x e^{S_E}$$

$$S_E = \int_0^\tau d\tau' \left[\frac{m}{2} \dot{x}^2 + V(x) \right]$$

where $S = iS_E$. Note evolution operator well defined bounded operator. Consider some operator A . Then

$$\text{Tr} (e^{-H\tau} A) = \sum_{n=0}^{\infty} e^{-E_n\tau} \langle n | A | n \rangle$$

$$Z(\tau) = \text{Tr} (e^{-H\tau}) = \sum_{n=0}^{\infty} e^{-E_n\tau}$$

For large τ the $n = 0$ term dominates, hence the ground state expectation value of A is

$$\langle 0 | A | 0 \rangle = \lim_{\tau \rightarrow \infty} \frac{1}{Z(\tau)} \text{Tr} (e^{-H\tau} A)$$

With

$$\mathbf{x}(\tau) = e^{H\tau} \mathbf{x} e^{-H\tau}$$

correlation functions are

$$\begin{aligned} \langle x(\tau_1) \dots x(\tau_n) \rangle &\equiv \langle 0 | \mathbf{x}(\tau_1) \dots \mathbf{x}(\tau_n) | 0 \rangle \\ &= \langle 0 | e^{E_0 \tau_1} \mathbf{x} e^{-H(\tau_1 - \tau_2)} \mathbf{x} \dots \mathbf{x} e^{-H(\tau_{n-1} - \tau_n)} | 0 \rangle \\ &= \lim_{\tau \rightarrow \infty} \frac{1}{Z(\tau)} \int dx \langle x | e^{-H(\tau/2 - \tau_1)} \mathbf{x} e^{-H(\tau_1 - \tau_2)} \mathbf{x} \dots e^{-H(\tau_n + \tau/2)} | x \rangle \\ &= \lim_{\tau \rightarrow \infty} \frac{1}{Z(\tau)} \int \mathcal{D}x \, x(\tau_1) \dots x(\tau_n) e^{-S_E[x(\tau)]} \end{aligned} \tag{1}$$

Schrödinger equation in Euclidean space is a diffusion eq.

$$\frac{\partial}{\partial \tau} \psi_E(x, \tau) + H \psi_E(x, \tau) = 0$$

Euclidean path integral is an average over random paths suitably weighted. Looks like a partition function (functional integral) with a Boltzmann weight S_E .

4-D STATISTICAL MECHANICS!!

Quantum Electro-Dynamics

Maxwell eqs. (here $c = \hbar/2\pi = 1$)

$$\vec{\nabla} \cdot \vec{E} = \rho, \quad \vec{\nabla} \times \vec{B} - \frac{\partial \vec{E}}{\partial t} = \vec{j}$$

can be written in a relativistic covariant form ($x_0 = t$, $\partial_\mu = \frac{\partial}{\partial x_\mu}$, $E_i = F_{0i}$, $B_i = \frac{1}{2} \sum_{jk=1}^3 \epsilon_{ijk} F_{jk}$, $j_0 = \rho$) as

$$\partial_\mu F_{\mu\nu}(x) = j_\nu(x), \quad F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x).$$

The covariant form of the Dirac equation is

$$\mathcal{D}\psi(x) \equiv \sum_{\mu} \gamma_{\mu} [\partial_{\mu} + ieA_{\mu}(x)] \psi(x) = 0.$$

These equations can be obtained from extremizing the action

$$S(A, \psi) = \int d^4x \left\{ \frac{1}{4} F_{\mu\nu}^2 + \bar{\psi}(x) \mathcal{D}\psi(x) \right\},$$

with the current-charge density $j_\mu(x) = i\bar{\psi}(x)\gamma_\mu\psi(x)$. In Euclidean space, the action is real.

Path Integral for QED

For a **quantum theory** of QED one integrates over fields $A_\mu(x)$, representing the **photons**, and fields $\psi(x)$, representing the **electrons**, as

$$\langle \mathcal{O}(A, \psi, \bar{\psi}) \rangle = \frac{1}{Z} \left\{ \prod_x \int dA(x) d\bar{\psi}(x) d\psi(x) \right\} \mathcal{O}(A, \psi, \bar{\psi}) e^{-\frac{1}{\hbar} S(A, \psi)} .$$

Z is a normalization factor defined by $\langle 1 \rangle = 1$.

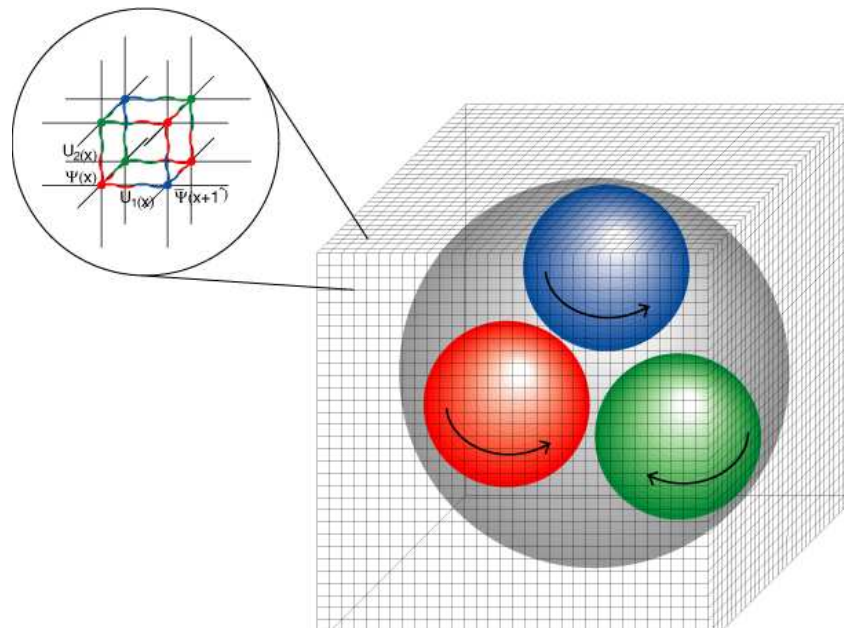
For **QCD**, the $\psi(x)$ represent quarks and the $A_\mu(x)$ represent gluons with suitable $S(A, \psi)$.

