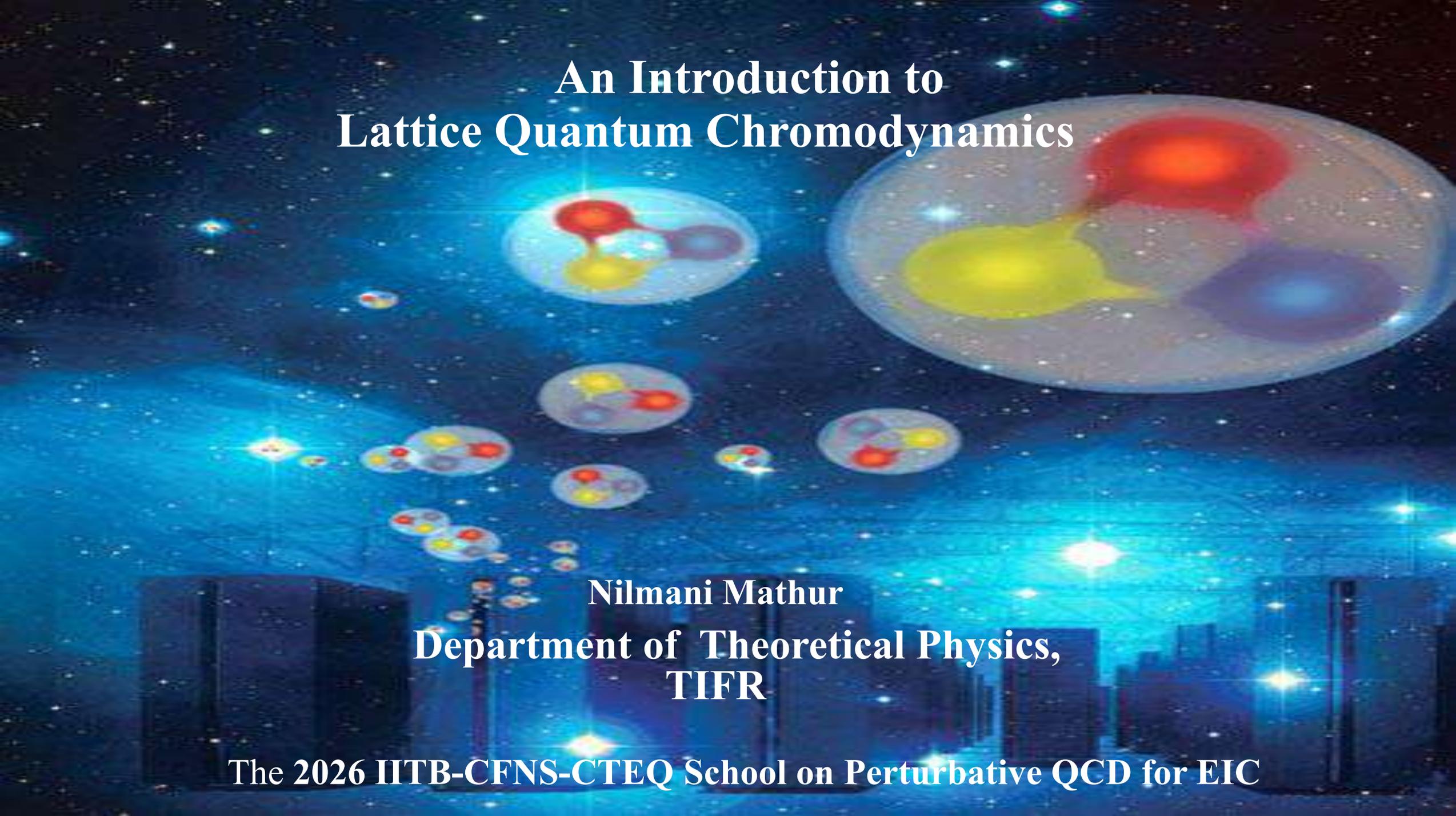


# An Introduction to Lattice Quantum Chromodynamics



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TIFR**

**The 2026 IITB-CFNS-CTEQ School on Perturbative QCD for EIC**

# Lecture 1

-  **Quantum Chromodynamics**  
Theory of quarks and gluons
-  **Introduction to lattice QCD**
  - **Gauge Action**
  - **Fermion Action**
-  **How to calculate an observable?**  
Numerical procedure
-  **Some results**
-  **Challenges**

$$\mathcal{L} = \frac{1}{4g^2} G_{\mu\nu}^a G_{\mu\nu}^a + \sum_j \bar{q}_j (i\gamma^\mu D_\mu + m_j) q_j$$

where  $G_{\mu\nu}^a \equiv \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + if_{bc}^a A_\mu^b A_\nu^c$

and  $D_\mu \equiv \partial_\mu + it^a A_\mu^a$

That's it!

FIGURE 1. THE QCD LAGRANGIAN  $\mathcal{L}$  displayed here is, in principle, a complete description of the strong interaction. But, in practice, it leads to equations that are notoriously hard to solve. Here  $m_j$  and  $q_j$  are the mass and quantum field of the quark of  $j$ th flavor, and  $A$  is the gluon field, with spacetime indices  $\mu$  and  $\nu$  and color indices  $a, b, c$ . The numerical coefficients  $f$  and  $t$  guarantee SU(3) color symmetry. Aside from the quark masses, the one coupling constant  $g$  is the only free parameter of the theory.

..Wilczek

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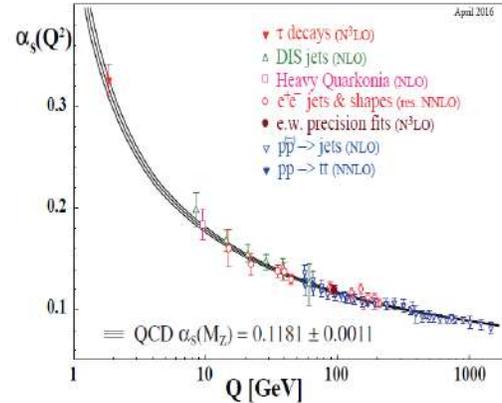
..Wilczek

# QCD

Quantum Chromodynamics is the gauge field theory of the strong interactions of nature

Strong interactions:

- Confining
- Asymptotically free
- Chirally broken



**SU(3)** component of the **SU(3) X SU(2) X U(1)** standard model of particle physics

To study the physics at hadronic scales, perturbative methods fail and we need a non-perturbative regulator

A good regulator should

- Interpret  $\int D\phi$
- Regularize momentum

**Lattice can do both**

$$\mathcal{L} = \sum_q \bar{\psi}_{q,a} (i\gamma^\mu \partial_\mu \delta_{ab} - g_s \gamma^\mu t_{ab}^C \mathcal{A}_\mu^C - m_q \delta_{ab}) \psi_{q,b} - \frac{1}{4} F_{\mu\nu}^A F^{A\mu\nu}$$

$$F_{\mu\nu}^A = \partial_\mu \mathcal{A}_\nu^A - \partial_\nu \mathcal{A}_\mu^A - g_s f_{ABC} \mathcal{A}_\mu^B \mathcal{A}_\nu^C \quad [t^A, t^B] = if_{ABC} t^C$$

□ Symmetries :

- SU(3) local gauge symmetry
- Lorentz, C, P, T and global flavor
- $\psi \rightarrow e^{i\alpha} \psi$
- In the  $m = 0$  chiral limit  $\psi \rightarrow e^{i\gamma_5 \alpha} \psi$

□ Need to preserve as much symmetries as possible on lattice

□ Fundamental free parameters in the theory :

The coupling between quarks and the gluons—dimensionless

The quark masses – dimensionfull

Lattice should not introduce more free parameters to be an *ab-initio* method

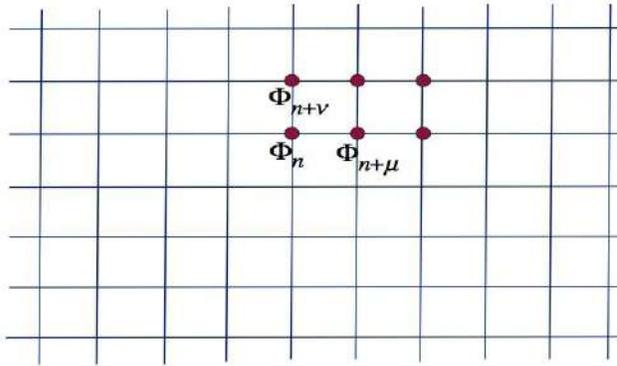
# Scalar Theory

Continuum Euclidean action :

$$Z = \int \mathcal{D}\phi e^{-S[\phi]}$$

$$S[\phi] = \int d^d x \left( \frac{1}{2} (\partial_\mu \phi(x))^2 + \frac{1}{2} m^2 \phi(x)^2 + \frac{\lambda}{4!} \phi(x)^4 \right)$$

Lattice action :



- Momentum is regularized
- A discrete set of integration points, that is finite dimensional integrals for finite lattice

Discretization of fields and derivatives :

$$\phi(x) \longrightarrow \phi_n, \quad x = na$$

$$\int dx_i \longrightarrow a \sum_{n_i}$$

$$\int \mathcal{D}\phi \longrightarrow \prod_n d\phi_n$$

$$\partial_\mu \phi(x) \longrightarrow \Delta_\mu \phi_n = \frac{1}{a} (\phi_{n+\hat{\mu}} - \phi_n)$$

$$\Delta_\mu^* \phi_n = \frac{1}{a} (\phi_n - \phi_{n-\hat{\mu}})$$

$$S[\phi] = a^4 \sum_n \left( \frac{1}{2} (\Delta_\mu \phi_n)^2 + \frac{1}{2} m^2 \phi_n^2 + \frac{\lambda}{4!} \phi_n^4 \right)$$

$$= a^4 \sum_n \left( -\frac{1}{2} \phi_n (\Delta_\mu^* \Delta_\mu) \phi_n + \frac{1}{2} m^2 \phi_n^2 + \frac{\lambda}{4!} \phi_n^4 \right)$$

Fourier transformation of discrete fields

$$\phi(x) = \int_{-\pi/a}^{\pi/a} \frac{d^4 p}{(2\pi)^4} e^{ipx} \tilde{\phi}(p)$$

$$\tilde{\phi}(p) = a^4 \sum_x e^{-ipx} \phi(x)$$

Fields are periodic in momentum space and are restricted to the first Brillouin zone

$$\phi(p) = \phi(p + \frac{2\pi}{a} n_\mu), \quad n_\mu \in \mathbb{Z}$$

$$p_\mu = \frac{2\pi}{a} \frac{n_\mu}{L} \quad |p_\mu| \leq \pi/a = \Lambda_{\text{cutoff}}$$

$$\int \frac{d^4 p}{(2\pi)^4} \rightarrow \frac{1}{a^4 L^3 T} \sum_{n_\mu} \quad L : \text{spatial size}, \quad T \rightarrow \text{temporal size}$$

Thus, Lattice provides a natural regulator for field theories.

Continuum limit can be obtained by taking the limit  $L$  and  $T \rightarrow \infty$ , and  $a \rightarrow 0$

**Does this method work for QCD?**

# Euclidean Formulation

$$\int \mathcal{D}x e^{iS(x)}$$

- \* Paths are weighted with an oscillating function and so is not suitable for numerical calculation!
- \* Change real time to imaginary time (Minkowski space to Euclidean space)

$$t \longrightarrow -i\tau,$$

$$\langle x_f, \tau_f | x_i, \tau_i \rangle = \int_{x_i}^{x_f} \mathcal{D}x e^{-S_E[x(\tau)]}$$

## Confinement of quarks\*

Kenneth G. Wilson

Laboratory of Nuclear Studies, Cornell University, Ithaca, New York 14850

(Received 12 June 1974)

A mechanism for total confinement of quarks, similar to that of Schwinger, is defined which requires the existence of Abelian or non-Abelian gauge fields. It is shown how to quantize a gauge field theory on a discrete lattice in Euclidean space-time, preserving exact gauge invariance and treating the gauge fields as angular variables (which makes a gauge-fixing term unnecessary). The lattice gauge theory has a computable strong-coupling limit; in this limit the binding mechanism applies and there are no free quarks. There is unfortunately no Lorentz (or Euclidean) invariance in the strong-coupling limit. The strong-coupling expansion involves sums over all quark paths and sums over all surfaces (on the lattice) joining quark paths. This structure is reminiscent of relativistic string models of hadrons.

### I. INTRODUCTION

The success of the quark-constituent picture both for resonances and for deep-inelastic electron and neutrino processes makes it difficult to believe quarks do not exist. The problem is that quarks have not been seen. This suggests that quarks, for some reason, cannot appear as separate particles in a final state. A number of speculations have been offered as to how this might happen.<sup>1</sup>

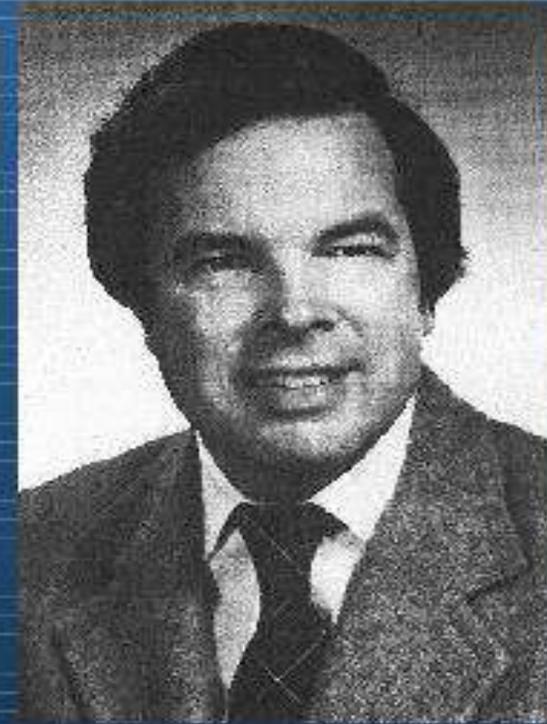
Independently of the quark problem, Schwinger observed many years ago<sup>2</sup> that the vector mesons of a gauge theory can have a nonzero mass if vacuum polarization totally screens the charges in a gauge theory. Schwinger illustrated this result

particles over short times and short distances. The polarization effects which prevent the appearance of electrons in the final state take place on a longer time scale (longer than  $1/m_\gamma$ , where  $m_\gamma$  is the photon mass).

A new mechanism which keeps quarks bound will be proposed in this paper. The mechanism applies to gauge theories only. The mechanism will be illustrated using the strong-coupling limit of a gauge theory in four-dimensional space-time. However, the model discussed here has a built-in ultraviolet cutoff, and in the strong-coupling limit all particle masses (including the gauge field masses) are much larger than the cutoff; in consequence the theory is far from covariant.

