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# **Lattice Field theory and Monte Carlo Simulations**

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# **Lattice Field theory and Monte Carlo Simulations**



Path integrals and QFT (introduction)



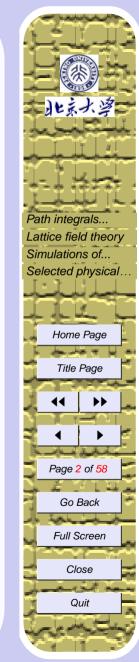
Lattice field theory (the name of the game)



Simulation of bosonic fields (fermions by A. Kennedy)



Some selected physical results (why doing all these)



# 1. Path integrals and Quantum Field Theory







# **Solution** Path integral: an alternative for quantization

Start with a one-dimensional harmonic oscillator with Hamiltonian:

$$H = \frac{p^2}{2} + \frac{\omega^2}{2}x^2 \,. \tag{1}$$

To quantize (1), we can either use:

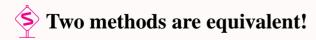
**A** Canonical quantization:

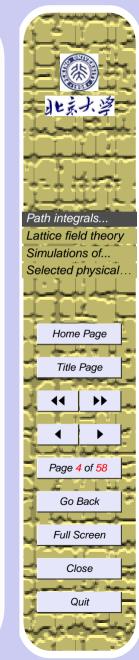
$$[\hat{x}, \hat{p}] = i\hbar , \Leftrightarrow [\hat{a}, \hat{a}^{\dagger}] = 1 , \qquad (2)$$

or:

**A** Path integral quantization:

$$\mathcal{Z} = \int \left[ \mathcal{D}x \right] e^{iS[x(t)]} . \tag{3}$$







# **Solution** More on path integral quantization (1)

We wish to find quantum-mechanical probability amplitude of finding the oscillator at position  $x_I$  at some initial time  $t_I$  and later on finding it at position  $x_F$ at some later time  $t_F$ . We set  $T \equiv t_F - t_I$  and this amplitude is given by:

$$\mathcal{Z}[x_I, t_I; x_F, t_F] = \langle x_F | e^{-iHT} | x_I \rangle . \tag{4}$$



### Caution: kinetic and potential energy do not commute!

therefore:

$$\exp\left(-iT\frac{\hat{p}^2}{2} - iT\frac{\omega^2}{2}\hat{x}^2\right) \neq \exp\left(-iT\frac{\hat{p}^2}{2}\right) \cdot \exp\left(-iT\frac{\omega^2}{2}\hat{x}^2\right) . \tag{5}$$

To work around this, one uses the trick:

$$e^{-i\hat{H}T} = e^{-i\hat{H}\epsilon} \cdot e^{-i\hat{H}\epsilon} \cdots e^{-i\hat{H}\epsilon}$$
, (6)

$$e^{-i\hat{H}\epsilon} = \exp\left(-i\epsilon\frac{\hat{p}^2}{2}\right) \cdot \exp\left(-i\epsilon\frac{\omega^2}{2}\hat{x}^2\right) + O(\epsilon^2),$$
 (7)

where  $\epsilon \equiv T/N_t$  is a small number.





### More on path integral quantization (2)

A common representation for momentum p is given by:

$$\hat{p} = -i\frac{\partial}{\partial x} \ . \tag{8}$$

Using this representation and inserting complete set of states in Eq. (6), one finally arrives at:

$$\mathcal{Z}[x_F, t_F; x_I, t_I] \equiv \langle x_F | e^{-iT\hat{H}} | x_I \rangle = \int \mathcal{D}x e^{iS[x(t)]} , \qquad (9)$$

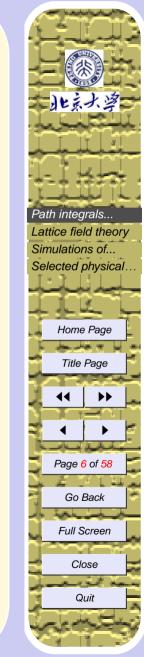
where S[x(t)] is the classical action of the harmonic oscillator:

$$S[x(t)] = \int_{t_I}^{t_F} dt L[x, \dot{x}, t] = \int_{t_I}^{t_F} dt \left[ \frac{1}{2} \dot{x}^2 - \frac{\omega^2}{2} x^2 \right] . \tag{10}$$

# Neat thing about path integral:

Operators: 
$$\hat{x}, \hat{p} \Rightarrow \text{Pure numbers: } x(t), \dot{x}(t)$$
. (11)

**Solution** Note: Eq. (9) is only a formal expression!





### Wick rotation

¶ If we take the "time" variable in our previous discussions to be pure imaginary, i.e. setting:  $(i\epsilon) = a_{\tau}$  and  $(iT) = N(i\epsilon) = Na_{\tau} = \beta$ , we have:

$$\left\langle x_F \left| e^{-\beta \hat{H}} \right| x_I \right\rangle = \int \left( \prod_{\tau=1}^{N-1} dx_\tau \right) \exp \left\{ -a_\tau \sum_{\tau=0}^{N-1} \left[ \frac{1}{2} \left( \frac{x_{\tau+1} - x_\tau}{a_\tau} \right)^2 + \frac{\omega^2}{2} x_\tau^2 \right] \right\} .$$

We find it resembles the form of the partition function in Statistical Physics, as long as we set  $x_I = x_F$  and integrate over it. Thus, the partition function:

$$\mathcal{Z} = Tre^{-\beta \hat{H}} = \int \mathcal{D}x e^{-S_E[x(\tau)]} , \qquad (12)$$

where  $S_E[x_\tau]$  is the (Euclidean space) action (which in fact is Hamiltonian):

$$S_E[x(\tau)] = a_\tau \sum_{\tau=0}^{N-1} \left[ \frac{1}{2} \left( \frac{x_{\tau+1} - x_\tau}{a_\tau} \right)^2 + \frac{\omega^2}{2} x_\tau^2 \right] , \qquad (13)$$



Rotation into pure imaginary time is called Wick rotation



 $\mathfrak{S}$  The partition function  $\mathcal{Z}$  in Eq. (12) is called Euclidean path integral



**Equivalence of quantum theory to statistical physics** 



# \$

### **Quantum Field Theory (QFT)**

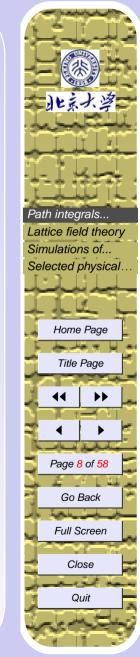
 $\clubsuit$  one (or a few) d.o.f. (QM)  $\Longrightarrow$  (infinitely) many d.o.f. (QFT)

If we label the degrees of freedom by  $\phi(\mathbf{x})$ , which are called *fields*, then probability amplitude similar to Eq. (9) is generalized to:

$$\mathcal{Z}[\phi^{(F)}, t_F; \phi^{(I)}, t_I] = \langle \{\phi^{(F)}(\mathbf{x})\}, t_F | e^{-iT\hat{H}} | \{\phi^{(I)}(\mathbf{x})\}, t_I \rangle = \int [\mathcal{D}\phi] e^{iS[\phi]} .$$
(14)

where  $\hat{H}$  and  $S[\phi]$  is the Hamiltonian and action for the field system, respectively.  $\mathcal{Z}$  is also known as the Schödinger functional.

