Introduction to Lattice Gauge Theories I

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   (d) How to compute typical QCD observables

Literature, text books:

Path integrals:

- R.P. Feynman, A.R. Hibbs, *Quantum mechanics and path integrals*, Mc Graw Hill, 1965
- L.D. Faddeev, in *Methods in field theory*, Les Houches School, 1975
- V. Popov, *Kontinualniye integraly v kvantovoi teorii polya i statisticheskoi fizikye*, Moskva Atomizdat, 1976
- H. Kleinert, *Path integrals in quantum mechanics, statistics, polymer physics*, World Scientific
- G. Roepstorf, *Path integral approach to quantum physics*, Springer
- J. Zinn-Justin, *Path integrals in quantum mechanics*, Oxford University Press (2005), translated into russian

Lattice field theory:

- K. G. Wilson, *Confinement of Quarks*, Phys. Rev. D10 (1974) 2445
- J. Kogut, L. Susskind, *Hamiltonian Formulation of Wilson's Lattice Gauge Theories.*, Phys. Rev. D11 (1975) 395
- M. Creutz, *Quarks, gluons and lattices*, Cambrigde Univ. Press (1983), translated into russian
- H. Rothe, *Lattice gauge theories - An introduction*, World Scientific
- I. Montvay, G. Münster, *Quantum fields on a lattice*, Cambrigde Univ. Press
- J. Smit, *Introduction to quantum fields on a lattice: A robust mate*, Cambridge Lect. Notes Phys. 15 (2002) 1-271
- C. Davies, *Lattice QCD*, Lecture notes, hep-ph/0205181 (2002)
- A. Kronfeld, *Progress in lattice QCD*, Lecture notes, hep-ph/0209231 (2002)
- T. DeGrand, C. E. DeTar, *Lattice methods for quantum chromodynamics*, World Scientific (2006)
- C. Gattringer, C.B. Lang, *Quantum Chromodynamics on the Lattice - An introductory presentation*, Springer (2010)

More general on non-perturbative methods:

- Yu. Makeenko, *Methods of contemporary gauge theory*, Cambrigde Univ. Press (2002)

1. Introductory remarks: Why lattice field theory?

Allows to understand non-perturbative phenomena and to carry out *ab initio* computations in strong interactions (and beyond):

- Spontaneous breaking of chiral symmetry:
  QCD Lagrangian for 3 zero-mass flavours - among other symmetries - symmetric with respect to $SU(3)_A$:

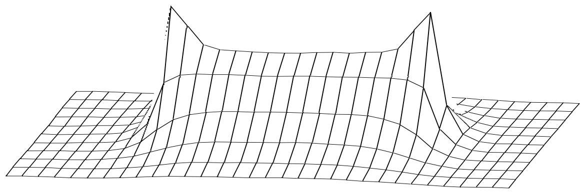
  $$\psi' = e^{i\xi_a \gamma_5 \lambda_a} \psi, \qquad \psi = (u, d, s)$$

  but $\quad < 0|\bar{\psi}\psi(x)|0 > \neq 0 \quad$ quark condensate
  $\Longrightarrow$ octet mesons (π's, K's, η) massless (Goldstone bosons).

- Quark confinement:
  Gluon field flux tube between static quarks:
  in pure gauge theory $\quad \Longrightarrow \quad F_{q\bar{q}}(r) = \frac{4}{3}\frac{\alpha_{q\bar{q}}(r)}{r^2} \quad \stackrel{r\to\infty}{\longrightarrow} \quad \sigma$ string tension

Scenarios for confinement made 'visible' in lattice QCD:

- flux tube structure visualized



From Abelian projection of SU(2) LGT [Bali, Schilling, Schlichter, '97]

- condensation of $U(1)$ monopoles: dual superconductor

  't Hooft; Mandelstam; Schierholz,. . ..; Bali, Bornyakov, M.-P., Schilling;

  Di Giacomo,. . .; . . .

- center vortices

  't Hooft; Mack; Greensite, Faber, Olejnik; Reinhardt,. . .; Polikarpov,. . .; . . .

- semiclassical approach via instantons, calorons, dyons $\cdots$
  solving e.g. the problem of large η'-mass ("$U_A(1)$-problem")
  better understood on the lattice, but responsibility for confinement **???**

but cf. lecture by V. Zakharov

- Hadron masses, hadronic matrix elements, ...:
  (cf. lectures by R. Sommer, M. Peardon, M. Göckeler, M. Polyakov)

  Not calculable within perturbation theory of continuum QCD,
  need non-perturbative (model) assumptions

  $\triangleright$ condensates $< \bar{\psi}\psi >, < \mathrm{tr}\, \mathrm{G}_{\mu\nu}\mathrm{G}_{\mu\nu} >, \cdots$

  $\Longrightarrow$ QCD sum rules

  Novikov, Shifman, Vainshtein, Zakharov; ...

  $\triangleright$ vacuum state scenarios: $\Longrightarrow$ most popular instanton liquid model

  Callan, Dashen, Gross; Shuryak; Ilgenfritz, M.-P.; Dyakonov, Petrov; ...

  $\triangleright$ Dyson-Schwinger and functional renormalization group equations

  or alternatively effective field theories or quark models ...

- Phase transitions:
  QCD: lattice predicts deconfinement or chiral transition:

  $$\text{hadrons} \quad \Longleftrightarrow \quad \text{quark-gluon plasma}$$

  under extreme conditions $T, \mu, \vec{B}$
  cf. lectures by P. Petreczky, F. Karsch, C. Schmidt, M. Polikarpov, O. Teryaev

- Standard model and beyond:
  Non-perturbative lattice approach very useful also for
  - strongly coupled QED Kogut,. . .; Schierholz,. . .; Mitrjushkin, M.-P.,. . .; . . .
  - Higgs-Yukawa model $\Longrightarrow$ e.g. bounds for Higgs mass, 4th generation ?
    K. Jansen,. . .; J. Kuti,. . .; . . . ,
  - (broken) SUSY
    cf. lectures by D. Kazakov, S. Catteral
  - lattice studies (large N_c, N_f) motivated by string theory and AdS/CFT correspondence M. Teper,. . .; J. Kuti,. . .; V. Zakharov,. . .; . . .
  - . . .

2. Path integrals in quantum (field) theory

2.1. Path integral and Euclidean correlation functions

Quantum physics mostly starts from hermitean, time-independent Hamiltonian

$$\hat{H}|n\rangle = E_n|n\rangle, \quad n = 0, 1, 2, \ldots \quad \text{with} \quad \langle m|n\rangle = \delta_{m,n}, \quad \sum_n |n\rangle\langle n| = \hat{\mathbf{1}}\,.$$

Schrödinger Equation for time evolution:

$$i\hbar\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle\,, \qquad |\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}|\psi(t_0)\rangle\,.$$

or

$$\psi(x,t) \equiv \langle x|\psi(t)\rangle = \int dx_0\ \langle x|e^{-\frac{i}{\hbar}\hat{H}(t-t_0)}|x_0\rangle\ \langle x_0|\psi(t_0)\rangle\,.$$

Standard task: find $\{E_n\}$, in particular ground state energy E_0.

Useful quantity for this: quantum statistical partition function:

$$Z = \mathrm{tr}\left(\ e^{-\beta\hat{H}}\right) = \int dx\ \langle x|e^{-\beta\hat{H}}|x\rangle \implies \text{free energy} \quad F(V,T) = -kT\log Z, \quad \beta \equiv \frac{1}{k_BT}$$

Note formal replacement: real time $\frac{i}{\hbar}\,t \quad \leftrightarrow \quad$ imaginary time $\beta \equiv \frac{1}{k_BT}$.

Extracting the ground state E_0 (Feynman-Kac formula):

$$Z = \sum_n e^{-\beta E_n} \quad \propto \quad e^{-\beta E_0} \left(1 + O(e^{-\beta(E_1 - E_0)})\right) \quad \text{for} \quad \beta \to \infty \,.$$

Extracting the energy (or mass) gap $E_1 - E_0$:

two-point correlation function in (Euclidean) Heisenberg picture ($\hbar = 1$):

operators: $\hat{X}(\tau) = e^{\hat{H}\tau} x e^{-\hat{H}\tau}$, states: $|\Psi\rangle = e^{\hat{H}\tau}|\psi(\tau)\rangle$,
quantum statistical mean values:

$$\langle \ldots \rangle \equiv Z^{-1} \text{ tr } (\ldots \; e^{-\beta \hat{H}}) \,.$$

$$\begin{aligned}
\langle \hat{X}(\tau) \rangle &= Z^{-1} \int dx \langle x | e^{-\hat{H}(\beta - \tau)} \hat{x} e^{-\hat{H}(\tau - 0)} | x \rangle \\
&= Z^{-1} \sum_n \langle n | \hat{x} | n \rangle e^{-E_n \beta} \propto Z^{-1} \, \langle 0 | \hat{x} | 0 \rangle e^{-E_0 \beta} + \ldots \\
&\propto \langle 0 | \hat{x} | 0 \rangle + \ldots \quad \text{for} \quad \beta \to \infty.
\end{aligned}$$

