# Introduction to Lattice QCD





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# Lecture 1: Introduction to the lattice formulation Outline



- Standard Model of Elementary Particles
- QCD versus QED
- Scalar field theory on a lattice



Bosons

4

Fermions

#### **Formulation of Lattice Gauge Theories**

- Local Gauge Symmetry
- U(1) gauge theory
- SU(N) Gauge Theory on a lattice
- String tension

#### 5 Continuum limit and Renormalization Asymptotic Freedom

Exercises

#### Standard model

The Standard Model (SM) is a synthesis of three of the four forces of nature described by gauge theories with coupling constants:

- Strong Interactions: α<sub>s</sub> ~ 1
- Electromagnetic interactions:  $\alpha_{em} \approx 1/137$
- Weak interactions:  $G_F \approx 10^{-5} \text{ GeV}^{-2}$ .

Basic constituents of matter:

- Six quarks, u, d, s, c, b, t, each in 3 colors, and six leptons e, ν<sub>e</sub>, μ, ν<sub>μ</sub>, τ, ν<sub>τ</sub>
- The quarks and leptons are classified into 3 generations of families.
- The interactions between the particles are mediated by vector bosons: the 8 gluons mediate strong interactions, the W<sup>±</sup> and Z mediate weak interactions, and the electromagnetic interactions are carried by the photon γ.
- The weak bosons acquire a mass through the Higgs mechanism.
- The SM is a local gauge field theory with the gauge group SU(3) × SU(2) × U(1) specifying the interactions among these constituents.

#### Masses in the Standard Model

Parameters	Number	Comments	n cha
Masses of quarks	6	u, d, s light	
		c, b heavy	n
		$t = 175 \pm 6 \; GeV$	
	•		
Masses of leptons	6	$e, \mu, \tau$	
		$M_{ u_e, \  u_\mu, \  u_ au}$ non-zero	
Mass of $W^{\pm}$	1	80.3 GeV	
Mass of Z	1	91.2 GeV	
Mass of gluons, $\gamma$		0 (Gauge symmetry)	
Mass of Higgs	1	125.35(15) GeV	
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# **QCD** – Gauge theory of the strong interaction

• Lagrangian: formulated in terms of quarks and gluons

$$egin{aligned} \mathcal{L}_{ ext{QCD}} &= -rac{1}{4}F^a_{\mu
u}F^{a\,\mu
u} + \sum_f \overline{\psi}_f \left(i\gamma^\mu D_\mu - m_f
ight)\psi_f, \quad f = u, d, s, c, b, t \ D_\mu &= \partial_\mu - ig(rac{1}{2}\lambda^a)A^a_\mu \end{aligned}$$



Harald Fritzsch



Murray Gell-Mann



Heinrich Leutwyler

#### **Properties of QCD**



"... for the discovery of asymptotic freedom in the theory of the strong interaction"



David Gross



Frank Wilczek



David Politzer

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Introduction to Lattice QCD

# **QCD versus QED**

- QCD is the theory of strong interactions formulated in terms of quarks and gluons as the basic degrees of freedom of hadronic matter.
- Conventional perturbative approach cannot be applied for hadronic process at scales <sup>5</sup> 1 GeV since the strong coupling constant α<sub>s</sub> ~ 1

 $\Longrightarrow$  we cannot calculate the masses of mesons and baryons from QCD even if we are given  $\alpha_s$  and the masses of quarks.

Bound state in QCD very different from QED e.g. the binding energy of a hydrogen atom is to a good approximation the sum of it constituent masses. Similarly for nuclei the binding energy is O(MeV). For the proton almost all the mass is attributed to the strong non-linear interactions of the gluons.



# **QCD** on the lattice

Why Lattice QCD?

- O Discrete space-time lattice acts as a non-perturbative regularization scheme with the lattice spacing a providing an ultraviolet cutoff at π/a → no infinities. Furthermore, renormalized physical quantities have a finite well behaved limit as a → 0.
- Can be simulated on the computer using methods analogous to those used for Statistical Mechanics systems. These simulations allow us to calculate correlation functions of hadronic operators and matrix elements of any operator between hadronic states in terms of the fundamental quark and gluon degrees of freedom.

Like continuum QCD lattice QCD has as unknown input parameters the coupling constant  $\alpha_s$  and the masses of the up, down, strange, charm and bottom quarks (the top quark is too short lived).  $\Rightarrow$ Lattice QCD provides a well-defined approach to calculate observables non-perturbative starting directly from the QCD Langragian.

#### Scalar field theory

Let the continuum  $\vec{r}$  be defined on lattice points i.e.  $\vec{r} \rightarrow \vec{n} \equiv (n_1, n_2, n_3)a$  where *a* is the lattice spacing.  $\implies$  equivalent to many-body problem where:

$$\hat{x}_i, \hat{p}_i 
ightarrow \hat{\phi}(\vec{n}), \hat{\pi}(\vec{n})$$
  $\hat{x}_i \ket{x} = x_i \ket{x} 
ightarrow \hat{\phi}(\vec{n}) = \phi(\vec{n}) \ket{\phi}.$ 

We then have

$$\int d^3r \left\{ \frac{1}{2} \pi^2(\vec{r}) + \frac{1}{2} |\vec{\nabla}\phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\} \rightarrow \sum_{\vec{n}} a^3 \left\{ \frac{1}{2} \pi^2(\vec{n}) + \frac{1}{2a^2} \sum_{i=1}^3 |\phi(\vec{n} + a\mu_i) - \phi(\vec{n})|^2 + V(\phi(\vec{n})) \right\}$$

where  $\mu_i$  denotes a displacement by one lattice site in the *i*<sup>th</sup> direction. The evolution operator in Euclidean time:

$$e^{-t\sum_{\vec{n}}a^3\left\{\frac{1}{2}\pi^2(\vec{n})+F(\phi(\vec{n}))\right\}} = \int \mathcal{D}[\phi(\vec{n})]e^{-\Delta t a^3\sum_{\vec{n},k}\left[\frac{1}{2\Delta t^2}\left(\phi_{k+1}(\vec{n})-\phi_k(\vec{n})\right)^2+F(\phi_k(\vec{n}))\right]}$$

Take isotropic lattice i.e.  $\Delta t = a$ 

 $\implies$  time slicing replaces  $\hat{\rho}^2(\vec{n})$  by  $\frac{1}{\Delta t}(\phi_{k+1}(\vec{n}) - \phi_k(\vec{n}))^2 \equiv \frac{1}{\Delta t}(\phi(n+a\mu_0) - \phi(n))^2$  which has the same structure as the discrete spatial derivative and where  $n = (n_0, n_1, n_2, n_3)a$ .