The confinement mechanism proposed here is

Among all time favorites



Ken Wilson

*Nobel Laureate 1982*

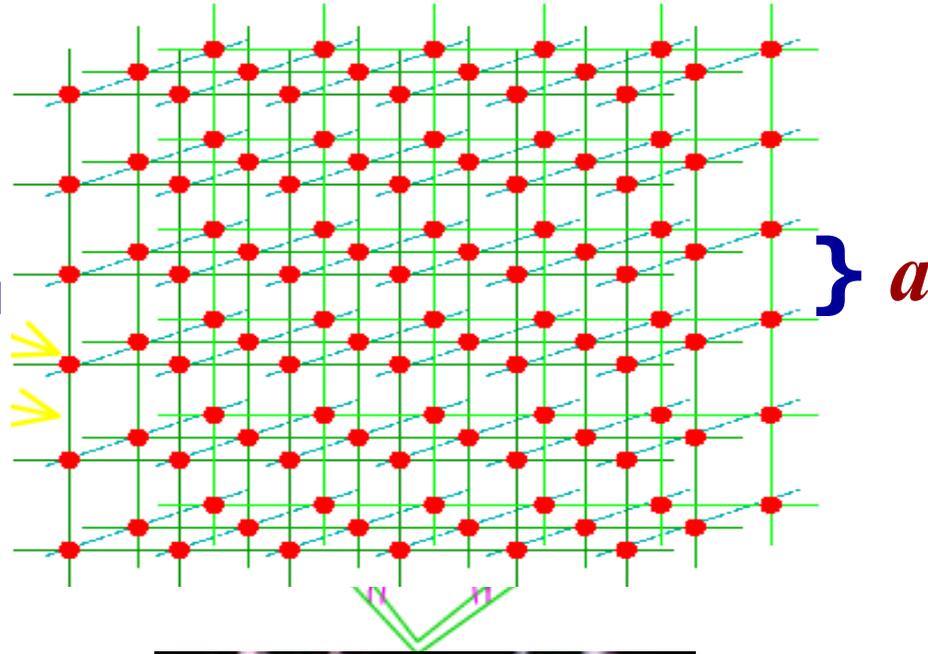
# Continuum to Lattice (Computer)

$$L_{QCD} = \frac{1}{2} \text{Tr} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} (\gamma^\mu D_\mu + m_q) \psi$$

Continuous space-time

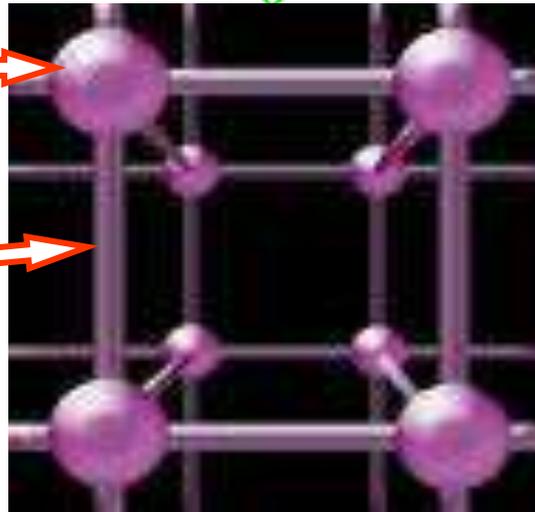
Euclidean  
path integral  
formulation

Discrete Euclidean space-time



Quark  
(on Lattice sites)

Gluon  
(on Links)



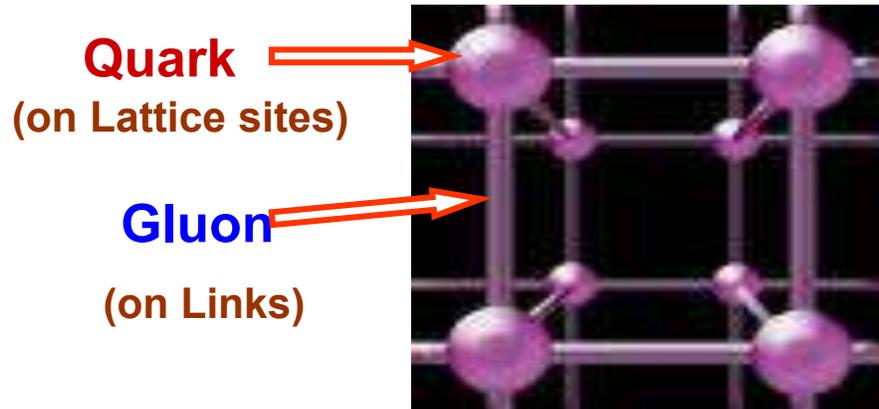
Quark  
Jungle  
Gym

# Life on a Lattice

- Quarks fields are on the lattice sites and carry colors, flavors and spin as like the continuum
- Gauge fields are links between sites and are SU(3) matrices. Continuum and lattice gauge fields are related by

$$A_\mu(x) \rightarrow U(x, \mu) = e^{-iagA_\mu^b(x)t^b}$$

- Under gauge transformation



$$\psi_n \rightarrow V_n \psi_n, \quad \bar{\psi}_n \rightarrow \bar{\psi}_n V_n^\dagger \quad V_n \in SU(3)$$

$$\bar{\psi}_n \psi_{n+\hat{\mu}} \longrightarrow \bar{\psi}_n U_{n,\mu} \psi_{n+\hat{\mu}}$$

$$U_{n,\mu} \rightarrow V_n U_{n,\mu} V_{n+\mu}^{-1}$$

- Make derivatives gauge invariants :

$$\nabla_\mu^{\text{fwd}} \psi(x) = \frac{1}{a} [U_\mu(x) \psi(x + a\hat{\mu}) - \psi(x)]$$

- Gauge invariant quantities are closed loops :

$$\prod_{\mathcal{P}} U_\mu(x)$$

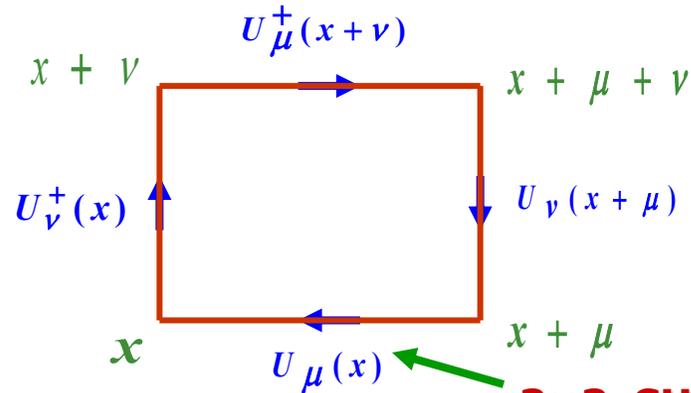
$$\bar{\psi}(x) \gamma_\mu U_\mu(x) \psi(x + a\hat{\mu})$$

# Lattice Formulation of QCD

- ❖ Preserve the symmetry on the lattice (QCD has gauge symmetry)

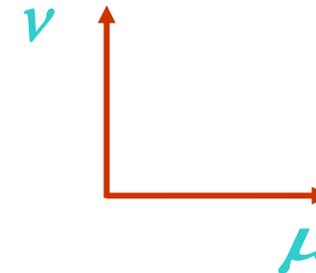
➤ Gauge Symmetry --- Wilson, 1974 ( $A_\mu \rightarrow U_\mu$ )

U : Link Variable



$$U_\mu(x) = e^{-iagA_\mu^a \lambda^a / 2}$$

**3x3 SU(3) matrices**



The simplest possible gauge invariant object (plaquette):

$$\text{Tr } \square_{\mu\nu}(x) \equiv \text{Tr } U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\mu)U_\mu^\dagger(x)$$

# Gauge Action

The simplest possible gauge invariant object (plaquette):

$$\text{Tr } \square_{\mu\nu}(x) \equiv \text{Tr } U_\nu(x)U_\mu(x+\hat{\nu})U_\nu^\dagger(x+\mu)U_\mu^\dagger(x)$$

Next to leading order expansion :

$$\begin{aligned} \square_{\mu\nu} &\simeq 1 + ia \left( A_\nu(x+\hat{\nu}/2) + A_\mu(x+\hat{\nu}+\hat{\mu}/2) - A_\nu(x+\hat{\nu}/2+\mu) - A_\mu(x+\hat{\mu}/2) \right) \\ &\simeq 1 + ia^2(\partial_\nu A_\mu - \partial_\mu A_\nu). \end{aligned}$$

Next order :

$$\begin{aligned} \square_{\mu\nu} &\simeq (\text{above}) - a^2 \left( A_\mu^2 + A_\nu^2 + A_\nu A_\mu - A_\nu A_\nu - A_\nu A_\mu - A_\mu A_\nu - A_\mu A_\mu + A_\nu A_\mu \right) \\ &= (\text{above}) - a^2 [A_\nu, A_\mu], \end{aligned}$$

$$\square_{\mu\nu} \simeq -ia^2 F_{\mu\nu}^a T^a$$

Reflection symmetry :  $\square_{\mu\nu} \simeq 1 - ia^2 F_{\mu\nu}^a T^a - \frac{a^4}{2} F_{\mu\nu}^a F_{\mu\nu}^b T^a T^b + \dots$

$$\sum_{x, \mu > \nu} [N_c - \text{Tr } \square_{\mu\nu}(x)] \simeq \int d^4x \frac{1}{8} F_{\mu\nu}^a F_{\mu\nu}^a$$

**Wilson Action:**  $S = \frac{\beta}{N_c} \sum_{x, \mu > \nu} (N_c - \text{Tr } \square_{\mu\nu}(x))$

**Improved action (1 X 2 boxes) :**

$$S_{\text{Symanzik}} : \sum_{\mu > \nu} \text{Tr } \square_{\mu\nu} \rightarrow \frac{5}{3} \sum_{\mu > \nu} \text{Tr } \square_{\mu\nu} - \frac{1}{12} \sum_{\mu > \nu} (\text{Tr } \square_{\mu\nu} + \text{Tr } \square_{\nu\mu})$$

# Continuum Limit

Relation between lattice spacing and gauge coupling,  $\beta = 6/g^2$  is

$$a = \frac{1}{\Lambda} e^{-1/2\beta_0 g^2} g^{-\beta_1/\beta_0^2} (1 + \mathcal{O}(g^2))$$

Lattice regularization generates a mass scale automatically!

$$\Lambda = \frac{1}{a} e^{-1/2\beta_0 g(a)^2} g(a)^{-\beta_1/\beta_0^2}$$

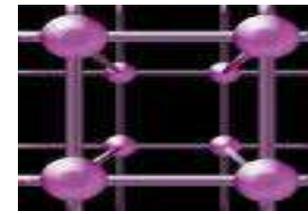
$a \rightarrow 0$  means  $g^2 \rightarrow 0$ ,  $\beta \rightarrow \infty$

$m_{lat}(g(a)) = am_{phy} \rightarrow 0$

So, the correlation length  $\xi \sim 1/m_{latt} \rightarrow \infty$

- A continuum limit of the lattice theory can be obtained by tuning the bare parameters to the critical surface of a lattice system.
- Use a few physical quantities, like masses/string tension to set the physical scale and quark masses.
- All other QCD observables will be prediction

# Fermion Actions



Quark  
Jungle  
Gym

$$\begin{aligned} \langle \hat{O} \rangle &= \text{Lim}_{\beta \rightarrow \infty} \frac{1}{Z} \text{Tr}[e^{-\beta H} \hat{O}(U, \bar{\psi}, \psi)] \\ &= \text{Lim}_{\beta \rightarrow \infty} \frac{\int \mathbf{D}U \mathbf{D}\bar{\psi} \mathbf{D}\psi \mathbf{O}[U, \bar{\psi}, \psi] e^{-S_g[U] - S_F[U, \bar{\psi}, \psi]}}{\int \mathbf{D}U \mathbf{D}\bar{\psi} \mathbf{D}\psi e^{-S_g[U] - S_F[U, \bar{\psi}, \psi]}} \end{aligned}$$

Integrating out the Grassmann variables is possible since  $S = \sum_{x,y} \bar{\psi}(x) M(x, y) \psi(y)$

**M is a complex matrix functional of the gauge fields**

$$\langle \hat{O} \rangle = \frac{\int \mathbf{D}U \{\det \mathbf{D}\}^{n_f} \mathbf{O}[U, \mathbf{D}^{-1}] e^{-S_g[U]}}{\int \mathbf{D}U \{\det \mathbf{D}\}^{n_f} e^{-S_g[U]}} = \prod_n \int \mathbf{d}U_n \underbrace{\frac{1}{Z} \{\det \mathbf{D}(U)\}^{n_f} e^{-S_g[U]}}_{\text{Fermion Action}} \mathbf{O}[U, \mathbf{D}^{-1}]$$

- **Traslational invariance**  $M(x, y) = D(x - y)$
- **Chiral symmetry**  $\{\tilde{D}(p), \gamma^5\} = 0$   $D(p) = \sum_{\mu} \gamma_{\mu} d_{\mu}(p)$
- **Locality** :  $D(p)$  is a regular function of  $p$  throughout the Brillouin zone

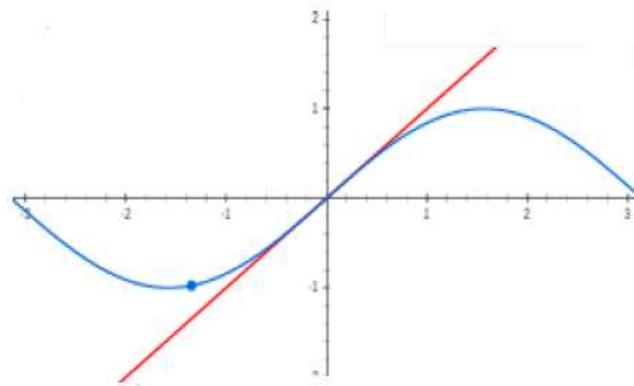
# Fermion Actions

Fermion action with naïve discretization :

$$S_f = a^4 \sum_{x,\mu} \left( \bar{\psi}(x) \gamma_\mu \left( \nabla_\mu^* + \nabla_\mu \right) \psi(x) + m \bar{\psi}(x) \psi(x) \right)$$
$$= a^4 \int_p \bar{\psi}(-p) \left[ \frac{i}{a} \sin(p_\mu a) \gamma_\mu + m \right] \psi(p)$$

Continuum to discrete momentum :

$$p_\mu \rightarrow \sin(p_\mu a)/a$$



- Very different at the Brillouin zone
- 16 ( $2^d$ ) poles of the propagator!
- Tried to describe one fermion, got 16!

## Fermion doubling problem

- Translational invariance  $M(x, y) = D(x - y)$
- Chiral symmetry  $\{\tilde{D}(p), \gamma^5\} = 0$   $D(p) = \sum_\mu \gamma_\mu d_\mu(p)$
- Locality :  $D(p)$  is a regular function of  $p$  throughout the Brillouin zone

# Neilsen-Ninomiya No-Go Theorem

**It is not possible to construct an action satisfying following properties :**

1.  $D(x)$  should be **local**, i.e.  $\|D(x)\| \leq C \exp(-\gamma x)$
2.  $D(p) = i \sum_{\mu} \gamma_{\mu} p_{\mu} + O((ap)^2)$  (cubic symmetry)
3. no doubler exist, i.e.  $D(p)$  is invertible for  $p \neq 0$
4.  $\gamma_5 D + D \gamma_5 = 0$  (chiral symmetry)

**That is, there is no doubler free, chirally symmetric, translation invariant, real-valued lattice action.**

# Wilson Fermions

Lift the fermion mass at the Brillouin zone by adding a term

$$S_W = a^4 \sum \bar{\psi}_n (D_W + m) \psi_n$$
$$D_W = \frac{1}{2} (\gamma_\mu (\Delta_\mu^* + \Delta_\mu) - ar \Delta_\mu^* \Delta_\mu)$$

## Wilson term

- Like a scalar kinetic term
- Lifts the doubler
- $O(a)$  irrelevant operator, additive mass renormalization
- Breaks chiral symmetry even in the chiral limit

Rescaling :  $\psi \rightarrow \sqrt{2\kappa} \psi$ ,  $\kappa = \frac{1}{2ma+8r}$  ← hopping parameter

$$S_W = a^4 \sum_n (\bar{\psi}_n \psi_n - \kappa (\bar{\psi}_n (r - \gamma_\mu) U_{n,\mu} \psi_{n+\mu} + \bar{\psi}_n (r + \gamma_\mu) U_{n,\mu} \psi_{n-\mu}))$$

# Staggered Fermions

- Distribute four spin components of the Dirac spinors on four different sites of the lattice.

$$\psi_n \rightarrow \Omega_n \psi'_n, \quad \Omega_n = \gamma_0^{n_0} \gamma_1^{n_1} \gamma_2^{n_2} \gamma_3^{n_3}$$

$$S = \frac{1}{2a} \sum_n \bar{\psi}'_n \alpha_\mu(n) [U_{n,\mu} \psi_{n+\hat{\mu}} - U_{n-\hat{\mu},\mu}^\dagger \psi_{n-\hat{\mu}}] + m \sum_n \psi'_n \psi'_n$$

Spin diagonal

phase  $\alpha_\mu(n) = (-1)^{n_0 + \dots + n_{\mu-1}} \pm 1$

Removing 3 of the four components of  $\psi \rightarrow \chi$

$$S = \frac{1}{2a} \sum_n \bar{\chi}_n \alpha_\mu(n) [U_{n,\mu} \chi_{n+\hat{\mu}} - U_{n-\hat{\mu},\mu}^\dagger \chi_{n-\hat{\mu}}] + m \sum_n \chi_n \chi_n$$

- Four tastes  $\rightarrow$  16 pions, only one is Goldstone boson. Taste changing interactions can be suppressed.
- Remnant **U(1) X U(1)** symmetry protects quark mass:

$$\chi_n \rightarrow e^{\pm i\theta} \chi_n, \quad n = \text{even or odd}$$

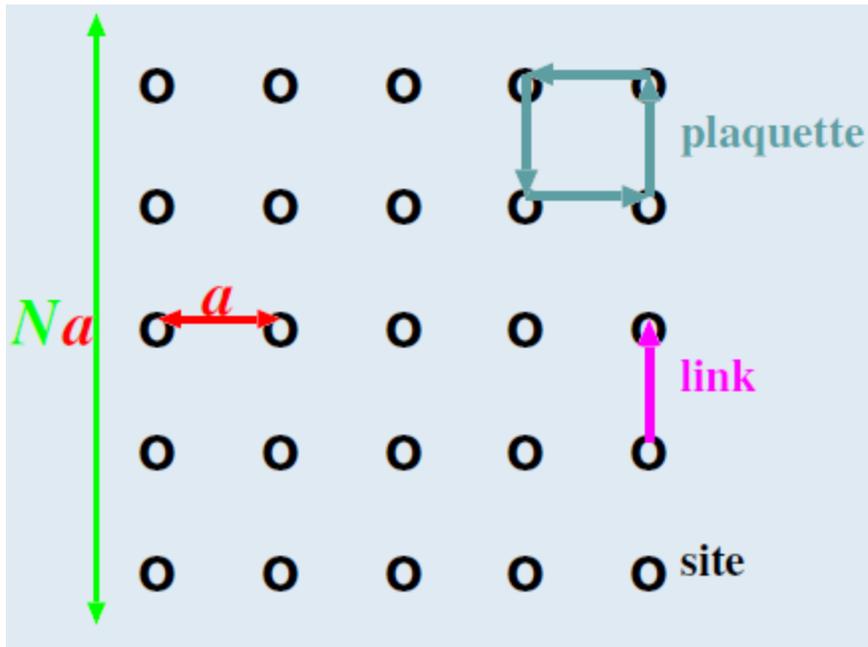
- However, four flavours to one flavour needs rooting. Breaking locality?