For two-point function assume $\beta \gg (\tau_2 - \tau_1) \gg 1$:

$$\begin{aligned}
\langle T\left(\hat{X}(\tau_2)\hat{X}(\tau_1)\right)\rangle &= Z^{-1}\int dx \langle x|e^{-\hat{H}(\beta-\tau_2)}\hat{x}e^{-\hat{H}(\tau_2-\tau_1)}\hat{x}e^{-\hat{H}(\tau_1-0)}|x\rangle \\
&\propto Z^{-1}\left\{\sum_n |\langle 0|\hat{x}|n\rangle|^2 e^{-(E_n-E_0)(\tau_2-\tau_1)}\right\} e^{-E_0\beta} + \ldots \\
&\propto Z^{-1}\left\{|\langle 0|\hat{x}|0\rangle|^2 + |\langle 0|\hat{x}|1\rangle|^2 e^{-(E_1-E_0)(\tau_2-\tau_1)}\right\} e^{-E_0\beta} + \ldots
\end{aligned}$$

Then connected two-point correlator:

$$\begin{aligned}
\langle\langle\ X(\tau_2)X(\tau_1)\ \rangle\rangle &\equiv \langle T\left(\hat{X}(\tau_2)\hat{X}(\tau_1)\right)\rangle - (\langle\hat{X}(\tau)\rangle)^2 \\
&\propto e^{-(\tau_2-\tau_1)(E_1-E_0)}(1+\ldots)
\end{aligned}$$

Higher order correlations can be defined.

Z and $\langle\langle\ldots\rangle\rangle$ allow path integral representations á la Feynman.

Path integral representation

Subdivide $\beta = N\epsilon = \text{fix}$ with $N \to \infty\,,\ \epsilon \to 0\,.$
Use $(N-1)$ times completeness relation $\int dx\ |x\rangle\langle x| = 1.$

$$Z = \int \prod_{i=1}^{N} dx_i\ \langle x_N|e^{-\hat{H}\epsilon}|x_{N-1}\rangle \cdot \langle x_{N-1}|e^{-\hat{H}\epsilon}|x_{N-2}\rangle \cdots \langle x_1|e^{-\hat{H}\epsilon}|x_0\rangle$$

with $x_0 \equiv x_N$, i.e. "periodic boundary condition".

For one degree of freedom: $\hat{H} = \hat{T} + \hat{V} = \hat{p}^2/2m + V(\hat{x})\,, \quad [\hat{x}, \hat{p}] = i$

Transfer matrix : $\langle x'|e^{-\hat{H}\epsilon}|x\rangle = \sqrt{\frac{\epsilon}{2\pi}}\, e^{-\frac{1}{2\epsilon}(x'-x)^2 - \frac{\epsilon}{2}[V(x)+V(x')]} + O(\epsilon^3)\,,$

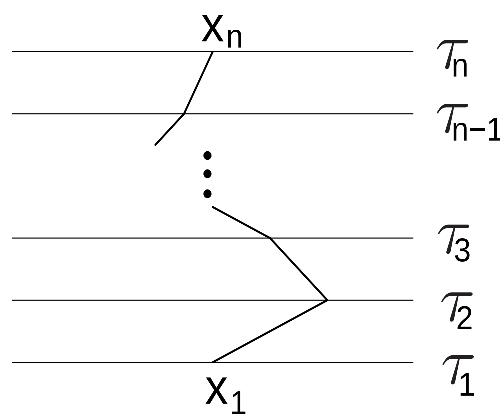
$$\Longrightarrow \qquad Z \sim \int Dx(\tau)\ e^{-S_E[x(\tau)]}$$

Proof applies Trotter product formula:

$$\exp(-\beta\hat{H}) \equiv \exp(-(\hat{T}+\hat{V})\epsilon)^N = \lim_{N\to\infty}\Big(\exp(-\epsilon\hat{T})\cdot\exp(-\epsilon\hat{V})\Big)^N$$

$$Dx(\tau) \equiv \lim_{N\to\infty}\left(\frac{\epsilon}{2\pi}\right)^{N/2}\prod_{i=1}^{N} dx_i, \qquad S_E[x(\tau)] \sim \int d\tau\left[\frac{m}{2}\left(\frac{dx(\tau)}{d\tau}\right)^2 + V(x(\tau))\right].$$

Result: summation over fictitious paths in imaginary time



Our main interest: correlation functions in Heisenberg picture:

$$\langle\ \Omega(\tau', \tau'', \ldots)\ \rangle = Z^{-1} \int Dx(\tau)\ \Omega(\tau', \tau'', \ldots)\ e^{-S_E[x(\tau)]}\ .$$

(Proof as for partition function Z.)

$\Longrightarrow$ no operators, but trajectories $x(\tau)$ and Euclidean action $S_E[x(\tau)]$,

$\Longrightarrow$ correlators resemble classical statistical averages,

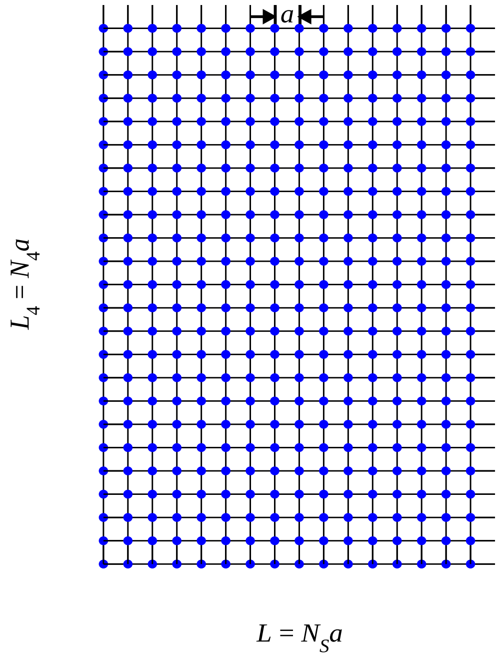
$\Longrightarrow$ we use $\beta = N\epsilon$ with N finite, but large, i.e. "lattice approximation".

2.2. Path integral quantization of scalar fields

- Lattice formulation allows non-perturbative computation from first principles.
- Axiomatic field theory starts from lattice formulation.

Illustration: scalar field, Euclidean space-time.

$$S[\phi] = \int d^4x \left[\frac{1}{2}(\partial_\mu \phi)^2 + V(\phi)\right], \quad V(\phi) = \frac{1}{2}m_0^2\phi^2 + \frac{1}{4!}g_0\phi^4.$$



["Lattice" taken from A. Kronfeld, hep-ph/0209231]

$$
\begin{aligned}
x &\longrightarrow x_n \\
\phi(x) &\longrightarrow \phi_n \equiv \phi(x_n) \\
\partial_\mu \phi(x) &\longrightarrow \tfrac{1}{a}(\phi_{n+\hat{\mu}} - \phi_n)
\end{aligned}
$$

$$S_{\text{Latt}} = a^4 \sum_n \left\{ \frac{1}{2} \sum_{\mu=1}^{4} (\phi_{n+\hat{\mu}} - \phi_n)^2 \frac{1}{a^2} + V(\phi_n) \right\}$$

$\Longrightarrow$ no unique discretization,

$\Longrightarrow$ even more - systematic improvement scheme exists (Symanzik).

Boundary condition: $\phi(x + L_\mu \cdot \hat{\mu}) = \phi(x)$

Spectrum: $-\frac{\pi}{a} \le k_\mu = \frac{2\pi}{L_\mu} n_\mu \le \frac{\pi}{a}$

Quantization:

Path integral for time ordered correlation functions and vacuum transition amplitude

$$
\begin{aligned}
< \phi(x_1 \cdots \phi(x_N) > &= Z^{-1} \int \prod_x d\phi(x) \{\phi(x_1) \cdots \phi(x_N)\} e^{-S[\phi]} && (1) \\
Z &= \int \prod_x d\phi(x)\; e^{-S[\phi]} && (2)
\end{aligned}
$$

$\Updownarrow$ lattice approximation and rescaling $\phi \longrightarrow \phi \cdot \sqrt{g_0}$.

$$
\begin{aligned}
< \phi_{n_1} \cdots \phi_{n_N} > &= Z_{\text{Latt}}^{-1} \int \prod_n d\phi_n \{\phi_{n_1} \cdots \phi_{n_N}\} e^{-\frac{1}{g_0} S_{\text{Latt}}} && (3) \\
Z_{\text{Latt}} &= \int \prod_n d\phi_n\; e^{-\frac{1}{g_0} S_{\text{Latt}}} && (4)
\end{aligned}
$$

Compare with: $\mathcal{Z}(T,V) = \int \prod_{i=1}^{f} dq_i\; dp_i\; e^{-\frac{1}{kT} H(q_i,p_i)}$

Scalar Higgs model in some detail:

$$\phi = \sqrt{2\kappa}\,\frac{\varphi}{a}\,, \quad g_0 = \frac{6\lambda}{\kappa^2}\,, \quad m_0^2 = \frac{1-2\lambda-8\kappa}{a^2\kappa}\,.$$

$$S_{\mathrm{Latt}} = -2\kappa \sum_{n,\mu} \varphi_n \varphi_{n+\hat{\mu}} + \lambda \sum_n (\varphi_n^2 - 1)^2 + \sum_n \varphi_n^2$$

(κ 'Hopping parameter')

No lattice spacing visible. How does the continuum limit occur?