$$\Longrightarrow \mathcal{O}(\phi) e^{-t \int d^3 r \left\{ \frac{1}{2} \pi^2(\vec{r}) + \frac{1}{2} |\vec{\nabla}\phi(\vec{r})|^2 + V(\phi(\vec{r})) \right\}} \to \int \mathcal{D}[\phi(n)] \mathcal{O}(\phi) e^{-S_{\text{cl}}[\phi]}$$

where  $S_{cl}[\phi] = \sum_{n} a^{4} \left\{ \sum_{i=0}^{3} \frac{(\phi(n+a\mu_{i})-\phi(n))^{2}}{a^{2}} + V(\phi(n)) \right\}.$ 

Note that  $S_{cl}$  is completely symmetric in time and space  $\rightarrow$  if we choose periodic b.c. then the shortest dimension acts as a finite temperature.

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#### **Coherent States for bosons**

For the Feynman path integral of the 1-d QM example we needed:

- Eigenstates of  $\hat{x}$ ,  $\hat{x} |x\rangle = x |x\rangle$  and
- Unity:  $\int dx |x\rangle \langle x| = 1$

The analogs for creation and annihilation operators are provided by boson coherent states. Consider a creation operator  $a^\dagger$  then

$$\left[\hat{a},\hat{a}^{\dagger}\right] = 1 \qquad \hat{a}^{\dagger} |n\rangle = \sqrt{n+1} |n+1\rangle \qquad \hat{a} |n\rangle = \sqrt{n} |n-1\rangle \qquad |n\rangle = \frac{1}{\sqrt{n!}} \left(\hat{a}^{\dagger}\right)^{n} |0\rangle$$

Define the coherent state  $|z\rangle$  by

$$|z\rangle \equiv e^{za^{\dagger}} |0\rangle = \sum_{n} \frac{z^{n}}{n!} \left(\hat{a}^{\dagger}\right)^{n} |0\rangle = \sum_{n} \frac{z^{n}}{\sqrt{n!}} |n\rangle$$

Properties:

$$\hat{a} |z\rangle = \sum_{n} \frac{z^{n}}{\sqrt{n!}} \hat{a} |n\rangle = z \sum_{n} \frac{z^{n-1}}{\sqrt{(n-1)!}} |n-1\rangle = z |z\rangle$$

$$\langle z|z'\rangle = \sum_{mn} \langle m| \frac{z^{*m}}{\sqrt{m!}} \frac{z'^{n}}{\sqrt{n!}} |n\rangle = e^{z^{*}z'}$$

$$\langle z|: A(\hat{a}^{\dagger}\hat{a}): |z\rangle' = e^{z^{*}z'} A(z^{*}, z')$$

$$1 = \int \frac{dzdz^{*}}{2\pi i} e^{-z^{*}z'} |z\rangle \langle z|$$
(1)

#### **Coherent States for bosons**

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Generalize for a set of creation operators  $\hat{a}^{\dagger}_{\alpha}$ 

$$\begin{split} |z\rangle &= e^{\sum_{\alpha} z_{\alpha} \hat{a}^{\dagger}_{\alpha}} |0\rangle \\ \hat{a_{\alpha}} |z\rangle &= z_{\alpha} |z\rangle \\ \langle z| : A(\hat{a}^{\dagger} \hat{a}) : |z\rangle' &= e^{\sum_{\alpha} z_{\alpha} Z'_{\alpha}} A(z^{*}, z') \\ 1 &= \int \prod_{\alpha} \frac{dz_{\alpha} z^{*}_{\alpha}}{2\pi i} e^{-z^{*}_{\alpha} z'_{\alpha}} |z\rangle \langle z| \equiv \int d\mu(z) |z\rangle \langle z| \end{split}$$

#### Path integral using coherent states

Time slicing the evolution operator:

$$\langle z_{f} | e^{-tH} | z_{i} \rangle = \langle z_{f} | e^{-\Delta tH} \int d\mu(z_{N-1}) | z_{N-1} \rangle \langle z_{N-1} | e^{-\Delta tH} \int d\mu(z_{N-2}) \cdots e^{-\Delta tH} | z_{i} \rangle$$

The matrix element of the infinitesimal evolution operator is

$$d\mu(z_k) \langle z_k | e^{-tH} | z_{k-1} \rangle = \prod_{\alpha} \frac{dz_{k,\alpha}^* dz_{k,\alpha}}{2i\pi} e^{-\sum_{\alpha} z_{k,\alpha}^* (z_{k,\alpha} - z_{k-1,\alpha}) - \Delta t H(z_{k,\alpha}^*, z_{k-1,\alpha})}$$

resulting in

$$\begin{aligned} \langle z_{f} | e^{-tH} | z_{i} \rangle &= \int \mathcal{D}[z_{k,\alpha}^{*}, z_{k,\alpha}] e^{-S(z_{k,\alpha}^{*}, z_{k,\alpha})} \\ S(z^{*}, z) &= \sum_{k} \Delta t \left\{ \sum_{\alpha} z_{k,\alpha}^{*} \left( \frac{z_{k,\alpha} - z_{k-1,\alpha}}{\Delta t} \right) + H(z_{k,\alpha}^{*}, z_{k-1,\alpha}) \right\} \end{aligned}$$

#### **Coherent states for fermions**

Fermions are represented by anti-commuting creation and annihilation operators  $c^{\dagger}_{\alpha}$  and  $c_{\alpha} \rightarrow$  need to introduce anti-commuting Grassmann variables  $\xi$  such that

 $\hat{c}_{lpha}\ket{\xi} = \xi_{lpha}\ket{\xi} \qquad \hat{c}_{lpha}\hat{c}_{eta}\ket{\xi} = \xi_{lpha}\xi_{eta}\ket{\xi} = -\xi_{eta}\xi_{lpha}\ket{\xi} = -\hat{c}_{eta}\hat{c}_{lpha}\ket{\xi}$ 

Since  $\xi_{\alpha}^2 = 0$  (Pauli principle) the only functions allowed are monomials. The rules for integration over a Grassmann variable  $\xi$  and  $\xi^*$  are

$$\int d\xi_{\alpha} = \int d\xi_{\alpha}^* = 0, \ \int d\xi_{\alpha}\xi_{\alpha} = \int d\xi_{\alpha}^*\xi_{\alpha}^* = 1$$

A fermion coherent state is defined by

 $|\xi\rangle \equiv e^{-\sum_{\alpha} \xi_{\alpha} c^{\dagger}_{\alpha}} |0\rangle$ 

with similar properties to bosons. The path integral have similar form to that for bosons with some minus signs that distinguish between bosons and fermions.