# Fermion Actions

- **Wilson** : Add a term to make doublers massive (proportional to inverse lattice spacing) –Wilson action. But it breaks chiral symmetry (quark mass is not protected from additive mass renormalization)
- **Staggered** : Put four spin component of the Dirac spinor on four different sites of the lattice. No breaking of chiral symmetry. Four tastes  $\rightarrow$  16 pions, only one is Goldstone boson. Taste changing interactions (Naik term) can be suppressed. However, four flavours to one flavour needs rooting. Breaking locality?
- **Clover fermions** : Wilson fermions with Symanzik type improvement. No  $O(a)$  term
- **Twisted mass** : a variety of Wilson action with flavour dependent chiral rotation of fermion fields. No  $O(a)$  term but breaks isospin symmetry.
- **HISQ** : Highly improved staggered quarks
- **Domain wall and Overlap fermions** : Exact extend chiral symmetry on the lattice. Not ultralocal. Extremely costly compared to Staggered and Wilson actions

# Fermion Actions

Action	Advantages	Disadvantages
Wilson	Computationally fast	Breaks chiral symmetry, $O(a)$ error, additive mass renormalization
Improved Wilson (Clover)	Computationally fast	Breaks chiral symmetry, operator improvement is necessary
Twisted mass	Computationally fast	Breaks chiral symmetry, Isospin breaking
Staggered	Computationally fast	Fourth root problem, taste breaking, complication in operator construction
Highly improved staggered (HISQ)	Computationally reasonably fast, lesser taste breaking	Fourth root problem, complication in operator construction
Domain wall	Improved Chiral symmetry	Computationally expensive
Overlap	Exact chiral symmetry	Computationally very expensive



**Typical values :**

$$a = 0.15\text{--}0.04 \text{ fm}$$

$$Na = 2\text{--}6 \text{ fm}$$

**Continuum limit :**

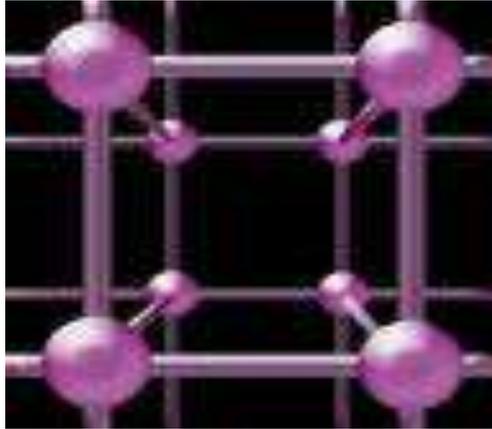
$$a \rightarrow 0, Na \text{ fixed}$$

**Infinite volume :**  $Na \rightarrow \infty$

**Inputs :**

Lattice spacing (coupling) : from known masses : say  $M_\Omega$   
 or static quark potential  
 heavy meson spectrum etc

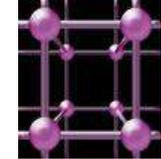
Quark mass :  $u(d) \leftarrow m_\pi$   
 $s \leftarrow m_k \text{ or } m(ss)$   
 $c \leftarrow \frac{1}{4}(3J/\Psi + \eta_c)$   
 $b \leftarrow Y_b$



**How to calculate an observable??**

**From statistical mechanical  
correlation functions**

# Too Many Integrations!!



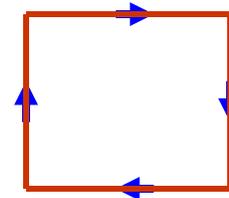
$$\langle 0 | \hat{Q}[\hat{\phi}(x)] | 0 \rangle \longrightarrow \langle Q(\phi_n) \rangle \equiv \frac{\int d\phi_n Q(\phi_n) e^{-S^{lat}(\phi_n)}}{\int d\phi_n e^{-S^{lat}(\phi_n)}}$$

We need lattice spacing as small as possible i.e., big volume.

Suppose we have a  $10^4$  lattice.

This has

- $10^4 = 10,000$  sites,
- $10^4 \times 4 = 40,000$  links (due to gluons)
- $10^4 \times 4 \times 8 = \mathbf{320,000}$  dimensional integral !!
- If we take only 2 points/dimension (very crude) sum will be with  $2^{320,000} = 3.8 \times 10^{96,329}$  terms!!



Age of the universe is only  $\sim 10^{27}$  nanoseconds!

# Statistical Evaluation -- Monte-Carlo Method

- ❖ The appearance of such large number immediately suggests a statistical treatment.
- ❖ These integrations can be avoided if we assume that the microscopic laws are defined in terms of probabilities and it is possible to generate a sequence of statistically independent configurations with that probability distribution over the possible paths or over the possible locations of the system in configuration space.
- ❖ These large number of integrations then reduce to an ensemble average

$$\langle O \rangle = \frac{1}{Z} \int [dU] [d\psi][d\bar{\psi}] O[U] e^{-S[U, \psi, \bar{\psi}]}$$

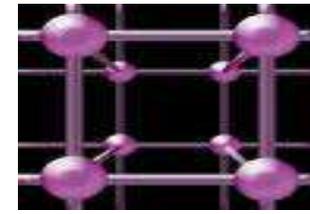
- ❖ **Measurement** : Average over a representative ensemble of gluon configurations  $\{U_i\}$  with probability

$$P(U_i) \propto \int [d\psi][d\bar{\psi}] e^{-S[U, \psi, \bar{\psi}]}$$

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^N O \{U_i\} + \Delta O \quad \Delta O \propto \frac{1}{\sqrt{N}} \xrightarrow{N \rightarrow \infty} 0$$

$\{U_i\}$ 's are the configurations generated by **Monte-Carlo Method**.

# Observables



Quark  
Jungle  
Gym

$$\begin{aligned} \langle \hat{O} \rangle &= \text{Lim}_{\beta \rightarrow \infty} \frac{1}{Z} \text{Tr}[e^{-\beta H} \hat{O}(U, \bar{\psi}, \psi)] \\ &= \text{Lim}_{\beta \rightarrow \infty} \frac{\int \mathbf{D}U \mathbf{D}\bar{\psi} \mathbf{D}\psi \mathbf{O}[U, \bar{\psi}, \psi] e^{-S_g[U] - S_F[U, \bar{\psi}, \psi]}}{\int \mathbf{D}U \mathbf{D}\bar{\psi} \mathbf{D}\psi e^{-S_g[U] - S_F[U, \bar{\psi}, \psi]}} \end{aligned}$$

Integrating out the Grassmann variables is possible since  $S_F = \bar{\psi} \mathbf{D} \psi$

$$\langle \hat{O} \rangle = \frac{\int \mathbf{D}U \{\det \mathbf{D}\}^{n_f} \mathbf{O}[U, \mathbf{D}^{-1}] e^{-S_g[U]}}{\int \mathbf{D}U \{\det \mathbf{D}\}^{n_f} e^{-S_g[U]}} = \prod_n \int \underbrace{dU_n \frac{1}{Z} \{\det \mathbf{D}(U)\}^{n_f} e^{-S_g[U]} \mathbf{O}[U, \mathbf{D}^{-1}]}_{\text{quark determinant}}$$

$$\langle \hat{O} \rangle = \frac{1}{N} \sum_{U \in \frac{1}{Z} e^{-S_g[U] + \ln \{\det \mathbf{D}\}^{n_f}}} \mathbf{O}[U, \mathbf{D}^{-1}] \quad \leftarrow \sum \mathbf{D}^{-1}(U) \mathbf{D}^{-1}(U) \dots \mathbf{D}^{-1}(U)$$

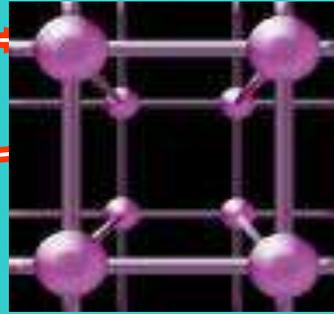
Parameters : gauge coupling  
and quark masses

# Rational Hybrid Monte Carlo Algorithm

- A state of the art Monte Carlo algorithm for lattice QCD which can generate gauge field configurations relatively faster way even at physical quark masses  
M. Clark: PoSLAT2006:004,2006
- Fermion determinant of very large matrices gets evaluated by a rational approximation
- Many supercomputers throughout the world are being used for generating these gauge configurations
- Huge amount of efforts go on to improve algorithms (by lattice gauge physicists, applied mathematicians, computer scientists)

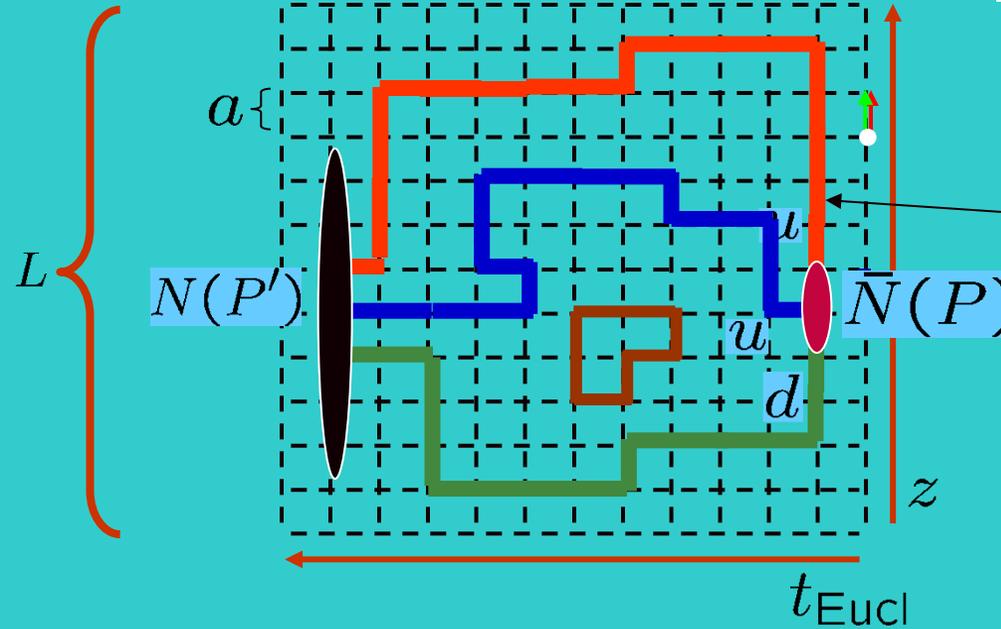
Quark  
(on Lattice  
sites)

Gluon  
(on  
Links)



Quark  
Jungle  
Gym

$$P_\alpha(x) = \epsilon_{abc} u_\alpha^a(x) u_\beta^b(x) (C\gamma_5)_{\beta\eta} d_\eta^c(x),$$



quark propagators :  
Inverse of very large  
matrix of space-time,  
spin and color

# Quark Propagator

$$L_{QCD} = \frac{1}{2} \text{Tr} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} (\gamma^\mu D_\mu + m_q) \psi$$

Fermion Action

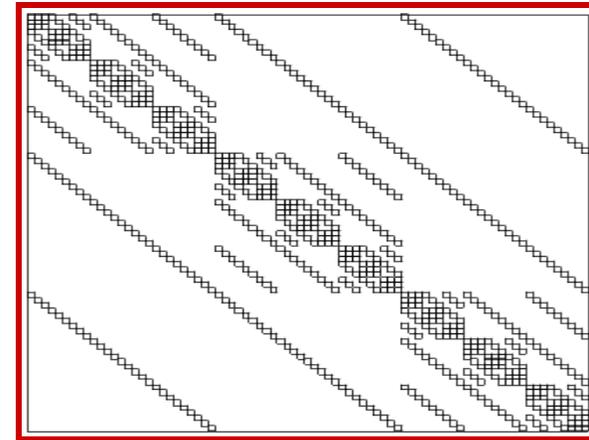
$$S_F = \sum_{x,y} \bar{\psi}(x) M(x,y) \psi(y)$$



Lattice size : **16<sup>3</sup> x 24**

Dimension of **M** : **16<sup>3</sup> x 24 x 2 x 3 x 4**  
 **$\approx 10^6 \times 10^6$  !!**

Need  **$M^{-1}(x,y)$ ,  $\text{Tr}[M^{-1}(x,y)]$ ,  $\text{Det}[M(x,y)]$**



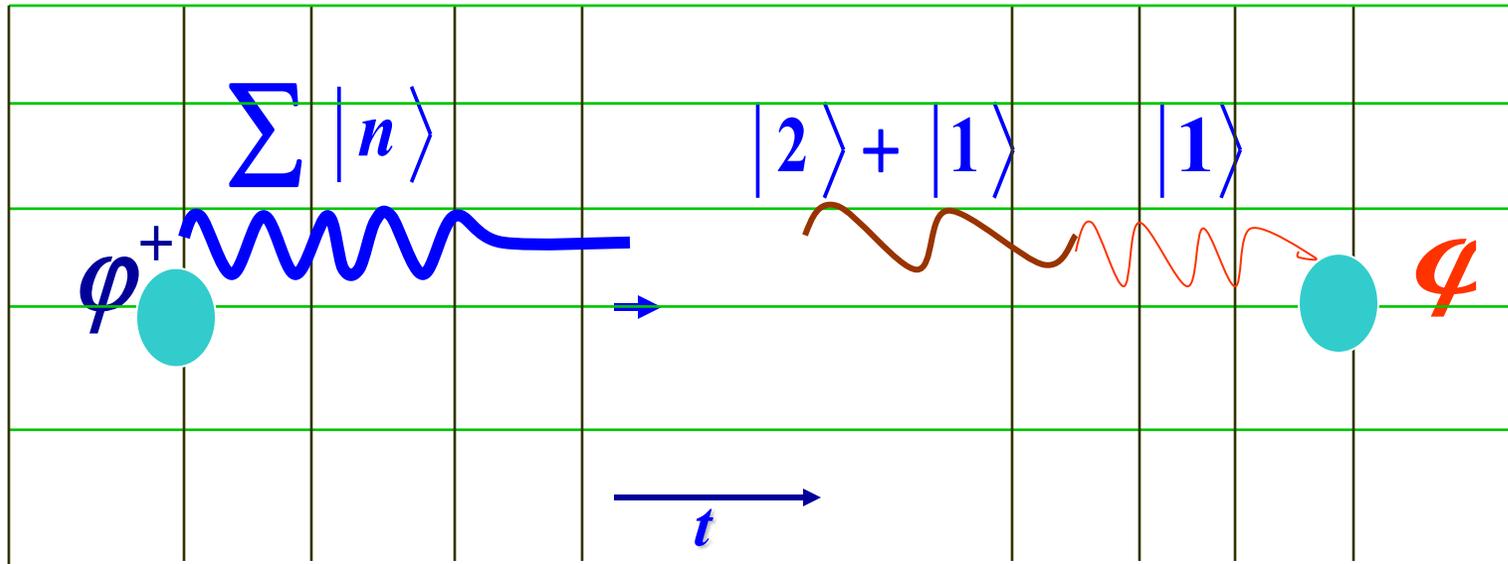
Translational invariance : need only  **$M^{-1}(x,0)$**