In practice need for determining correlation lengths

$$L_4 = N_4 a \;\gg\; \zeta \equiv m^{-1} \;\gg\; a$$

Continuum limit corresponds to 2^{nd} order phase transition:

$$\zeta/a \to \infty \quad \text{whereas} \quad m_1/m_2 \to \text{const.}$$

$\lambda \to \infty$: $\quad \kappa = \text{fixed} \quad \Longrightarrow \quad \varphi_n = \pm 1\,.$

$$Z_{\mathrm{Latt}} \to \text{const.} \cdot \sum_{\varphi_{\mathrm{n}}=\pm 1} \exp\left(-2\kappa \sum_{\mathrm{n},\mu} \varphi_{\mathrm{n}} \varphi_{\mathrm{n}+\hat{\mu}} \right)$$

$\Longrightarrow$ Ising model in 4D,

$\Longrightarrow$ 2^{nd} order phase transition at $\kappa_c = 0.0748$.

$\lambda < \infty$: find critical line $\kappa = \kappa_c(\lambda)$.

Comment:

renormalized coupling $\quad \lambda_{ren} \to 0$ for $\kappa \to \kappa_c$

$\Longrightarrow$ non-interacting theory in the continuum limit or

$\Longrightarrow$ effective theory at finite cutoff.

3. Discretizing gauge fields

3.1. QCD: a short introduction

The strong force of hadrons realized by quarks interacting with gluons

- Quarks (= fermionic matter field) occur with
  - $N_c = 3$ "colour" states (gauge group $SU(N_c)$),
  - $N_f = 6$ (?) "flavour" states (up, down, strange, charm, bottom, top, ...),
  - 4 "spinor" states.
- Gluons (= bosonic gauge field) occur with
  - $N_c^2 - 1 = 8$ "colour" states (adjoint repr. of $SU(N_c)$),
  - 4 space-time components.

Colour neutral bound states:

$$qqq: \text{ baryons} - \ p,\ n,\ \ldots,$$
$$q\bar{q}: \text{ mesons} - \ \pi,\ \rho, K,\ \ldots.$$

QCD: quark fields $\psi_f(x) \equiv \{(\psi_f(x))_s^\alpha\ ,\ \alpha = 1, \ldots, N_c,\ s = 1, \ldots, 4\}$

minimally coupled to gluon fields $A_\mu^a(x), \mu = 0, .., 3\ ,\ x = (\vec{x}, t)$.

$$S[\bar{\psi},\psi,A] = \int d^4x \left(-\frac{1}{2}\mathrm{tr}\; G^{\mu\nu}G_{\mu\nu} + \sum_{f=1}^{N_f} \bar{\psi}_f(i\gamma_\mu D^\mu - m_f)\psi_f \right)$$

$$G_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + ig_0[A_\mu, A_\nu]\,, \quad D_\mu = \partial_\mu \mathbf{1} + ig_0 A_\mu\,, \quad A_\mu = A_\mu^a T^a\,,$$

$$T^a \;\; (a = 1, \ldots, N_c^2 - 1) \;\; \text{– generators of } SU(N_c),$$
$$\text{with} \;\; [T^a, T^b] = if^{abc}T^c, \;\; 2\mathrm{tr}(T^aT^b) = \delta_{ab}, \;\; \mathrm{tr}T^a = 0.$$

- local gauge invariance – the main principle of the standard model

  $$\psi'(x) = g(x)\psi(x), \quad A'_\mu(x) = g(x)A_\mu g^\dagger(x) - \frac{i}{g_0}(\partial_\mu g(x))g^\dagger(x), \quad g(x) \in SU(N_c)$$

  leaves action $S[\bar{\psi},\psi,A]$ invariant for any $g(x)$.

- quantization with Euclidean path integral analogously to QM:

  $$\langle\; \Omega(\bar{\psi},\psi,A)\;\rangle = Z^{-1}\int DA_\mu D\bar{\psi}D\psi \;\; \Omega(\bar{\psi},\psi,A) \;\; e^{-S_E[\bar{\psi},\psi,A]}$$

  $$DA_\mu = \prod_x dA_\mu(x)\,; \quad D\psi = \prod_x d\psi(x) \quad - \quad \text{Grassmannian measure}$$

$\Longrightarrow$ weak coupling ($\alpha_s \ll O(1)$): perturbation theory, requires gauge fixing;

$\Longrightarrow$ stronger coupling ($\alpha_s \simeq O(1)$): lattice theory, Dyson-Schwinger eqs., ...

3.2. Gauge fields on a lattice

K. Wilson '74:
Local $SU(N_c)$ gauge symmetry kept exact by non-local prescription on a 4d Euclidean lattice $\Longrightarrow$ link variables

$$
\begin{aligned}
A_\mu(x_n) \Longrightarrow U_{n,\mu} \quad &\equiv \quad P \exp i g_0 \int_{x_n}^{x_n+\hat{\mu}a} A_\mu(x) dx_\mu \ \in \ SU(N_c) \\
&\simeq \quad e^{iag_0 A_\mu(x_n)} \simeq \mathbf{1} + iag_0 A_\mu(x_n) + O(a^2)
\end{aligned}
$$

Gauge transformation $\quad g_n \equiv g(x_n) \in \ SU(N_c)$ for $a \to 0$:

$$
\begin{aligned}
A'_\mu(x_n) \quad &\simeq \quad g_n A_\mu g_n^\dagger - \frac{i}{ag_0}(g_{n+\hat{\mu}} - g_n) g_n^\dagger \\
U'_{n,\mu} \quad &= \quad \mathbf{1} + iag_0 A'_\mu(x_n) + O(a^2) \\
&= \quad iag_0 \, g_n A_\mu g_n^\dagger + g_{n+\hat{\mu}} g_n^\dagger + O(a^2), \qquad g_n = g_{n+\hat{\mu}} + O(a) \\
&= \quad g_{n+\hat{\mu}}(\mathbf{1} + iag_0 A_\mu(x_n) + O(a^2)) g_n^\dagger \\
&= \quad g_{n+\hat{\mu}} \, U_{n,\mu} \, g_n^\dagger
\end{aligned}
$$

Transformation of a product of variables of connected links

$$U'(n+\hat{\mu}+\hat{\nu},n) \equiv U'_{n+\hat{\mu},\nu}U'_{n,\mu} = g_{n+\hat{\mu}+\hat{\nu}}U_{n+\hat{\mu},\nu}U_{n,\mu}g_n^\dagger = g_{n+\hat{\mu}+\hat{\nu}}U(n+\hat{\mu}+\hat{\nu},n)g_n^\dagger$$

can be generalized to arbitrary continuum path:
"Schwinger line" (parallel transporter)

$$\begin{aligned} U(x_2,x_1) &= P\exp\left\{ig_0\int_{x_1}^{x_2} A_\mu dx_\mu\right\}, \\ \Longrightarrow \quad U'(x_2,x_1) &= g(x_2)U(x_2,x_1)g^\dagger(x_1). \end{aligned}$$

$$\Longrightarrow \quad \mathrm{tr}\left(P\exp\left\{ig_0\oint A_\mu dx_\mu\right\}\right) = \text{invariant}.$$

Combination with matter field: $\psi'(x) = g(x)\psi(x), \quad \psi'^\dagger(x) = \psi^\dagger(x)g^\dagger(x)$

$$\Longrightarrow \quad \psi^\dagger(x_2)U(x_2,x_1)\psi(x_1) = \text{invariant}.$$

Lattice gauge action: from elementary closed (Wilson) loops ("plaquettes")

$$
\begin{aligned}
U_{n,\mu\nu} &\equiv U_n \; U_{n+\hat{\mu},\nu} \; U^\dagger_{n+\hat{\nu},\mu} \; U^\dagger_{n,\nu} \, , \\
S_G^W &= \bar{\beta} \sum_{n,\mu<\nu} \left(1 - \frac{1}{N_c} \text{ Re tr } U_{n,\mu\nu} \right) , \quad \bar{\beta} = \frac{2N_c}{g_0^2} \\
&= \frac{1}{2} \sum_n a^4 \text{ tr } G^{\mu\nu} G_{\mu\nu} + O(a^2), \\
&\to \frac{1}{2} \int d^4x \text{ tr } G^{\mu\nu} G_{\mu\nu} .
\end{aligned}
$$

Proof: $\longrightarrow$ homework, tutorial.