- **..** For relativistic QFT, the action  $S[\phi]$  should respect Lorentz symmetry in Minkowski space
- **.\*** For non-relativistic QFT, the action  $S[\phi]$  should respect corresponding symmetry





### **Relativistic QFT and Particles**



**Dynamical variables (fields)** Quantized Particles

♣ Scalar fields ⇔ Scalar Particles (spin=0, boson)

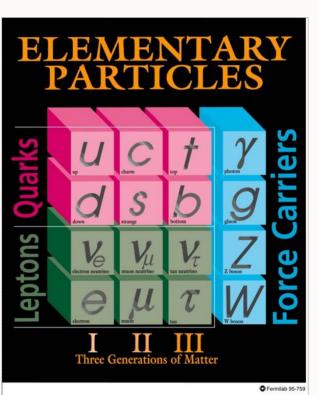
Examples: Higgs, phonon, etc.

♣ Spinor fields ⇒ Fermion Particles (spin=1/2, fermion)

Examples: leptons (electron, muon, tau and their neutrinos), quarks (which form protons and neutrons).

♣ Gauge fields ⇔ Gauge Particles (spin=1, boson)

Examples: photons, W and Z boson, gluons.





Non-relativistic QFT and quasi-particles





# **QFT and Statistical Physics**



# Wick rotate to Euclidean space

$$\mathcal{Z} = \int \mathcal{D}\phi \exp\left(-S_E[\phi]\right) , \qquad (15)$$

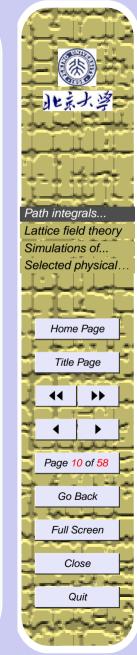
where  $S_E[\phi]$  is the Euclidean action (energy) of the system.

Physical observables are given by:

$$\mathcal{O} = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \mathcal{O}[\phi] \exp\left(-S_E[\phi]\right) , \qquad (16)$$

The most common observables are correlation (Green's) functions.

- $\clubsuit$  Quantum Field Theory (QFT)  $\stackrel{\text{Equivalent}}{\Longleftrightarrow}$  Statistical Physics (SP)
- To be more precise:
- $\clubsuit d + 1$  dimensional QFT  $\overset{\text{Wick}}{\Longleftrightarrow}$  (d+1) dimensional SP





# **Role of correlation functions**

Lots of info is encoded in various correlation functions

$$\langle \mathcal{O}[\phi(t)]\mathcal{O}[\phi(0)]\rangle = \int \mathcal{D}\phi \mathcal{O}[\phi(t)]\mathcal{O}[\phi(0)] \exp\left(-S_E[\phi]\right) . \tag{17}$$

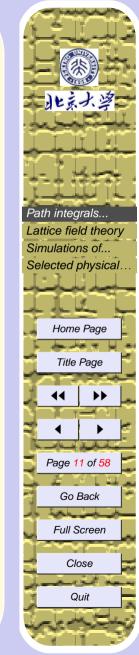
The same correlator can be understood from canonical quantization:

$$\langle \mathcal{O}[\phi(t)]\mathcal{O}[\phi(0)]\rangle = Tr\left(\hat{\mathcal{O}}_H[\phi(t)]\hat{\mathcal{O}}_H[\phi(0)]e^{-\beta H}\right).$$
 (18)

where  $\hat{\mathcal{O}}_H[\phi(t)]$  represents the operator in Heisenberg picture. Inserting a complete set of states for the Hamiltonian, one gets in the large  $\beta$  limit:

$$\langle \mathcal{O}[\phi(t)]\mathcal{O}[\phi(0)]\rangle \simeq \sum_{n} |\langle 0|\hat{\mathcal{O}}[\phi]|n\rangle|^2 e^{-tE_n},$$
 (19)

where  $|n\rangle$  is the *n*-th eigenstate of the Hamiltonian and we have taken  $E_0 = 0$ . Therefore, the correlator of a particular operator reflects the energy gap of the state which that operator can create from vacuum.

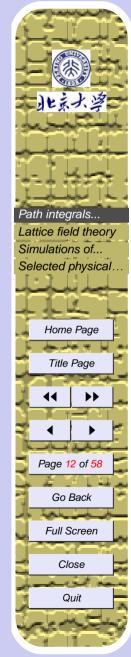


# Summary

- **QFT** is important: It offers the theoretical framework for:
  - particle physics &
  - nuclear physics &
  - condensed matter physics & ...

# **S** QFT is hard!

- ♣ Too many d.o.f.
  - \* Exact solutions rare, except special cases.
  - \* Ultra-violet divergences (regularization, renormalization).
- **&** Limitations of perturbative study
  - \* Non-perturbative features exist for QFT. Perturbative expansions are at best asymptotic expansions.
  - \* Non-perturbative phenomena exist in Nature.



- **Solution Lattice field theory: the non-perturbative prescription of QFT**
- **Solution** Path integral is the non-perturbative definition of QFT
- **Solution** Euclidean path integral is where computers can help!







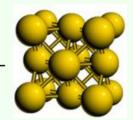
# 2. Lattice field theory





### 2.1. Definition of lattice field theory

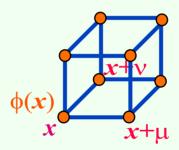
**..** Dynamical variables – fields  $\phi(x)$  - are defined on the lattice

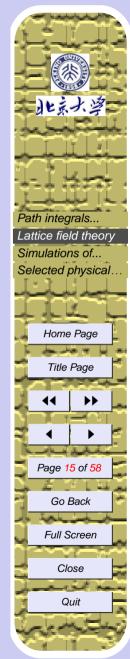


- **4** d.o.f: finite but many
- **.** Action of system  $S[\phi(x)]$  given.
- **♣** Path Integral Quantization

$$\mathcal{Z} = \int [\mathcal{D}\phi] e^{-S[\phi]} . \tag{20}$$

**.** For finite number of  $\phi(x)$ , Eq. (20) is just a multi-dimensional ordinary integral.





#### 2.2. Dual view of the lattice



# High energy physicists:

- Lattice is a virtual tool (ultra-violet regulator)
- Lattice is usually 4dimensional
- Simple lattice structure is usually enough
- Dump lattice eventually



- Lattice is real life (real crystals)
- Lattice is less than 4dimensional
- Have to study various lattice structures
- **.** Live happily ever after



#### 2.3. Scalar lattice field theory

The action (energy):

$$S = -\kappa \sum_{x,\mu} \left[ \phi_x (\phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}}) \right] + \sum_x \left[ \phi_x^2 + \lambda (\phi_x^2 - 1)^2 \right] , \qquad (21)$$

 $\kappa$ : hopping parameter;  $\lambda$ : self-coupling.

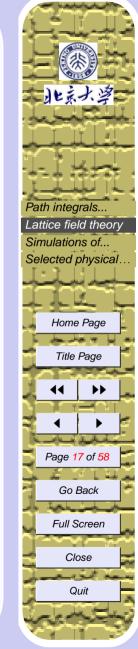
Continuum counterpart:

$$S = \int d^4x \frac{1}{2}\phi(x)(-\partial^2 + m_0^2)\phi(x) + \frac{\lambda_0}{4!}\phi^4(x) . \tag{22}$$

 $m_0$ : (bare) mass;  $\lambda_0$ : self-coupling.