$$M_{\alpha\beta}^{ab}(x,y)$$

Different type of algorithms for different fermionic action

**Conjugate gradient** is the best for Hermitian positive definite matrix.

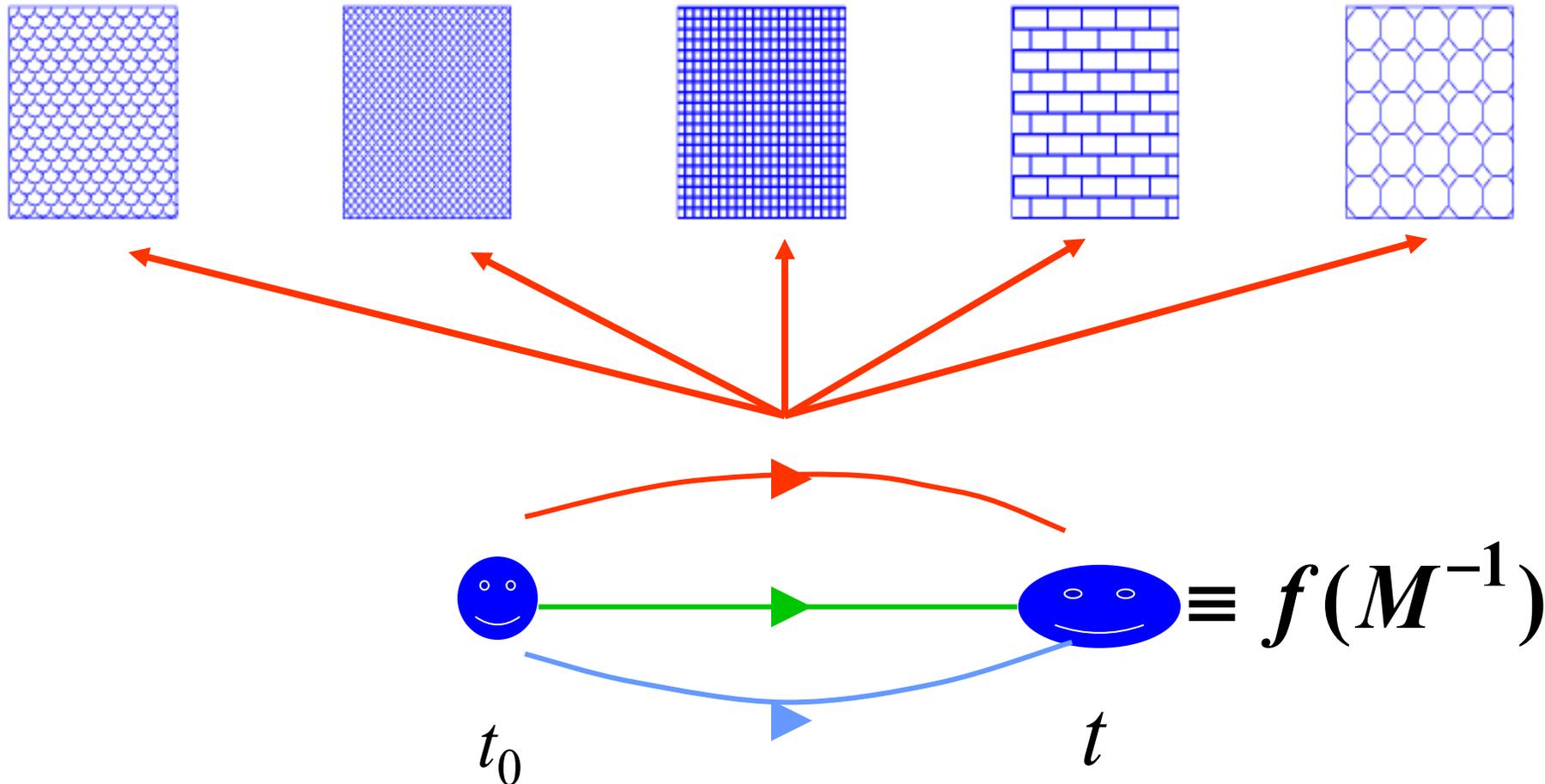
Here also algorithms are constantly being improved



$$\varphi(t) = e^{Ht} \varphi(0) e^{-Ht}$$

$$\begin{aligned}
 G(t, \vec{p}) &= \sum_{\vec{x}} e^{-i\vec{p} \cdot (\vec{x} - \vec{x}_0)} \sum_{n, \vec{q}} \langle \mathbf{0} | \varphi(x) | n, \vec{q} \rangle \langle n, \vec{q} | \varphi(x_0) | \mathbf{0} \rangle \\
 &= \sum_{\vec{x}} e^{-i\vec{p} \cdot (\vec{x} - \vec{x}_0)} \sum_{n, \vec{q}} \langle \mathbf{0} | e^{H(t-t_0) - i\vec{p}' \cdot (\vec{x} - \vec{x}_0)} \varphi(x_0) e^{-H(t-t_0) + i\vec{p}' \cdot (\vec{x} - \vec{x}_0)} | n, \vec{q} \rangle \langle n, \vec{q} | \varphi(x_0) | \mathbf{0} \rangle \\
 &= \sum_{\vec{x}} e^{-i\vec{p} \cdot (\vec{x} - \vec{x}_0)} \sum_{n, \vec{q}} e^{i\vec{q} \cdot (\vec{x} - \vec{x}_0) - E_q^n (t-t_0)} \langle \mathbf{0} | \varphi(x_0) | n, \vec{q} \rangle \langle n, \vec{q} | \varphi(x_0) | \mathbf{0} \rangle \\
 &\approx \sum_{n, \vec{q}} \delta(\vec{p} - \vec{q}) e^{i(\vec{p} - \vec{q}) \cdot \vec{x}_0 - E_q^n (t-t_0)} \langle \mathbf{0} | \varphi(x_0) | n, \vec{q} \rangle \langle n, \vec{q} | \varphi(x_0) | \mathbf{0} \rangle \\
 &= \sum_n e^{-E_p^n (t-t_0)} \left| \langle \mathbf{0} | \varphi(x_0) | n, \vec{p} \rangle \right|^2 \quad \text{Determines how effectively this operator} \\
 &= \sum_n W_n e^{-E_p^n (t-t_0)} \xrightarrow{t \rightarrow \infty} W_1 e^{-E_1^n (t-t_0)} \quad \text{interpolates states 'n' from the vacuum}
 \end{aligned}$$

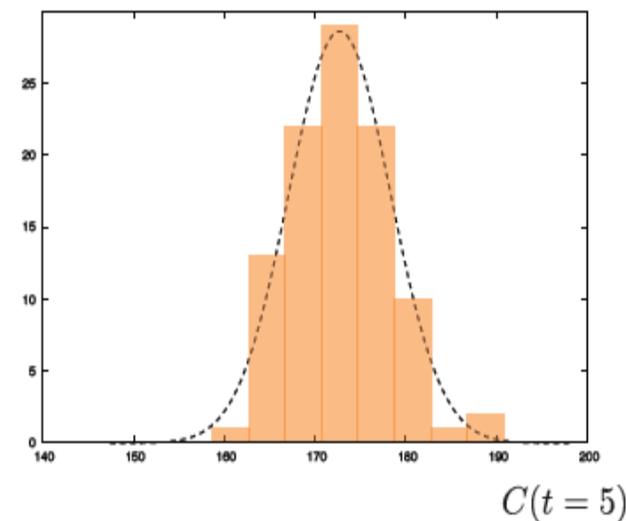
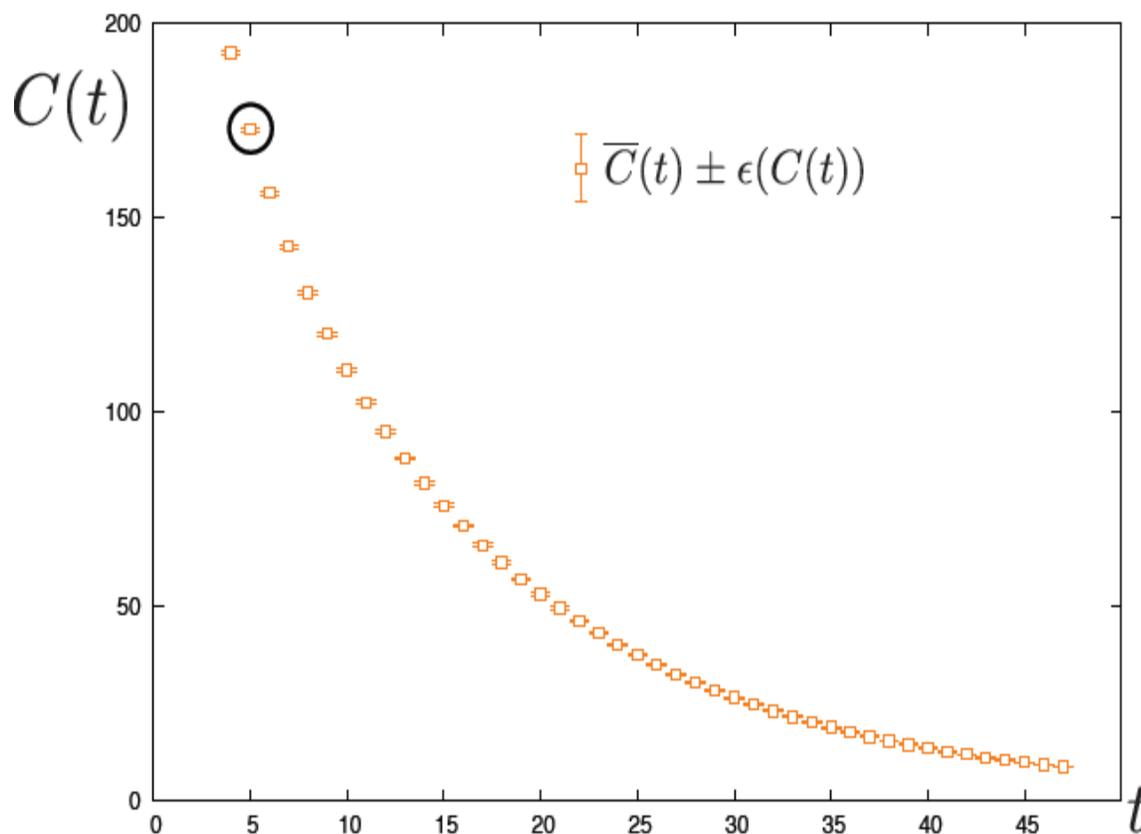
# Measure observable on many independent configurations (ensemble)



$$C(t) = \langle 0 | \sum_{\vec{x}} \bar{\psi}_{\vec{x},t} \gamma_5 \psi_{\vec{x},t} \cdot \bar{\psi}_{\vec{0},0} \gamma_5 \psi_{\vec{0},0} | 0 \rangle$$

so we actually obtain an ensemble  $C^{(i)}(t)$

one entry for each gauge-field configuration  $\{U_{x\mu}\}_{i=1\dots N}$



... how do we relate this information to the mass of the pion ?

# Analysis (Extraction of Mass)

$$G(\tau) = \sum_{i=1}^N W_i e^{-m_i \tau} \underset{\tau \rightarrow \infty}{\approx} W_1 e^{-m_1 \tau}$$

Effective mass :

$$\frac{G(\tau)}{G(\tau+1)} = e^{-m_1 \tau + m_1 (\tau+1)}$$

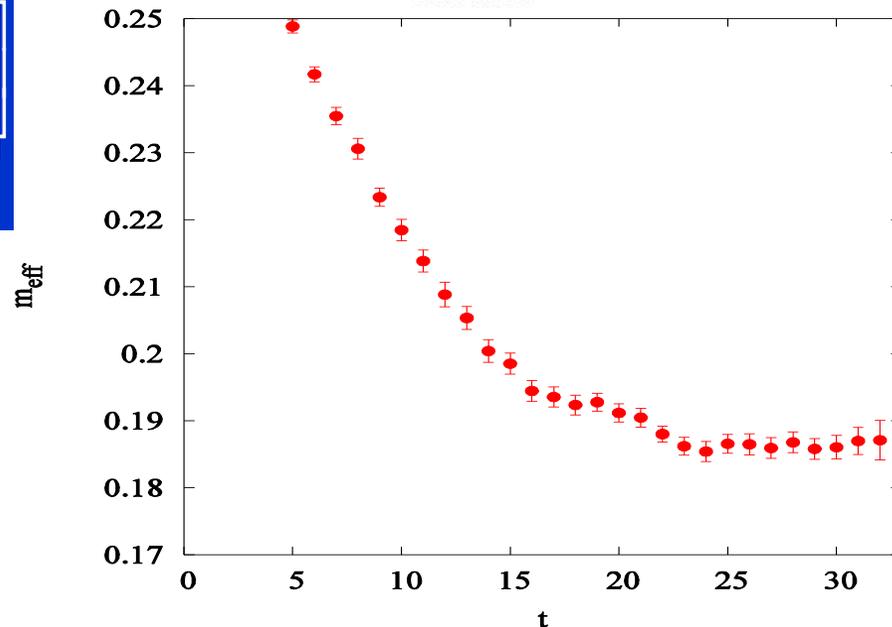
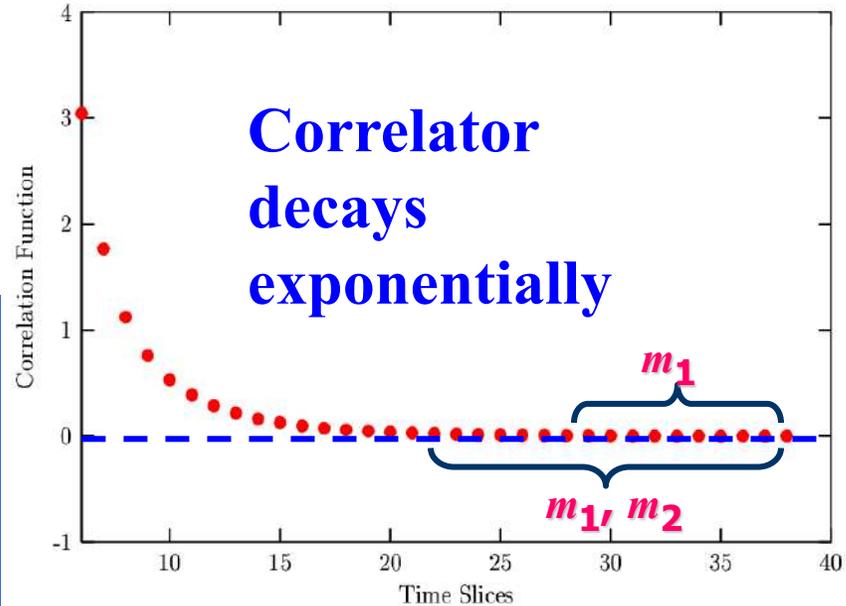
$$m(\tau) = \ln \left[ \frac{G(\tau)}{G(\tau+1)} \right]$$

$$\chi^2 = \sum_{i=1}^N \left[ \frac{f(t_i) - \langle G(t_i) \rangle}{\varepsilon(t_i)} \right]^2$$