#### Integration over fermions

For numerical evaluation we can not have the path integrals in terms of Grassmann variables. Fortunately for normalizable field theories we can integrate analytically over the fermionic degrees of freedom Recall Gaussian integral

$$\int \prod_{i} \frac{dz_{i}^{*} dz_{i}}{2i\pi} e^{-z_{i}^{*} H_{ij} z_{j} + J_{i}^{*} z_{i} + z_{i}^{*} J_{j}} = [detH]^{-1} e^{J_{i}^{*} H_{ij}^{-1} J_{j}}$$

An analogous result is obtained for Grassmann "Gaussian": For one pair of Grassmann variables we have

$$\int d\xi^* d\xi \, e^{-\xi^* \mathbf{a}\xi} = \int d\xi^* d\xi (1-\xi^* \mathbf{a}\xi) = \mathbf{a}$$

This generalizes to

$$\int \prod_{i} d\xi_{i}^{*} d\xi_{i} e^{-\xi_{i}^{*} H_{ij}\xi_{j} + \eta_{i}^{*}\xi_{i} + \xi_{i}^{*} \eta_{i}} = [detH] e^{\eta_{i}^{*} H_{ij}^{-1} \eta_{j}}$$

i.e. the only difference is that *detH* appears in the numerator  $\rightarrow$  accounts for the minus sign of fermion loops. If our action is of the form  $S(\xi^*, \xi, \phi) = \xi_i^* M(\phi)_{ij}\xi_j + S_B(\phi)$  then

$$\int d\xi^* d\xi d\phi \, e^{\xi_i^* M(\phi)_{ij}\xi_j + S_{\mathcal{B}}(\phi)} = \int d\phi \, det \mathcal{M}(\phi) \, e^{S_{\mathcal{B}}(\phi)}$$

i.e.  $S_{\text{eff}}(\phi) = \ln det M(\phi) + S_B(\phi)$ 

#### **Fermion propagators**

Consider the time ordered product of field creation and annihilation operators at space-time points  $j = (x_j, t_j)$  and  $i = (x_i, t_j)$  respectively:

$$\langle \hat{T}\psi_i \bar{\psi}_j \rangle = \operatorname{Tr} \hat{T}\psi_i \bar{\psi}_j \, e^{-\bar{\psi} M(\phi)\psi + S_{\mathcal{B}}(\phi)} = \int \mathcal{D}[\phi] \mathcal{D}[\bar{\xi}\xi] \xi_i \bar{\xi}_j \, e^{-\bar{\xi} M(\phi)\xi + S_{\mathcal{B}}(\phi)} = \int \mathcal{D}[\phi] \, M_{ij}^{-1}(\phi) \, e^{S_{\mathrm{eff}}(\phi)}$$

In general for n pairs of creation and annihilation operators

$$\int \mathcal{D}(\xi^{*},\xi) \,\xi_{i_{1}} \cdots \xi_{i_{n}} \xi_{j_{n}}^{*} \cdots \xi_{j_{1}} \,e^{-\xi^{*}M\xi}$$

$$= \frac{\delta^{2n}}{\delta\eta_{i_{1}}^{*} \cdots \delta\eta_{i_{n}}^{*}\delta\eta_{j_{n}} \cdots \delta\eta_{j_{1}}} \int \mathcal{D}(\xi^{*},\xi) \,e^{-\xi_{i}^{*}M_{ij}\xi_{j}+\eta_{i}^{*}\xi_{i}+\xi_{i}^{*}\eta_{i}} |_{\eta=\eta^{*}=0}$$

$$= \frac{\delta^{2n}}{\delta\eta_{i_{1}}^{*} \cdots \delta\eta_{i_{n}}^{*}\delta_{j_{n}} \cdots \delta\eta_{j_{1}}} \det M \,e^{\eta_{i}^{*}M_{ij}^{-1}\eta_{j}} |_{\eta=\eta^{*}=0}$$

$$= \sum_{P} (-1)^{P} M_{i_{P}n}^{-1} \cdots M_{i_{P}1}^{-1} e^{\ln \det M}$$

where *P* denotes a permutation of the indices. This is nothing else but Wick's theorem.

⇒ fermions can be integrated out and we left only with an effective action with the bosonic degrees of freedom.

Boundary conditions:

$$Tre^{-tH} = \int dz_0^* dz_0 e^{-z_0^* z_0} \langle \pm z_0 | e^{-tH} | z_0 \rangle = \int dz_0^* dz_0 e^{-z_0^* z_0} \int d\mathcal{D}[z^*, z] e^{-S(z^*, z)}$$

where the plus is for bosons and minus for fermions and  $S(z^*, z) = \pm z_0^* (\pm z_0 - z_{N-1}) + H_{0.N-1} + z_{N-1}^* (z_{N-1} - z_{N-2}) + H_{N-1,N-2} + \dots + z_1^* (z_1 - z_0) H_{1,0}.$ 

#### Lattice Gauge theories

- K. Wilson: 1974 formulated Euclidean gauge theories on the lattice as a tool for the study of confinement and non-perturbative properties of QCD.
- M. Creutz: 1980 perform the first numerical implementation of the path integral for gauge theories.
- The set-up for the numerical evaluation requires
  - Discretization of space-time: Discretize space-time in 4 Euclidean dimensions → simplest isotropic hypercubic grid with spacing a = a<sub>S</sub> = a<sub>T</sub> and size N<sub>S</sub> × N<sub>S</sub> × N<sub>S</sub> × N<sub>T</sub>
  - Definition of the gauge and fermion degrees on the discrete space-time: The quark field is represented by anticommuting Grassmann variables defined at each site of the lattice. They belong to the fundamental representation of SU(3). The gauge field is discussed below.
  - Construction of an appropriate action
  - Definition of the measure of integration in the path integral.
  - Construction of the operators used to probe the physics

#### Gauge degrees of freedom

In the continuum a fermion moving from site x to y in the presence of a gauge field  $A_{\mu}(x)$  picks up a phase factor given by the path ordered product

$$\psi(\mathbf{y}) = \mathcal{P} \, e^{i \int_{\mathbf{x}}^{\mathbf{y}} g A_{\mu}(\mathbf{x}) d\mathbf{x}_{\mu}} \, \psi(\mathbf{x}) \, .$$

⇒ associate gauge fields with links that connect sites on the lattice. So, with each link associate a discrete version of the path ordered product:

$$U(x; x + \hat{\mu}) \equiv U_{\mu}(x) = e^{iagA_{\mu}(x)},$$

U is a  $3 \times 3$  unitary matrix with unit determinant. It follows that

$$U(x; x - \hat{\mu}) \equiv U_{-\mu}(x) = e^{-iagA_{\mu}(x)} = U^{\dagger}(x - \hat{\mu}; x)$$
.