Comments:

- Improvement of S_G^W: suppression of $O(a)$-corrections by adding contributions from larger loops (e.g. various 6-link loops) or contributions of loops in higher group representations (e.g. adjoint representation)
- Test: non-trivial vacuum field $=$ pure gauge

$$
\begin{aligned}
U^{(vac)}_{n\mu} &\equiv g_{n+\hat{\mu}} \; g_n^\dagger , \quad \text{for arbitrary } \; g_n \in SU(N_c) \\
\text{Re tr } U_{n,\mu\nu} &= N_c \implies S_G^W = 0.
\end{aligned}
$$

Path integral quantization:

replacement $\int \prod_{x,\mu} dA_\mu(x) \quad \longrightarrow \quad \int \prod_{n,\mu} [dU]_{n,\mu}$, $[dU]$ "Haar measure".

Properties: $U, V \in G = SU(N_c)$ in fundamental representation, then

- $\int_G [dU] = 1$ normalization,
- $\int_G f(U)[dU] = \int_G f(VU)[dU] = \int_G f(UV)[dU], \quad [d(UV)] = [d(VU)] = [dU]$,
- $\int_G f(U)[dU] = \int_G f(U^{-1})[dU]$.

Examples:

$U(1): \quad U = e^{i\varphi} \quad \Longrightarrow \quad [dU] = \frac{1}{2\pi} d\varphi, \quad \int f(U)[dU] \equiv \frac{1}{2\pi} \int_0^{2\pi} d\varphi \; f(U(\varphi))$;

$SU(2): \quad U = B^0 + i\vec{\sigma} \cdot \vec{B}, \; \sum_i (B^i)^2 = 1 \quad \Longrightarrow \quad [dU] = \frac{1}{\pi^2} \; \delta(B^2 - 1) \; d^4B$,

$\vec{\sigma}$ – Pauli matrices.

Expectation values, correlation functions in pure gauge theory:

$$\langle W \rangle = \frac{1}{Z} \int (\prod_{n,\mu} [dU_{n\mu}]) \; W[U] \; e^{-S_G[U]}, \quad Z = \int (\prod_{n,\mu} [dU_{n\mu}]) \; e^{-S_G[U]} \, .$$

Gauge invariance:

$U'_{n\mu} = g_{n+\hat{\mu}}\ U_{n\mu} g_n^\dagger \quad \Longrightarrow \quad dU'_{n\mu} = dU_{n\mu}, \quad S_G[U'] = S_G[U]$

Then immediately

$$\begin{aligned} \langle W' \rangle &= \frac{1}{Z'} \int (\prod_{n,\mu} [dU'_{n\mu}])\ W[U']\ e^{-S_G[U']} \\ &= \frac{1}{Z} \int (\prod_{n,\mu} [dU_{n\mu}])\ W[U']\ e^{-S_G[U]} \end{aligned}$$

$\Longrightarrow$ invariant, if $W[U]$ itself is gauge invariant.

Fortunately, holds in most of the applications of lattice gauge theory !

Exceptions:

Quark, gluon, ghost propagators or various vertex functions.

Gauge fixing is required, e.g. Landau/Lorenz gauge, as in perturbation theory.

However, gauge condition not uniquely solvable - “Gribov problem”.

Lattice discretized path integral allows to study analytically:

- $\bar{\beta} \to \infty, \; g_0 \to 0$: *(lattice) perturbation theory* by expanding all link variables $U_{n\mu} = e^{iag_0\,A_\mu(x_n)}$ in powers of g_0.
  Inverse lattice spacing a^{-1} acts as UV cutoff.

- $\bar{\beta} \to 0, \; g_0 \to \infty$: *strong coupling expansion* by expanding in powers of $\bar{\beta}$

$$\exp\left\{-\bar{\beta}\sum_{n,\mu<\nu}\left(1 - \frac{1}{N_c}\,\mathrm{Re}\;\mathrm{tr}\;U_{n,\mu\nu}\right)\right\}.$$

Mostly we have to rely on $g_0 \simeq O(1) \implies$ Monte Carlo simulation.

3.3. Wilson and Polyakov loops

Closed *Wilson loops*

$$W[U] \equiv \mathrm{tr}\left(P \exp\left\{ i g_0 \oint A_\mu dx_\mu \right\} \right)$$

play important rôle for explaining quark confinement.

Sketch of the proof [cf. book H. Rothe, '92]:

Consider (infinitely) heavy $Q\bar{Q}$-pair. Gauge-invariant state at fixed t':

$$\bar{\psi}_\alpha^{(Q)}(\vec{x}, t')\ U(\vec{x}, t'; \vec{y}, t')\ \psi_\beta^{(Q)}(\vec{y}, t')\ |\Omega\rangle$$

with

$$U(\vec{x}, t'; \vec{y}, t') = P \exp\left\{ i g_0 \int_{\vec{x}}^{\vec{y}} A_\mu(\vec{z}, t')\ dz_\mu \right\} .$$

Compute 2-pt. function for $Q\bar{Q}$-pair - propagation from 0 to t:

$G_{\alpha', \beta'; \alpha, \beta}(\vec{x}', \vec{y}', t;\ \vec{x}, \vec{y}, 0)$

$= \langle \Omega | \, T \, \{ \bar{\psi}_{\beta'}^{(Q)}(\vec{y}', t) U(\vec{y}', t; \vec{x}', t) \psi_{\alpha'}^{(Q)}(\vec{x}', t) \cdot \bar{\psi}_\alpha^{(Q)}(\vec{x}, 0) U(\vec{x}, 0; \vec{y}, 0) \psi_\beta^{(Q)}(\vec{y}, 0) \} \, |\Omega\rangle \, .$

Euclidean time $t = -i\tau$; for $\tau \to \infty$, $M_Q \to \infty$ expect

$$G_{\alpha',\beta';\alpha,\beta} \propto \delta^{(3)}(\vec{x} - \vec{x}')\, \delta^{(3)}(\vec{y} - \vec{y}')\, C_{\alpha',\beta';\alpha,\beta}(\vec{x}, \vec{y}) \exp(-E(R)\tau)$$

$E(R)$ = energy of the lowest state (above vacuum), i.e. $Q\bar{Q}$-potential.

Path integral representation:

$$G_{\alpha',\beta';\alpha,\beta} = \frac{1}{Z} \int DA \int D\psi^{(Q)} D\bar{\psi}^{(Q)} \left(\bar{\psi}^{(Q)}_{\beta'}(\vec{y}', \tau) \ldots \psi^{(Q)}_{\beta}(\vec{y}, 0) \right) \exp(-S[\bar{\psi}^{(Q)}, \psi^{(Q)}, A])$$

Carry out (Grassmanian) fermion integration

$\longrightarrow$ product of Green's functions for Q, $\bar{Q}$ and Det $\to$ const for $M_Q \to \infty$.

Static limit – neglect spatial derivatives $(i\gamma^\mu D_\mu) \to (i\gamma^4 D_4)$

$\longrightarrow$ Green's function:

$$[i\gamma^4 D_4(A) - M_Q]\; K(z, z'; A) = \delta^{(4)}(z - z').$$

Solution:

$$K(z, z'; A) \sim P \exp\left\{ i g_0 \int_0^\tau A_0(\vec{z}, t')\, dt' \right\} \delta^{(3)}(\vec{z} - \vec{z}') \cdot \mathbf{K}$$

with $\mathbf{K}$ containing projectors $P_\pm = \frac{1}{2}(1 \pm \gamma^4)$.

Combine time-like phase factors at $\vec{z} = \vec{x}, \vec{y}$ with space-like ones
$U(\vec{x}, 0; \vec{y}, 0), \quad U(\vec{y}, \tau; \vec{x}, \tau)$.

Result:

$$G_{\alpha', \beta'; \alpha, \beta} \sim \langle W \rangle \equiv \left\langle \mathrm{tr}\ P \exp \left\{ i g_0 \oint A_\mu dx_\mu \right\} \right\rangle$$

with closed rectangular path of extension $R \times \tau$.

For $\tau \to \infty$: $\quad \langle W \rangle \propto \exp(-E(R) \cdot \tau)$.

Confinement:

$E(R) \propto \sigma R$ for large $R \quad \Longleftrightarrow \quad \langle W \rangle \propto \exp(-\sigma \cdot (R \cdot \tau))$ (area law)

Polyakov loops and non-zero temperature QCD [cf. lecture by P. Petreczky]

[Gross, Pisarski, Yaffe, Rev.Mod.Phys. 53 (1981) 43;
Svetitsky, Yaffe, Nucl.Phys. B210 (1982) 423; Svetitsky, Phys.Rept. 132 (1986) 1]

Partition function:

$$\begin{aligned}
Z &= \mathrm{Tr}\exp(-\beta\hat{H}), \qquad \beta = 1/k_B T, \\
&= \sum_x \langle x|(\exp(-\epsilon\hat{H}))^N|x\rangle, \qquad N\epsilon = \beta, \\
&= C\int Dx\exp(-S_E[x(t)]), \qquad S_E = \int_0^\beta dt\,[\frac{m}{2}\dot{x}(t)^2 + V(x(t))]
\end{aligned}$$

with $x(0) = x(\beta)$, i.e. periodicity.

For Yang-Mills theory analogous proof of path integral representation is non-trivial:

– Hamiltonian approach within gauge $A_0^a = 0$,

– trace integration produces integration over auxiliary field A_4^a,

$\Longrightarrow$ full Euclidean Yang-Mills action recovered.