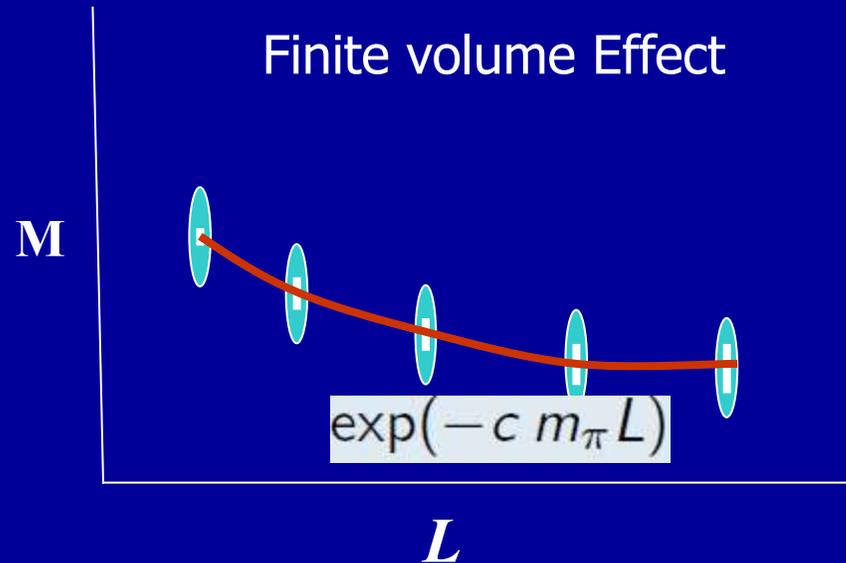
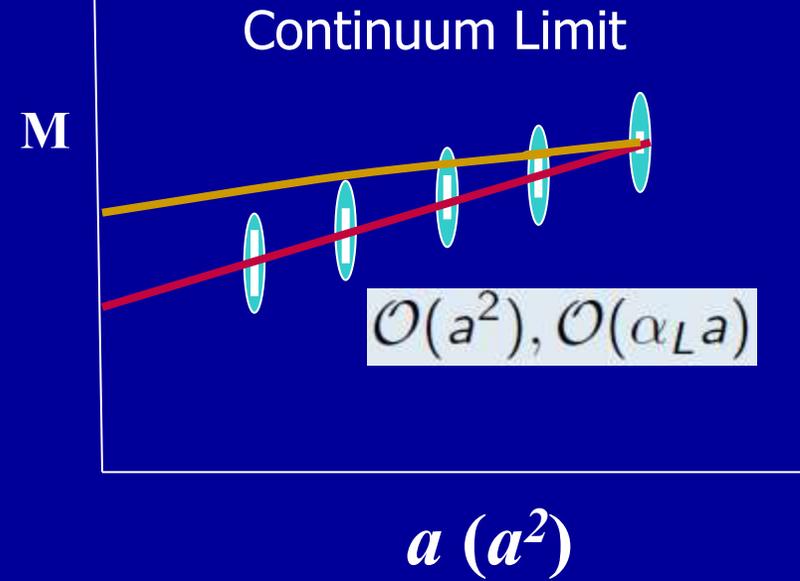
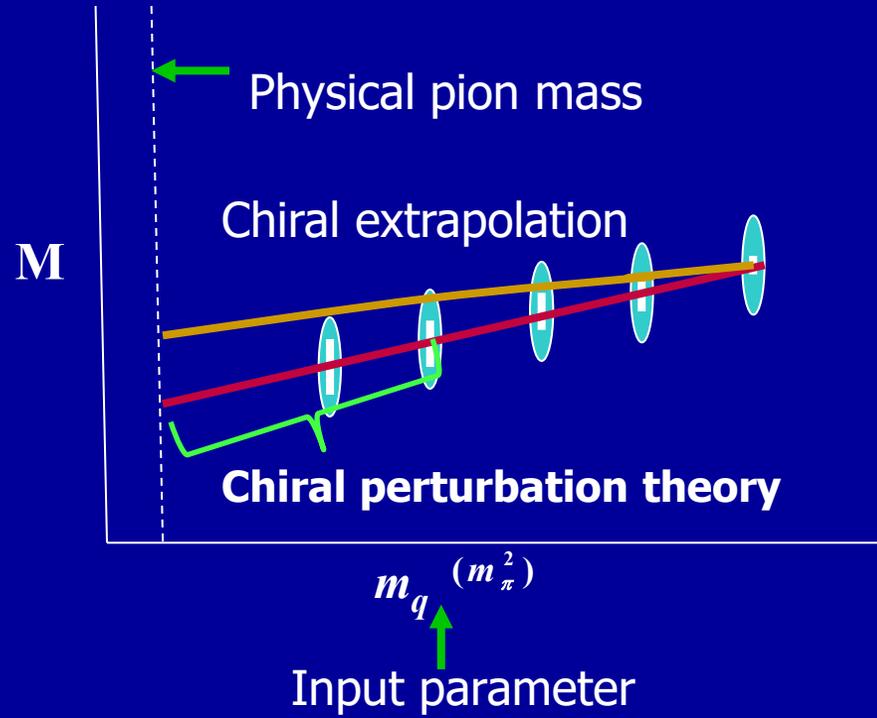
$$e^{-mt} = e^{-(ma)(t/a)}$$

dimensionless integer  
mass timeslices

Determine  $a$  by measuring some physical quantity and compare that to expt, like parameter tuning in any renormalized field theory

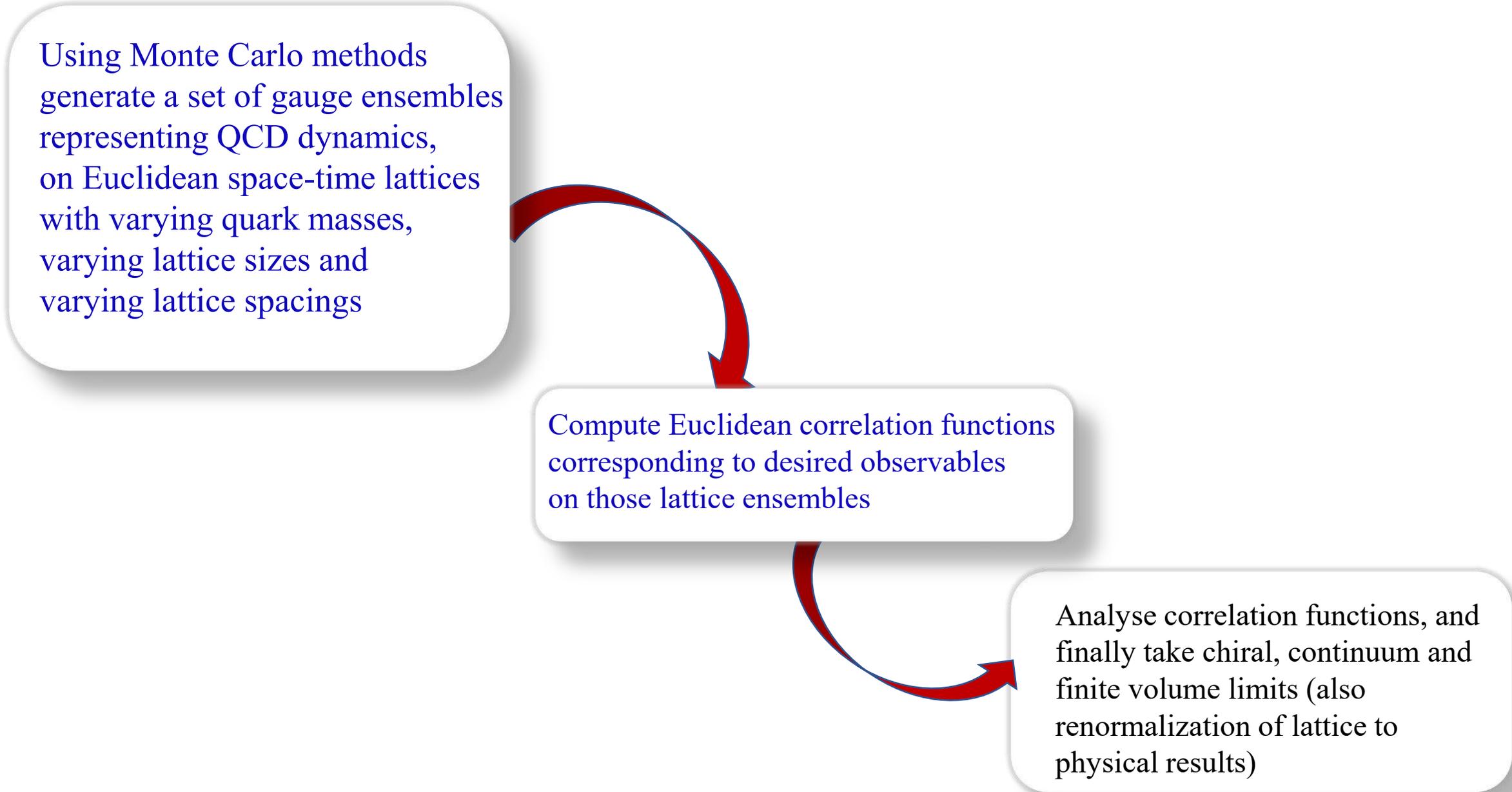


# Control of Sytemetics



# Lattice QCD Workflow

Using Monte Carlo methods generate a set of gauge ensembles representing QCD dynamics, on Euclidean space-time lattices with varying quark masses, varying lattice sizes and varying lattice spacings



```
graph LR; A[Using Monte Carlo methods generate a set of gauge ensembles representing QCD dynamics, on Euclidean space-time lattices with varying quark masses, varying lattice sizes and varying lattice spacings] --> B[Compute Euclidean correlation functions corresponding to desired observables on those lattice ensembles]; B --> C[Analyse correlation functions, and finally take chiral, continuum and finite volume limits (also renormalization of lattice to physical results)];
```

Compute Euclidean correlation functions corresponding to desired observables on those lattice ensembles

Analyse correlation functions, and finally take chiral, continuum and finite volume limits (also renormalization of lattice to physical results)

**QCD**

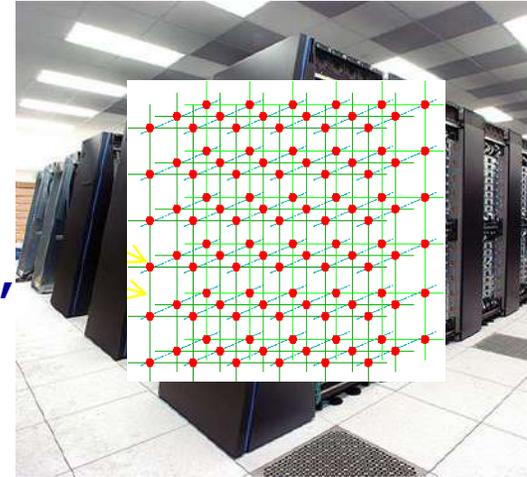


**LQCD**



Euclidian time  
Improved  
discretization

Inputs : lattice spacing,  
quark masses



Algorithmic developments  
AI-ML applications, Algorithms for QC

Continuum,  
Chiral,  
finite volume  
inter-extra-  
polations

Experiments :  
(postdictions,  
predictions)

**Spectra, matrix elements,  
scattering lengths,  
thermodynamic properties  
vacuum structure etc.**

Models (validity)

**Weak decays and  
matrix elements**

**Hadron  
Structure**

**Chiral symmetry**

**Hadron spectroscopy  
and interactions**

**Hadron tomography**

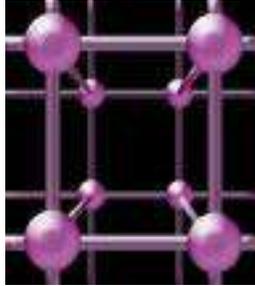
**Nonzero temperature  
and density**

**Physics Beyond  
the Standard Model,  
Supersymmetry**

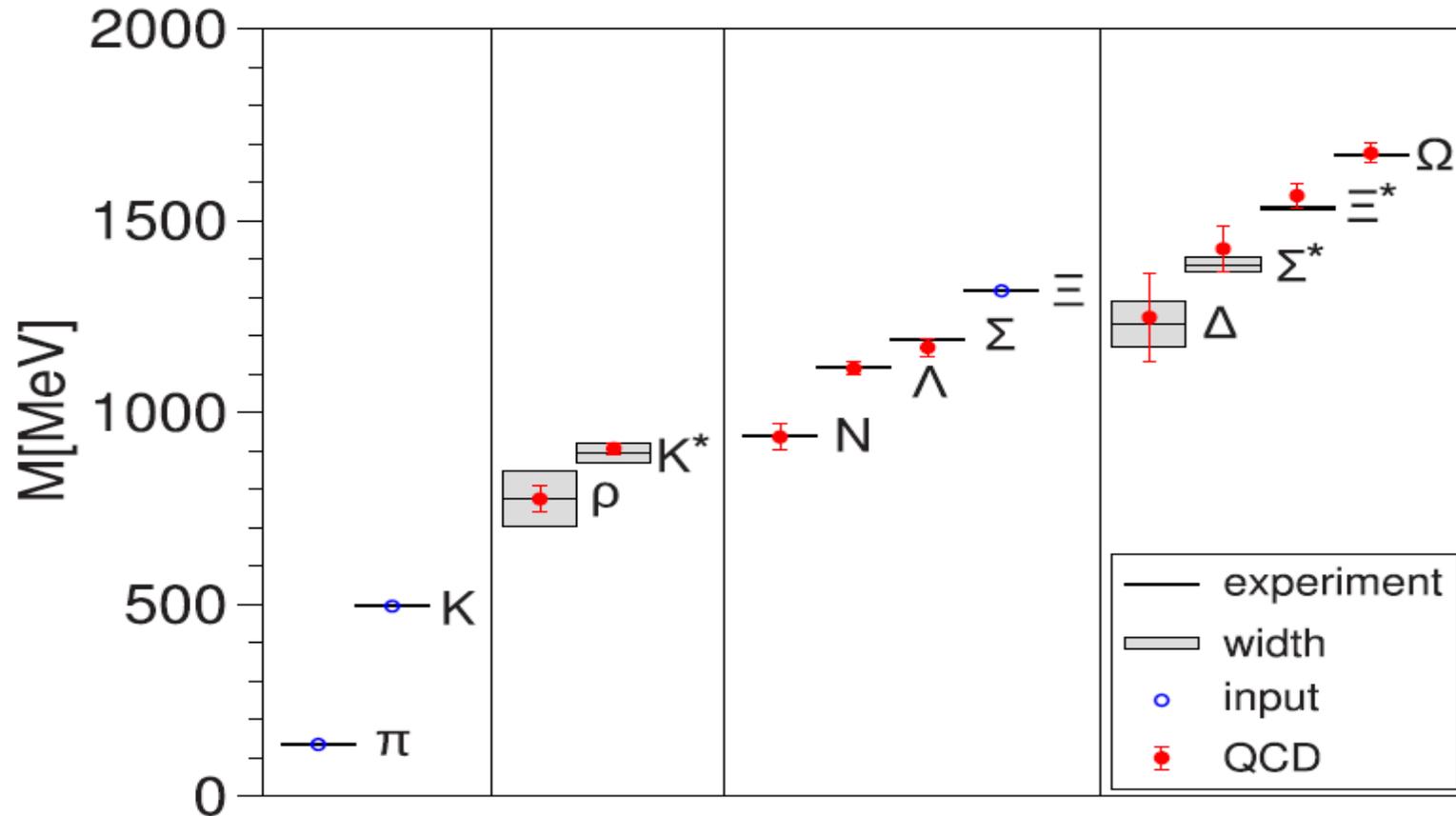
**Standard model  
parameters  
and renormalization**

**Nuclear Physics**

**Vacuum structure  
and confinement**

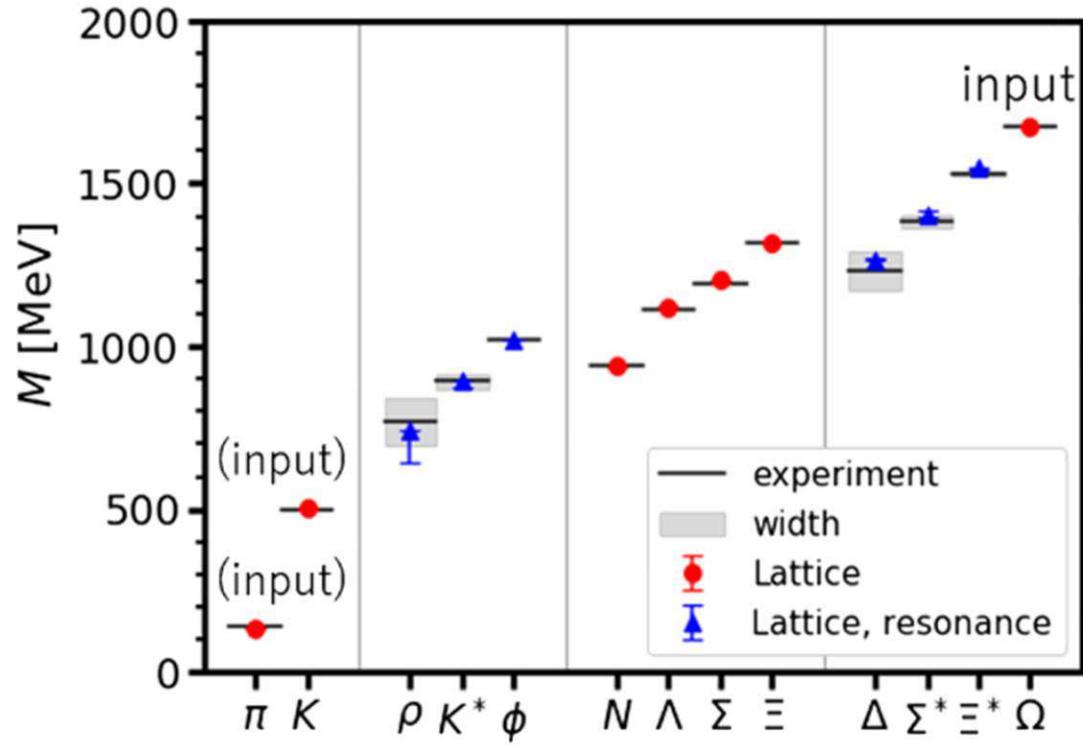


# Hadronic mass generation

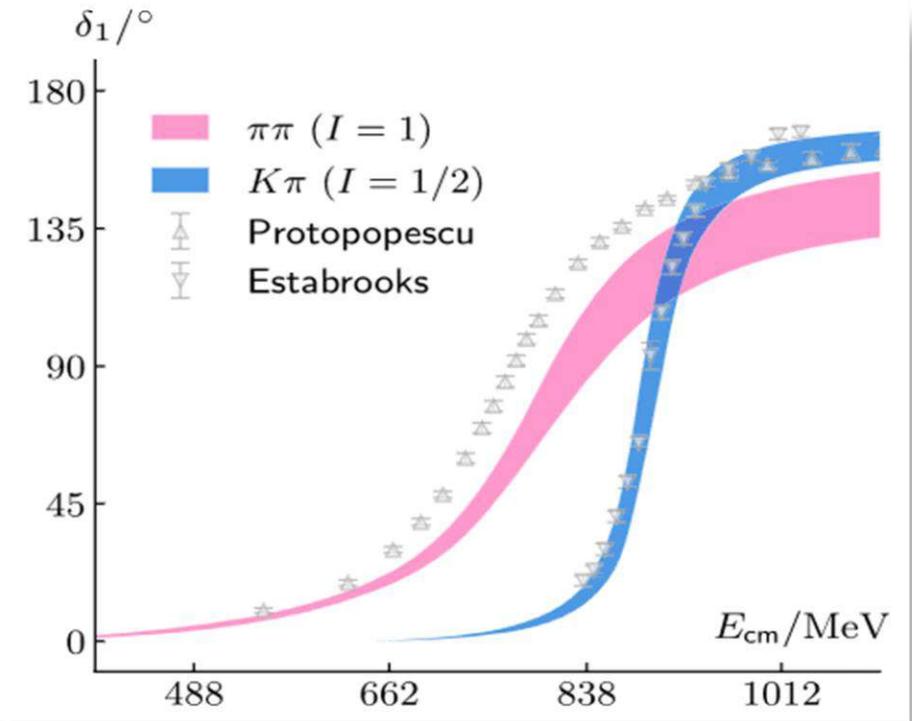


**S. Durr et.al, Science 322, 1224 (2008)**

# Some up-to-date results (incomplete list)



HALQCD: Phys. Rev. D 110, 094502 (2024)



