

# Introduction to lattice QCD

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## Plan for first lecture

1. Scalar field theory in the path integral formulation on the lattice;
2. Dirac fermion on the lattice;
3. Gauge fields in the continuum, and on the lattice;
4. The QCD path integral on the lattice;
5. Perturbation theory in lattice regularisation;
6. The static potential & asymptotic freedom;
7. Computing hadron masses;
8. Aspects of importance sampling Monte-Carlo.

## Scalar field theory

Expectation values in the Euclidean path integral for a real scalar field  $\phi$ :

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \exp(-S[\phi]) \mathcal{O}[\phi], \quad Z \text{ such that } \langle 1 \rangle = 1, \quad (1)$$

with the measure formally defined as  $D\phi = \prod_x d\phi(x)$ .

In continuum field theory, the action in  $d$  spacetime dimensions is defined as

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

The parameter  $m$  corresponds to the mass of the scalar particle and  $\lambda$  to the strength of its self-interaction.

The lattice regularization

- renders the number of degrees of freedom countable
- makes all correlation functions finite.

Here: consider only cubic lattices,

$$\Lambda = \left\{ x \in \mathbb{R}^d \mid x = an, n \in \mathbb{Z}^d \right\}. \quad (3)$$

The length  $a$  is referred to as the lattice spacing. A lattice field  $\phi(x)$  is the assignment of a real number to every point on the lattice.

We write unit vectors in the four directions as  $\hat{\mu}$ ,  $\mu = 0, 1, \dots, d$ .

Introduce the discretized forward and backward derivatives,

$$\partial_{\mu}\phi(x) = \frac{1}{a}(\phi(x + a\hat{\mu}) - \phi(x)), \quad \partial_{\mu}^*\phi(x) = \frac{1}{a}(\phi(x) - \phi(x - a\hat{\mu})), \quad (4)$$

as well as the symmetric derivative  $\tilde{\partial}_{\mu} = \frac{1}{2}(\partial_{\mu} + \partial_{\mu}^*)$ .

Making the simplest choice to discretize the continuum action:

$$S[\phi] = a^d \sum_x \left( \frac{1}{2}(\partial_{\mu}\phi(x))^2 + \frac{1}{2}m^2\phi(x)^2 + \frac{1}{4!}\lambda\phi(x)^4 \right). \quad (5)$$

## Analysis in momentum space

Representation of lattice fields in momentum space,

$$\tilde{\phi}(p) = a^d \sum_x e^{-ipx} \phi(x), \quad (6)$$

then clearly  $\tilde{\phi}(p + \frac{2\pi}{a}n) = \tilde{\phi}(p)$  for  $n \in \mathbb{Z}^d$ .

The independent momenta are therefore restricted to the **Brillouin zone**,

$$\mathcal{B} = \left\{ p \in \mathbb{R}^d \mid |p_\mu| \leq \frac{\pi}{a} \right\} \quad (7)$$

and the position-space field can be written as

$$\phi(x) = \int_{\mathcal{B}} \frac{d^d p}{(2\pi)^d} e^{ipx} \tilde{\phi}(p). \quad (8)$$

$\rightsquigarrow$  The lattice introduces a momentum cutoff of order  $\frac{1}{a}$ , since higher-momentum modes do not appear in Eq. (8).

## Exercises

Show that in momentum space the lattice Laplacian acts like

$$\Delta \equiv \sum_{\mu} \partial_{\mu}^* \partial_{\mu} \longrightarrow -\hat{p}^2,$$

where  $\hat{p}_{\mu} \equiv \frac{2}{a} \sin(\frac{1}{2}ap_{\mu})$ .

Show (by contour integration) that the scalar propagator on the lattice is given by

$$\langle \phi(x)\phi(y) \rangle = \int_{\mathcal{B}} \frac{d^d p}{(2\pi)^d} \frac{e^{ip(x-y)}}{\hat{p}^2 + m^2} = \int_{-\pi/a}^{\pi/a} \frac{d^{d-1} \vec{p}}{(2\pi)^{d-1}} \frac{e^{-\Omega_{\vec{p}}|x_0-y_0| + i\vec{p}(\vec{x}-\vec{y})}}{\frac{2}{a} \sinh(a\Omega_{\vec{p}})} \quad (9)$$

with  $\Omega_{\vec{p}} = \frac{2}{a} \operatorname{asinh}(\frac{a}{2} \sqrt{\hat{p}^2 + m^2})$ .