#### Local gauge symmetry

The effect of a local gauge transformation V(x) on the variables  $\psi(x)$  and U is defined as

 $\begin{array}{lll} \psi(x) & \to & V(x)\psi(x) \\ \bar{\psi}(x) & \to & \bar{\psi}(x)V^{\dagger}(x) \\ U_{\mu}(x) & \to & V(x)U_{\mu}(x)V^{\dagger}(x+\hat{\mu}) \end{array}$ 

where V(x) is in the same representation as the  $U_{\mu}(x)$ , *i.e.*, temporisize it is an SU(3) matrix. With these definitions there are two types of gauge invariant objects that one can construct on the lattice.



A string consisting of a path-ordered product of links capped by a fermion and an antifermion e.g.

Tr  $\overline{\psi}(x) U_{\mu}(x) U_{\nu}(x + \hat{\mu}) \dots U_{\rho}(y - \hat{\rho}) \psi(y)$ 

where the trace is over the color indices.

If the string stretches across the lattice and is closed by the periodicity are called Polyakov lines.

The simplest example of closed Wilson loops is the plaquette, a 1 × 1 loop,

$$W_{\mu\nu}^{1\times 1} = P_{\mu\nu}(x) = \text{Re Tr} \left( U_{\mu}(x) U_{\nu}(x+\hat{\mu}) U_{\mu}^{\dagger}(x+\hat{\nu}) U_{\nu}^{\dagger}(x) \right)$$

Preserve gauge invariance at all  $a \rightarrow$  protects from having many more parameters to tune (the zero gluon mass, and the equality of the quark-gluon, 3-gluon, and 4-gluon couplings) and there would arise many more operators at any given order in *a*.

# U(1) gauge theory

Consider a Lagrangian of a complex field  $\phi: L = \partial_{\mu} \phi^* \partial^{\mu} \phi - V(\phi^*, \phi)$ . If we require that the Lagrangian is invariant under a local gauge transformation  $\phi'(x) = e^{-i\alpha(x)}\phi(x)$  then we need a field  $A_{\mu}(x)$  to compensate the change in the derivative  $\partial_{\mu}\phi$  that transforms as

$$A'_{\mu}(x) = A_{\mu}(x) + rac{1}{g} \partial_{\mu} \alpha(x) \; \partial_{\mu} 
ightarrow D_{\mu} \equiv \partial_{\mu} + igA_{\mu}(x)$$

The gauge invariant Lagrangian is written as

$$L = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} + (D_{\mu}\phi)^*D_{\mu}\phi - V(\phi^*,\phi)$$

A scalar moving from site x to y in the presence of a gauge field  $A_{ii}(x)$  picks up a phase factor given by

$$U(x; y) = e^{ig \int_{x}^{y} dx_{\mu} A^{\mu}(x)}$$

which removes the phase between the value of the field at the two points and yields a gauge invariant result.





The link variable from site *n* in the  $\mu$  direction to site  $n + a\hat{e}_{\mu}$  is defined as the discrete approximation to the integral  $e^{ig \int_{n}^{n+\mu}}$ :  $U_{\mu}(n) = e^{i\theta_{\mu}(n)}$  with  $\theta_{\mu}(n)$ the approximation of  $g \int_{a}^{a+\mu} dx_{\mu} A^{\mu}(x)$ .



The integral over the field variables is the invariant group measure for U(1):  $\frac{1}{2\pi}\int_{-\pi}^{\pi}d\theta.$ The action is the sum of all plaquettes  $P_{\mu\nu} = U(n)_{\mu}U_{\nu}(n+\mu)U_{\mu}^{\dagger}(n+\nu)U_{\nu}^{\dagger}(n)$ .

For U(1):  $P_{\mu\nu}(n) = e^{i\theta_{\mu}(n)}e^{i\theta_{\nu}(n+\mu)}e^{-i\theta_{\mu}(n+\mu)}e^{-i\theta_{\nu}(n)} \equiv e^{iB_{\mu\nu}}, B_{\mu\nu} = \Delta_{\mu}\theta_{\nu} - \Delta_{\nu}\theta_{\mu} \xrightarrow{a \to 0} F_{\mu\nu}.$ 

#### Lattice action of U(1)

Since a plaquette produces  $F_{\mu\nu}$  the action can be constructed by choosing a function of the plaquette such that it generates  $F_{\mu\nu}^2$  in the continuum limit.

$$S = \beta \sum_{n} \sum_{\mu > \nu} \left( 1 - \operatorname{Re} P_{\mu\nu}(n) \right) = \beta \sum_{n} \sum_{\mu > \nu} \left( 1 - \cos B_{\mu\nu} \right),$$

where  $\beta = \frac{1}{g^2}$  and  $B_{\mu\nu} = \Delta_{\mu}\theta_{\nu} - \Delta_{\nu}\theta_{\mu} \stackrel{a\to 0}{\to} F_{\mu\nu}$ .

In the limit  $a \to 0$  we recover continuum QED: Taking  $\theta_{\mu}(n) = agA_{\mu}(n)$  and expanding  $\theta_{\nu}(n + \hat{e}_{\mu}a) = \theta_{\nu}(n) + a\partial_{\mu}\theta_{\nu}(n) + O(a^2)$ 

$$S \sim \frac{1}{g^2} \sum_{P} [1 - \cos(a\partial_{\mu}\theta_{\nu} - a\partial_{\nu}\theta_{\mu})] = \frac{1}{g^2} \sum_{P} \left[1 - \cos(a^2 g F_{\mu\nu})\right] = \frac{1}{g^2} \sum_{n} \sum_{\mu > \nu} \left[\frac{a^4 g^2}{2} F_{\mu\nu}^2 + \cdots\right]$$
  
$$\rightarrow \frac{1}{4} \int d^4 x F_{\mu\nu}^2(x)$$

#### SU(N) Gauge Theory on a lattice

The generalization to non-Abelian gauge theory is straightforward. The link variable is

$$U_{\mu}(n) = e^{iag\lambda^{C}A_{\mu}^{C}(n)} = e^{iagA_{\mu}(n)}$$
 and  $U_{-\mu}(n) = e^{-iag\lambda^{C}A_{\mu}^{C}(n)} = U_{\mu}^{\dagger}(n-\mu)$ 