- **\*** Relation to spin models:  $\lambda = \infty$  is Ising model
- Physics: correlation functions

$$\langle \phi_x \phi_y \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi(\phi_x \phi_y) e^{-S[\phi]} , \quad \mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]} .$$
 (23)



# **Phase structure**

Two phases: symmetric (paramagnetic) & broken (ferromagnetic)

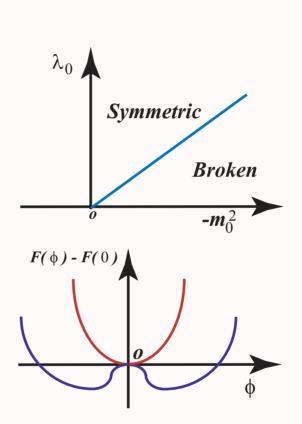
The order parameter  $\langle \phi \rangle$  has zero and non-zero values respectively.

Second order phase transition line (critical line):

$$\xi \simeq (1/m) \to \infty$$
. (24)

Two types of effective action (free energy in Landau theory) in two phases:

A good example to study spontaneous symmetry breaking.





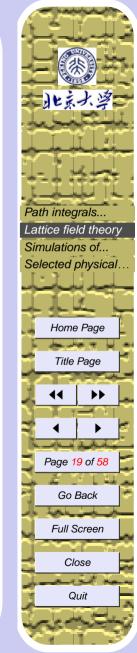
# $\bigcirc O(N)$ model

**Action for** O(N) **model** Consider the scalar field theory with O(N) symmetry.

$$S = -\kappa \sum_{x,\mu} \left[ \phi_x^a (\phi_{x+\hat{\mu}}^a + \phi_{x-\hat{\mu}}^a) \right] + \sum_x \left[ \phi_x^a \phi_x^a + \lambda (\phi_x^a \phi_x^a - 1)^2 \right] , \quad (25)$$

where  $\phi_x^a$  is an N-component field. This action has a global O(N) symmetry.

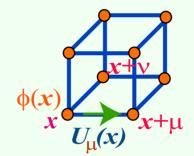
- ♣ Special cases:  $\lambda = \infty$  gives non-linear O(N)  $\sigma$ -model (For N=2 it is XY-model; for N=3 it is Heisenberg model).
- **.\* Two phases:** symmetric phase (symmetry O(N)) and broken phase (symmetry O(N-1)), separated by a second-order phase transition line.
- Massless Goldstone modes: also known as spin waves dominates the lowenergy behavior.



### 2.4. Lattice gauge fields

Gauge fields live on the link.

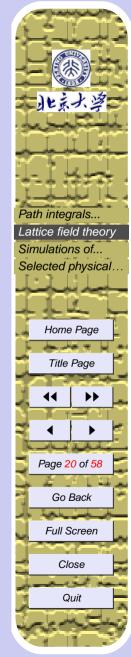
 $U_{\mu}(x)$  defined on the link pointing from point x to its neighboring point  $x + \hat{\mu}$  in the positive  $\mu$  direction.



- **\$\rightarrow\$ Group valued:**  $U_{\mu}(x) \in G$  where G is the *gauge group*. Particle physicists usually play with Lie groups while solid state physicists prefer point groups.
- ♣ Gauge transformation: let  $\phi_x$  forms basic rep. of G. A common example is the gauge group SU(N), then  $\phi_x$  is N component complex field:  $\phi_x^a$ ,  $a = 1, 2, \dots, N$ . Gauge transformation is (with  $g(x) \in G$ ):

$$\phi_x \to \phi_x' = g(x) \cdot \phi_x \,, \tag{26}$$

$$U_{\mu}(x) \rightarrow U'_{\mu}(x) = g(x) \cdot U_{\mu}(x) \cdot g^{-1}(x + \hat{\mu})$$
 (27)





### Gauge invariance

**&** Covariant lattice derivatives:

$$(\nabla_{\mu}\phi)_{x} = U_{\mu}(x)\phi_{x+\hat{\mu}} - \phi_{x} , (\nabla_{\mu}^{*}\phi)_{x} = \phi_{x} - U_{\mu}^{\dagger}(x-\hat{\mu})\phi_{x-\hat{\mu}} , \qquad (28)$$

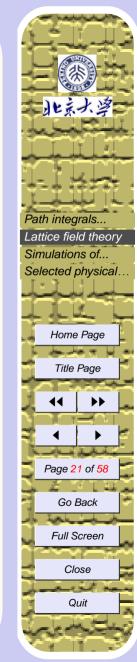
♣ Pure gauge part: Characters of gauge fields products along any closed loops is gauge invariant.

$$S_g[U_\mu(x)] = -\frac{\beta}{2N} \sum_P Tr(U_P) \ .$$
 (29)

where  $U_P$  stands for the product of gauge fields along a plaquette on the lattice.

**&** Gauge invariant action:

$$S = S_g[U_\mu(x)] + \sum_x \frac{1}{2} (\nabla_\mu \phi)_x^* (\nabla_\mu \phi)_x + \frac{m_0^2}{2} \phi_x^2 + \frac{\lambda_0}{4!} (\phi_x^2)^2 , \qquad (30)$$





# Continuum counterparts (SU(N))

Gauge potential:

$$U_{\mu}(x) = \exp(g_0 a A_{\mu}(x + (a/2)\hat{\mu})) , \qquad (31)$$

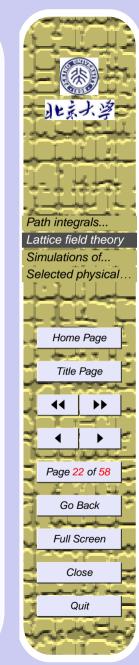
where  $A_{\mu}(x)$  takes value in the corresponding Lie algebra.

**.** Naive continuum limit: Assuming  $a \to 0$ , we find:

$$S_g[U_\mu(x)] \simeq \frac{1}{2} \int d^4x Tr(F_{\mu\nu}F_{\mu\nu}) ,$$
 (32)

where  $F_{\mu\nu}$  is the field:

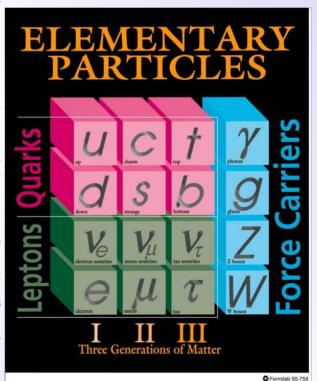
$$F_{\mu\nu}(x) = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu} + g_0[A_{\mu}, A_{\nu}]. \tag{33}$$

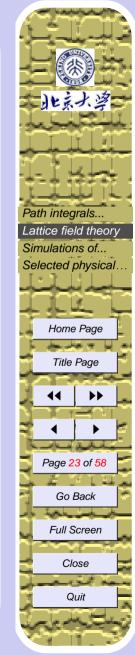




### Why gauge fields?

- ♣ Fundamental interactions in Nature: Strong, Weak, Electromagnetic and Gravitational.
- ♣ Gauge bosons mediate fundamental interactions Not including gravity which we don't know much about.
- ♣ The celebrated Standard Model (SM): A quantum gauge field theory which unifies strong, weak and electromagnetic interactions. The gauge group for the SM is:  $SU(3) \times SU(2) \times U(1)$ .
- ♣ Verified experimentally to good precision The only missing part is the symmetry breaking mechanism, which will be tested starting next year at Large Hadron Collider (LHC) at CERN.