## Symmetries

A very important aspect of any regularization is, how much symmetry of the original action it preserves.

Translations, rotations and boosts are no longer continuous symmetries of the lattice action.

The lattice regularization breaks space-time symmetries, leaving only a discrete subgroup intact.

↪ There is no strictly conserved energy-momentum tensor on the lattice.

## Symmetries (2)

Complex scalar field on the lattice:  $Z = \int D[\phi]D[\phi^*] e^{-S[\phi, \phi^*]}$ ,

$$S[\phi, \phi^*] = a^d \sum_x \left( \partial_\mu \phi(x) \partial_\mu \phi(x)^* + m^2 \phi(x) \phi(x)^* + \frac{1}{4} \lambda (\phi(x) \phi(x)^*)^2 \right).$$

Exercise: Give the expression of the conserved current associated with the U(1) symmetry transformation

$$\phi'(x) = e^{i\alpha} \phi(x), \quad (\phi^*)'(x) = \phi^*(x) e^{-i\alpha}. \quad (10)$$

Answer:

$$j_\mu(x) = i \left( (\partial_\mu \phi)(x) \phi(x + \hat{\mu})^* - (\partial_\mu \phi)(x)^* \phi(x + \hat{\mu}) \right) \quad (11)$$

$$= \frac{i}{a} \left( \phi(x)^* \phi(x + \hat{\mu}) - \phi(x + \hat{\mu})^* \phi(x) \right). \quad (12)$$

Conservation equation in correlation functions: if  $\mathcal{O}_1(x_1), \dots, \mathcal{O}_n(x_n)$  are local operators located at a fixed distance from  $x$ ,

$$\langle \partial_\mu^* j_\mu(x) \mathcal{O}_1(x_1) \dots \mathcal{O}_n(x_n) \rangle = 0.$$



## Fermions (in 4d)

Continuum Euclidean space: the action for a Dirac fermion of mass  $m$  reads

$$S_f[\psi, \bar{\psi}] = \int d^4x \bar{\psi}(x)(\gamma_\mu \partial_\mu + m)\psi(x) \quad (13)$$

where all four  $4 \times 4$  matrices  $\gamma_\mu$  are hermitian and satisfy  $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$ .

Correspondingly, the propagator, which coincides with the Green's function of  $(\gamma_\mu \partial_\mu + m)$ , reads

$$\langle \psi(x)\bar{\psi}(y) \rangle = \int \frac{d^4p}{(2\pi)^4} \frac{e^{ip(x-y)}}{i\not{p} + m} \quad (14)$$

with  $\not{p} \equiv p_\mu \gamma_\mu$ .

Wick's theorem:  $n$ -point functions can be expressed as a sum of products of propagators with appropriate minus signs.

## Wilson's lattice action for fermions

The original 1974 Wilson action for fermions on the lattice reads

$$S_f[\psi, \bar{\psi}] = a^4 \sum_x \bar{\psi}(x) (D_w + m) \psi(x), \quad (15)$$

$$D_w = \sum_{\mu} \left( \gamma_{\mu} \tilde{\partial}_{\mu} - \frac{a}{2} \partial_{\mu}^* \partial_{\mu} \right), \quad \tilde{\partial}_{\mu} = \frac{1}{2} (\partial_{\mu} + \partial_{\mu}^*). \quad (16)$$

- The first-order derivatives are discretized symmetrically in the first term;
- an additional term proportional to the lattice Laplacian operator has been added;
- the first-order derivatives alone would not couple neighbouring points;
- this would lead to unwanted additional light degrees of freedom called 'doublers';
- This problem is fixed by the (dimension-five) Laplacian term.