Result:

$$Z_G = C \int DA e^{-S_G[A]}, \qquad S_G[A] = \int_0^\beta dt \int d^3x \; \frac{1}{2} \mathrm{tr}(G_{\mu\nu} G_{\mu\nu})$$

with $A^a_\mu(\vec{x},0) = A^a_\mu(\vec{x},\beta)$, and $G_{\mu\nu} = G^a_{\mu\nu} T^a$ Euclidean.

Applied to lattice pure gauge theory:

$$Z_G \equiv \int [dU] e^{-S_G[U]}, \;\; \text{with} \;\; U_\mu(\vec{x},0) = U_\mu(\vec{x},\beta), \;\; \beta = aN_4 = \frac{1}{k_B T}.$$

We are interested in the thermodynamic limit: $V^{(3)} \to \infty$.
In practice, "aspect ratio" $N_s/N_4 \gg 1$ and periodic b.c.'s in spatial directions.

Extension to full QCD: time-antiperiodic boundary conditions for fermionic fields from trace of statist. operator: $\psi(\vec{x},0) = -\psi(\vec{x},\beta)$, $\overline{\psi}(\vec{x},0) = -\overline{\psi}(\vec{x},\beta)$.

Polyakov loop:

$$L(\vec{x}) \equiv \frac{1}{N_c} \mathrm{tr} \prod_{x_4=1}^{N_4} U_4(\vec{x},x_4), \qquad (a=1),$$

invariant w.r. to time-periodic gauge transformations $g(\vec{x},1) = g(\vec{x},N_4+1)$.

Physical interpretation:

$$\langle L(\vec{x})\rangle = \exp(-\beta F_Q),$$

with F_Q free energy of an isolated infinitely heavy quark.
Proof goes analogously as for Wilson loop expectation value.

$\Longrightarrow$ $F_Q \to \infty$, i.e. $\langle L(\vec{x})\rangle \to 0$ within the confinement phase.
$\Longrightarrow$ $\langle L(\vec{x})\rangle$ order parameter for the deconfinement transition.

Spontaneous breaking of $\mathbf{Z}_N$ center symmetry:

$$z_\nu = e^{2\pi i \frac{\nu}{N}}\,\mathbf{1} \in \mathbf{Z}_N \subset SU(N), \quad \nu = 0, 1, \ldots, N-1$$

commute with all elements of $SU(N)$. For $SU(2)$: $z_\nu = \pm\mathbf{1}$.

Global $\mathbf{Z}_N$-transformation:

$$U_4(\vec{x}, x_4) \to z \cdot U_4(\vec{x}, x_4) \quad \text{for all} \quad \vec{x} \quad \text{and fixed } x_4$$

$\Longrightarrow$ $L(\vec{x}) \to zL(\vec{x})$ not invariant.
$\Longrightarrow$ Plaquette values $U_{n,i4} \to zz^\star U_{n,i4} = U_{n,i4}$, i.e. S_G invariant.

$SU(2)$-case:

$L(\vec{x}) \to -L(\vec{x})$. Both states have same statistical weight.

$\Longrightarrow \quad \langle L(\vec{x}) \rangle = 0$.

$\Longrightarrow$ Order parameter for the deconfinement transition:

$$\langle |\overline{L}| \rangle \equiv \left\langle | \frac{1}{V^{(3)}} \sum_{\vec{x}} L(\vec{x}) | \right\rangle \sim \begin{cases} 0 & \text{confinement} \\ 1 & \text{deconfinement} \end{cases}$$

analogously to spin magnetization for 3d Ising model.

$SU(3)$-case: $\overline{L}$ complex-valued.

$$\begin{aligned} \text{Confinement} \quad &\to \quad \overline{L} \simeq 0, \\ \text{Deconfinement} \quad &\to \quad \overline{L} \simeq z_\nu, \;\; \nu = 0, 1, 2. \end{aligned}$$

Notice: fermions break center symmetry. Then

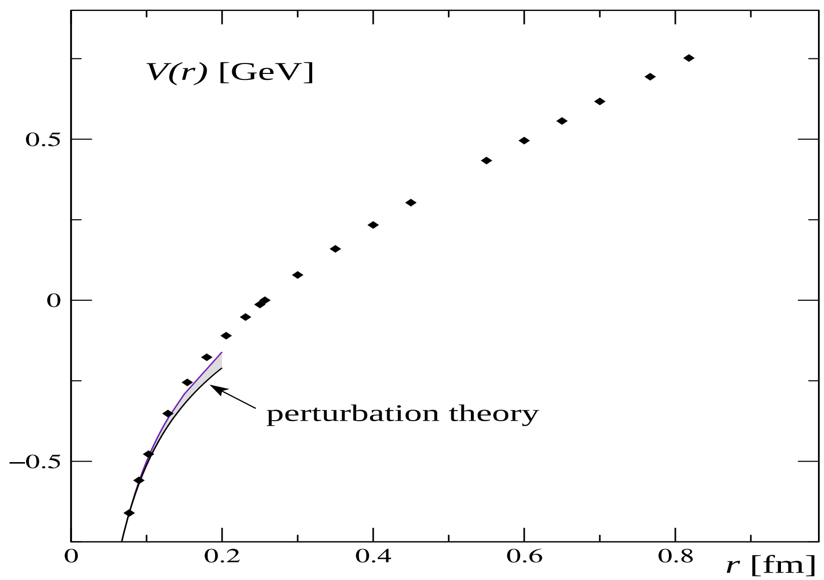
$\Rightarrow$ Polyakov loop – no order parameter, but still useful indicator.

$\Rightarrow$ Condensate $\langle \bar{\psi} \psi \rangle$ – order parameter for chiral symmetry restoration.

3.4. Fixing the QCD scale

Expectation values $\langle W \rangle$ (of Wilson loops etc.) in pure gauge theory only depend on parameter $\bar{\beta} \equiv 2N_c/g_0^2$ (and linear lattice extensions N_μ).

View some Monte Carlo results in gluodynamics.

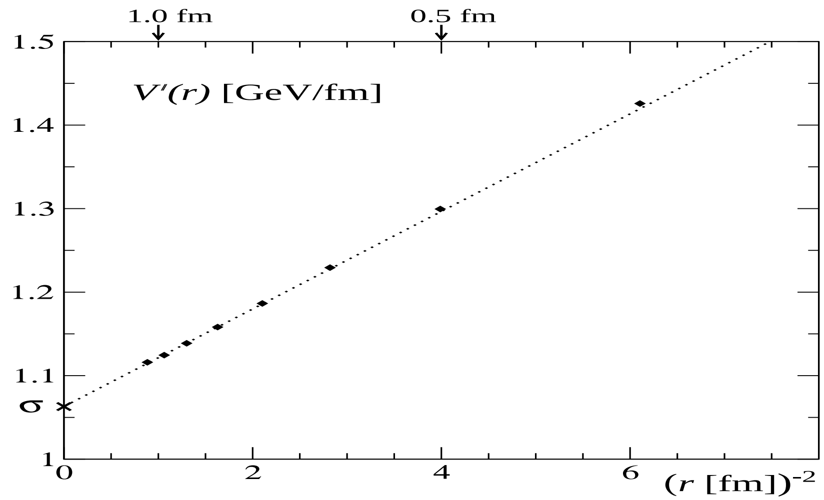


Static $Q\bar{Q}$ potential $V(r)$ ($\equiv E(R)$) at small distances from Wilson loops.

Necco, Sommer, '02

Alternative method: Polyakov loop correlator

$\langle L(\vec{x_1} L(\vec{x_2}^{\dagger}) \rangle \propto \exp(-\beta V(r))(1 + \ldots), r \equiv |\vec{x_1} - \vec{x_2}|$



Static $Q\bar{Q}$ force $F(r) \equiv dV/dr$ from Polyakov loop correlators at $T = 0$.

$\Longrightarrow$ in perfect agreement with string model prediction

$$V(r) \sim \sigma r + \mu - \frac{\pi}{12\,r} + O(r^{-2}).$$

Lüscher, Weisz, '02

$F(r)$ allows to fix the scale by comparing with phenomenologically known $\bar{c}c$- or $\bar{b}b$-potential [R. Sommer, '94]:

$$F(r_0)\; r_0^2 \;=\; 1.65 \quad \leftrightarrow \quad r_0 \simeq 0.5 \text{ fm}$$

If *Sommer scale* r_0 is determined in lattice units a for certain $\bar{\beta}$, spacing $a(\bar{\beta})$ can be fixed in physical units.