#### 2.5. Fermion fields

Fermions are drastically different from bosons:

Fermions obey Pauli's exclusion principle. In canonical quantization procedure, this is represented by the anti-commutation relation:

$$\{\hat{c}_i, \hat{c}_i^{\dagger}\} = \delta_{ij} , \qquad (34)$$

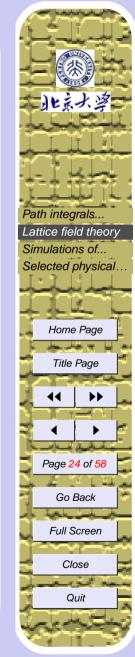
where  $\hat{c}_i$  and  $\hat{c}_i^{\dagger}$  corresponds to fermion annihilation and creation operators.

\* How to cope with fermions in path integral quantization? The following observation will help:

Canonical quantization 
$$\Rightarrow$$
 Path integral quantization operators:  $a_i$ ,  $a_i^{\dagger}$   $\Rightarrow$  numbers:  $\phi_i$ ,  $\phi_i^*$ ,  $a_i a_j^{\dagger} - a_j^{\dagger} a_i = \delta_{ij} \Rightarrow \phi_i \phi_j^* - \phi_j^* \phi_i = 0$  (35)

We anticipate fermions are represented by anti-commuting numbers (Grassmann variables).

$$\hat{c}_i \hat{c}_j^{\dagger} + \hat{c}_j^{\dagger} \hat{c}_i = \delta_{ij} \quad \Rightarrow \quad \psi_i \bar{\psi}_j + \bar{\psi}_j \psi_i = 0 \ . \tag{36}$$



# 客 Grassmann path integrals

. In path integral, fermion fields are Grassmann numbers:

$$\psi_i \psi_j \equiv -\psi_j \psi_i \;, \tag{37}$$

Note that:  $\psi^2 \equiv 0$ .

**\*** We can set up rules for integration (differentiation):

$$\int d\psi = 0 \; , \quad \int d\psi \psi = 1 \; , \tag{38}$$

**&** Lattice field theory for fermion is represented by:

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S_f[\bar{\psi},\psi]} , \qquad (39)$$

**A useful formula:** Usually, fermion action can be brought into a form that is bilinear in fermion fields:  $S_f[\bar{\psi}, \psi] = \sum_{i,j} \bar{\psi}_i \mathcal{M}_{ij} \psi_j$ , thus:

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\bar{\psi}_i\mathcal{M}_{ij}\psi_j} = \det \mathcal{M} , \langle \psi_i\bar{\psi}_j\rangle = \left(\mathcal{M}^{-1}\right)_{ij} . \tag{40}$$



#### 2.6. Some Examples



# Gauged scalar models

#### **&** Lattice actions:

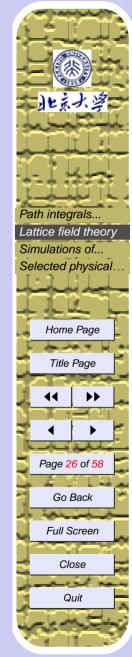
$$S = S_H[\phi] + S_g[U_\mu] , S_g[U_\mu] = -\frac{\beta}{2N} \sum_P Tr(U_P) . \tag{41}$$

$$\Phi_{\parallel} = -\kappa \sum_{P} Tr(\Phi, U, (\pi)\Phi^{\dagger}, \Gamma) + \sum_{P} [Tr(\Phi^{\dagger}\Phi) + \Gamma(Tr(\Phi^{\dagger}\Phi), \Gamma)^2] . \tag{41}$$

$$S_H[\Phi] = -\kappa \sum_{x,\mu} Tr(\Phi_x U_\mu(x) \Phi_{x+\hat{\mu}}^{\dagger}) + \sum_x \left[ Tr(\Phi^{\dagger} \Phi) + \lambda (Tr(\Phi^{\dagger} \Phi) - 1)^2 \right] ,$$

#### **Anderson-Higgs Mechanism: broken gauge symmetry**

- In particle physics, this is the model relevant for the study of eletro-weak symmetry breaking. The gauge group is taken to be SU(2) and the nature of the phase transition is intimately related to the asymmetry of matter and anti-matter in the universe.
- In condensed matter physics, this is the Ginzburg-Landau theory of superconductors.  $\Phi_x$  is a complex field (order parameter) and the gauge field is the ordinary electromagnetic field.





#### **...** Lattice actions:

$$S = S_H[\phi] + S_f[\bar{\psi}, \psi, \phi] ,$$
  

$$S_f[\bar{\psi}, \psi, \phi] = \sum_{x,y} \bar{\psi}_x \mathcal{M}_{xy}[\phi] \psi_y,$$
(42)

where  $S_H[\phi]$  is the action for scalar fields.  $\mathcal{M}[\phi]$  is the fermion matrix.

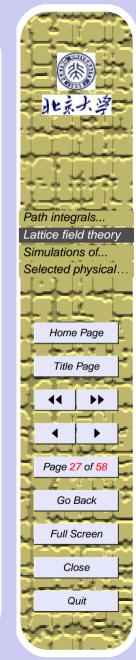
#### **...** Integrating out the fermions:

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

$$= \int \mathcal{D}\phi e^{-S_H[\phi]} \det \mathcal{M}[\phi]. \tag{43}$$

The fermion determinant  $\det \mathcal{M}[\phi]$  can be problematic (sign problem and/or resource demanding).

Relevant in both condensed matter and particle physics
Yukawa model in particle physics, electrons interacting with phonons.





# **Example 2** Lattice Quantum Chromodynamics (QCD)

#### **Lattice actions:**

$$S_{LQCD} = S_{g}[U_{\mu}(x)] + S_{f}[\bar{\psi}, \psi, U_{\mu}], \qquad (44)$$

$$S_{g}[U_{\mu}] = -\frac{\beta}{2N} \sum_{P} Tr(U_{P}), \quad S_{f}[\bar{\psi}, \psi, U_{\mu}] = \sum_{x,y} \bar{\psi}_{x} \mathcal{M}_{xy}[U_{\mu}] \psi_{y},$$

$$\mathcal{M}_{xy} = \delta_{xy} - \kappa \sum_{\mu} \left[ (1 - \gamma_{\mu}) U_{\mu}(x) \delta_{x+\hat{\mu},y} + (1 + \gamma_{\mu}) U_{\mu}^{\dagger}(x - \hat{\mu}) \delta_{x-\hat{\mu},y} \right].$$

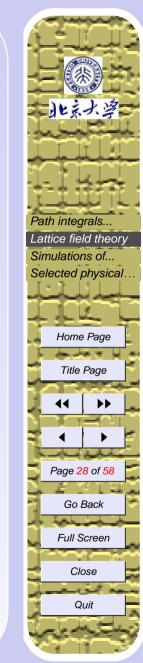
#### Simulations of LQCD:

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}U_{\mu}e^{-S_{LQCD}[\bar{\psi},\psi,U_{\mu}]},$$

$$= \int \mathcal{D}U_{\mu}e^{-S_{g}[U_{\mu}]}\det\mathcal{M}[U_{\mu}]. \tag{45}$$

It requires tremendous amount of computer resources to really take into account det  $\mathcal{M}[U_{\mu}]$ , if it can be done at all.