## Discrete symmetries of the Wilson fermion action

1. Verify that the following transformations are symmetries of the Wilson action: Parity:

$$\psi(x) \rightarrow \gamma_0 \psi(x_0, -\vec{x}), \quad \bar{\psi}(x) \rightarrow \bar{\psi}(x_0, -\vec{x}) \gamma_0 ; \quad (17)$$

Euclidean time reversal: with  $\gamma_5 \equiv \gamma_0 \gamma_1 \gamma_2 \gamma_3$ ,

$$\psi(x) \rightarrow \gamma_0 \gamma_5 \psi(-x_0, \vec{x}), \quad \bar{\psi}(x) \rightarrow \bar{\psi}(-x_0, \vec{x}) \gamma_5 \gamma_0 ; \quad (18)$$

Charge conjugation<sup>1</sup>:

$$\psi(x) \rightarrow (\bar{\psi}(x) \gamma_0 \gamma_2)^\top, \quad \bar{\psi}(x) \rightarrow (\gamma_0 \gamma_2 \psi(x))^\top. \quad (19)$$

2. With respect to the obvious scalar product of lattice fermion fields, show that the Wilson-Dirac operator satisfies the  $\gamma_5$ -hermiticity relation

$$D_w^\dagger = \gamma_5 D_w \gamma_5. \quad (20)$$

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<sup>1</sup>This transformation law applies for certain representations of the Dirac matrices, e.g.

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} 0 & -i\sigma^i \\ i\sigma^i & 0 \end{pmatrix}$$

with  $\sigma^i$  the Pauli matrices.

Wick's theorem for fermionic correlation functions has a representation in terms of a path integral over Grassmann variables.

Let  $\eta_1, \dots, \eta_n$  and  $\bar{\eta}_1, \dots, \bar{\eta}_n$  be anticommuting generators of a Grassmann algebra.

Let also  $\zeta$  and  $\bar{\zeta}$  be vectors of anticommuting variables and  $A$  an  $n \times n$  c-number matrix.

Define the 'integration' rules as

$$\int d\eta_i = \int d\bar{\eta}_i = 0, \quad \int d\eta_i \eta_j = \int d\bar{\eta}_i \bar{\eta}_j = \delta_{ij}, \quad \int d\eta_i \bar{\eta}_j = \int d\bar{\eta}_i \eta_j = 0 ;$$

then the Gaussian integral for the generating functional

$$Z[\zeta, \bar{\zeta}] \equiv \int d\eta_1 \dots d\eta_n d\bar{\eta}_1 \dots d\bar{\eta}_n \exp \left( - \sum_{i,j} (\bar{\eta}_i A_{ij} \eta_j) + \sum_i (\bar{\eta}_i \zeta_i + \bar{\zeta}_i \eta_i) \right) \quad (21)$$

is given by

$$Z[\zeta, \bar{\zeta}] = c \cdot \det(A) \exp \left( \sum_{i,j} \bar{\zeta}_i (A^{-1})_{ij} \zeta_j \right). \quad (22)$$

NB. The determinant appears in the numerator rather than in the denominator!

## Path-integral representation of fermionic $n$ -point functions

$$\begin{aligned} & \langle \psi(x_1) \dots \psi(x_n) \bar{\psi}(y_1) \dots \bar{\psi}(y_n) \rangle \\ &= \frac{1}{Z[0,0]} \int D[\psi] D[\bar{\psi}] \psi(x_1) \dots \psi(x_n) \bar{\psi}(y_1) \dots \bar{\psi}(y_n) \exp(-S_f[\psi, \bar{\psi}]) \end{aligned} \quad (23)$$

with

$$D[\psi] = \prod_{\alpha,x} d\psi_{\alpha}(x), \quad D[\bar{\psi}] = \prod_{\alpha,x} d\bar{\psi}_{\alpha}(x). \quad (24)$$

Since Wick's theorem gives all correlation functions in terms of the propagator, only the latter remains to be specified:

$$\langle \psi(x) \bar{\psi}(y) \rangle = \int_{\mathcal{B}} \frac{d^4 p}{(2\pi)^4} \frac{e^{ip(x-y)}}{i \sum_{\mu} (\hat{p}_{\mu} \gamma_{\mu}) + \frac{1}{2} a \hat{p}^2 + m}. \quad (25)$$

where  $\hat{p}_{\mu} = \frac{1}{a} \sin(ap_{\mu})$ .

## Gauge fields in the continuum

If the fermion field is replaced by an  $N$ -tuple (corresponding to  $N$  'colors'), the global symmetry becomes  $U(N)$ . Here we will focus on the  $SU(N)$  subgroup.

We will use traceless hermitian generators  $T^a$ , normalized according to  $\text{Tr} \{T^a T^b\} = \frac{1}{2} \delta^{ab}$  and satisfying the commutation relations  $[T^a, T^b] = i f^{abc} T^c$ .