Regularization of QCD on a lattice

We approximate **continuous space-time** with a **4-dim lattice**, and derivatives by finite differences. Quarks are put on sites, gluons on links. They are represented by 3×3 complex unitary matrices $U_{x,\mu} = \exp(igaA_{x,\mu})$, elements of the group $SU(3)$. Then

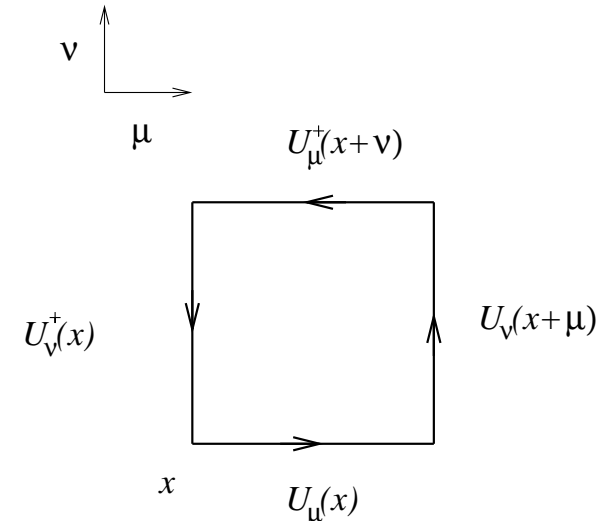
$$\begin{aligned} \langle \mathcal{O}(U, \psi, \bar{\psi}) \rangle &= \frac{1}{Z} \int dU_\mu d\bar{\psi} d\psi \mathcal{O}(U, \psi, \bar{\psi}) e^{-S_G(U) + \bar{\psi} M(U) \psi} \\ &\rightarrow \frac{1}{Z} \int dU_\mu \mathcal{O}(U, M^{-1}(U)) e^{-S_G(U)} \det M(U) \end{aligned}$$

The Gaussian integration over the anti-commuting fermion fields ψ and $\bar{\psi}$ was done, resulting in the $\det M(U)$ and $M^{-1}(U)$ factors.



The *lattice gauge action* is constructed from elementary **plaquettes**

$$U_{\square_{\mu\nu}}(x) = U_{\mu}(x)U_{\nu}(x + \hat{\mu})U_{\mu}^{\dagger}(x + \hat{\nu})U_{\nu}^{\dagger}(x)$$



The **gauge action** is

$$S_G = \frac{2N_c}{g^2} \sum_x \sum_{\mu > \nu} \left[1 - \frac{1}{N_c} \Re \text{Tr} U_{\square_{\mu\nu}}(x) \right] \equiv -\frac{\beta}{N_c} \sum_x \sum_{\mu > \nu} \Re \text{Tr} U_{\square_{\mu\nu}},$$

where we have ignored the constant term, and introduced

$$\beta = \frac{2N_c}{g^2}$$

with, for QCD, $N_c = 3$. β assumes the rôle of *inverse temperature*.

Exercise: Show that

$$S_G = \frac{1}{4} \int d^4x F_{\mu\nu}^a F_{\mu\nu}^a + \mathcal{O}(a^2),$$

i.e. that the lattice gauge action has $\mathcal{O}(a^2)$ **discretisation errors**.

Gauge invariance: the action is invariant under

Monte Carlo method

On a finite lattice need to compute integral over **large**, but **finite**, number U -fields.
Can be done numerically, though not by direct integration.

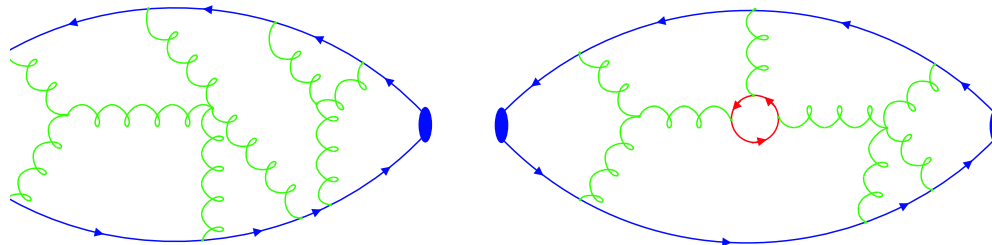
Stochastic Monte Carlo method: generate series of configurations $U_\mu^{(i)}(x)$ distributed with probability $e^{-S_G(U)} \det M(U)/Z$ and compute expectation values as averages over those configurations:

$$\langle \mathcal{O}(U, \psi, \bar{\psi}) \rangle = \frac{1}{N} \sum_{i=1}^N \mathcal{O}(U^{(i)}, M^{-1}(U^{(i)})).$$

Statistical errors go like $1/\sqrt{N}$, for N configurations

The $\det M(U)$ is a big computational cost since the (sparse) matrix M is order $V \times V$.

Quenched approximation., set $\det M = 1$, *i.e.* **neglect internal quark loops**.

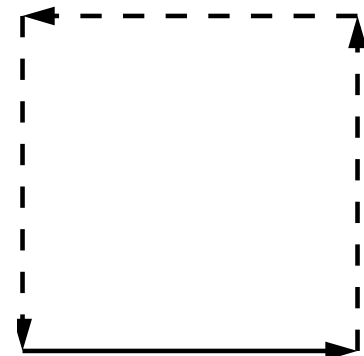


Metropolis algorithm - highly simplified

- Start with some “trial” configuration $\{U(x)\}$
- Go through sites of lattice $x_i, i = 1, \dots, N$ in some order.
 - Choose new local gauge field $U'(x_i)$ - keep others fixed
 - Calculate change in action ΔS
 - Accept the new configuration with probability $\min\{1, e^{-\Delta S}\}$
- One complete pass through the lattice is a **sweep**.

There are two crucial features that simplify the calculation.

- The change in the energy can be calculated *locally*.
- “Independent” sites can be updated *in parallel*
- Well suited for **parallel computers**