For SU(3)  $\lambda^c$  are the Gell-Mann matrices and  $c = 1, \dots, 8$  is a color label. The 8 group generators are normalized as  $Tr\lambda_a\lambda_b = 2\delta_{ab}$  and U is a 3  $\times$  3 unitary matrix with unit determinant. The action is given in terms of the product of SU(N) group elements around an elementary plaquette

$$P_{\mu
u}(n) = U_{\mu}(n)U_{\nu}(n+\mu)U_{\mu}^{\dagger}(n+
u)U_{\nu}^{\dagger}(n) = e^{iagA_{\mu}(n)}e^{iagA_{\nu}(n+\mu)}e^{-iagA_{\mu}(n+
u)}e^{-igA_{\nu}(n)}$$

In order to find the continuum limit of this plaquette we expand A by applying the the Baker-Hausdorff identity  $e^{X}e^{Y} = e^{X+Y+\frac{1}{2}[X,Y]+\cdots}$ 

$$\begin{array}{lcl} \mathcal{D}_{\mu\nu} & \sim & e^{iagA_{\mu}(n)}e^{iag(A_{\nu}(n)+a\partial_{\mu}A_{\nu}(n))}e^{-iag(A_{\mu}(n)+a\partial_{\nu}A_{\mu}(n))}e^{-iagA_{\nu}(n)} \\ & \sim & e^{iag\left(A_{\mu}(n)+A_{\nu}(n)+a\partial_{\mu}A_{\nu}(n)+\frac{1}{2}iag[A_{\mu},A_{\nu}]\right)}e^{-iag\left(A_{\mu}(n)+A_{\nu}(n)+a\partial_{\nu}A_{\mu}(n)-\frac{1}{2}iag[A_{\mu},A_{\nu}]\right)} \\ & \sim & e^{ia^{2}g\left(\partial_{\mu}A_{\nu}(n)-\partial_{\nu}A_{\mu}(n)+ig[A_{\mu},A_{\nu}]\right)}=e^{ia^{2}gF_{\mu\nu}} \end{array}$$

and therefore we may define the SU(N) action by choosing a function of the plaquette which yields  $F_{\mu\nu}^2$ :

$$S(U) = \beta \sum_{n} \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \operatorname{Re} \operatorname{Tr} P_{\mu\nu} \right), \ \beta = \frac{2N}{g^2},$$

#### SU(N) Gauge Theory

$$S(U) = \beta \sum_{n} \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \operatorname{Re} \operatorname{Tr} P_{\mu \nu} \right), \ \beta = \frac{2N}{g^2},$$

Using the continuum limit of the plaquette we can easily obtain the continuum limit of the above action:

$$S(U) = \beta \sum_{n} \sum_{\mu > \nu} \left( 1 - \frac{1}{N} \operatorname{Re} \operatorname{Tr} \left( 1 + ia^{2} F_{\mu\nu} - \frac{1}{2} a^{4} g^{2} F_{\mu\nu}^{2} + \cdots \right) \right)$$
  
$$\sim \frac{1}{2} \beta a^{4} g^{2} \sum_{n} \sum_{\mu > \nu} \frac{1}{N} \operatorname{Tr} \left( \frac{1}{2} \lambda^{c} F_{\mu\nu}^{c}(n) \frac{1}{2} \lambda^{b} F_{\mu\nu}^{b}(n) \right) \sim \beta \frac{g^{2}}{2N} \sum_{n} a^{4} \sum_{\mu\nu} \frac{1}{2} F_{\mu\nu}^{c} F_{\mu\nu}^{c}(n)$$
  
$$\rightarrow \frac{1}{4} \int d^{4} x F_{\mu\nu}^{c}(x) F_{\mu\nu}^{c}$$

The fact that the generators  $\lambda^c$  are traceless is used to eliminate linear terms. The relation  $\text{Tr}\lambda^b\lambda^c = 2\delta^{bc}$  has been used to get the diagonal piece.

There is a great freedom to construct other expressions with the same continuum limit. E.g. considering a product of link variables around a larger rectangle  $ja \times ka$  we obtain

$$\frac{1}{a^4}\left(1-\frac{1}{N}\operatorname{ReTr} W^{j\times k}\right) = c_{jk}F_{\mu\nu}^2 + a^2\sum_m d_{jk}^m f^m(D_\mu, D_\nu, F_{\alpha\beta}, F_{\gamma\delta}) + \mathcal{O}(a^4)$$

where  $I^m$  denotes an invariant from two derivatives and two *F*'s and the coefficients *c* and *d* are calculable  $\rightarrow$  we can construct improved actions by taking linear combinations for various rectangles.

#### **Gauge action**

There are four important points to note based on the above construction of the lattice action.

- The leading correction is  $O(a^2)$ : The term  $\frac{a^2}{6}F_{\mu\nu}(\partial^3_{\mu}A_{\nu} \partial^3_{\nu}A_{\mu})$  is present in the expansion of all planar Wilson loops. Thus at the classical level it can be gotten rid of by choosing an action that is a linear combination of say 1 × 1 and 1 × 2 Wilson loops with the appropriate relative strength given by the Taylor expansion
- **2** Quantum effects will give rise to corrections, *i.e.*  $a^2 \rightarrow X(g^2)a^2$  where in perturbation theory  $X(g^2) = 1 + c_1g^2 + \ldots$ , and will bring in additional non-planar loops. Improvement of the action will consequently require including these additional loops, and adjusting the relative strengths which become functions of  $g^2$ .
- The reason for defining the action in terms of small loops is computational speed and reducing the size of the discretization errors. For example the leading correction to 1 × 1 loops is proportional to a<sup>2</sup>/6 whereas for 1 × 2 loops it increases to 5a<sup>2</sup>/12. Also, the cost of simulation increases by a factor of 2 3.
- The electric and magnetic fields *E* and *B* are proportional to  $F_{\mu\nu}$ . They are are given in terms of the imaginary part of Wilson loops: Im $P_{\mu\nu} \stackrel{a=0}{=} a^2 g F_{\mu\nu}$ .