The structure constants  $f^{abc}$  are real and totally antisymmetric. With  $\Lambda(x) \in SU(N)$ , the gauge-transformed fields are defined as

$$\begin{aligned}\psi^\Lambda(x) &= \Lambda(x)\psi(x), & \bar{\psi}^\Lambda(x) &= \bar{\psi}(x)\Lambda(x)^{-1}, \\ A_\mu^\Lambda(x) &= \Lambda(x)A_\mu(x)\Lambda(x)^{-1} + i\Lambda(x)\partial_\mu\Lambda(x)^{-1}.\end{aligned}\tag{26}$$

The covariant derivative of the fermion field

$$D_\mu\psi(x) = (\partial_\mu - iA_\mu(x))\psi(x)\tag{27}$$

then transforms like  $\psi(x)$  and the fermion action

$$S_f[\psi, \bar{\psi}] = \int d^4x \bar{\psi}(x)(\gamma_\mu D_\mu + m)\psi(x)\tag{28}$$

is gauge invariant.

## Gauge fields in the continuum (2)

The field strength tensor

$$G_{\mu\nu} = G_{\mu\nu}^a T^a \equiv \partial_\mu A_\nu - \partial_\nu A_\mu - i[A_\mu, A_\nu] \quad (29)$$

transforms covariantly,

$$G_{\mu\nu}^\Lambda(x) = \Lambda(x) G_{\mu\nu}(x) \Lambda(x)^{-1}. \quad (30)$$

In particular, the gauge action

$$S_g[A] = \frac{1}{2g_0^2} \int d^4x \operatorname{Tr} \{ G_{\mu\nu}(x) G_{\mu\nu}(x) \} \quad (31)$$

is gauge invariant.

## Gauge fields on the lattice

We follow the same logic on the lattice. The *raison d'être* of the gauge field is to make finite-difference operators gauge covariant.

If  $U_\mu(x) \in SU(N)$  is a variable which transforms as

$$U_\mu^\Lambda(x) = \Lambda(x)U_\mu(x)\Lambda(x + a\hat{\mu})^{-1}, \quad (32)$$

then

$$\nabla_\mu \psi(x) \equiv \frac{1}{a} (U_\mu(x)\psi(x + a\hat{\mu}) - \psi(x)), \quad (33)$$

$$\nabla_\mu^* \psi(x) \equiv \frac{1}{a} (\psi(x) - U_\mu(x - a\hat{\mu})^{-1}\psi(x - a\hat{\mu})) \quad (34)$$

transform like  $\psi(x)$  itself.

$U_\mu(x)$  is naturally associated with the 'link' joining the points  $x$  and  $x + a\hat{\mu}$ . It is therefore called a 'link variable'.

It can be thought of as the Wilson line  $\exp(i \int A_\mu dx_\mu)$  from  $x$  to  $x + a\hat{\mu}$ .



## The QCD action on the lattice

Gauge invariant lattice fermion action:

$$S_f[\psi, \bar{\psi}, U] = a^4 \sum_x \bar{\psi}(x)(D_w + m_0)\psi(x), \quad D_w = \sum_{\mu} (\gamma_{\mu} \tilde{\nabla}_{\mu} - \frac{a}{2} \nabla_{\mu} \nabla_{\mu}^*). \quad (35)$$

Gauge invariant operators made solely of the link variables:  
the trace of a product of link variables along a *closed* loop is gauge invariant.

The shortest non-trivial Wilson loop on the lattice is the *plaquette*

$$P_{\mu\nu}(x) = U_{\mu}(x)U_{\nu}(x + a\hat{\mu})U_{\mu}(x + a\hat{\nu})^{-1}U_{\nu}(x)^{-1}. \quad (36)$$

The simplest lattice action for the gauge fields is

$$S_g[U] = \frac{2}{g_0^2} \sum_x \sum_{\mu < \nu} \text{Re Tr} \{1 - P_{\mu\nu}(x)\}. \quad (37)$$

QCD action on the lattice:

$$S[U, \psi, \bar{\psi}] = S_f[U, \psi, \bar{\psi}] + S_g[U]. \quad (38)$$

## Lattice QCD path integral

Fermions are represented by Grassmann variables in the path integral.

What about the gauge field measure  $D[U] = \prod_{x,\mu} dU_\mu(x)$  ?