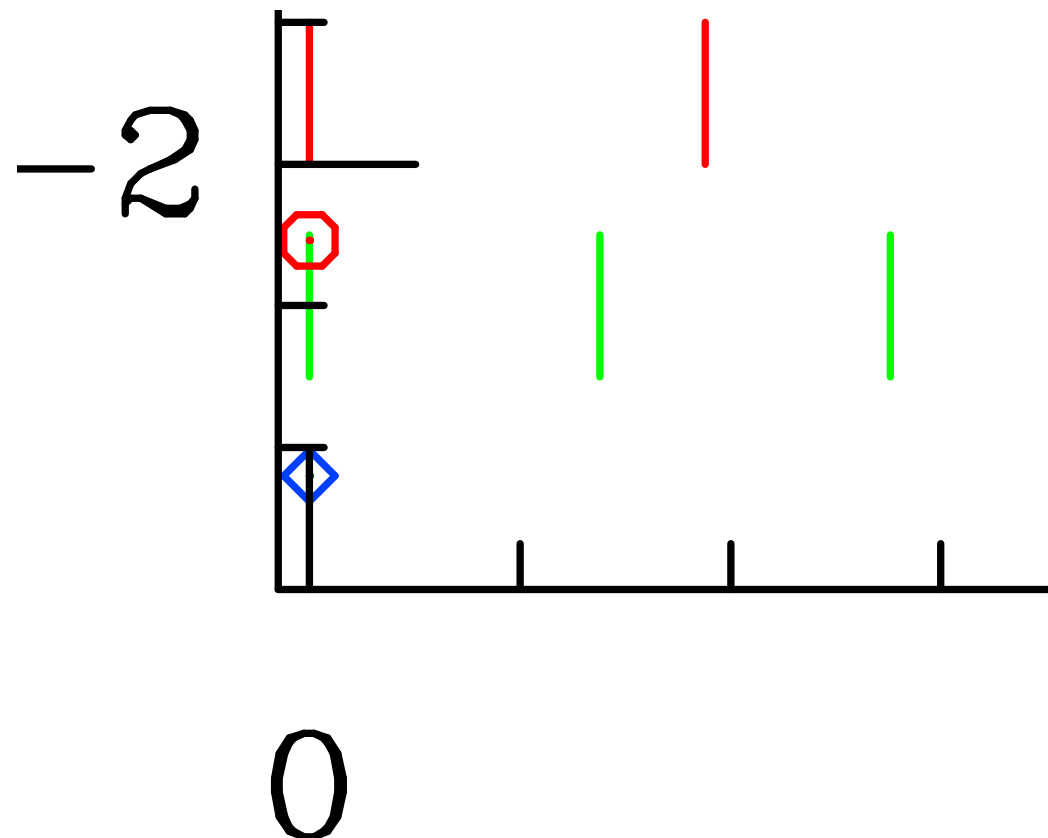
Statistical and Systematic Uncertainties

- Procedure is in principle exact after systematic errors are controlled
- **Statistical uncertainties**
 - Statistical errors go like $1/\sqrt{N}$, for N configurations
 - Including determinant, cost of producing each configuration $\mathcal{O}(100)$ times more expensive.
- **Systematic Uncertainties**
 - *Finite volume*: lattice box must hold a hadron state, typically $L \sim 2fm$ or more. Need $m_\pi L \sim 4$ (several pion Compton wavelengths)
 - *Chiral extrapolations*: calculations with small quark masses expensive - observables to physical quark mass region (delicate!).
 - *Discretization effects*: inherent $\mathcal{O}(a)$ or $\mathcal{O}(a^2)$ lattice uncertainty. Must extrapolate to continuum limit ($a \rightarrow 0$) to recover physical quantities.

The static quark potential

Confinement was the first property of QCD demonstrated by numerical simulations in (quenched) lattice QCD, by M. Creutz, *Phys. Rev. Lett.* **43** (1979) 553.

Confinement is seen as a linear rise of the static potential at large distances. It is by now the best studied property of QCD. Here I shall use it to illustrate the effect of **quenching**, *i.e.*, of neglecting internal quark loops.

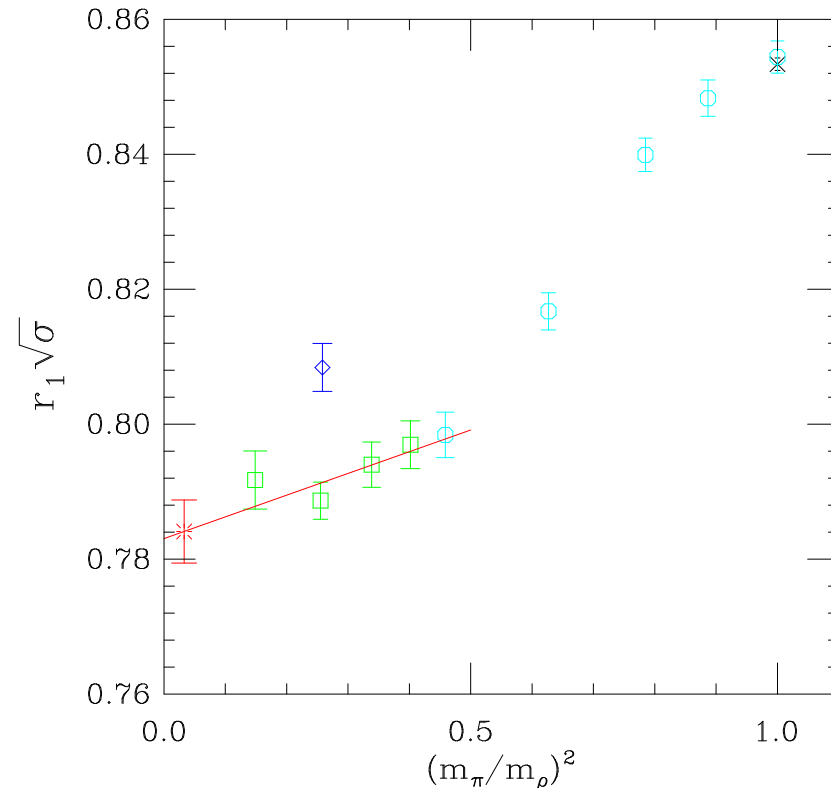


r_1 is the distance defined by the condition $r_1^2 F_{Q\bar{Q}}(r_1) = 1$. The potentials are matched at r_1 .

The Coulomb well is deeper with dynamical fermions, and the string tension slightly

The difference in the **short distance behavior**, corresponding to **high energies**, is due to the different running of the **strong coupling constant α_s** in the presence of **dynamical quarks**.