Boyle et al: Phys. Rev. Lett. 134, 111901 (2025)

# Today's common practice

Construct the correlator matrix with your favorite interpolators

$$\begin{bmatrix} C(t)_{00} & C(t)_{01} & \dots \\ \vdots & \ddots & \\ C(t)_{N0} & & C(t)_{NN} \end{bmatrix} v_a = \lambda_a(t, t_0) \begin{bmatrix} C(t_0)_{00} & C(t_0)_{01} & \dots \\ \vdots & \ddots & \\ C(t_0)_{N0} & & C(t_0)_{NN} \end{bmatrix} v_a$$

Distillation:  
[Peardon et al.  
PRD 09]  
[Morningstar et al  
PRD 11]  
CODE: Chroma,  
[github:paboyle  
/grid]  
[github:aportelli  
/hadrons]

# Today's common practice

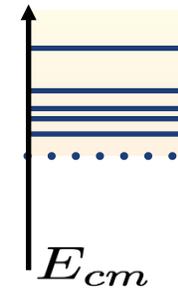
Construct the correlator matrix with your favorite interpolators

$$v_a = \lambda_a(t, t_0) \begin{bmatrix} C(t)_{00} & C(t)_{01} & \dots \\ \vdots & \ddots & \\ C(t)_{N0} & & C(t)_{NN} \end{bmatrix} v_a = \begin{bmatrix} C(t_0)_{00} & C(t_0)_{01} & \dots \\ \vdots & \ddots & \\ C(t_0)_{N0} & & C(t_0)_{NN} \end{bmatrix} v_a$$

Distillation:  
[Peardon et al. PRD 09]  
[Morningstar et al PRD 11]  
CODE: Chroma,  
[github:paboyle/grid]  
[github:aportelli/hadrons]

Fit the principal correlators and extract the finite volume spectra

$$\lambda_\alpha(t, t_0) \sim e^{-E_\alpha(t-t_0)}$$



# Today's common practice

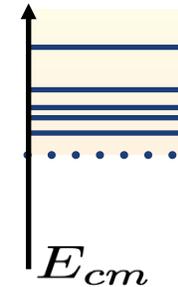
Construct the correlator matrix with your favorite interpolators

$$\begin{bmatrix} C(t)_{00} & C(t)_{01} & \dots \\ \vdots & \ddots & \\ C(t)_{N0} & & C(t)_{NN} \end{bmatrix} v_a = \lambda_a(t, t_0) \begin{bmatrix} C(t_0)_{00} & C(t_0)_{01} & \dots \\ \vdots & \ddots & \\ C(t_0)_{N0} & & C(t_0)_{NN} \end{bmatrix} v_a$$

Distillation:  
 [Peardon et al. PRD 09]  
 [Morningstar et al. PRD 11]  
 CODE: Chroma, [github:paboyle/grid]  
 [github:aportelli/hadrons]

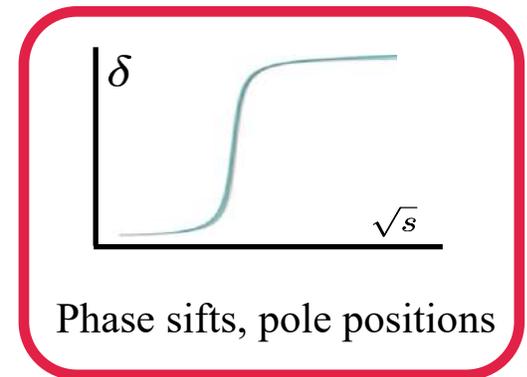
Fit the principal correlators and extract the finite volume spectra

$$\lambda_\alpha(t, t_0) \sim e^{-E_\alpha(t-t_0)}$$



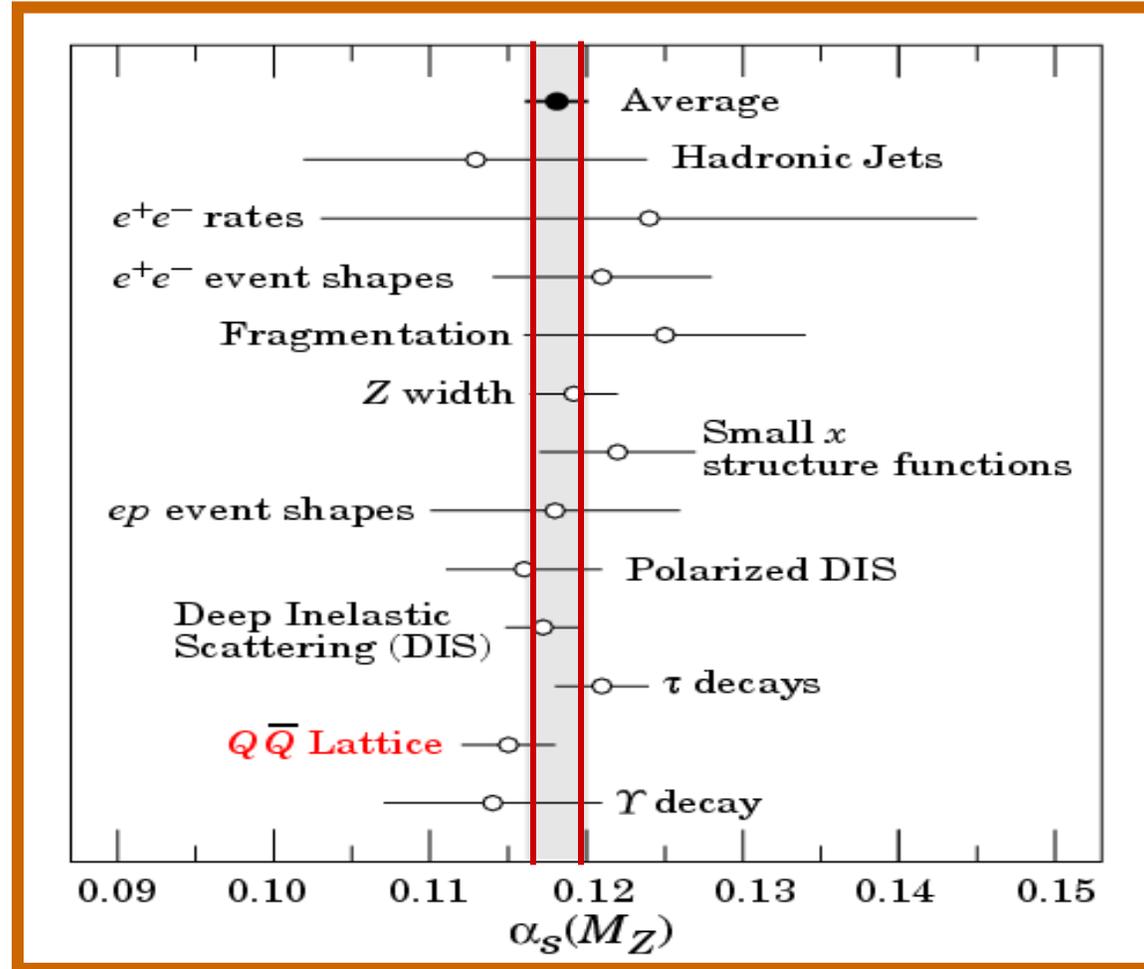
Solve for the quantization condition, Analytically continue the amplitudes, look for poles in the complex energy plane

$$\det [F^{-1} + \mathcal{M}] = 0 \longrightarrow$$

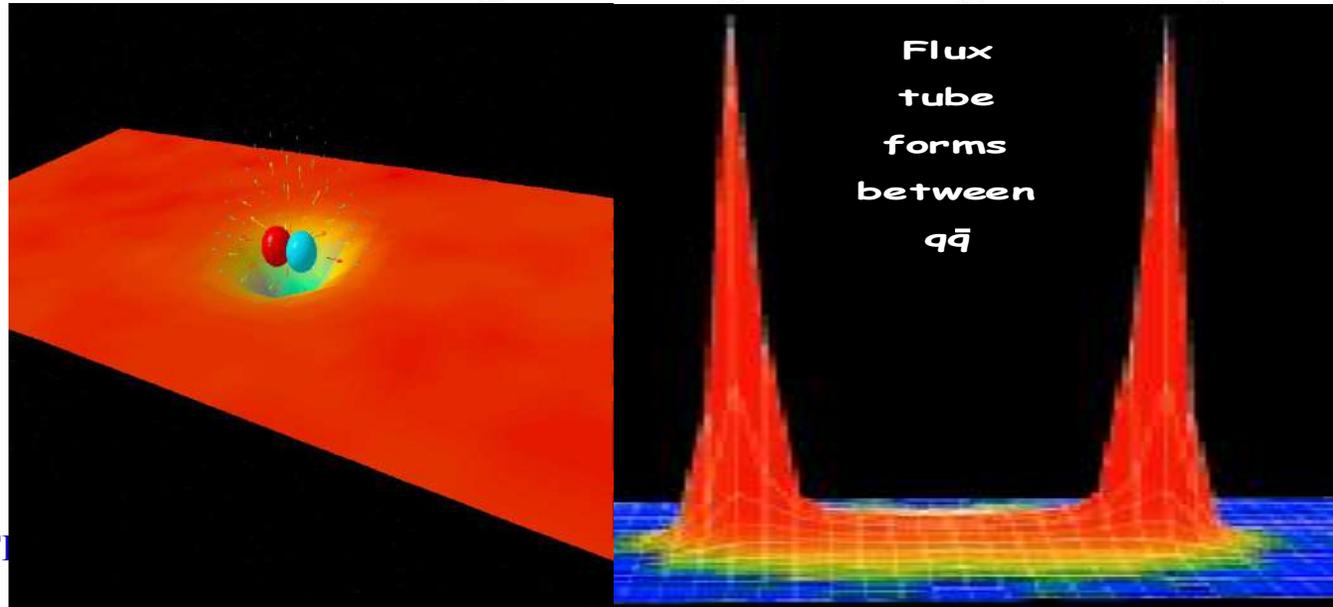
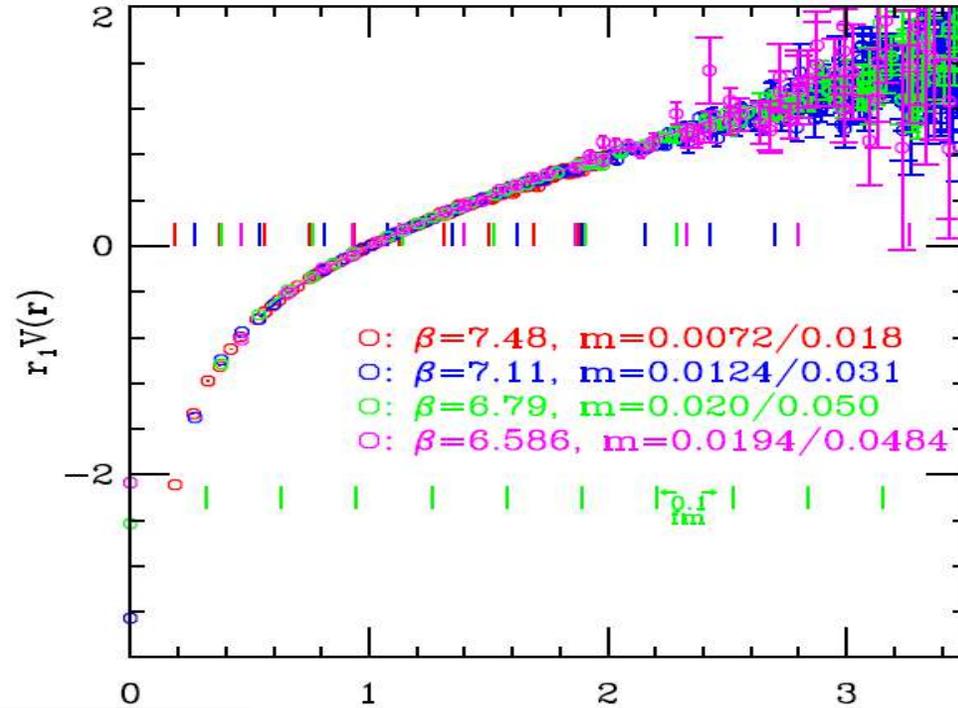