**4 Quenching LQCD:** Set  $\det \mathcal{M}[U_{\mu}] = 1$ .



#### 2.7. Fermions: the trouble-maker

#### **&** Computers do not know about Grassmann numbers:

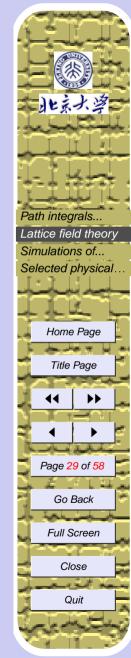
There is no "Grassmannian chips". One always has to integrate out fermions (to get a fermion determinant).

#### **\*** The notorious sign problem:

Fermion determinant can be non-positive definite (in fact, it can even be complex, as in finite density QCD). If this happens, ordinary Monte Carlo breaks down (probability must be positive). Even if the fermion determinant *is* positive definite, it is usually quite expensive!

#### **...** Lattice Fermions have doubling problems:

- Fermions have handedness.
- Naive lattice fermions have doubling problem
- Way out: Wilson fermions, staggered fermions, domain wall fermions, overlap fermions, etc.
- The problem remains for chiral gauge theories.



#### 2.8. Continuum Limit

#### Naively speaking:

Continuum limit is a limit where we take the lattice spacing  $a \to 0$ , relative to the typical physical length scale that we are considering.

### For particle physicists:

This is equivalent to sending the corresponding ultra-violet cut-off  $\Lambda \simeq \pi/a$  to infinity relative to our physical energy scales.

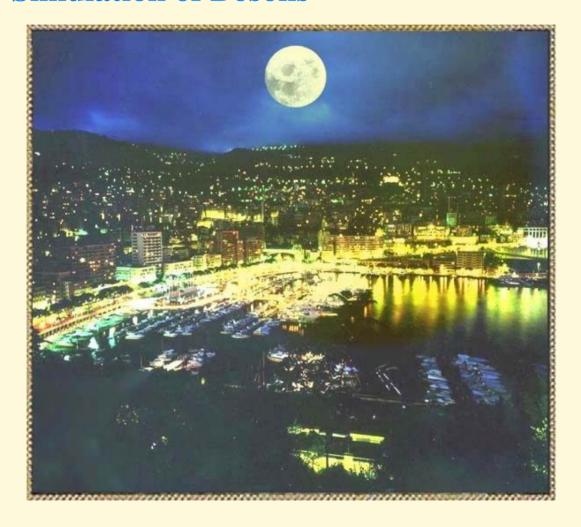
#### For condensed matter physicists:

This amounts to going to the <u>critical region</u> where the typical correlation length in the system diverges (<u>critical phenomena</u>).

♣ The essence of continuum limit lies in renormalization (and renormalization group)



# 3. Simulation of Bosons





### **3.1.** Monte Carlo integration

QFT/SP is defined via path integral:

$$\mathcal{Z} = \int \mathcal{D}\phi e^{-S[\phi]} , \langle \mathcal{O}[\phi] \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}\phi \mathcal{O}[\phi] e^{-S[\phi]} , \qquad (46)$$

- When we don't know how to integrate something, we hand it over to the computers:
  - However, brut-force numerical integration simply does not work! The configuration space in which we are integrating over is too large for brutforce numerical integration.
  - Note that Eq. (46) looks like an ensemble average with probability distribution:

$$P[\phi] = \frac{1}{\mathcal{Z}} e^{-S[\phi]} . \tag{47}$$

- This suggests stochastic methods: important sampling with Markov chain (Monte Carlo).
- One iterates a Markov chain which generates field configurations (samples) whose probability distribution is the Boltzmann distribution (47).
- Then physical quantities in Eq (46) can be obtained by averaging over the corresponding values from the samples.



# Markov chain and exact algorithms

**4** A Markov chain is a stochastic process characterized by a transition probability function  $W[\{\phi\} \to \{\phi'\}]$  such that:

$$P^{(j+1)}[\phi'] = \int \mathcal{D}\phi W[\{\phi\} \to \{\phi'\}] P^{(j)}[\phi] . \tag{48}$$

We need specific Markov chains:

Since we are aiming to generate distribution (47), our choice of  $W[\{\phi\} \rightarrow \{\phi'\}]$  has to satisfy the following two conditions (an *exact algroithm*):

**Stability condition:** 

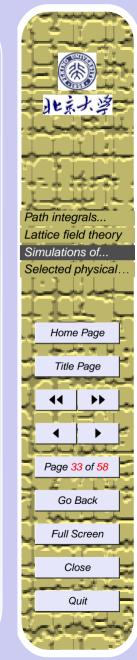
$$e^{-S[\phi']} = \int \mathcal{D}\phi W[\{\phi\} \to \{\phi'\}] e^{-S[\phi]}$$
 (49)

**Ergodic condition:** 

 $W[\{\phi\} \to \{\phi'\}]$  can reach anywhere in configuration space.

**A** sufficient replacement of the stability condition is the well-known detailed balance condition:

$$e^{-S[\phi']}W[\{\phi'\} \to \{\phi\}] = W[\{\phi\} \to \{\phi'\}]e^{-S[\phi]}$$
 (50)





# Standard steps (CMD) to take in Monte Carlo simulations

- Collection of field configurations: generate the right probability distribution (47) using an exact algorithm and store the field configuration samples.
- Measurements of physical observables: measure relevant physical quantities from the stored configurations. Suppose we have N samples measured, then an estimate for the physical observable is given by:

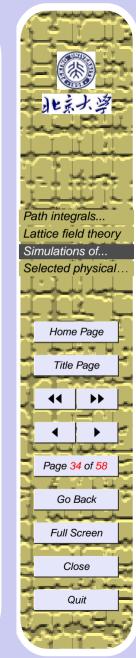
$$\langle \mathcal{O}[\phi] \rangle \simeq \bar{\mathcal{O}} = \frac{1}{N} \sum_{j=1}^{N} \mathcal{O}_j ,$$
 (51)

where  $\mathcal{O}_j$  is the measured value of  $\mathcal{O}$  from the j-th configuration sample.

• *Data analysis*: analyze the output and obtain estimates for physical quantities (with errors). The naive error for physical observable is given by:

$$(\Delta \mathcal{O})^2 = \frac{1}{N(N-1)} \sum_{j=1}^{N} (\mathcal{O}_j - \bar{\mathcal{O}})^2 .$$
 (52)

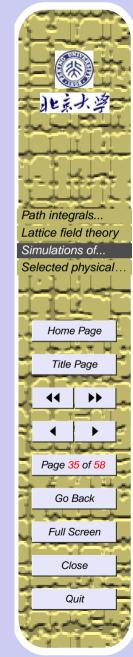
One usually needs data-fitting processes to obtain secondary physical quantities (those that are not directly measured).





#### The pros and cons for simulating lattice field theories

- △ Memory consumption is moderate, typically proportional to the lattice size.
- $\triangle$  Floating point computation is also proportional to the size of the lattice.
- △ The action of the theory is always local (not including some statistical physics systems which can have non-local interaction). This is a restriction for QFT to have universal continuum limit. The locality property makes lattice simulations easily (well, relatively speaking...) implemented on parallel machines.
- ∇ Monte Carlo cannot escape the fate of fighting statistical errors. Typically
  to reduce the statistical error by a factor of two, one needs 4 times computer
  time consumption.
- ∇ Lattice is four-dimensional. Increasing the size by a factor of two thus increase the memory consumption by a factor of 16. Similarly for the CPU consumption.
- ∇ Usually, one is interested in a parameter region where simulation is getting expensive.