#### Wilson loops

In the pure gauge theory the only gauge invariant objects are closed loops. The Wilson loop

$$W = \operatorname{Tr} U_i(x) U_k(x + ja) \cdots U_i(x - ia)$$

Consider a space-time Wilson loop: Under a gauge transformation a product of gauge links becomes

$$U_i(x) \cdots U_i(x + ka) \rightarrow V(x)U_i(x) \cdots U_i(x + ka)V^{\mathsf{T}}(x + ka)$$

whereas

$$\psi(x)\overline{\psi}(x+ka) \rightarrow V(x)\psi(x)\overline{\psi}(x+ka)V^{\dagger}(x+ka).$$

i.e as far as the gauge fields are concerned the ends of a chain of link variables are equivalent to an external quark-antiquark source  $\rightarrow$  response of system to an external quark-antiquark source.

The expectation of the space-time Wilson loop

$$\langle W \rangle = \frac{\int \mathcal{D} U e^{-S(u)} W}{\int \mathcal{D} U e^{-S(u)}}$$

gives the time evolution of the system: Prior to  $t_i$  there are no color sources  $\rightarrow |0\rangle = e^{-t_i H} |Q = 0\rangle$ .

- At time t<sub>i</sub> the line of link variables between 0 and R creates an external antiquark source at 0 and a quark source at R.
- The links in the time direction between t<sub>i</sub> and t<sub>i</sub> maintain these sources at 0 and R → state evolves to the lowest gluon state in the presence of a quark-antiquark source.
- The  $q \bar{q}$  pair is annihilated at time  $t_f$ .

 $\implies \langle W \rangle \propto e^{-(t_f - t_i)V(R)}$  where V(R) is the potential between two static quarks.



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gives the time evolution of the system: Prior to  $t_i$  there are no color sources  $\rightarrow |0\rangle = e^{-t_i H} |Q = 0\rangle$ .

- At time t the line of link variables between 0 and R creates an external antiquark source at 0 and a quark source at R.
- The links in the time direction between t and t maintain these sources at 0 and  $B \rightarrow$  state evolves to the lowest gluon state in the presence of a quark-antiquark source.
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#### Area law

Consider a non-relativistic particle

$$H=\frac{p^2}{2m}+V(r)$$

Propagator:

$$G(\vec{r}',t;\vec{r},0) = \left\langle r' \right| e^{-iHt} \left| r \right\rangle \stackrel{m \to \infty}{\longrightarrow} \delta^{3}(r'-r)e^{-iV(r)t}$$

Wick rotation:  $t \rightarrow -it$ 

$$\implies G_E(r',t;r,0) \stackrel{m\to\infty}{\longrightarrow} \delta^3(r'-r)e^{-V(r)t}$$

#### i.e. the potential is determined by the exponential behavior of the propagator of a static particle.

In the gauge theory we need to generate the eigenstate of the QCD Hamiltonian for static quark-antiquark  $\rightarrow$  e.g.time evolving the Wilson loop or correlation between two Polyakov loops. If there are J links in the time direction and K links in the space direction then

$$\langle W^{J \times K} \rangle \stackrel{J \to \infty}{\sim} e^{-aJV(aK)} \stackrel{K \to \infty}{\sim} e^{-a^2 \sigma JK}$$

where we used the fact that at large distances the potential is linear since in pure gauge no quark-antiquark can be produced.

#### Area law - Signature of confinemen

Note that this holds in the limit of large Wilson loops and for the Wilson loops considered one has corrections that are proportional to the perimeter of the loop as well as a constant term. Take ratios to eliminate these:

$$\Longrightarrow \chi(I,J) = -\log\left(\frac{W^{I\times J}W^{J-1\times J-1}}{W^{I\times J-1}W^{J-1\times J}}\right) \sim a^2\sigma.$$

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#### Wilson loop revisited

Consider a heavy quark Q and a heavy antiquark  $\overline{Q}$ . Construct a gauge invariant state at t = 0

$$|\phi_{\alpha,\beta}\rangle\left(\vec{x},\vec{y}\right) = \bar{Q}_{\alpha}\left(\vec{x},0\right)U(\vec{x},0;\vec{y},0)Q_{\beta}\left(\vec{y},0\right)|\Omega\rangle$$

Propagate at later time t and annihilate the  $Q\bar{Q}$ :

$$\begin{aligned} G_{\beta',\alpha';\alpha,\beta}(y'x';x,y) &\equiv & \langle \Omega | \,\hat{T}\bar{Q}_{\beta'}(\vec{y}',t)U(\vec{y}',t;\vec{x}',t)Q_{\alpha'}(\vec{x}',t)\bar{Q}_{\alpha}(\vec{x},0)U(\vec{x},0;\vec{y},0)Q_{\beta}(\vec{y},0) | \Omega \rangle \\ &= & \frac{1}{Z}\int \mathcal{D}U\mathcal{D}(\bar{Q},Q)\bar{Q}_{\beta'}(y')\cdots Q_{\beta}(x) \, e^{iS} \end{aligned}$$

where  $x = (\vec{x}, 0), y = (\vec{y}, 0), x' = (\vec{x}', t)$  and  $y' = (\vec{y}', t)$ . Do in the continuum theory, *i.e.* 

$$S = S_G(A) + S_Q(\bar{Q}, Q, A), \quad S_Q = \int d^4 x \bar{Q}(x) \left( i \gamma_\mu D^\mu - M_Q \right) Q(x)$$

Integrate over heavy fermions:

$$\begin{aligned} G_{\beta',\alpha';\alpha,\beta}(y'x';x,y) &= \frac{1}{Z}\int \mathcal{D}(A)\left[S_{\beta\beta'}(y,y';A)S_{\alpha'\alpha}(x',x;A) - S_{\alpha'\beta'}(x',y';A)S_{\beta\alpha}(y,x;A)\right] \\ &= U(x;y)U(y';x')\operatorname{Det} D^Q(A)\,e^{iS_G} \end{aligned}$$