3.5. Renormalization group and continuum limit

Assume for a physical observable Ω (e.g. string tension σ, critical temperature T_c, glueball mass $M_g, \ldots$) in the continuum limit

$$\lim_{a \to 0} \Omega\left(g_0(a), a\right) = \Omega_c$$

Then *renormalization group Eq.*

$$\frac{d\,\Omega}{d(\ln a)} = 0 \quad \Longrightarrow \quad \left(\frac{\partial}{\partial(\ln a)} - \beta(g_0)\frac{\partial}{\partial g_0}\right)\Omega\left(g_0, a\right) = 0$$

with $\quad \beta(g_0) \equiv -\frac{\partial\, g_0}{\partial(\ln\, a)}$ known from perturbation theory

$$\beta(g)/g^3 = -\beta_0 - \beta_1 g^2 + O(g^4).$$

For $SU(N_c)$ and N_f massless fermions, independent on renormalization scheme:

$$\begin{aligned} \beta_0 &= \frac{1}{(4\pi)^2}\left(\frac{11}{3}N_c - \frac{2}{3}N_f\right), \\ \beta_1 &= \frac{1}{(4\pi)^4}\left(\frac{34}{3}N_c^2 - \frac{10}{3}N_c N_f - \frac{N_c^2 - 1}{N_c}N_f\right). \end{aligned}$$

For pure gluodynamics: $N_c = 3, \quad N_f = 0 \quad \Rightarrow \quad \beta_0 > 0.$

Solution yields continuum limit

$$a(g_0) = \frac{1}{\Lambda_{Latt}} (\beta_0 g_0^2)^{-\frac{\beta_1}{2\beta_0^2}} \exp\left(-\frac{1}{2\beta_0 g_0^2}\right)(1 + O(g_0^2)).$$

$\Longrightarrow \qquad 1/a \to \infty$ for $g_0 \to 0$ (or $\bar{\beta} \to \infty$), *asymptotic freedom*.

Corresponds to second order phase transition.

In practice, tune g_0, N_4 for getting correlation lengths ξ, such that:

$$N_4 \gg \xi/a(g_0) \gg 1\,.$$

At non-zero $T = 1/L_4 = 1/(N_4 a(\bar{\beta}))$:

T can be varied by changing $\bar{\beta}$ at fixed N_4 or N_4 at fixed $\bar{\beta}$.

4. Simulating gauge fields

4.1. How does Monte Carlo work?

Realization in quantum mechanics:

M. Creutz, B. Freedman, A stat. approach to quantum mechanics, Annals Phys. 132(1981)427

Here consider n-dim. integral:

$\langle f \rangle \;=\; \int_\Omega d^n x\, f(x) w(x)$ with $0 \le w(x) \le 1$, $\int_\Omega w(x)\, d^n x = 1$.

$$\langle f \rangle = \int_\Omega d^n x\, f(x) \int_0^{w(x)} d\eta = \int_\Omega d^n x \int_0^1 d\eta\, f(x)\, \Theta(w(x) - \eta)$$

Importance sampling by selecting x in acc. with $w(x)$:

(a) choose randomly: $x \in \Omega$ and $\eta \in [0, 1]$,

(b) acceptance check: accept x, if η satisfies $\eta < w(x)$, otherwise reject.

$\Longrightarrow$ From accepted $x^{(i)}$'s estimate $\langle f \rangle \simeq (1/N) \sum_{i=1}^N f(x^{(i)})$.

$\Longrightarrow$ However, efficiency small, if acceptance rate in large areas of Ω is low.

More efficient: appropriate Markov chain $x^{(1)}, x^{(2)}, \ldots$

generated with transition probability $P(x^{(i)} \to x^{(i+1)})$
satisfying *detailed balance condition*

$$w(x)P(x \to x') = w(x')P(x' \to x)$$

- sufficient for $w(x)$ becoming fix-point of the Markov chain,
- obviously satisfied for $P(x \to x') \equiv w(x')$.

Markov chains realizable step-by-step by selecting
single components x_ν keeping all $x_\mu, \mu \neq \nu$ fixed.

Heat bath method:
- If possible determine x'_ν with probability $\omega(x'_\nu) \sim w(x_1, \ldots, x'_\nu, \ldots, x_n)$.
- Replace old value x_ν by x'_ν.
- Repeat procedure for other component x_μ.

Metropolis method:

- random shifts $x_\nu \to x'_\nu = x_\nu + \eta$, $\eta \in (-\epsilon, +\epsilon)$ with ϵ approp. chosen,
- if $\omega(x'_\nu) > \omega(x_\nu)$, then accept x'_ν,
- if $\omega(x'_\nu) < \omega(x_\nu)$, then accept with probability $\omega(x'_\nu)/\omega(x_\nu)$,
- accepted values x'_ν replace x_ν.

4.2. Creutz' heat bath method

Assume statistical weight $w[U] \sim e^{-S_G[U]}$ with plaquette action

$$S_G[U] = \bar{\beta} \sum_{n,\mu<\nu} \left(1 - \frac{1}{N_c} \text{ Re tr } U_{n,\mu\nu}\right).$$

Select a single link variable: $U_{n_0,\mu_0} \equiv U_0$. There are 6 plaquettes containing this link and contributing to S_G:

$$\begin{aligned} S_G[U_0; \{U\} \setminus U_0] &= C[\{U\} \setminus U_0] - \frac{\bar{\beta}}{N_c} \sum_{S=1}^{6} \text{Re tr } (U_0 U_S) \\ &= C - \frac{\bar{\beta}}{N_c} \text{Re tr } (U_0 A), \quad A = \sum_{S=1}^{6} U_S \end{aligned}$$

Call open plaquette $U_S =$ "staple".
Assume A be fixed ("heat bath") $\Longrightarrow$ link variable U_0 to be determined with probability

$$w(U_0)\ [dU_0] \sim \exp\left(\frac{\bar{\beta}}{N_c} \text{Re tr } (U_0 A)\right)\ [dU_0]$$

.

Metropolis:

- apply random shifts $U_0 \to U_0' = GU_0$, with $G \in U_\epsilon(\mathbf{1}) \subset SU(N_c)$,
- carry out Metropolis acceptance steps.

Heat bath for $SU(2)$:

Normalize $V = A/\sqrt{\det A} \in SU(2)$, put $VU_0 \equiv U$ and use invariance of Haar measure

$$w(U)[dU] \ \sim \exp\left(\rho \ \mathrm{tr}\ U\right)[dU], \quad \rho = \frac{\bar{\beta}\sqrt{\det A}}{2}$$

$$U \equiv B^0 \mathbf{1} + i\sigma\vec{B}, \quad [dU] = \frac{1}{\pi^2}\ \delta(B^2-1)\ d^4B, \quad \mathrm{tr}\ U = 2B^0$$

$$\Longrightarrow \qquad w(U)[dU] \ \sim \exp\left(2\rho B^0\right)\delta(B^2-1)\ d^4B$$

$$\Longrightarrow \qquad \text{determine } \ U \ \text{ and } \ U_0 = V^\dagger U.$$

Heat bath for $SU(N_c)$ [Cabibbo, Marinari, '82]

Use $SU(2)$ heat bath algorithm for various subgroup embeddings into $SU(N_c)$.

5. Fermions on the lattice

5.1. Naive discretization and fermion doubling

Path integral for fermions requires anticomm. variables – Grassmann algebra:

$$\eta_i, \bar{\eta}_i, i = 1, 2, \ldots, N \quad \text{with} \quad \bar{\eta}_i \text{ adjoint to } \eta_i,$$

$$\begin{aligned}
\{\eta_i, \eta_j\} &\equiv \eta_i \eta_j + \eta_j \eta_i \\
&= \{\bar{\eta}_i, \eta_j\} = \{\bar{\eta}_i, \bar{\eta}_j\} = \ldots = 0, \\
\eta_i^2 &= 0,
\end{aligned}$$

such that any function has representation

$$f(\eta) = f_0 + \sum_i f_i \; \eta_i + \sum_{i \neq j} f_{ij} \; \eta_i \eta_j + \ldots f_{12\ldots N} \; \eta_1 \eta_2 \ldots \eta_N,$$

correspondingly for $f(\eta, \bar{\eta})$.

E.g. $\quad g(\eta, \bar{\eta}) = \exp(-\sum_{i,j} \bar{\eta}_i A_{ij} \eta_j) = \prod_{ij=1}^{N} (1 - \bar{\eta}_i A_{ij} \eta_j)$.