### 3.2. Basic algorithms for scalar fields



# The Metropolis algorithm

We take the one component scalar lattice field theory as an illustration. The action is:

$$S[\phi] = -\kappa \sum_{x,\mu} \left[ \phi_x (\phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}}) \right] + \sum_x \left[ \phi_x^2 + \lambda (\phi_x^2 - 1)^2 \right] , \qquad (53)$$

The Metropolis algorithm amounts to changing one particular  $\phi_x$  at a time. The change is accepted/rejected according to the change of the action which depends on values of its neighboring fields.

• For a given site x, update  $\phi_x$  according to:

$$\phi_x \to \phi_x' = \phi_x + \Delta\epsilon \;, \tag{54}$$

where  $\Delta > 0$  is a tunable parameter and  $\epsilon$  is a random number uniformly distributed in the interval [-1, +1].

- Calculate the change in the action of the system:  $\Delta S = S[\phi'] S[\phi]$ . The update  $\phi_x \to \phi'$  is accepted according to the probability:  $\min(1, e^{-\Delta S})$ .
- Repeat the above steps for every site. This completes a *sweep*.





#### Heatbath algorithm

For the Ising model:

$$S[\phi] = -\kappa \sum_{x,\mu} \left[ \phi_x (\phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}}) \right] , \qquad (55)$$

where  $\phi_x = \pm 1$ , heatbath algorithm is available. Note that for a given site x, the probability distribution we wish to generate is proportional:

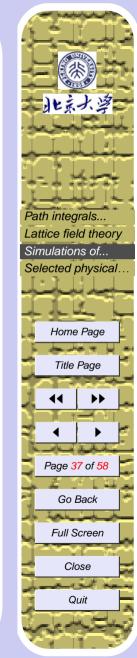
$$\exp\left(2\kappa\phi_x\bar{\phi}\right) \ . \tag{56}$$

where  $\bar{\phi} = \sum_{\mu} (\phi_{x+\hat{\mu}} + \phi_{x-\hat{\mu}})$  Since the neighboring fields are fixed and  $\phi_x$  can take only  $\pm 1$ , so the probability of  $\phi_x$  taking values +1 and -1 respectively:

$$P_{+} = \frac{e^{2\kappa\bar{\phi}}}{e^{2\kappa\bar{\phi}} + e^{-2\kappa\bar{\phi}}} , \quad P_{-} = \frac{e^{-2\kappa\bar{\phi}}}{e^{2\kappa\bar{\phi}} + e^{-2\kappa\bar{\phi}}} . \tag{57}$$

So the heatbath algorithm consists of the following two steps:

- For a given site x, update  $\phi_x = \pm 1$  with corresponding probabilities given by Eq. (57).
- Repeat the above steps for every site. This completes a *sweep*.





#### **Correlation of measurements**

• As a stochastic process, the error for physical quantities typically goes to zero as:

$$\frac{\Delta \mathcal{O}}{\bar{\mathcal{O}}} \simeq \frac{1}{\sqrt{N}} \ . \tag{58}$$

where N is the number of measurements. Note that resource consumption is proportional to N.

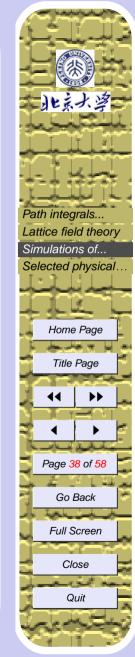
• However, the above error estimate is only valid when the samples are *statistically independent*. In practice, since Markov chain has memories, the configuration samples have correlations. This correlation typically vanishes exponentially as the "Monte Carlo time" interval  $\tau$  gets large:

$$\langle (\mathcal{O}(\tau) - \langle \mathcal{O} \rangle)(\mathcal{O}(0) - \langle \mathcal{O} \rangle) \rangle \propto e^{-\tau/\tau_a},$$
 (59)

where  $\tau_a$  is called the auto-correlation time for the observable  $\mathcal{O}$ .

• Roughly speaking, only every  $\tau_a$  measurements are statistically independent and a better error estimate is:

$$\frac{\Delta \mathcal{O}}{\bar{\mathcal{O}}} \simeq \frac{1}{\sqrt{N/\tau_a}} \,, \tag{60}$$





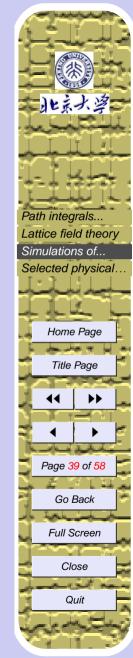
#### **Critical slowing-down**

- Auto-correlation time depends crucially on the algorithm. Good algorithms have shorter auto-correlation time while bad algorithms have longer auto-correlation time.
- Auto-correlation time also depends on the parameter of the theory. In particular, near the critical line it typically behaves like:

$$\tau_a \simeq \xi^z$$
, or  $\tau_a \simeq L^z$ , (61)

with  $\xi$  being the correlation length and z>0 being the dynamical critical exponent. The second behavior applies when finite lattices are considered.

- Near the critical line where  $\xi \to \infty$ ,  $\tau_a$  also diverges. This means that it is more time-consuming to generate a statistically independent configuration near the critical line. This phenomenon is called critical slowing-down.
- It is known that for scalar field theories, Metropolis and the heatbath algorithm gives z > 1.
- For scalar field theories, the most powerful algorithm to fight critical slowing down is the cluster algorithm whose z is substantially less than 1.



#### 3.3. Cluster algorithm for scalar fields



### The Swendsen-Wang algorithm for Pott's model

The q-state Pott's model is a spin model with spin variables  $\sigma_i$  defined at the lattice site i can take q different values. The action (Hamiltonian) of the system is given by:

$$S = -K \sum_{\langle ij \rangle} \delta_{\sigma_i \sigma_j} , \qquad (62)$$

The Swendsen-Wang algorithm corresponds to the following steps:

• For each pair of neighboring sites i, j, create the bond between the two sites with probability:

$$p(\sigma_i, \sigma_j) = \delta_{\sigma_i \sigma_j} (1 - e^{-K}) .$$
(63)

The connected bonds thus created forms a *cluster*.

- For each cluster created on the lattice, generate a random spin value and assign it to *all* the spins in the cluster.
- Repeat the above two steps.





### Wolff's algorithm for $\mathcal{O}(N)$ model

Wolff's single cluster algorithm is a generalization of SW to O(N) model.

- Choose a random direction with unit vector  $\mathbf{r}$  in N-dimensional space and a random site x from the lattice to be the first member of the cluster c.
- Flip the component of  $\phi_x$  that is parallel to r:

$$\phi_x \to (R(\mathbf{r}) \cdot \phi_x)^a \equiv \phi_x^a - 2(\mathbf{r} \cdot \phi_x)\mathbf{r}^a$$
, (64)

with  $\mathbf{r} \cdot \phi_x = \mathbf{r}^b \phi_x^b$  being the inner product in O(N) space.

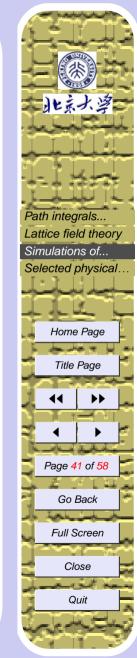
• Go to a nearest neighbor point y of x and activate the bond  $\langle xy \rangle$  with probability:

$$P(\phi_x, \phi_y) = 1 - \exp\left(\min\{0, 4\kappa(\mathbf{r} \cdot \phi_x)(\mathbf{r} \cdot \phi_y)\}\right). \tag{65}$$

If the bond is activated, flip  $\phi_y$  according to Eq. (64) as well and then join y to the cluster c.