It is required to be 'SU(N) invariant'; that is

$$\int dU f(UV) = \int dU f(VU) = \int dU f(U) \quad \forall V \in SU(N). \quad (39)$$

Expectation values are then defined as<sup>2</sup>

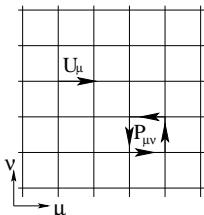
$$\langle \mathcal{O}_1 \dots \mathcal{O}_n \rangle = \frac{1}{Z} \int D[U] \int D[\psi] D[\bar{\psi}] \mathcal{O}_1 \dots \mathcal{O}_n \exp(-S[U, \psi, \bar{\psi}]). \quad (40)$$

**No gauge fixing is needed**, because the volume of the gauge group is finite!

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<sup>2</sup>The partition function  $Z$  is chosen such that  $\langle 1 \rangle = 1$ .

## Recap: discretisation of QCD on a four-dimensional lattice



**Gluons:**  $U_\mu(x) = e^{iag_0 A_\mu(x)} \in SU(3)$

**Quarks:**  $\psi(x) = \text{Dirac Fermion}$

**Gauge invariance** is preserved by the discretisation.

$\rightsquigarrow$  Lattice QCD = 4d statistical mechanics system

Starting point for **Monte-Carlo simulations**, similar to Ising model.

## Perturbation theory in lattice regularisation

The perturbative expansion is based on the idea that for  $g_0$  very small, the path integral should be dominated by the fields that minimize the action. Perturbation theory is then a saddle point expansion around such field configurations.

The gauge fields minimizing  $S_g[U]$  are of the form  $U_\mu(x) = \Lambda(x)\Lambda(x + a\hat{\mu})^{-1}$  and are thus gauge-equivalent to the 'unit-configuration'  $U_\mu(x) = 1 \forall \mu, x$ . The small fluctuations of the link variables are then parametrized by a gauge potential,

$$U_\mu(x) = \exp(ig_0 a A_\mu(x)), \quad A_\mu(x) = A_\mu^a(x) T^a. \quad (41)$$

Jacobian of the change of integration variables is

$$dU_\mu(x) = \left( \prod_{a=1}^{N^2-1} dA_\mu^a(x) \right) \left( 1 + \frac{g_0^2 N}{12} a^2 A_\nu^b(x) A_\nu^b(x) + \dots \right). \quad (42)$$

## Perturbation theory in lattice regularisation (2)

Natural gauge-fixing condition  $\partial_\mu^* A_\mu = 0$ : it is equivalent to the condition that the variation  $\epsilon \partial_\omega A_\mu(x)$  of the field  $A_\mu(x)$  under any infinitesimal gauge transformation  $\Lambda(x) = 1 + i\epsilon\omega(x)$  is orthogonal to  $A_\mu(x)$  itself<sup>3</sup>.

Perturbative expansion of an observable  $\mathcal{O}$ :

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D[U] D[c] D[\bar{c}] \mathcal{O}[U] \exp(-S_{\text{tot}}[A, c, \bar{c}]), \quad (43)$$

where  $c$  and  $\bar{c}$  are Fadeev-Popov ghosts, and

$$S_{\text{tot}}[A, c, \bar{c}] = S_g[U] + S_{\text{gf}}[A] + S_{\text{FP}}[A, c, \bar{c}], \quad (44)$$

$$S_{\text{FP}}[A, c, \bar{c}] = a^4 \sum_x \bar{c}^a(x) \Delta_{\text{FP}}^{ab} c^b(x), \quad \Delta_{\text{FP}}\omega(x) \equiv g_0 \partial_\mu^* \partial_\omega A_\mu(x), \quad (45)$$

$$S_{\text{gf}}[A] = \frac{\lambda_0 a^4}{2} \sum_x \partial_\mu^* A_\mu^a(x) \partial_\nu^* A_\nu^a(x) \quad (46)$$

where it is understood that  $U_\mu(x) = \exp(ig_0 a A_\mu(x))$  and that the integration measure is given by Eq. (42).

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<sup>3</sup>With respect to the scalar product  $(A, B) = a^4 \sum_{x, \mu, a} A_\mu^a(x) B_\mu^a(x)$ .