Integration rules (same as differentiation):

$$\int d\eta_i = \int d\bar{\eta}_i = 0, \qquad \int d\eta_i \eta_i = \int d\bar{\eta}_i \bar{\eta}_i = 1,$$

$$\{d\eta_i, d\eta_j\} = \{d\bar{\eta}_i, d\eta_j\} = \{d\bar{\eta}_i, d\bar{\eta}_j\} = \{d\eta_i, \eta_j\} = \ldots = 0.$$

Most important for us:

$$
\begin{aligned}
I[A] &= \int \prod_{l=1}^{N} d\bar{\eta}_l d\eta_l \ \exp\left(- \sum_{ij=1}^{N} \bar{\eta}_i A_{ij} \eta_j \right) = \det A, \\
Z[A;\rho,\bar{\rho}] &= \int \prod_{l=1}^{N} d\bar{\eta}_l d\eta_l \ \exp\left(- \sum_{ij=1}^{N} \bar{\eta}_i A_{ij} \eta_j + \sum_i (\bar{\eta}_i \rho_i + \bar{\rho}_i \eta_i) \right), \\
&= \det A \cdot \exp\left(\sum_{ij=1}^{N} \bar{\rho}_i A^{-1}_{ij} \rho_j \right), \\
\langle \eta_i \bar{\eta}_j \rangle &= \frac{\int D(\bar{\eta}\eta) \ \eta_i \bar{\eta}_j \exp(-\bar{\eta} A \eta)}{\int D(\bar{\eta}\eta) \ \exp(-\bar{\eta} A \eta)} = A^{-1}_{ij}.
\end{aligned}
$$

Dirac Propagator (with Euclidean: $\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}$, $\gamma_4 \equiv \gamma_M^0, \gamma_i \equiv -i\gamma_M^i$)

$$
\begin{aligned}
\langle \psi_\alpha(x) \bar{\psi}_\beta(y) \rangle &= \frac{\int D\bar{\psi} D\psi \ \psi_\alpha(x) \bar{\psi}_\beta(y) \exp\left(-S_F[\bar{\psi}\psi]\right)}{\int D\bar{\psi} D\psi \ \exp\left(-S_F[\bar{\psi}\psi]\right)}, \\
S_F[\bar{\psi}\psi] &= \int d^4x \ \bar{\psi}(x)(\gamma_\mu \partial_\mu + m)\psi(x).
\end{aligned}
$$

Naive lattice discretization:

rescale $\quad m \to M/a, \quad \psi_\alpha(x_n) \to \frac{1}{a^{3/2}}\hat{\psi}_\alpha(n), \quad \partial_\mu \psi_\alpha(x_n) \to \frac{1}{a^{5/2}}\hat{\partial}_\mu \hat{\psi}_\alpha(n)$

$$\hat{\partial}_\mu \hat{\psi}_\alpha(n) = \frac{1}{2}\,[\hat{\psi}_\alpha(n+\hat{\mu}) - \hat{\psi}_\alpha(n-\hat{\mu})]$$

$$S_F[\bar{\psi}\psi] \simeq \sum_{n,m;\alpha,\beta} \hat{\bar{\psi}}_\alpha(n) K_{\alpha\beta}(n,m) \hat{\psi}_\beta(m)$$

with $\quad K_{\alpha\beta}(n,m) = \frac{1}{2}\sum_\mu (\gamma_\mu)_{\alpha\beta}\,[\delta_{m,n+\hat{\mu}} - \delta_{m,n-\hat{\mu}}] + M\,\delta_{mn}\delta_{\alpha\beta}$

Free lattice Dirac propagator:

$$\langle \psi_\alpha(x)\bar{\psi}_\beta(y)\rangle = \lim_{a\to 0}\int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4}\,\frac{[-i\sum_\mu \gamma_\mu \tilde{p}_\mu + m]_{\alpha\beta}}{\sum_\mu \tilde{p}_\mu^2 + m^2}\, e^{ip(x-y)}$$

with $\tilde{p}_\mu = \frac{1}{a}\sin(p_\mu a)$ to be compared with scalar case $\tilde{k}_\mu = \frac{2}{a}\sin(k_\mu a/2)$.

For $M = 0$ in momentum space we get poles at all 2^d corners of the Brillouin zone $[(0000), (\pi/a\ 000), \ldots]$. $\Longrightarrow$ "Doubling of fermion degrees of freedom".

Theorem by Nielsen, Ninomiya, '81:

Doubling problem can be avoided only by giving up at least one of:

- reflexion positivity,
- cubic symmetry,
- locality,
- chiral invariance in the zero mass case.

5.2. Wilson fermions and improvements

Wilson's choice – break chiral symmetry even at $m = 0$:

$$D_F = \gamma_\mu \partial_\mu \quad \longrightarrow \quad D_{\mathrm{Latt}} \equiv D_F^W = \frac{1}{2}\left[\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - ar\nabla_\mu^* \nabla_\mu\right],$$

where ∇_μ (∇_μ^*) forward (backward) gauge covariant derivatives

$$\nabla_\mu \psi(x_n) = \frac{1}{a}\Big[U_{n,\mu}\psi(n+\hat{\mu}) - \psi(n)\Big]$$

r – arbitrary real parameter, often chosen to be $r = 1$.

Lattice free Wilson fermion action:

$$S_F^W[\bar{\psi}\psi] \simeq \sum_{n,m;\alpha,\beta} \overline{\hat{\psi}}_\alpha(n) K^W_{\alpha\beta}(n,m) \hat{\psi}_\beta(m),$$

$$K^W_{\alpha\beta}(n,m) = (M+4r)\delta_{mn}\delta_{\alpha\beta} - \frac{1}{2}\sum_\mu \left[(r-\gamma_\mu)_{\alpha\beta}\ \delta_{m,n+\hat{\mu}} + (r+\gamma_\mu)_{\alpha\beta}\ \delta_{m,n-\hat{\mu}}\right]$$

Propagator:

$$\langle \psi_\alpha(x)\bar{\psi}_\beta(y)\rangle = \lim_{a\to 0}\int_{-\pi/a}^{\pi/a} \frac{d^4p}{(2\pi)^4} \frac{[-i\sum_\mu \gamma_\mu \tilde{p}_\mu + m(p)]_{\alpha\beta}}{\sum_\mu \tilde{p}_\mu^2 + m(p)^2} e^{ip(x-y)},$$

$\tilde{p}_\mu$ as before, but $m(p) = m + \frac{2r}{a}\sum_\mu \sin^2(p_\mu a/2)$

For $a \to 0$

$$m(p) \to m \quad \text{for} \quad p_\mu \neq \pm\frac{\pi}{a},$$

$$m(p) \to \infty \quad \text{for} \quad p_\mu = \pm\frac{\pi}{a}.$$

Problems:

- Chiral $SU(3)_A$ flavor symmetry explicitly broken.
- Eigenvalue value spectrum of D_F^W strongly differs from continuum spectrum.
- Discretization error $\delta S_F^W \sim O(a)$ compared with $\delta S_G^W \sim O(a^2)$

$\Longrightarrow$ improvement possible with clover term

$$S_F^{clover} = S_F^W + a^5 \sum_n c_{sw} \psi(x_n) \frac{i}{4} \sigma_{\mu\nu} \hat{F}_{\mu\nu} \psi(x_n) \,.$$

Sheikholeslami, Wohlert '85

$\Longrightarrow$ alternative: twisted-mass fermions at maximal twist (cf. K. Jansen).

Chiral improvement: Ginsparg-Wilson fermions

Any lattice Dirac operator satisfying the Ginsparg-Wilson relation (GWR)

Ginsparg, Wilson '82

$$\gamma_5 D_{\mathrm{Latt}} + D_{\mathrm{Latt}}\gamma_5 = a D_{\mathrm{Latt}}\gamma_5 D_{\mathrm{Latt}}$$

guaranties approximately local ($\sim O(a)$), but exact chiral symmetry.

Lüscher '98

Topological charge becomes well defined

$$a^4 q_t(x_n) \sim \mathrm{Tr}\left[\gamma_5 \mathrm{D_{Latt}}(\mathrm{x_n}, \mathrm{x_n})\right] ,$$

Atiyah-Singer Index theorem holds

$$n_- \; - \; n_+ \; = \; \mathrm{index}(\mathrm{D_{Latt}}) \; = \; \mathrm{a}^4 \sum_{\mathrm{n}} \mathrm{q_t}(\mathrm{x_n})\,.$$

$\Longrightarrow$ tool for investigating topological excitations (instantons etc.).

Strategies to solve GWR:

- Neuberger's operator: exact solution of GWR

$$D + m \quad \rightarrow \quad D_N = \left\{ 1 + \frac{m}{2} (1 + \, A \, (A^\dagger A)^{-\frac{1}{2}} \,) \right\}, \quad A = 1 + s - D_F^W$$

Neuberger '98

Properties:

  - $(\sqrt{A^\dagger A})^{-1}$ numerically involved:
    approximation by polynomials (Chebyshev approx.).
  - Det $\mathrm{D_N}$ hard to compute, but required for full fermionic simulation.
  - Discretization error still $O(a^2)$.

- Equivalent alternative domain wall fermions: extension to 5 dimensions

$$D_{\mathrm{Latt}} = \frac{1}{2} \left[\gamma_5 (\partial_s^* + \partial_s) - a_s \partial_s^* \partial_s \right] + D_F^W - \frac{\rho}{a}, \quad 0 < \rho < 2$$

with boundary condition

$$P_+ \psi(\, o, x) = P_- \psi(\, (N_s + 1) \, a_s, x) = 0 \,, \qquad P_\pm = (1 \pm \gamma_5)/2$$

and limit $N_s \rightarrow \infty$ and $a_s \rightarrow 0$

Kaplan '92; Shamir '93

- Approximative methods:
  - Renormalization group based perfect action approach

    P. Hasenfratz, Niedermayer '94; DeGrand, ... '94
  - generalized (less local) ansatzes for D_{Latt} with parameters fixed from GWR

    Gattringer '01

5.3. Staggered fermions

Kogut, Susskind, '75

- Use naive discretization and diagonalize action w.r. to spinor degrees of freedom.
- Neglect three of four degenerate Dirac components.
- Attribute the 16 fermionic degrees of freedom localized around one elementary hypercube to four *tastes* with four Dirac indices each.