• Continue for all neighboring sites of the cluster until the cluster growth stops.

It can be shown that is algorithm is both ergodic and detailed-balanced.



#### **3.4.** Simulation of Gauge fields



### The Creutz heatbath algorithm for SU(2) pure gauge theory

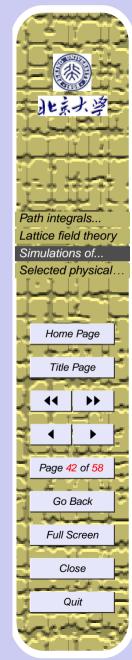
An SU(2) matrix is represented by:  $U(x) = a_0 + i\boldsymbol{\sigma} \cdot \mathbf{a}$ , with  $a_0^2 + \mathbf{a}^2 = 1$ .  $\boldsymbol{\sigma}$  are the Pauli matrices. Then in the plaquette action, terms that depend on a specific gauge link reads:

$$S(U_{\mu}(x)) = -\beta Tr(U_{\mu}(x) \cdot R) , \qquad (66)$$

where  $R = \sum_s U_s$  represents the sum of all staples containing the link. We may write:  $R = k \cdot R'$ , with R' in SU(2). k is the norm of R. Then, heatbath algorithm requires to generate the probability distribution for  $a_0$  of the form:

$$P(a_0) \propto (1 - a_0^2)^{1/2} e^{\beta k a_0} , \qquad (67)$$

a is then generated uniformly on the surface of a 3-sphere with radius  $\sqrt{1-a_0^2}$ .





#### The pseudo-heatbath and over-relaxation for SU(3)

#### Pseudo-heatbath:

For group SU(N), one can embed several SU(2) subgroups into SU(N). For SU(3) we can take the following two embedding:

$$c_1 = ((\alpha_1)_{2 \times 2}, 1) , c_2 = (1, (\alpha_2)_{2 \times 2}) ,$$
 (68)

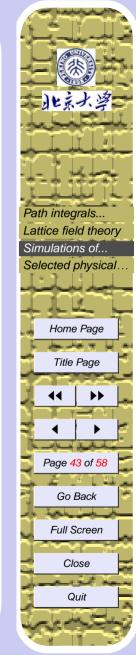
where  $\alpha_1$  and  $\alpha_2$  are SU(2) matrices. The update of the gauge link is done by:

$$U_{\mu} \to U'_{\mu} = c_2 \cdot c_1 \cdot U_{\mu} ,$$
 (69)

where  $c_2$  and  $c_1$  can be generated using Creutz heatbath algorithm for SU(2). This is the pseudo-heatbath algorithm due to Cabbibo-Mariani.

#### Over-relaxation:

The pseudo-heatbath algorithm has rather long auto-correlation length. To fight this bad feature, one can mix it with the so-called over-relaxation algorithm, which is a micro-canonical (meaning keeping the action unchanged) update of the gauge fields.





#### The new and the old algorithms





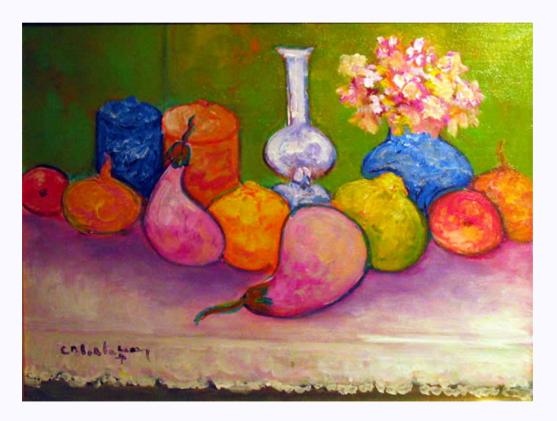
- Modern algorithms are more efficient to fight critical slowingdown.
- Good things are always fragile. They are working only for some particular models. For example, cluster algorithms for gauge theories and for other systems are not well developed.
- Old-fashioned algorithms usually have rather serious critical slowing-down. Not recommended for sophisticated study.
- However, they usually can be applied widely to almost all models. For example, Metropolis seems to be working even for non-local theories.



Fermion algorithms: Tony's talk.



## 4. Selected physical results



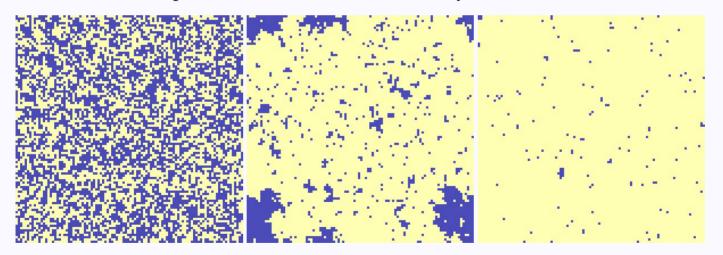


#### 4.1. Spin models



### The 2D Ising model can be solved analytically

On the other hand, it can be simulated using the most efficient algorithm (cluster). Comparison of Monte Carlo with analytic results is fun.







#### Triviality and the Higgs mass bound

- Scalar field theory was extensively studied using lattice techniques in the 1980's using two type of methods: 1) high temperature expansion and RG;
  2) Monte Carlo simulations. These methods provide a numerical solution to scalar field theory. A remarkable feature of scalar field theory in four dimensions is *triviality*, i.e. renormalized quatic coupling λ<sub>R</sub> is a marginal coupling which goes to zero logarithmically in the critical region as: λ<sub>R</sub> ≃ 1/ln ξ.
- In Minimal SM, eletro-weak symmetry is broken via Anderson-Higgs mechanism, which is similar to the case in BCS superconductors. Higgs particle which corresponds to the scalar field (called the Higgs field) is the only missing particle in Minimal SM. The mass of the Higgs particle is roughly related to the quatic coupling via:

$$m_H^2 \simeq \lambda_R v^2 \,, \tag{70}$$

where  $v=246 {\rm GeV}$  is a fixed physical scale. Therefore, triviality implies an upper bound for the mass of the Higgs particle in the range of  $600-800 {\rm GeV}$ . Maybe we will witness the discovery of this particle in the future LHC run.



#### 4.2. QCD and Lattice QCD



#### Hadrons at low and high energies

#### **...** Low energy hadrons

Before 1960, elementary particles refers to those microscopic particles which does not show structure: electrons, protons, neutrons, pions, etc. But soon, so many of them have been found in the experiment that it is hard to believe that they are all elementary.

By studying the mass of the hadrons, underlying symmetries emerge. These symmetries can be better understood by assuming hadrons made up of more elementary constituents called quarks. Quarks are bound together via strong interaction in a hadron. This is the so-called Quark Model. It also suggests quarks have another charge called "color". However, quarks have never been found individually. It seems that they are always confined in the hadron. This is called confinement.

#### **4** Hadrons at high energies

Deep inelastic scattering (DIS) experiments in the late 60's verified that hadrons have internal structure. Some scaling behavior (Bjorken scaling) was found which suggests that hadrons are made of almost free (non-interacting) constituents called partons.