## Feynman rules (3)

The gauge-field and ghost propagators read

$$\langle A_\mu^a(x) A_\nu^b(y) \rangle = \delta^{ab} \int_{\mathcal{B}} \frac{d^4 p}{(2\pi)^4} \frac{e^{i(p(x-y) + \frac{1}{2}ap_\mu - \frac{1}{2}ap_\nu)}}{\hat{p}^2} \left( \delta_{\mu\nu} - (1 - \lambda_0^{-1}) \frac{\hat{p}_\mu \hat{p}_\nu}{\hat{p}^2} \right), \quad (47)$$

$$\langle c^a(x) c^b(y) \rangle = \delta^{ab} \int_{\mathcal{B}} \frac{d^4 p}{(2\pi)^4} \frac{e^{ip(x-y)}}{\hat{p}^2}. \quad (48)$$

Vertices: e.g. quark-quark-gluon vertex is given by

$$ig_0(T^a)_{ij} \left( \gamma_\mu \cos\left(\frac{1}{2}a(p+p')_\mu\right) - i \sin\left(\frac{1}{2}a(p+p')_\mu\right) \right), \quad (49)$$

with  $p$  the incoming momentum of a quark with color index  $j$  and  $p'$  the outgoing momentum of the other quark line.

## The force between two static quarks

Rectangular Wilson loop of size  $d \times d'$ :

$$W_{\mu\nu}(x, d, d') \equiv \mathcal{L}_\mu(x, d)\mathcal{L}_\nu(x + d\hat{\mu}, d')\mathcal{L}_\mu(x + d'\hat{\nu}, d)^{-1}\mathcal{L}_\nu(x, d')^{-1}, \quad (50)$$

$$\mathcal{L}_\mu(x, d) \equiv U_\mu(x)U_\mu(x + a\hat{\mu}) \dots U_\mu(x + (d - a)\hat{\mu}). \quad (51)$$

Define a *static potential*  $V(R)$  from the loop of size  $R \times T$  via

$$\langle W_{0k}(x, R, T) \rangle \stackrel{T \rightarrow \infty}{\equiv} c(R) \exp(-TV(R)) + \dots \quad (52)$$

It has the interpretation of the potential energy between two static (= infinitely massive) quarks.

To remove an ultraviolet-divergent additive constant, consider the 'static force'

$$F(R) \equiv -\frac{\partial V}{\partial R}.$$

We expect  $R^2 \cdot F(R)$  for a fixed separation  $R$  to reach a finite limit when  $a \rightarrow 0$ .

## One-loop calculation of the static force

A one-loop calculation in the pure SU(N) gauge theory yields the result

$$F(R, g_0, a) \stackrel{R \gg a}{\cong} \frac{C_F}{4\pi R^2} \left( g_0^2 + \frac{11N}{24\pi^2} g_0^4 (\log(R/a) + \bar{c}) + O(g_0^6) \right) \quad (53)$$

with  $C_F = (N^2 - 1)/(2N)$  and  $\bar{c}$  a numerical constant. The form (53) clearly shows that  $R^2 \cdot F(R)$  only has a finite limit when  $a \rightarrow 0$  if  $g_0$  is adjusted as a function of  $a$ .

How exactly it must be adjusted can be worked out by requiring that  $F$  be independent of  $a$  (Callan-Symanzik equation),

$$0 = a \frac{d}{da} F(R, g_0(a), a) = \left( a \frac{\partial}{\partial a} - \beta(g_0) \frac{\partial}{\partial g_0} \right) F(R, g_0, a) \Big|_{g_0=g_0(a)}, \quad (54)$$

with

$$\beta(g_0) \equiv -a \frac{\partial g_0}{\partial a}. \quad (55)$$



## Asymptotic freedom

Inserting the one-loop expression (53) into Eq. (54), one finds

$$\beta(g_0) = -b_0 g_0^3, \quad b_0 = \frac{11N}{48\pi^2}. \quad (56)$$

The definition (55) of  $\beta(g_0)$  can now be read as a differential equation for  $g_0$ . The negative value of the beta function means that  $g_0$  must be made smaller in order to reduce the lattice spacing. The asymptotic solution of the differential equation is