# The Strong Coupling Constant

Lattice result :  $0.115 \pm 0.03$ , Combined average :  $0.118 \pm 0.002$

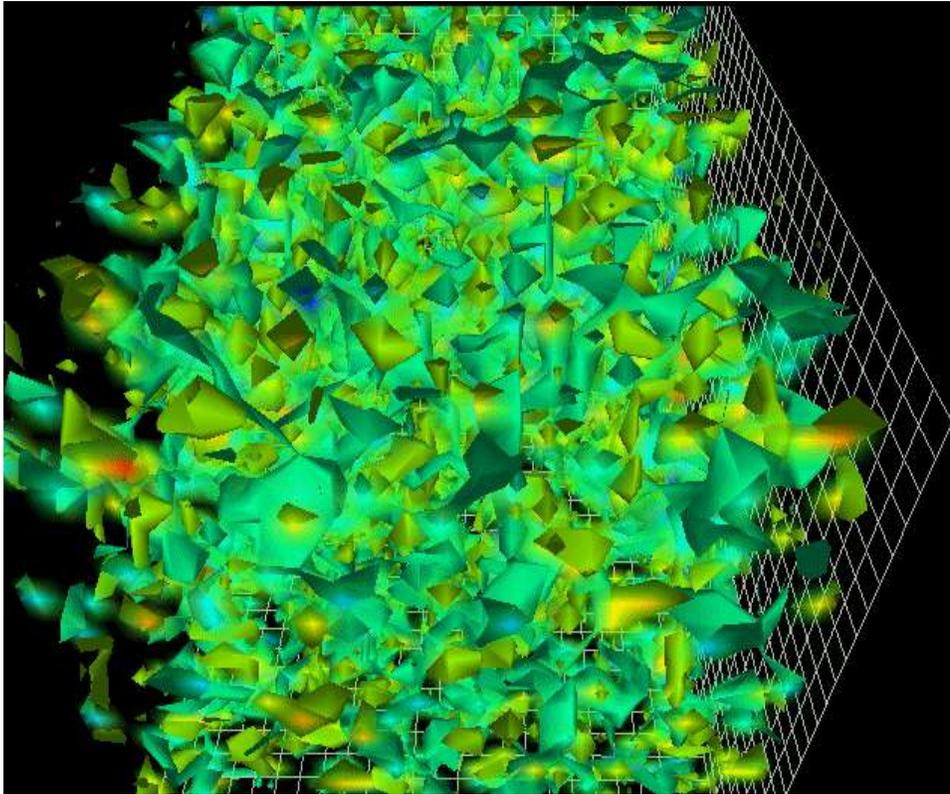


# Static Quark Potential

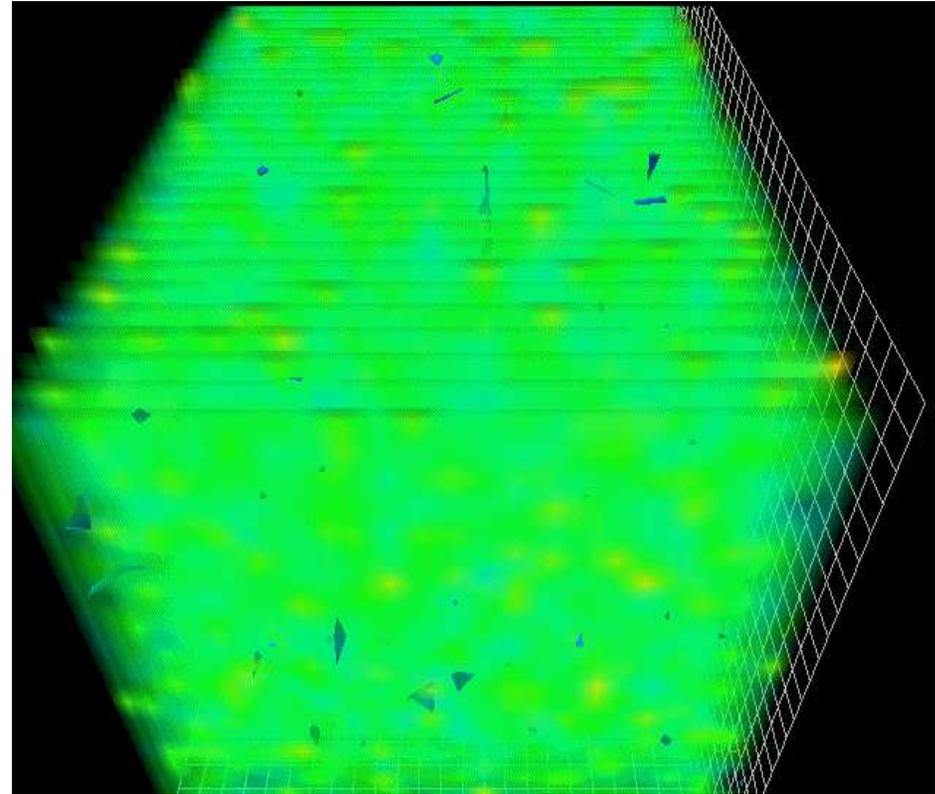


Action density  
Bali et. al

# Topological Structure of QCD vacuum



**Topological charge density**



**Action density**

**@D. Lienweber**

**Topological charge can be calculated  
by measuring zero modes using overlap action**

# Decay constants from Lattice QCD

In SM :

$$\Gamma(H \rightarrow \ell\nu) = \frac{M_H}{8\pi} f_H^2 |G_F V_{Qq}^* m_\ell|^2 \left(1 - \frac{m_\ell^2}{M_H^2}\right)^2,$$

**Pseudoscalar to vacuum matrix element of the axial current  $\longrightarrow$  pseudoscalar decay constant**

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle = i p^\mu f_H,$$

$$\langle 0 | \mathcal{A}^\mu | H(p) \rangle (M_H)^{-1/2} = i(p^\mu / M_H) \phi_H$$

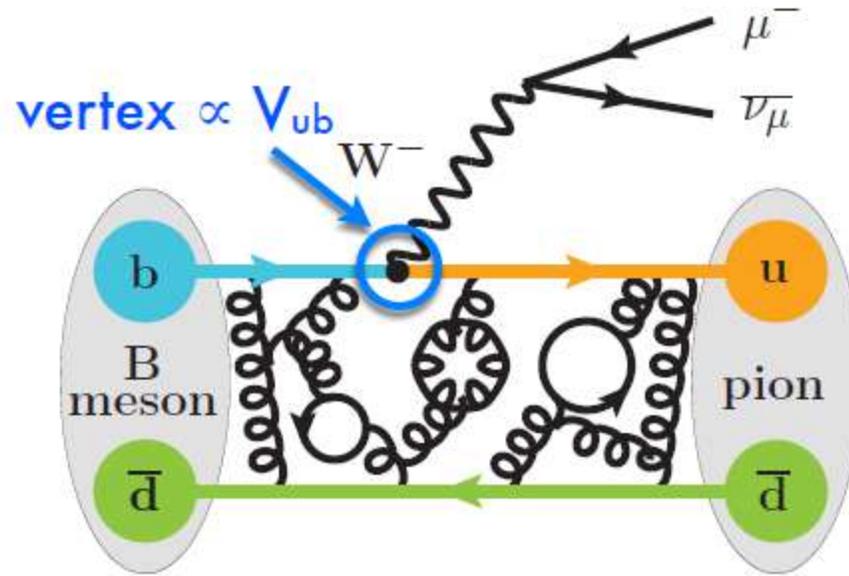
$$f_H = \phi_H / \sqrt{M_H}$$

$H$	$\mathcal{A}^\mu$	$V$
$D$	$\bar{d}\gamma^\mu\gamma^5 c$	$V_{cd}^*$
$D_s$	$\bar{s}\gamma^\mu\gamma^5 c$	$V_{cs}^*$
$B$	$\bar{b}\gamma^\mu\gamma^5 u$	$V_{ub}$
$B_s$	$\bar{b}\gamma^\mu\gamma^5 s$	—

**Renormalization constant (to match with continuum physics) :**

$$Z_{A^\mu} A^\mu \doteq \mathcal{A}^\mu + \mathcal{O}(\alpha_s a \Lambda f_i(m_Q a)) + \mathcal{O}(a^2 \Lambda^2 f_j(m_Q a))$$

# Weak matrix elements



$$\frac{d\Gamma(B \rightarrow \pi l \nu)}{dq^2}, \frac{d\Gamma(B \rightarrow D^{(*)} l \nu)}{dw}, \dots$$



$$(\text{Experiment}) = (\text{known}) \times (\text{CKM factors}) \times (\text{Hadronic Matrix Element})$$

Compute nonperturbative QCD parameters  
(decay constants, form factors, B-parameters,...)  
numerically with **LATTICE QCD**



@Van de Water

# CKM matrix elements and lattice calculations

$$\left( \begin{array}{ccc} \mathbf{V}_{ud} & \mathbf{V}_{us} & \mathbf{V}_{ub} \\ \pi \rightarrow l\nu & K| \rightarrow l\nu & B \rightarrow l\nu \\ & K \rightarrow \pi l\nu & B \rightarrow \pi l\nu \\ \\ \mathbf{V}_{cd} & \mathbf{V}_{cs} & \mathbf{V}_{cb} \\ D \rightarrow l\nu & D_s \rightarrow l\nu & B \rightarrow D l\nu \\ D \rightarrow \pi l\nu & D \rightarrow K l\nu & B \rightarrow D^* l\nu \\ \\ \mathbf{V}_{td} & \mathbf{V}_{ts} & \mathbf{V}_{tb} \\ \langle B_d | \bar{B}_d \rangle & \langle B_s | \bar{B}_s \rangle & \\ B \rightarrow \pi ll & B \rightarrow K ll & \end{array} \right)$$

**"Gold plated"**

processes on the lattice  $\rightarrow$  **CKM matrix elements**

- One hadron in the initial state and zero or one hadron in the final state
- Stable hadrons (that is narrow or far from threshold  $\rightarrow$  easier to study on lattice)
- Chiral extrapolation is controllable



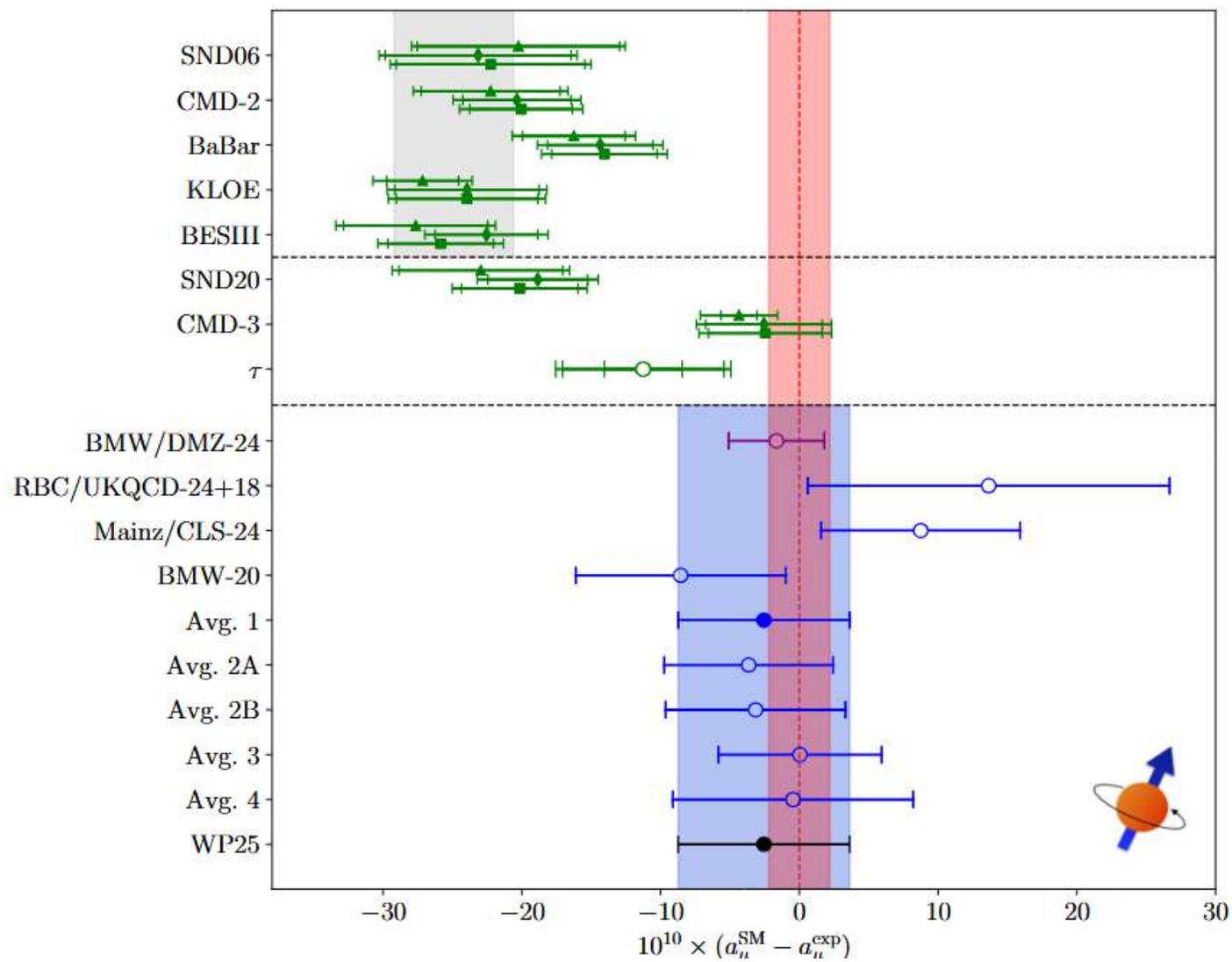
# Various matrix elements

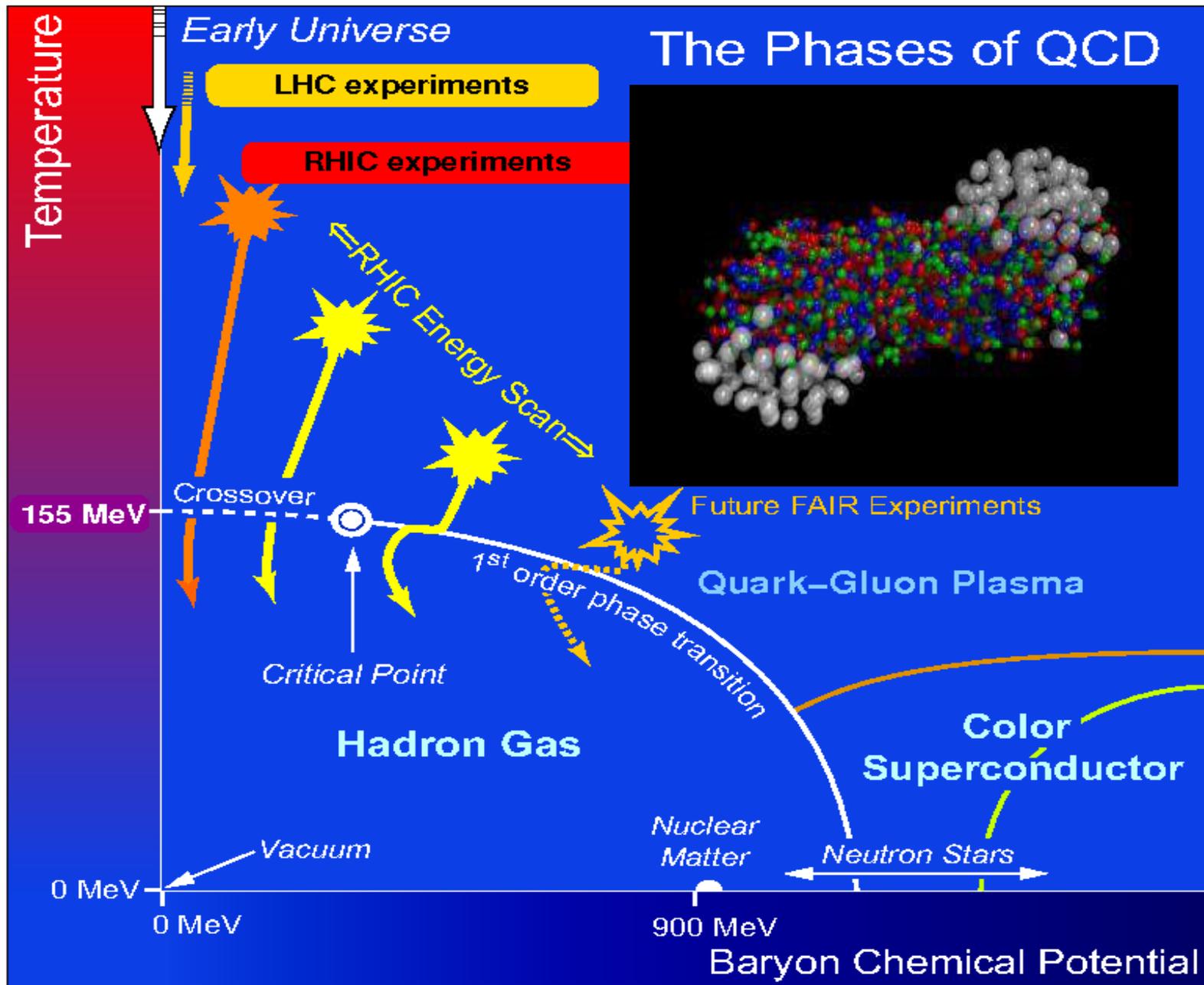
- Electromagnetic, scalar, axial and tensor form factors are being investigated rigorously by various lattice groups.
- Quark-gluon spin and orbital angular momentum are also being studied on lattice. Matrix elements of energy momentum tensor ((Liu), PRL 118, 102001(2017))
- GPD, TMD and also PDFs are being investigated using lattice QCD

## Some other lattice calculations :

- Muon  $g-2$ ,
- $K_0$  oscillation,
- $\epsilon/\epsilon'$

# Muon $g-2$





# Lattice QCD and Cosmology-Astrophysics

## Matter at extreme conditions

- Extreme temperature : Study of early Universe : QGP, equation of state, Phase diagram, Phase transition, Critical Point
- Extreme density : Neutron star
- Extreme magnetic fields : Magnetars, early universe?
- Search for dark matter

# QCD properties

## ➤ Quark confinement :

- No quarks and gluons in the physical spectrum
- The physical degrees of freedom are hadrons
- Order parameter : Polyakov Loop