A more detailed comparison of the behavior of a **long distance scale $\sqrt{\sigma}$** and a **shorter distance scale $r_1 \approx 0.35$ fm** as function of **quark mass, $m_q \propto (m_\pi/m_\rho)^2$** , is shown in

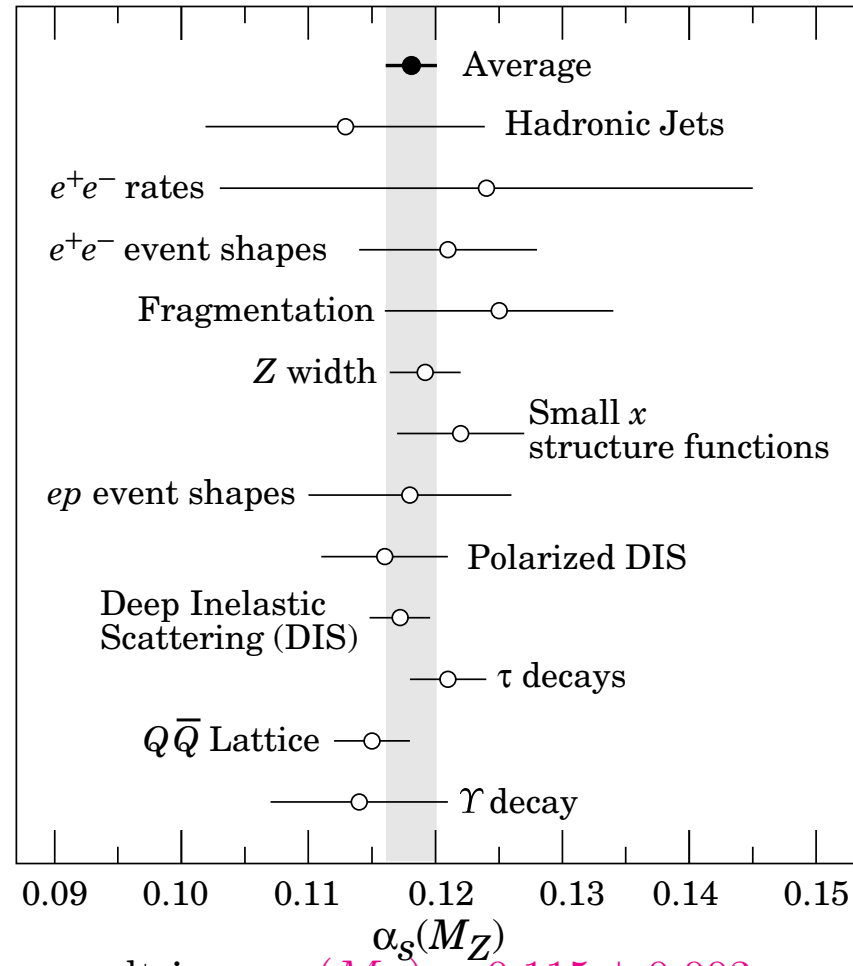


The **effects** of the **dynamical quarks** are **clearly seen**.

Ref.: C. Bernard *et al.* (MILC), *Phys. Rev.* **D62** (2000) 034503.

Strong coupling constant

A comparison of **lattice calculations** of α_s with **experimental determinations**



The combined lattice result is: $\alpha_s(M_Z) = 0.115 \pm 0.003$.

The complete average is: $\alpha_s(M_Z) = 0.118 \pm 0.002$.

Problem of Chiral Symmetry

- Naive lattice discretization of free Dirac operator

$$\sum_{\mu} \gamma_{\mu} \partial_{\mu} \rightarrow \frac{1}{2a} \sum_{\mu} \gamma_{\mu} [\delta_{x+a\hat{\mu},y} - \delta_{x-a\hat{\mu},y}]$$

- In momentum space

$$G^{-1}(p) = \frac{i}{a} \sum_{\mu} \gamma_{\mu} \sin(ap_{\mu}) = i \sum_{\mu} \gamma_{\mu} p_{\mu} \left[1 + O\left((ap_{\mu})^2\right) \right]$$

- Additional zeros, e.g. $a * p_{\mu} = 0, \dots, \pi$ - infamous doubling problem. Can lift doublers - add Laplacian term that breaks chiral symmetry.
- Nielsen-Ninomia no-go theorem - can not avoid both doubling and chiral symmetry breaking with a local, hermitian action analytic in gauge fields. *Major theoretical problem.*
- Problem has been **solved** with recent advent of chiral fermion actions (e.g., Domain-Wall fermions). Crucial for matrix elements.

Hadron Spectrum

In principle, the method to determine the mass of particle P is straightforward:

- Choose an *interpolating operator* \mathcal{O}_P such that $\langle 0|\mathcal{O}_P|P\rangle \neq 0$
- Construct the time-sliced correlator $C(t) = \sum_{\vec{x}} \langle \mathcal{O}(\vec{x}, t) \mathcal{O}^\dagger(\vec{0}, 0) \rangle$
- Insert a complete set of states

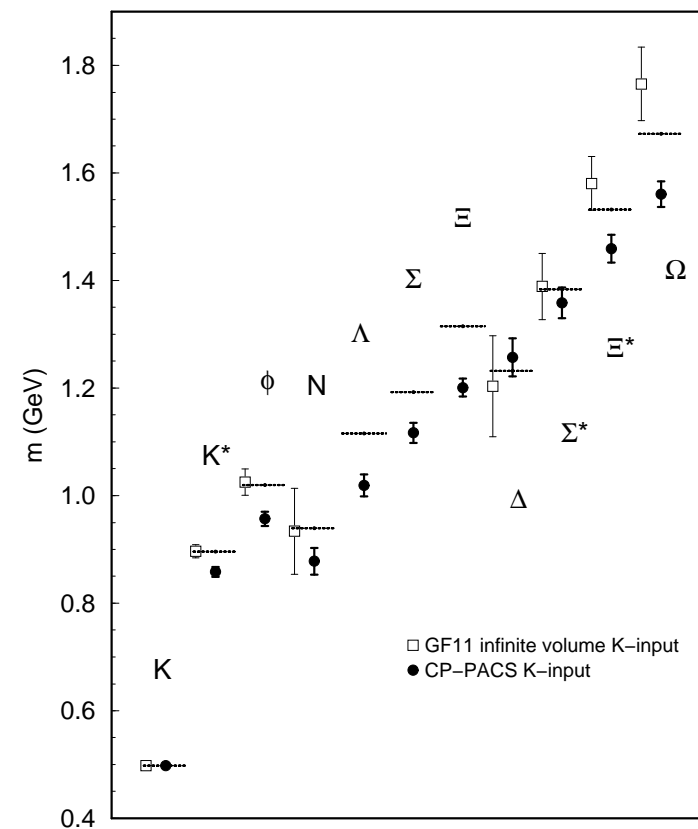
$$\begin{aligned}
 C(t) &= \sum_{\vec{x}} \sum_P \int \frac{d^3k}{(2\pi)^3 2E(\vec{k})} \langle 0|\mathcal{O}(\vec{x}, t)|P(\vec{k})\rangle \langle P(\vec{k})|\mathcal{O}^\dagger(\vec{0}, 0)|0\rangle \\
 &= \sum_{\vec{x}} \sum_P \int \frac{d^3k}{(2\pi)^3 2E(\vec{k})} \langle 0|\mathcal{O}|P(\vec{k})\rangle \langle P(\vec{k})|\mathcal{O}^\dagger|0\rangle e^{ik \cdot x} \\
 &= \sum_P \int \frac{d^3k}{2E(\vec{k})} \delta^3(\vec{k}) \langle 0|\mathcal{O}|P(\vec{k})\rangle \langle P(\vec{k})|\mathcal{O}^\dagger|0\rangle e^{iE(\vec{k})t} \\
 &= \sum_P \frac{|\langle 0|\mathcal{O}|P\rangle|^2}{2m_P} e^{iM_P t}
 \end{aligned}$$