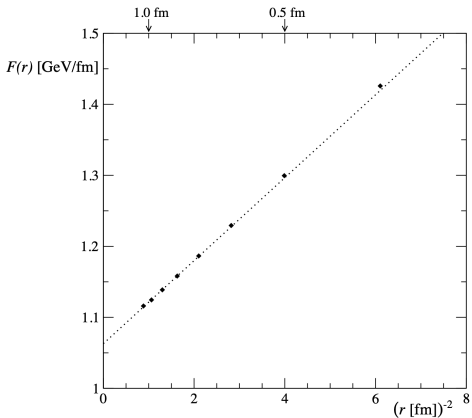
$$g_0^2 = -\frac{1}{2b_0 \log(a\Lambda)} + \dots \quad (57)$$

This is the expression of the **asymptotic freedom** property of QCD at the level of the bare regularized theory: in order to send  $a \rightarrow 0$ , you need to take  $g_0 \rightarrow 0$ .

NB. A mass scale  $\Lambda$  had to be introduced (the ‘Lambda parameter’).

NB. With  $N_f$  quarks:  $b_0 = \frac{11N - 2N_f}{48\pi^2}$ .

## Illustration: Monte-Carlo evaluation of $F(r)$ at long distances



$F(r)$  tends to a finite value at large  $r$ : the 'string tension'.

Fig. from M. Lüscher & P. Weisz, hep-lat/0207003 (pure SU(3) gauge theory simulations).

## Continuum limit and universality

In the statistical-mechanics language, the 'critical point'  $g_0 = 0$ , where correlation lengths in lattice units diverge, is a trivial or Gaussian one.

However, we are interested in non-trivial ratios of correlation lengths, or equivalently ratios of hadron masses, which tend to a finite value when  $a \rightarrow 0$ .

There is a degree of arbitrariness in the choice of the discretization. Ratios of correlation lengths associated with source fields of different quantum numbers do not depend on the details of the discretization (**universality**).

Add suitable terms that accelerate the approach to the continuum: lattice artefacts can be made to vanish as  $a^2$  instead of as  $a$  by adding the Pauli term

$$S \rightarrow S + \frac{i}{4} c_{sw} a^5 \sum_x \bar{\psi}(x) \sigma_{\mu\nu} \hat{G}_{\mu\nu} \psi(x). \quad (58)$$

with a suitable **improvement coefficient**  $c_{sw}$ .

## Hadron spectroscopy: how to compute the pion mass

Heisenberg representation of operator  $\hat{\phi}$  in Euclidean time:

$$\hat{\phi}(x) = e^{Hx_0 - i\vec{P}\cdot\vec{x}} \hat{\phi}(0) e^{-Hx_0 + i\vec{P}\cdot\vec{x}} \quad (59)$$

Suppose we use as an interpolating operator  $\hat{\phi}(x) = \bar{d}\gamma_5 u$  and write

$$\langle 0 | \hat{\phi}(x) | \vec{p} \rangle = \sqrt{\phi_\pi} e^{-E_{\vec{p}}x_0 + i\vec{p}\cdot\vec{x}}.$$

$$\Rightarrow G(x_0, \vec{p}) \equiv \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle 0 | \hat{\phi}(x) \hat{\phi}(0)^\dagger | 0 \rangle \stackrel{x_0 \geq 0}{=} \int d^3x e^{-i\vec{p}\cdot\vec{x}} \langle \phi(x) \phi(0)^\dagger \rangle. \quad (60)$$

Inserting a complete set of states<sup>4</sup> of total momentum  $\vec{p}$ ,

$$1 = \int \frac{d^3\vec{p}}{(2\pi)^3 2E_{\vec{p}}} |\vec{p}\rangle \langle \vec{p}| + (\text{projector onto states of energy } > 3m_\pi), \quad (61)$$

we have

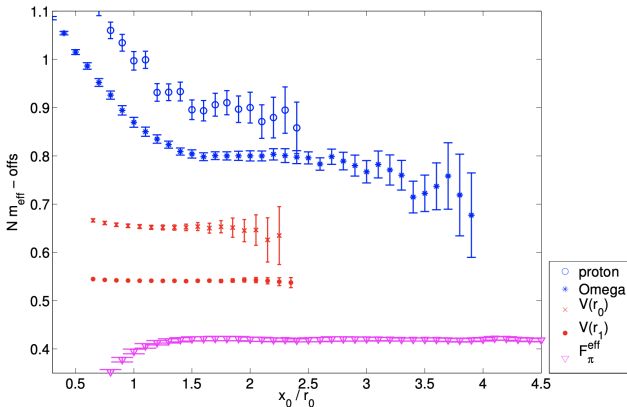
$$G(x_0, \vec{0}) \stackrel{|x_0| \rightarrow \infty}{=} \phi_\pi \frac{e^{-m_\pi |x_0|}}{2m_\pi} + \mathcal{O}(e^{-3m_\pi |x_0|}). \quad (62)$$