#### **Dual face of QCD**

#### Asymptotic freedom and QCD

In 1972, a feature called asymptotic freedom was found for non-abelian gauge theories which was able to explain major features (scaling) found in the DIS experiments. This leads to the belief that Quantum Chromodynamics (QCD) is the theory for strong interactions, that is, the field theoretical framework for strong interaction is a non-abelian gauge theory which becomes almost free (no interactions) at high energies where perturbative methods (perturbative QCD) is applicable.

#### Confinement and QCD

At low energies, however, the interaction of QCD becomes so strong that it finally confines the quarks into colorless hadrons. This regime is totally non-perturbative and only non-perturbative methods like Lattice QCD can provide physical understanding. This is non-perturbative QCD.

♣ As the fundamental theory of strong interaction, QCD should explain both asymptotic freedom at hight and confinement at low energies





#### Confinement and the static quark potential

#### Quarks are confined:

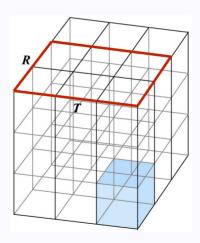
The force between quarks and anti-quarks are so strong that non-perturbative study (using lattice) is necessary.

# The static quark potential and Wilson loop:

To provide confinement, the potential V(r) between a static (infinitely heavy) quark and a static anti-quark should grow linearly with the distance r at long distances. The potential is related to the so-called *Wilson loop* via:

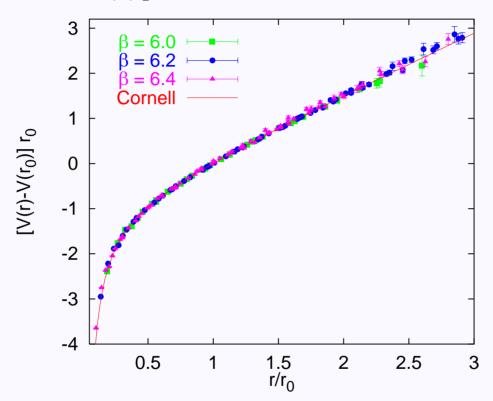
$$\langle W(r,T)\rangle \propto e^{-V(r)T}$$
, (71)

where r and T being the spatial and temporal side of the rectangular loop, respectively.





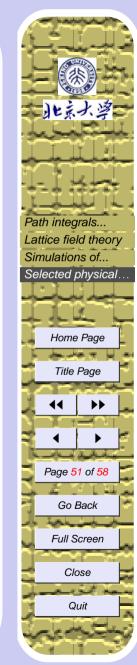
### ightharpoonup An illustration of <math>Qar Q potential



Taken from G. Bali hep-ph/0001312

#### **...** Linear behavior observed for large distances:

$$V(r) = V_0 + \frac{\alpha}{r} + \sigma r \ . \tag{72}$$





#### The mass of hadrons can be predicted

If QCD were the right theory for strong interactions, we should be able to *predict* the mass of the hadrons since they are bound states of quarks.

#### **4** Hadron masses can be obtained in Lattice QCD:

To obtain these, one constructs a suitable operator  $\mathcal{O}$  which carries the right quantum number of the hadron being studied. Therefore,  $\mathcal{O}|0\rangle$  will have a non-zero overlap with the hadron state whose energy is  $E_n$ . Then we measure the following correlation function:

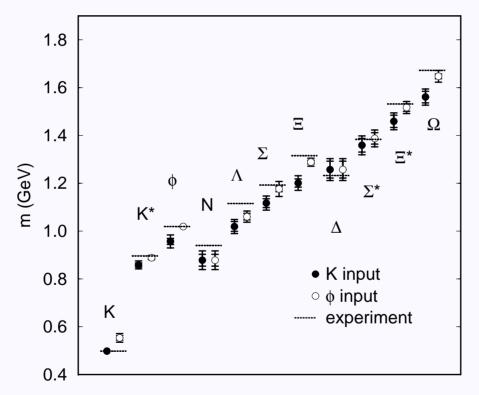
$$\langle \mathcal{O}(t)\mathcal{O}(0)\rangle = \sum_{n} e^{-E_n t} |\langle 0|\mathcal{O}|n\rangle|^2$$
 (73)

By measuring the exponential decay rate of this function, one obtains the energy of the hadronic state:  $E_n$ .



## \$

### An illustration of quenched hadron spectrum

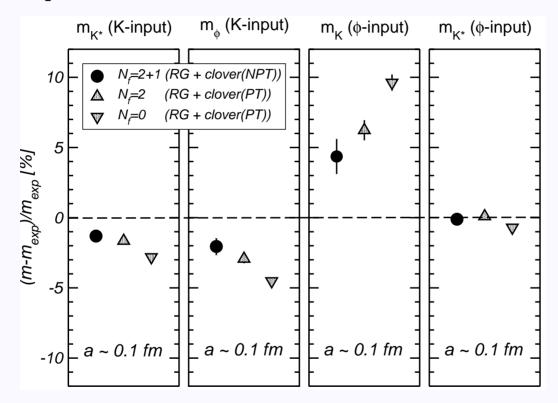


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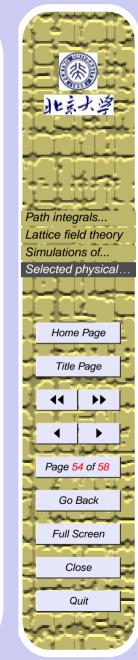


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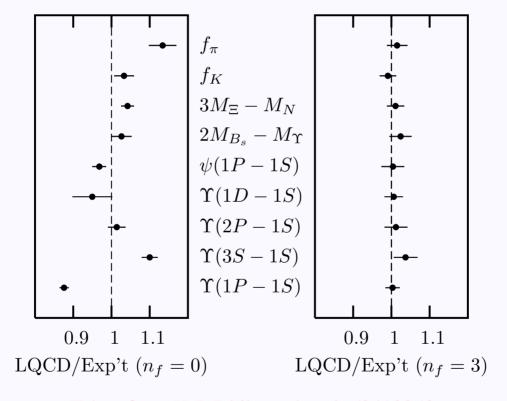
### The unquenched results



Taken from K-I. Ishikawa hep-lat/0410050



### The unquenched results

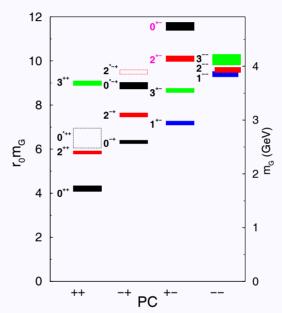


Taken from K-I. Ishikawa hep-lat/0410050





- Non-abelian (pure) gauge theories can have bound states known as *glueballs*.
- Glueballs come in as different quantum numbers of  $J^{PC}$ .
- They can be studied by forming appropriate glueball operators with definite quantum numbers and measure correlation functions among these operators.
- Glueball correlators are noisy objects. To get a descent signal for them, one needs large amount of gauge configurations.
- Other techniques are also needed: lat/9901004. smearing, fuzzying, anisotropic lattices, variational methods, etc.



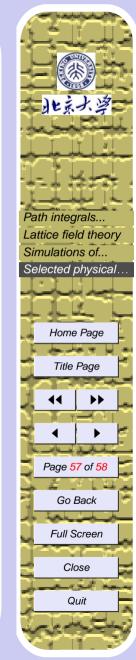
Taken from Morningstar and Peardon hep-lat/9901004.



### **\$**

### What's not included...





# Thank you!

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