S(z, z'; A) is the quark propagator in an external field  $A_{\mu}$  *i.e.* 

$$(i\gamma^{\mu}D_{\mu}-M_{Q})S(z,z';A)=\delta^{4}(z-z')$$

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Take  $M_Q \rightarrow \infty$ :

$$S(z, z'; A) = P e^{ig \int_0^t dt' A_0(\vec{x}, t')} S(z - z'), \quad (i\gamma_0 \partial_0 - M_Q) S(z - z') = \delta^4(z - z')$$

$$\implies iS(z, z'; A) = \delta^{(3)}(\vec{z} - \vec{z}')P e^{ig \int_0^t dt' A_0(\vec{z}, t')} \left\{ \Theta(z_0 - z'_0) \left(\frac{1 + \gamma_0}{2}\right) e^{-iM_Q(z_0 - z'_0)} + \Theta(z'_0 - z_0) \left(\frac{1 - \gamma_0}{2}\right) e^{iM_Q(z_0 - z'_0)} \right\}$$

$$G_{\beta',\alpha';\alpha,\beta}(y'x';x,y) \xrightarrow{M_Q \to \infty} \delta^{(3)}(\vec{x} - \vec{x}') \delta^{(3)}(\vec{y} - \vec{y}') \left(\frac{1 + \gamma_0}{2}\right)_{\alpha'\alpha} \left(\frac{1 - \gamma_0}{2}\right)_{\beta\beta'} e^{-2iM_Q t} \langle P e^{ig \oint dx^{\mu}A_{\mu}} \rangle$$

Rotate in Euclidean time and discretize:

$$G_{\beta',\alpha';\alpha,\beta}(\mathbf{y}'\mathbf{x}';\mathbf{x},\mathbf{y}) \xrightarrow{M_Q \to \infty} \delta^{(3)}(\vec{\mathbf{x}} - \vec{\mathbf{x}}')\delta^{(3)}(\vec{\mathbf{y}} - \vec{\mathbf{y}}') \left(\frac{1 + \gamma_0}{2}\right)_{\alpha'\alpha} \left(\frac{1 - \gamma_0}{2}\right)_{\beta\beta'} e^{-2M_Q t} \langle W_C(U) \rangle$$

where  $W_C$  is the Wilson loop:  $\langle W_C \rangle = \frac{1}{Z} \int \mathcal{D}(U) W_C(u) e^{-S_G(U)} \rightarrow e^{-V(R)t}$ .

### String tension

Can we relate the string tension extracted from the Wilson loop to a quantity measured in experiment? Families of mesons with a given set of quantum numbers have masses obeying the Regge formula

$$M_J^2 = \frac{1}{\alpha} J, \qquad \alpha = 0.9 \, \mathrm{GeV}^{-1}$$

Consider a simple model:

[J. W. Negele]

- A massless quark and an antiquark connected by a string of length 2L.
- Since they are massless they are moving with the speed of light and the speed of a segment of string a distance x from the origin is v = <sup>x</sup>/<sub>1</sub>c
- σ=energy per unit length of the flux in its rest frame
- Contribution to energy and angular momentum of the element dx:

$$dE = \gamma \sigma dx, \ dJ = \gamma \sigma v x dx$$



$$\implies M = \int_{-L}^{L} dx \frac{\sigma}{\sqrt{1 - \left(\frac{x}{L}\right)^2}} = \pi \sigma L, \quad J = \int_{-L}^{L} dx \frac{\sigma x^2 / L}{\sqrt{1 - \left(\frac{x}{L}\right)^2}} = \frac{\pi}{2} \sigma L^2 \implies M^2 = 2\pi \sigma J$$
  
or  $\sqrt{\sigma} = 2\pi \alpha^{-1/2} = 420$  MeV.

Note that this is a rough model and disagreement to the 10% level will not come as a surprise.

Introduction to Lattice QCD

# Results

G. Bali, K. Schilling, C. Schlichter, 1995





[S. Necco and R. Sommer, NPB622 (2002)]  $r_0$  extracted from the  $q\bar{q}$  force:  $r^2 \frac{\partial V(r)}{\partial r}|_{r=r_0} = 1.65$ .

#### **Continuum limit**

Pure gauge on a lattice has only two parameters: the dimensionless bare coupling constant g and the lattice spacing a.

As we change a, g must be adjusted to keep physical quantities fixed.

The renormalization procedure is in principle simple:

- Pick an initial value of g
- Calculate a set of dimensionful physical quantities  $\langle O_i \rangle$ . These can be written in the form:

 $\langle \mathcal{O}_i \rangle = a^{-d_i} \langle O_i^L(g) \rangle, \ d_i = \text{dimension of operator, and } O_i^L \text{dimensionless.}$ 

e.g. the string tension has the form  $\sigma = a^{-2}\chi$ 

- Use the physical value of one operator, e.g.  $\mathcal{O}_1$  to determine *a* that corresponds to the particular value of *g* e.g. if we choose  $\sigma$  then  $a = \sqrt{\chi}/0.420 \text{ GeV}^{-1}$
- All other observables are then determined

One should then repeat the above steps for smaller values of g to determine g(a) and the physical quantities  $\langle \mathcal{O}_2 \rangle \cdots \langle \mathcal{O}_N \rangle$ .

The existence of a continuum limit implies that

$$\langle O_i(g(a), a) \rangle = a^{-d_i} \langle O_i^L(g) \rangle \stackrel{a \to 0}{\longrightarrow} O_i^{phys.}$$

*i.e.* the values of these observables should approach a limit as  $g \to 0$  and agree with experiment. All dimensionful quantities in lattice simulations are measured in units of the lattice spacing e.g. for masses one measures  $m^L \equiv Ma$  and not M. As  $a \to 0$   $Ma \to 0$  or the correlation length  $\xi^L \equiv 1/Ma$  diverges. This is precisely what one wants to happen so that the system looses memory of the lattice.

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#### Asymptotic freedom

Asymptotic freedom: the running coupling  $g \to 0$  as the momentum scale of the probe  $\mu$  or  $1/a \to \infty$ . It is characterized by renormalization group function  $a \frac{dg}{da}$  or the  $\beta$ -function

$$-arac{\partial g}{\partial a}\equiveta(g)=-eta_0g^3-eta_1g^5+\ldots$$

The perturbative  $\beta$ -function satisfies for N colors and  $n_f$  active flavors ['t Hooft, Politzer, Gross and Wilczek]  $\beta_0 = \left(\frac{11N-2n_f}{3}\right) \frac{1}{16\pi^2} \ , \ \beta_1 = \left(\frac{34N^2}{3} - \frac{10Nn_f}{3} - \frac{n_f(N^2-1)}{N}\right) \frac{1}{(16\pi^2)^2} \ .$ 

The point is that these two leading terms in the expansion of  $\beta(q)$  are gauge and regularization scheme invariant  $\rightarrow$  can be used in lattice regularization. Integration of this relation yields

$$a(g^{2}) = \frac{1}{\Lambda_{L}} \left(\beta_{0}g^{2}\right)^{-\frac{\beta_{1}}{2\beta_{0}^{2}}} e^{-\frac{1}{2\beta_{0}g^{2}}} \equiv \frac{1}{\Lambda_{L}}f(g),$$

where  $n_f = 0$  for pure gauge and  $\Lambda_I$  is an integration constant which is regularization scheme dependent. Inverting we obtain:

$$g(a)^{-2} = \beta_0 \ln(a^{-2} \Lambda_L^{-2}) + \frac{\beta_1}{\beta_0} \ln\left(\ln(a^{-2} \Lambda_L^{-2})\right) + \cdots$$

i.e. changing a one must tune g such that physical observables remain independent. Vanishing a corresponds to vanishing  $q \rightarrow asymptotic freedom$ .