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<sup>4</sup>One-particle states are normalized according to  $\langle \vec{p}' | \vec{p} \rangle = (2\pi)^3 2E_{\vec{p}} \delta(\vec{p} - \vec{p}')$ .

## Illustration: effective mass plots

$$m_{\text{eff}}(x_0) = -\frac{d}{dx_0} \log G(x_0, \vec{0})$$



The quality of the signal depends strongly on the hadronic channel.

NB. The length scale  $r_0 \approx 0.5$  fm is defined by the property  $r_0^2 F(r_0) = 1.65$ .

Fig. from R. Sommer 1401.3270. Data is for  $m_{\pi} = 340$  MeV.

## Importance sampling Monte-Carlo methods

First consider the case of the pure gauge theory.

1. Interpret

$$p[U] = \frac{1}{Z} D[U] \exp(-S_g[U]) \quad (63)$$

as a normalized probability distribution on the space of all gauge fields.

2. Generate a representative sample of field 'configurations'  $\{U_1, \dots, U_{N_c}\}$ , meaning that the fraction of the number of configurations belonging to a domain  $\mathcal{D}$  of field space is given by

$$\int_{\mathcal{D}} D[U] p[U],$$

with an error of order  $N_c^{-1/2}$ .

3. Estimate the path-integral expectation value of observables according to

$$\langle \mathcal{O}[U] \rangle = \frac{1}{N_c} \sum_{i=1}^{N_c} \mathcal{O}[U_i] + \mathcal{O}(N_c^{-1/2}). \quad (64)$$

One thus needs a methods of generating the probability distribution (63).

## Importance sampling Monte-Carlo methods (2)

- Usually, a complicated probability distribution must be generated iteratively; a Markov chain is a general method that achieves this.
- The chain starts from an initial configuration and then visits a sequence of configurations according to a given transition probability.
- General criteria exist that guarantee that the configurations visited after a sufficient number of iterations are indeed distributed according to the desired probability distribution

See M. Lüscher, 1002.4232 for details. In recent years, machine-learning techniques have been applied to 'learn' the probability distribution.

## Including dynamical quarks in the simulation

- Fermions are integrated out, yielding the determinant of the Dirac operator in the numerator of the path integral
- The determinant can be treated as part of the probability distribution  $p[U]$ , provided it is positive on all gauge-field configurations.
- The  $\gamma_5$  hermiticity of the Dirac operator implies that the determinant is real. For a doublet of mass-degenerate quarks, the square of the determinant is thus positive.
- Standard algorithm to generate the distribution of gauge fields including the effect of the quarks: hybrid Monte-Carlo algorithm (1987).
- Many important refinements for speed-up and better stability (see e.g. St. Schaefer 1211.5069).
- The generated sample of gauge-field configurations (an 'ensemble') is stored on disk, so that observables can be calculated on the configurations at a later stage.



## Example: two-point function of quark bilinears $\mathcal{O}(x) = \bar{u}(x)\Gamma u(x)$

$\mathcal{O}'(x) = \bar{u}(x)\Gamma' u(x)$  (with  $\Gamma, \Gamma'$  some Dirac matrices) are evaluated as

$$\begin{aligned} \langle \mathcal{O}(x) \mathcal{O}'(y) \rangle &= \frac{1}{N} \sum_{i=1}^{N_c} \left( -\text{Tr}\{\Gamma D^{-1}([U_i]; x, y)\Gamma' D^{-1}([U_i]; y, x)\} \right. \\ &\quad \left. + \text{Tr}\{\Gamma D^{-1}([U_i]; x, x)\} \text{Tr}\{\Gamma' D^{-1}([U_i]; y, y)\} \right) + \mathcal{O}(N_c^{-1/2}), \end{aligned} \quad (65)$$

where  $D$  is the lattice Dirac operator and the traces are taken with respect to color and spin indices.