- Go to *Euclidean space*

$$C(t) \rightarrow \sum_P \frac{|\langle 0|\mathcal{O}|P\rangle|^2}{2m_P} e^{-M_P t}$$

Quenched hadron spectrum

- Spectrum of lowest lying states is the benchmark of LQCD
- Most extensively pursued lattice calculation
- Quenched spectrum agrees with experiment to 10%
- Inconsistency in meson sector apparently resolved in full QCD
- *Systematic uncertainties:*
 - Finite volume: $V \rightarrow \infty$
 - Continuum extrapolation: $a \rightarrow 0$
 - Chiral extrapolations: $m_{PS} \rightarrow m_{\pi}$



Glueballs

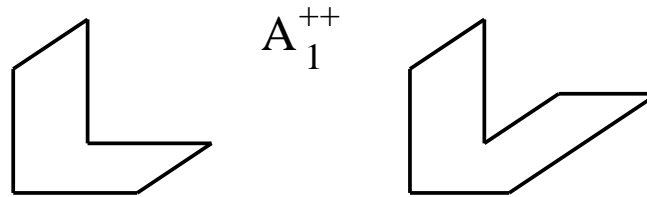
- Gluon **self-coupling** admits existence of **purely gluonic bound states** - **glueballs**.
- Only true states in quenched QCD are glueballs!
- Quenched light-hadron spectrum agrees well with experiment - better than $1/N_c$. Zweig's rule - hadronic decays where initial quarks annihilate are strongly suppressed. Glueball ball mixing with quarks should be similarly suppressed.
- Therefore, much research into quenched calculations
- Glueball calculations are plagued by two problems:
 - Glueballs are **heavy** - correlation functions die rapidly at increasing separations,
 - Glueball operators have large **vacuum fluctuations**.
 - Hence, signal-to-noise ratio for glueball correlators is terrible.

Solutions

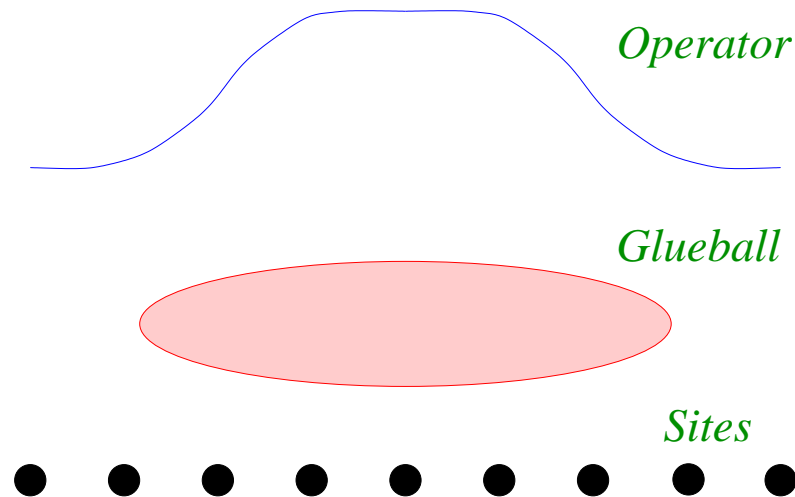
Fuzzed operators: Recall our technique for extracting hadron masses:

$$C(t) = \sum_{\vec{x}} \langle 0 | \mathcal{O}(\vec{x}, t) | 0 \rangle = \mathcal{A}_0 e^{-m_0 t} + \mathcal{A}_1 e^{-m_1 t} + \dots$$

Typical glueball operators



Try to make overlap of **ground state** to \mathcal{O} **large**, and overlap with **excited states** **small**
 – can then **determine mass** at **smaller t**.



Improved Gluon Action

C. Morningstar and M. Peardon By working on a coarser lattice, fewer sites are needed, and the computational cost is greatly reduced.

Discretisation errors for the Wilson action are already $O(a^2)$. But we have seen that there are still *substantial discretisation errors*.

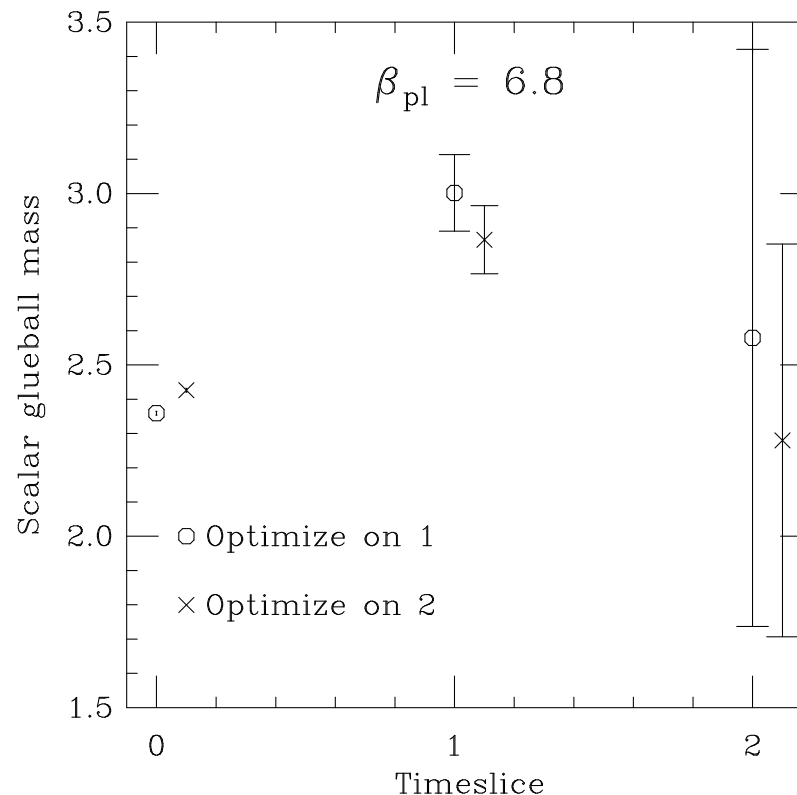
Solution: use $O(a^2)$ -improved gluon action.