Chiral symmetry restored $\Longleftrightarrow$ flavor symmetry broken.
Naturally the mass-degenerated four-flavor case is described.

Rooting prescription:
for $N_f = 2 + 1(+1)$ 4th-root of the fermionic determinant is taken.
$\Longrightarrow$ Locality violated (??)

Improvement possible by 'smearing' link variables.

5.4. How to compute typical QCD observables

Path integral quantization for Euclidean time $\Longrightarrow$ 'statistical averages'.

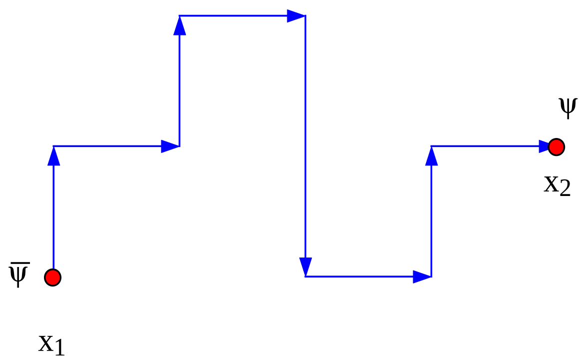
Fermions as anticommuting Grassmann variables
$\Longrightarrow$ analytically integrated $\Rightarrow$ non-local effective action $S^{eff}(U)$.

'Partition function' for $f = 1, \cdots, N_f$ light quark flavors:

$$\begin{aligned} Z &= \int [dU] \prod_f [d\psi_f]\, [d\bar{\psi}_f]\; e^{-S^G(U) + \sum_f \bar{\psi}_f M_f(U) \psi_f} \\ &= \int [dU]\; e^{-S^G(U)} \prod_f \mathrm{Det} M_f(U) \\ &= \int [dU]\; e^{-S^{eff}(U)}, \quad S^{eff}(U) = S^G(U) - \sum_f \log(\mathrm{Det} M_f(U)) \end{aligned}$$

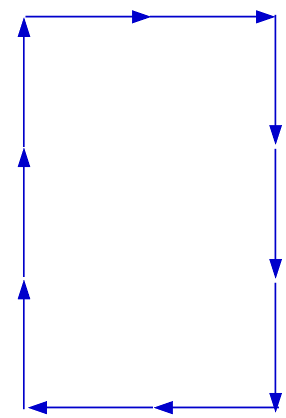
with $\quad M_f(U) \equiv D_{\mathrm{Latt}}(U) + m_f$.
To be simulated on a finite lattice $N_t \times N_s^3$, mostly with periodic boundary conditions for gluons (anti-periodic for quarks).

Observables: mostly gauge invariant.



$\bar{\psi}_u(x_1)\; U(x_1,x_2)\; \Gamma\; \psi_d(x_2)$

Non-local fermionic current



$\Omega(U) = \mathrm{tr} \prod_l \mathrm{U}_l$

Wilson loop

[These and the following diagrams taken from C. Davies, hep-ph/0205181]

Pure gauge observables:

$$\begin{aligned}
\langle \Omega \rangle &= \frac{1}{Z} \int [dU] \prod_f [d\psi_f]\, [d\bar{\psi}_f]\; \Omega(U)\; e^{-S^G(U) + \sum_f \bar{\psi}_f M(U) \psi_f} \\
&= \frac{1}{Z} \int [dU]\; \Omega(U)\; e^{-S^{eff}(U)}
\end{aligned}$$

Fermionic observables through correlators,
e.g. for local (u,d)-meson current $H(x) = \bar{\psi}_u^a(x)\,\Gamma\,\psi_d^a(x)$

$$\langle\, H^\dagger(x) H(y)\,\rangle = \frac{1}{Z}\int [dU] \prod_f [d\psi_f][d\bar{\psi}_f]\; H^\dagger(x) H(y)\; e^{-S^G + \sum_f \bar{\psi}_f M(U)\psi_f}$$

$$= \frac{1}{Z}\int [dU]\; (M(U)^{-1}(x,y))_u^{ab}\;\Gamma\;(M(U)^{-1}(y,x))_d^{ba}\;\Gamma\; e^{-S^{eff}(U)}$$

propagator $(M(U)^{-1}(x,y))_f\,,\;\; f = u,d$ computed with conj. gradient method.

Quenched approximation: put Det $M(U) \equiv 1$, i.e. pure gauge field simulation.

Det $M(U) \neq 1$ can be taken into account, but time consuming
$\Longrightarrow$ Hybrid Monte Carlo, multibosonic algorithms,...
$\Longrightarrow$ massively parallel supercomputers required.

The 3 critical limites:

$$CPU \simeq F_{\mathrm{per}} \left(\frac{m_\rho}{m_\pi}\right)^{z_\pi} \left(\frac{L}{a}\right)^{z_L} \left(\frac{r_0}{a}\right)^{z_a}$$

Exponents depend on algorithms. To be determined empirically. E.g.

$$F_{\mathrm{per}} \simeq 6 \cdot 10^6 \text{ flops}, \qquad \mathrm{z}_\pi \simeq 6, \quad \mathrm{z_L} \simeq 5, \quad \mathrm{z_a} \simeq 2, \quad \mathrm{r_0} \simeq 0.5 \text{ fm}$$

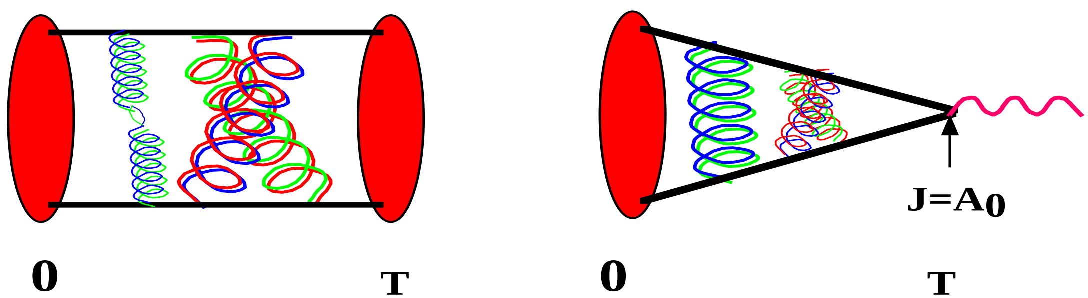
Ukawa, LATTICE 2001; in the meantime much improved, cf. C. Urbach's lecture

Our aim: computation of hadronic masses and matrix elements from various 2-point or 3-point functions

2-point functions:

$$\langle O_f(T) O_i(0)\rangle - \langle O_f\rangle\langle O_i\rangle = \sum_n \frac{\langle \mathrm{vac}|\mathrm{O_f}|\mathrm{n}\rangle\langle \mathrm{n}|\mathrm{O_i}|\mathrm{vac}\rangle}{2M_n} e^{-M_n T} \ \overset{T\to\infty}{\sim} \ e^{-M_0 T}$$

- $O_f \equiv H^\dagger, \quad O_i \equiv H \quad \Longrightarrow$ extract masses of hadrons with quantum numbers related to non-local current H.
- $O_f \equiv J, \quad O_i \equiv H \quad \Longrightarrow$ extract vacuum-to-hadron matrix elements (decay constants) with local current J.

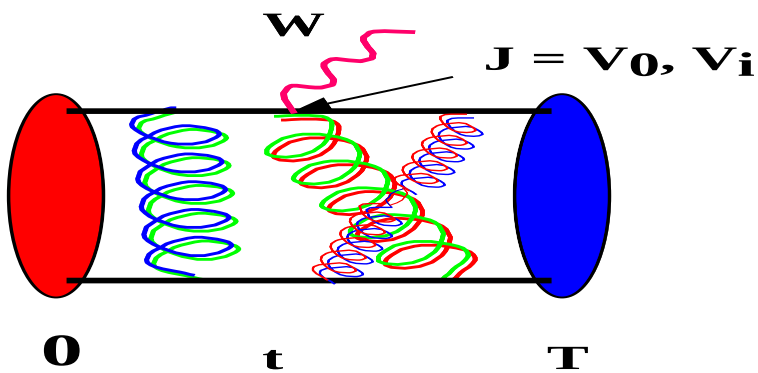


2pt function for spectrum 2pt function for decay constant

3-point functions:

$$\langle H'^{\dagger}(T)J(t)H(0)\rangle = \sum_n \sum_m \frac{\langle \mathrm{vac}|\mathrm{H}^{\dagger}|\mathrm{m}\rangle \langle \mathrm{m}|\mathrm{J}|\mathrm{n}\rangle \langle \mathrm{n}|\mathrm{H}|\mathrm{vac}\rangle}{2M_n 2M_m} e^{-M_n t} e^{-M_m (T-t)}$$

- allow to extract experimentally relevant hadron-to-hadron matrix elements for decay constants, moments of structure functions and form factors of hadrons.



3pt function for SL decay