From our lattice calculation we can calculate  $a(q^2)$  e.g.

$$a(g^2) = \left[\frac{a^2\sigma|_{g^2}}{\sigma_{\text{exper.}}}\right]^{1/2} = \frac{\sqrt{\chi}}{0.42 \,\text{GeV}}$$

should coincide with the perturbative result as  $a \rightarrow 0$  and be independent of the obsrvable used. This is called asymptotic scaling.

#### Mass scale $\Lambda_{QCD}$

Asymptotic freedom implies that QCD dynamically generates a mass scale. Consider:  $\mu \frac{\partial g}{\partial \mu} = \beta = -\beta_0 g^3 - \beta_1 g^5$ . Integrate from momentum scale  $\mu_1$  to  $\mu_2$  with  $\mu_2 > \mu_1$  keeping only the  $\beta_0$  term:

$$\frac{1}{2\beta_0 g^2(\mu_2)} - \frac{1}{2\beta_0 g^2(\mu_1)} = \log \frac{\mu_2}{\mu_1} ,$$

*i.e.* the coupling constant of non-abelian gauge theories depends logarithmically on the momentum scale of the process. Equivalently:

$$\frac{1}{2\beta_0 g^2(\mu)} - \log \mu = \log \Lambda_{QCD} \implies \exp \left\{ \frac{1}{2\beta_0 g^2(\mu)} \right\} = \frac{\mu}{\Lambda_{QCD}}$$
$$\implies \alpha_s(\mu) = \frac{g^2(\mu)}{4\pi} = \frac{1}{8\pi\beta_0 \log \frac{\mu}{\Lambda_{QCD}}}$$

introduces  $\Lambda_{QCD}$ , the invariant scale of the theory with dimensions of mass.  $\implies$  QCD in pure gauge with *g* dimensionless dynamically generates a mass scale. This happens because to specify *g* we need a momentum scale at which it is defined.

#### Mass scale $\Lambda_{QCD}$

Extending the above analysis to include  $\beta_1$  gives

$$\Lambda_{QCD} = \lim_{\mu \to \infty} \mu \left( \frac{1}{\beta_0 g^2(\mu)} \right)^{\frac{\beta_1}{2\beta_0^2}} \exp[-\frac{1}{2\beta_0 g^2(\mu)}] \equiv \mu f(g(\mu)) \ .$$

This 2-loop definition of  $\Lambda_{QCD}$  is not unique; the value of  $\Lambda_{QCD}$  depends on the the precise relation between g and  $\mu$ . However, once the value of  $\Lambda$  is determined in one scheme it can be related to that in any other perturbative scheme. For example, in the lattice regularized theory  $\Lambda_{latt}$  is also defined by the same equation but with  $\mu$  replaced by 1/a. Then to 1-loop

$$\frac{\Lambda_{QCD}}{\Lambda_{latt}} = \mu a \exp\left\{-\frac{1}{2\beta_0}\left[\frac{1}{g^2(\mu)} - \frac{1}{g^2(a)}\right]\right\}.$$

In perturbation theory the two coupling constants are related as

$$g^{2}(\mu) \;=\; g^{2}(a) igg\{ 1 - eta_{0}g^{2}(a) igg( \log(\mu a)^{2} - \log C^{2} igg) + O(g^{4}) igg\}$$

and

$$\Lambda_{QCD} = C \Lambda_{latt}$$

*i.e.* the two constants,  $\Lambda_{QCD}$  and  $\Lambda_{latt}$ , are related by a multiplicative constant. To calculate *C* requires knowing the finite part of the coupling constant renormalization to 1-loop in both the lattice and continuum regularization schemes.

The results are listed in the following Table for  $\Lambda_{MOM}$  and  $\Lambda_{\overline{MS}}$ .

n <sub>f</sub>	0	1	2	3	4
$\Lambda_{\overline{MS}}/\Lambda_{latt}$	28.8	34.0	41.1	51.0	65.5
$\Lambda_{MOM}/\Lambda_{latt}$	83.4	89.4	96.7	105.8	117.4

#### **Exercises**

Using fermion coherent states find the path integral representation of the evolution operator. Then find the partition function and propagator for a non-interacting many partice system.

Uisng the SPA evaluate the 1-D integral

$$I(l) = \int_{-\infty}^{\infty} dx \, e^{-lf(x)}$$

to O(1/I) assuming  $I \gg 1$  and f(x) a real function with a minimum at  $x = x_0$ . Try to use a diagramatic expression and then give the diagrams for the  $O(1/I^2)$ -terms.

Write a computer program to implement the Metropolis Monte Carlo algorithm for the one dimensional harmonic oscillator  $V(x) = \frac{x^2}{2}$  with m = 1. Compare your results with those of standard quantum mechanics:

 $\langle x | e^{-HT} | x \rangle \approx |\langle x | E_0 \rangle|^2 e^{-E_0 T}$ 

where  $E_0 = 1/2$  and  $\langle x | E_0 \rangle = \frac{e^{-x^2/2}}{\pi^{1/4}}$ .

Extract the energy and wave-function from your numerical result. In addition calculate

$$G(t) = \frac{1}{N} \sum_{j} \langle x(t_j + t) x(t_j) \rangle$$

for all  $t = 0, a, 2a \dots (N-1)a$ ; i.e. calculate  $G_n = \frac{1}{N} \sum_j \langle x_{(j+n) \mod N} x_j \rangle$  for  $n = 0 \dots N-1$  with periodic boundary conditions. Try N = 20 lattice sites with lattice spacing a = 1/2, and set  $\epsilon = 1.4$  and  $N_{cor} = 20$ . Try  $N_{cf}$ 's of 25, 100, 1000 and 10000. Use the results to compute the excitation energy from

$$\Delta E_n \equiv \log(G_n/G_{n+1}) \stackrel{n \text{ large}}{\longrightarrow} (E_1 - E_0) a$$

Repeat this exercise for  $V(x) = x^4/2$ .