Problem: too few lattice sites in temporal direction to isolate the *heavy* ground state.

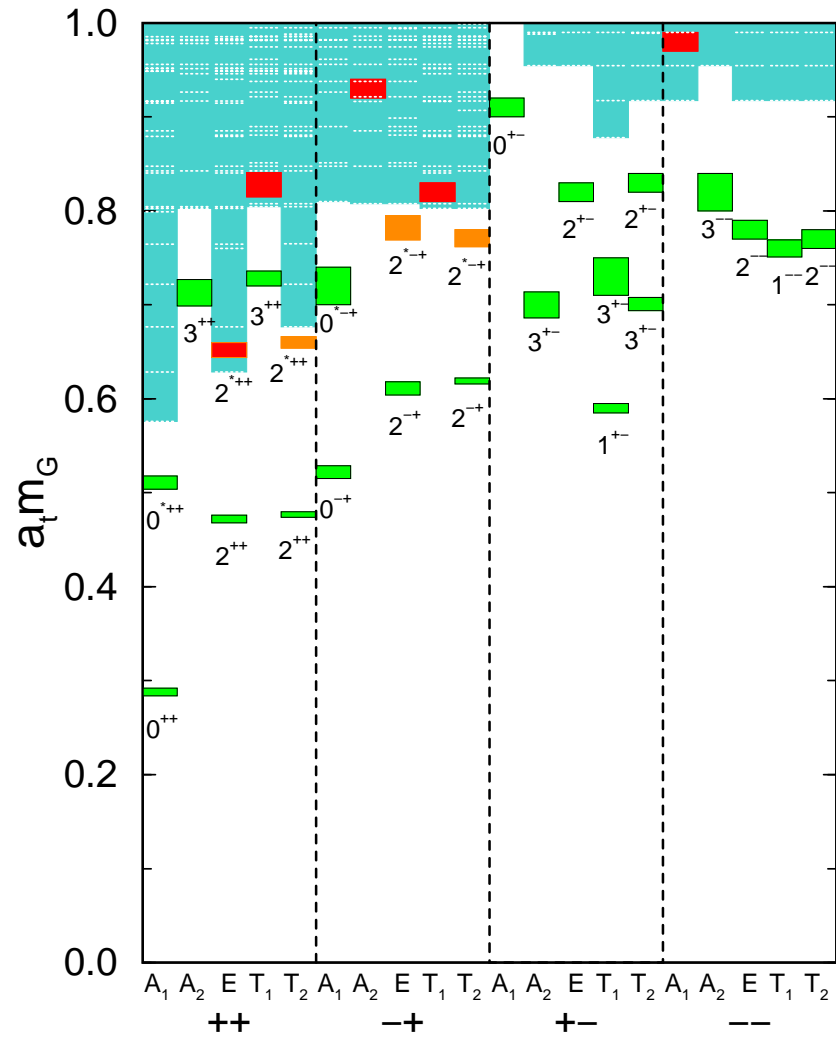
The **effective mass**

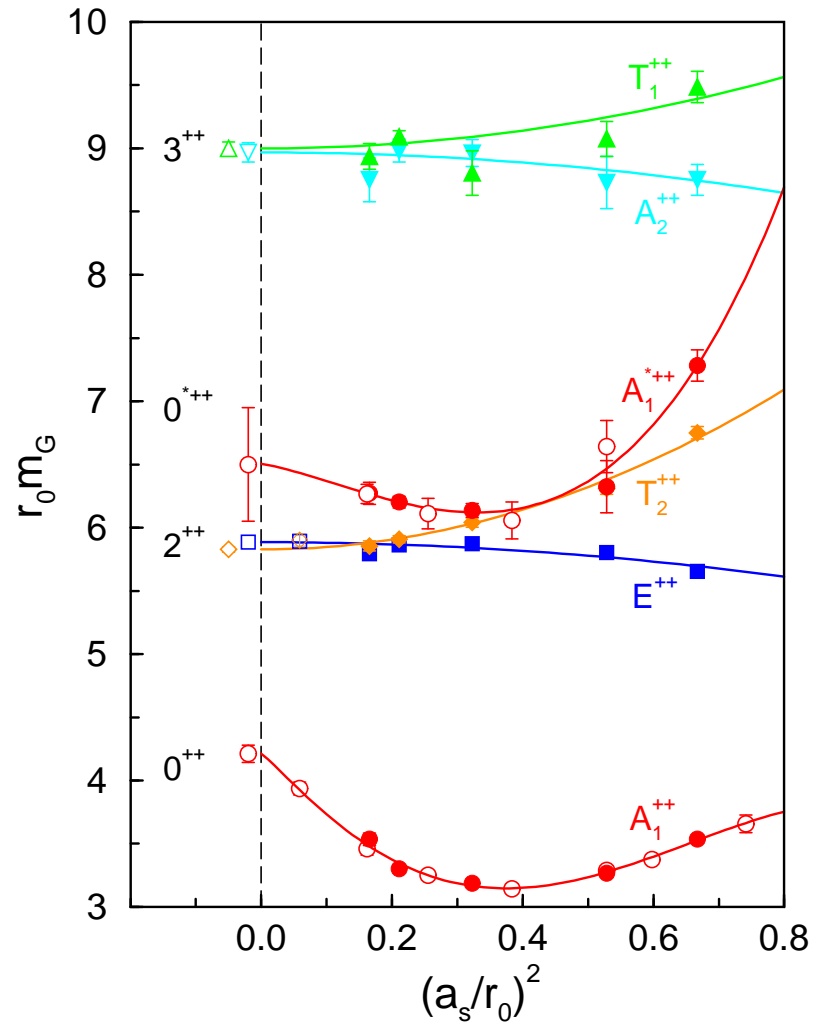
$$m_{\text{eff}} = \ln C(t)/C(t+1)$$

Morningstar and Peardon,
Lattice 94



On lattice, **rotational symmetry** becomes a **cubic symmetry**, representations A_1, A_2, E, T_1, T_2 .