## ➤ Chiral symmetry breaking :

- Hadrons are massive
- Order parameter : quark condensate

The relevant order parameter : Polyakov loop

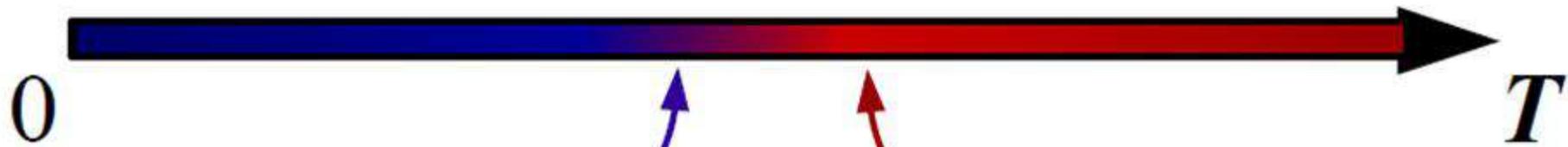
$$L(x) = \frac{1}{3} \text{Tr} \mathcal{P} \exp \left[ i \int_0^{1/T} d\tau A_4(x, \tau) \right]$$

Related to the free energy of a single quark

$$\langle L \rangle = \exp(-F_q/T)$$

Confinement-deconfinement :

$$\begin{aligned} \langle L \rangle &= 0, & \text{low } T, \\ \langle L \rangle &\neq 0, & \text{high } T \end{aligned}$$

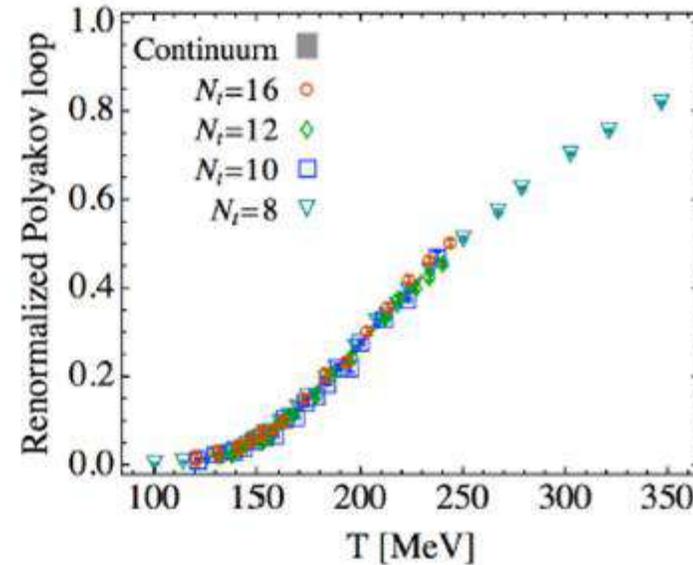
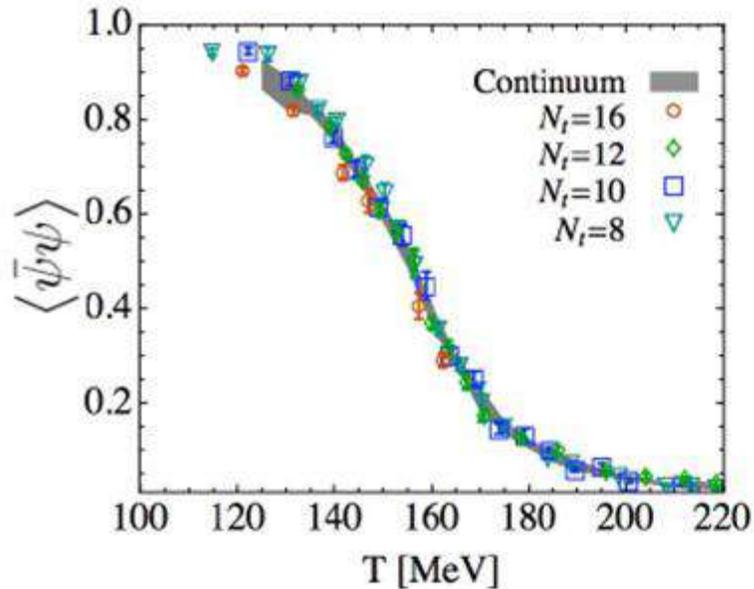


Restoration of  
the chiral symmetry

Deconfinement  
transition

$$T_{\text{chiral}} \approx 155 \text{ MeV}$$

$$T_{\text{deconf}} \approx 170 \text{ MeV}$$



@BMW, HOTQCD

$$T_c(\bar{\psi}\psi) = 155(3)(3) \text{ MeV} = 1.95(5) \cdot 10^{12} \text{ K.}$$

(Cross-over: other quantities may have different pseudocritical temperatures.)

# Finite density – sign problem

Partition function with chemical potential :

$$\begin{aligned} Z &= \text{Tr} e^{-\beta(H-\mu N)} = \int DUD\bar{\psi} D\psi e^{-(S_G + \bar{\psi}\Delta\psi)} \\ &= \int DU \det \Delta e^{-S_G} \quad \Delta = D_\nu \gamma_\nu + m + \mu\gamma_0 \end{aligned}$$

Now,

$$\begin{aligned} U_\mu(x) &= e^{iA_\mu(x)} \\ U_t(x) &\rightarrow e^\mu U_t(x) \\ U_t^\dagger(x) &\rightarrow e^{-\mu} U_t^\dagger(x) \end{aligned}$$

At  $\mu = 0$

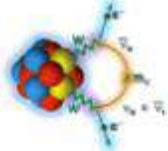
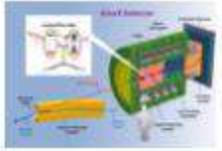
$$(\det \Delta)^* = \det \Delta^\dagger = \det \gamma_5 \Delta \gamma_5 = \det \Delta \quad \Rightarrow \det \Delta : \text{real}$$

However, at  $\mu \neq 0$

$$\Delta^\dagger = -D_\nu \gamma_\nu + m + \mu\gamma_0 \neq \gamma_5 \Delta \gamma_5 \Rightarrow \det \Delta : \text{complex}$$

**Cannot do Monte-Carlo : Sign problem**

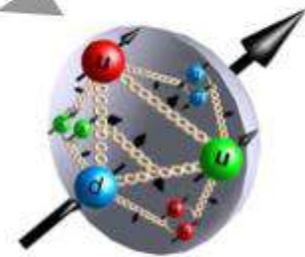
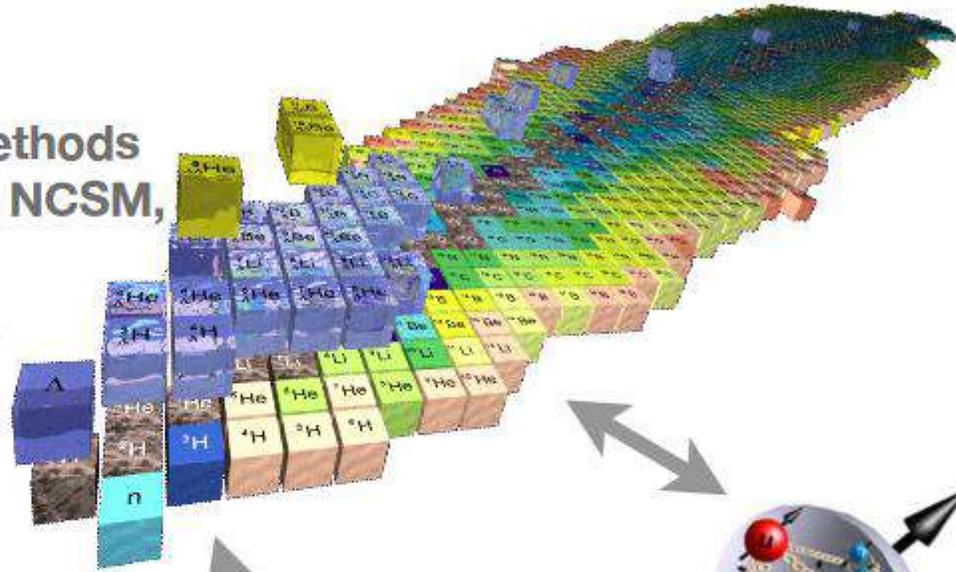
# Emergence of Nuclei from QCD



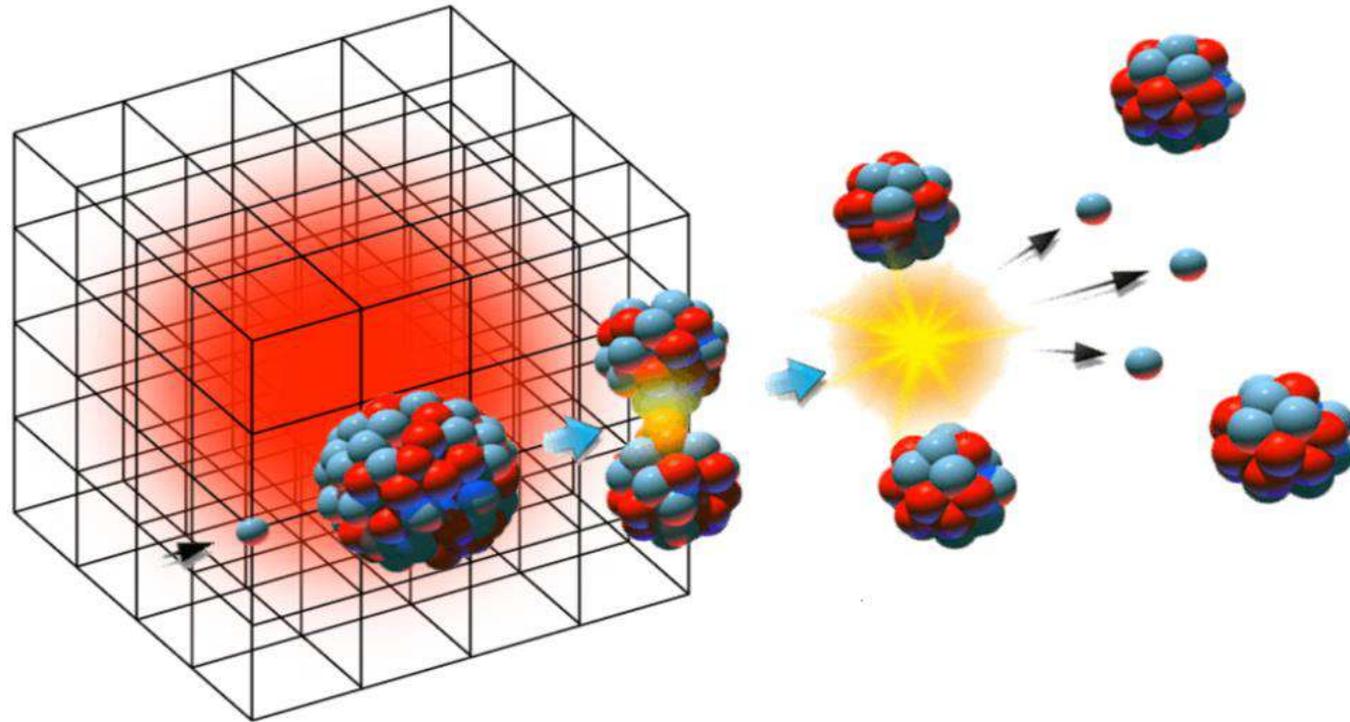
	2N force	3N force	4N force
LO		—	—
NLO		—	—
		—	—
N <sup>2</sup> LO			—
N <sup>3</sup> LO			—

Nuclear Forces

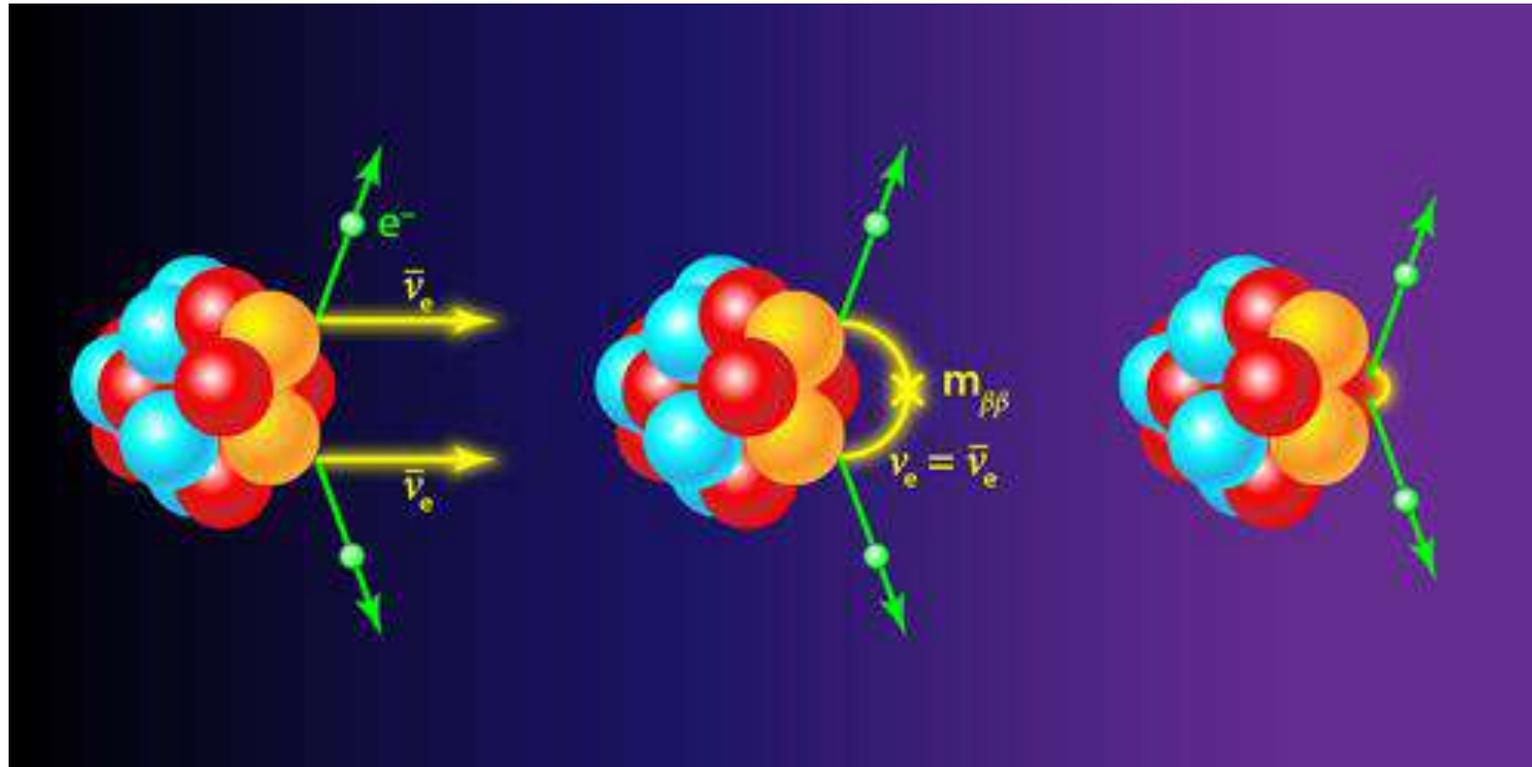
Many-Body Methods  
e.g. SM, GFMC, NCSM,  
DFT,...



# Can we study light nuclei and their properties from first-principles?



# Weak nuclear processes: BSM Physics and Various nuclear matrix elements



# Challenges in Lattice QCD

- How to go to smaller lattice spacings (freezing topology) with reasonable computing time? AI-ML
- How to compute nuclear tomography with precision?
- How to solve sign problem? (physics of neutron star, QCD phase diagram, condensed matter systems with fermions). Is it an unsolvable problem with classical computers? Quantum computing?
- How to calculate precision spectra of multi-hadron states in nuclear physics, Deuteron to Carbon, with reasonable computing time? Quantum computing?
- How to deal nuclear physics reactions with precision?
- How to deal with chiral gauge theories?



**Computing resources for LQCD**



# Books

- **M. Creutz: *Quarks, Gluons and Lattices*; (Cambridge Univ. Press: Cambridge, 1983)**
- **C. Rebbi: *Lattice Gauge Theories and Monte Carlo Simulations*; (World Scientific: Singapore, 1983)**
- **M. Creutz: *Quantum Fields on the Computer*; (World Scientific: Singapore, 1992)**
- **H. J. Rothe: *Lattice Gauge Theories - An Introduction*; (World Scientific: Singapore, 1992)**
- **I. Montvay and G. Münster: *Quantum Fields on a Lattice*; (Cambridge University Press: Cambridge, 1994)**
- **J. Smit : *Introduction to Quantum Fields on a Lattice*; (Cambridge University Press: Cambridge, 2002)**
- **T. DeGrand and C. DeTar : *Lattice Methods for Quantum Chromodynamics*; (World Scientific: Singapore, 2007)**
- **C. Gattringer and C. B. Lang : *Quantum Chromodynamics on the Lattice (An introductory presentation)*; (Springer: Berlin, Heidelberg, New York, 2009)**