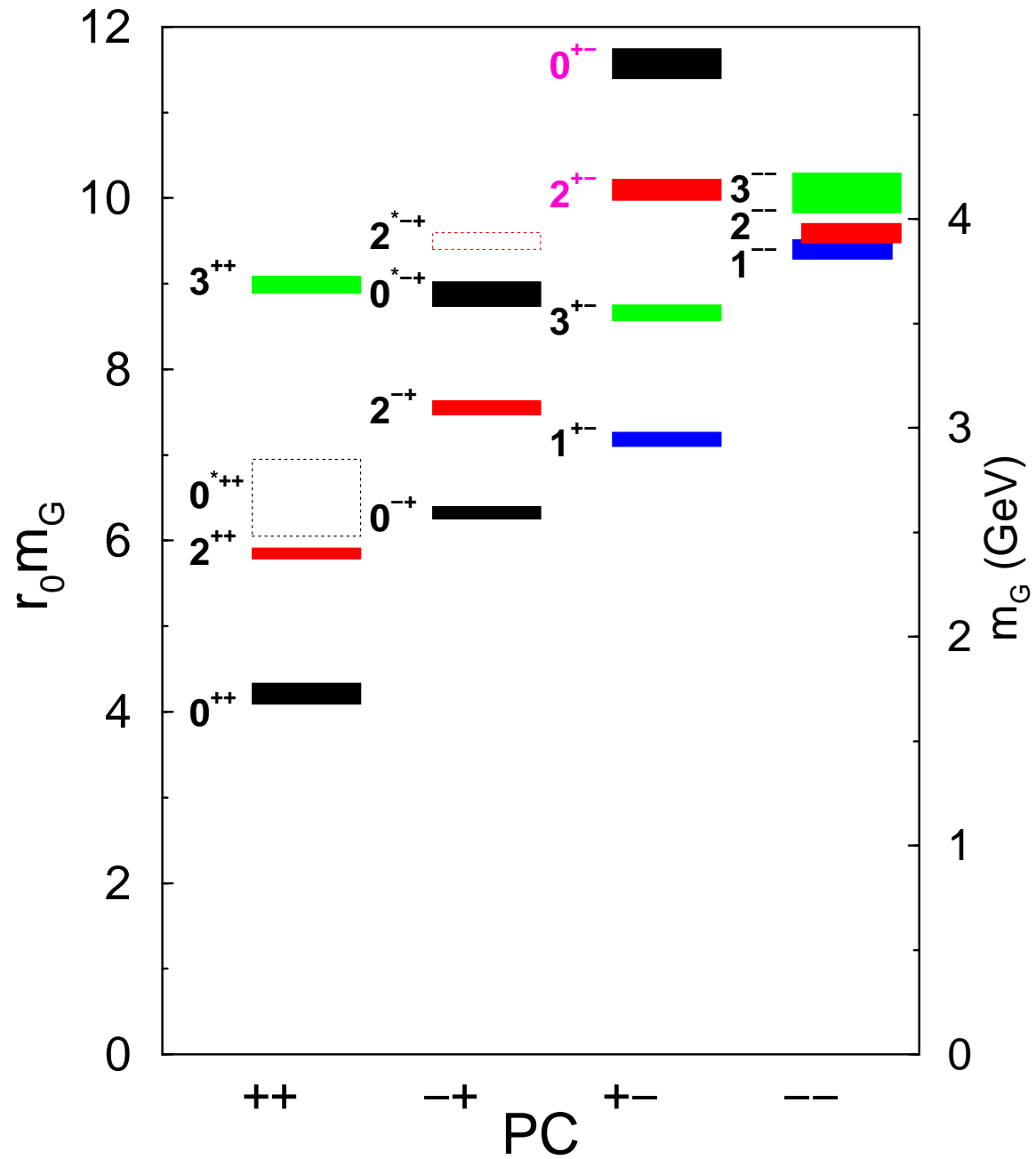




Continuum extrapolations for the $PC = ++$ states

Morningstar and Peardon, hep-lat/9901004

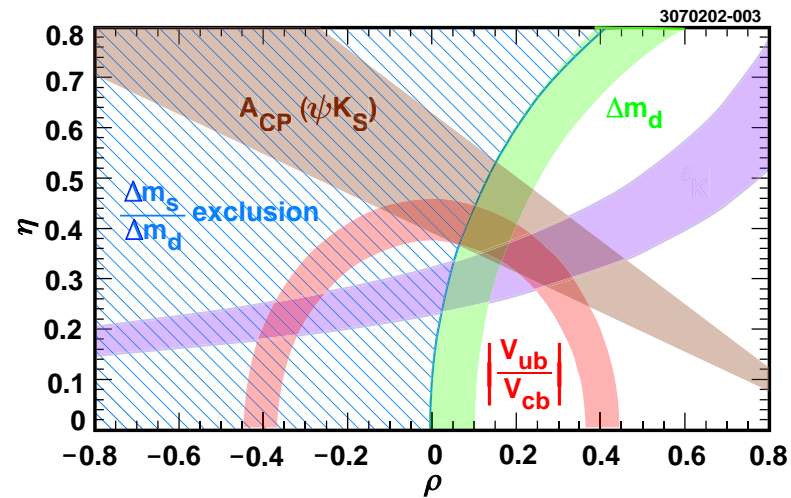
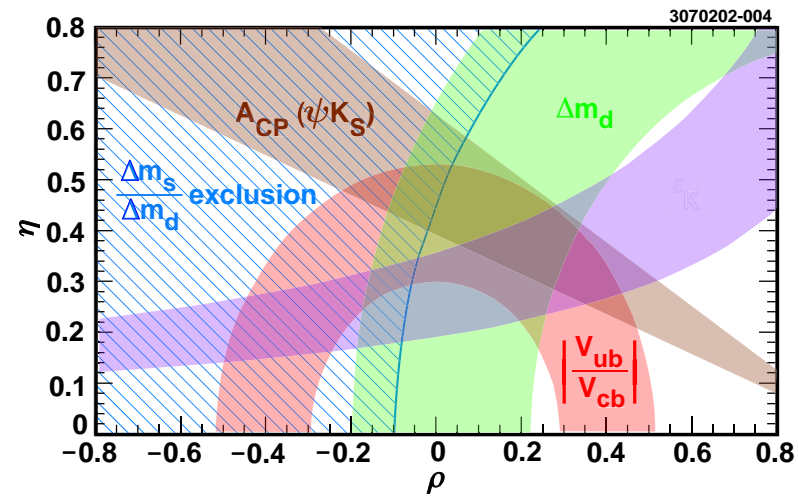
The glueball spectrum after extrapolation to the continuum ($a \rightarrow 0$)



Precision Tests of the Standard Model

- Lattice calculations of weak matrix elements are needed to relate experimental results to underlying parameters of the Standard Model
- Multiple measurements of the same Standard Model parameters in different experiments and calculations will lead to crucial consistency tests
- In many cases the greatest challenge is to reduce the uncertainties in the lattice calculations

Constraints on Standard Model Parameters

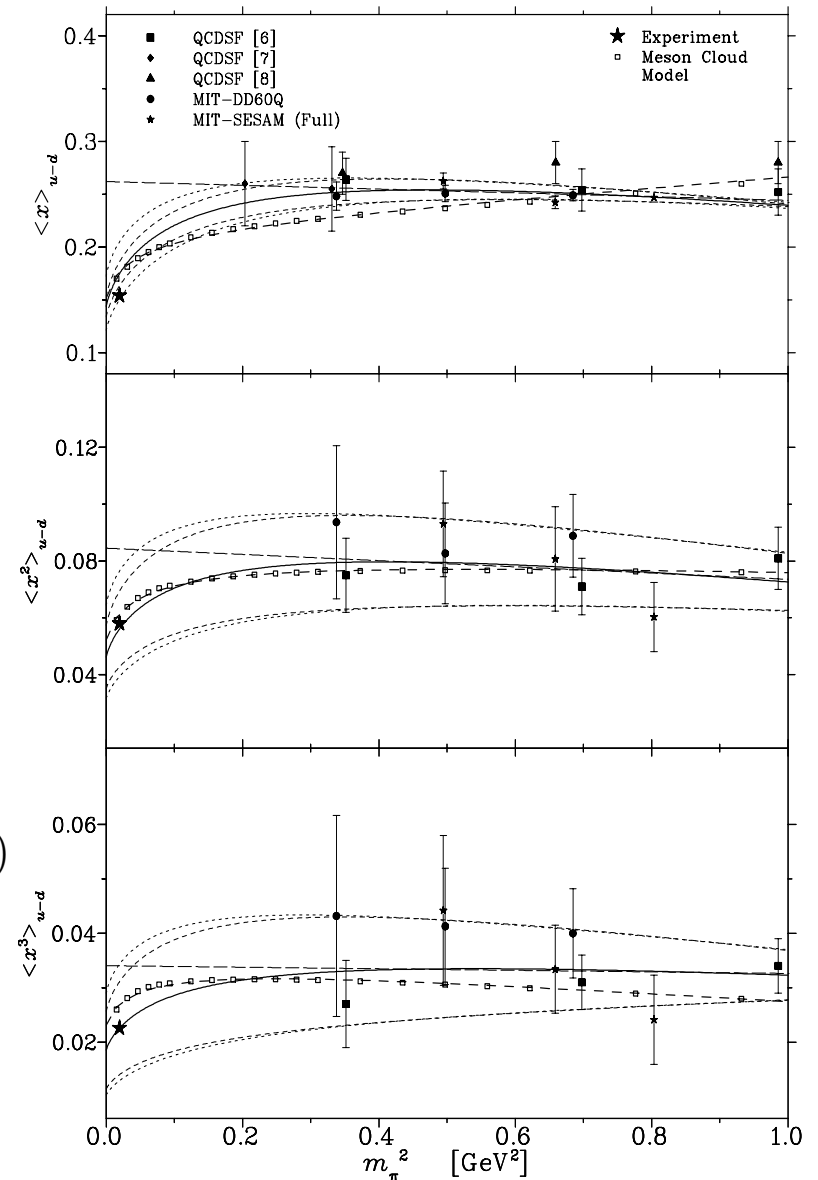


Constraints on the Standard Model parameters ρ and η (one sigma confidence level). For the Standard Model to be correct, they must be restricted to the region of overlap of the solidly colored bands. The figure on the top shows the constraints as they exist today. The figure on the bottom shows the constraints as they would exist with no improvement in the experimental errors, but with lattice gauge theory uncertainties reduced to 3%. R. Patterson, Cornell University.

Moments

- JLab/MIT-Adelaide: 1st three non-trivial moments of non-singlet unpolarized quark distribution u-d in the proton:
- Calculation 10's of Gflops-years
- Chiral extrapolation sensitive to small quark mass
- Prediction for transversity dist

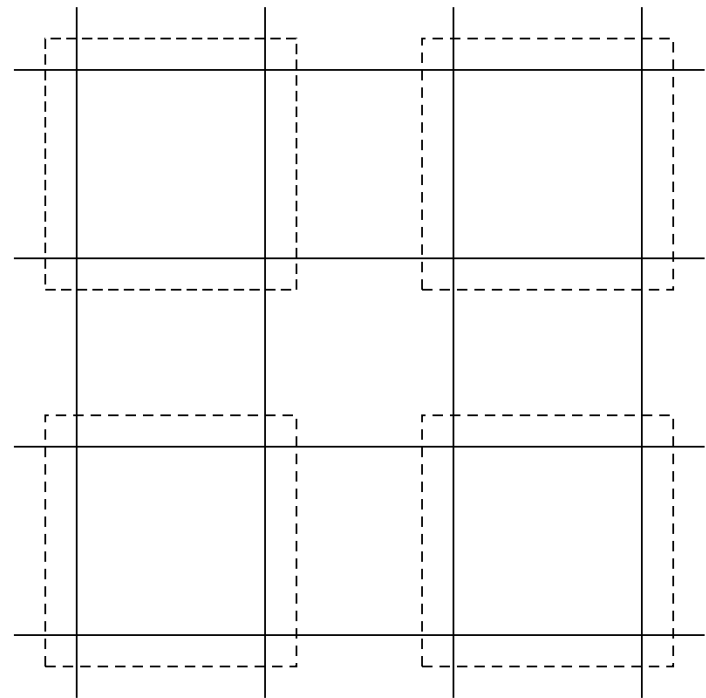
$$\langle 1 \rangle_{\delta u - \delta d} = 1.224(57), \quad \langle x \rangle_{\delta u - \delta d} = 0.506(89)$$



QCD on a Parallel Computer

- Want to decrease runtime for a fixed problem size - increase # of processors N .
- Consider a 2 dimensional problem. Use a grid mapping.

- Data to communicate proportional to surface area
- Limit of scalability is communication / computation ratio
- Overlap communication and computations
- For a Teraflop scale computer, typically exchange a few hundred bytes between processors.



- Researchers build dedicated or commodity optimized facilities

SciDAC

Scientific Discovery through Advanced Computing

- DOE program supporting national effort by US lattice community to develop software and hardware infrastructure for next generation computers
- Physics efforts centered around JLab (hadron physics), FNAL (weak matrix elements), BNL (high temperature)
- Current funding only supports software developers - \$2M to Jlab over 3 years
- Recently installed 128 node Pentium 4 cluster ~ roughly 130 GigaFlop/sec.
- Two more purchases - roughly 256 node P4 arranged in
- Goal is a coordinated three 10 TerFlop/sec computing facilities for national community by 2005.