Introduction to Lattice QCD (part1)

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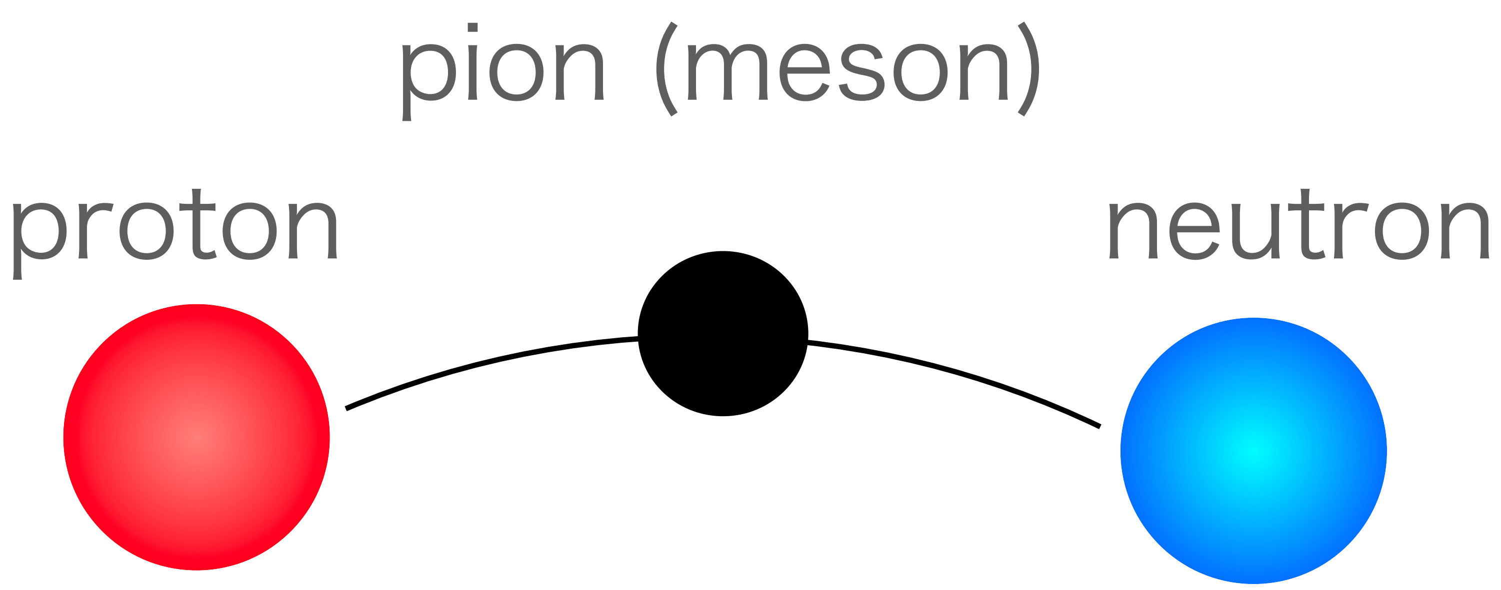
YITP long-term workshop
Hadrons and Hadron Interactions in QCD 2024 (HHIQCD2024)@ YITP, Kyoto U., 2024/10/16

1. Introduction

YITP and Yukawa theory

- Yukawa Institute for theoretical physics, Kyoto University (1952 -)
- Yukawa theory (1935)
  introduce a new particle (meson) to explain the nuclear force  (1949)
- Discovery of the neutron (1932) by James Chadwick  (1935)
- You can see his note in the salon in front of this lecture hall

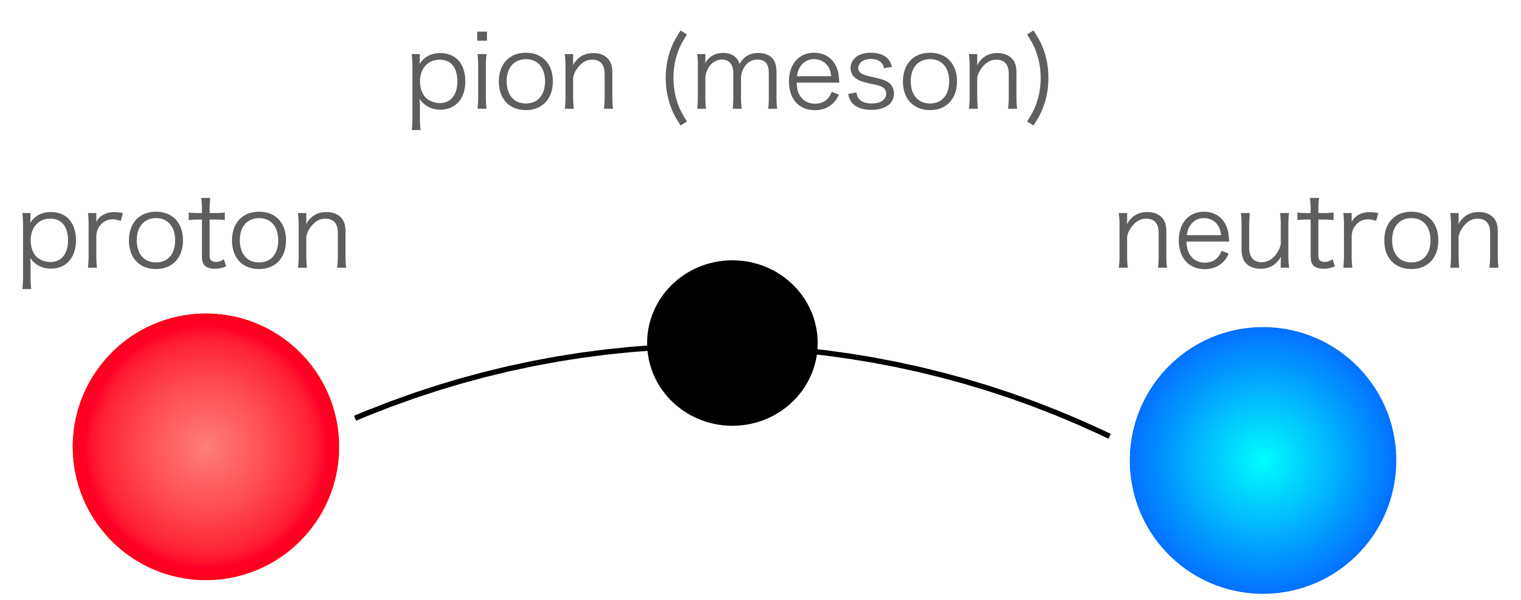
Yukawa interaction



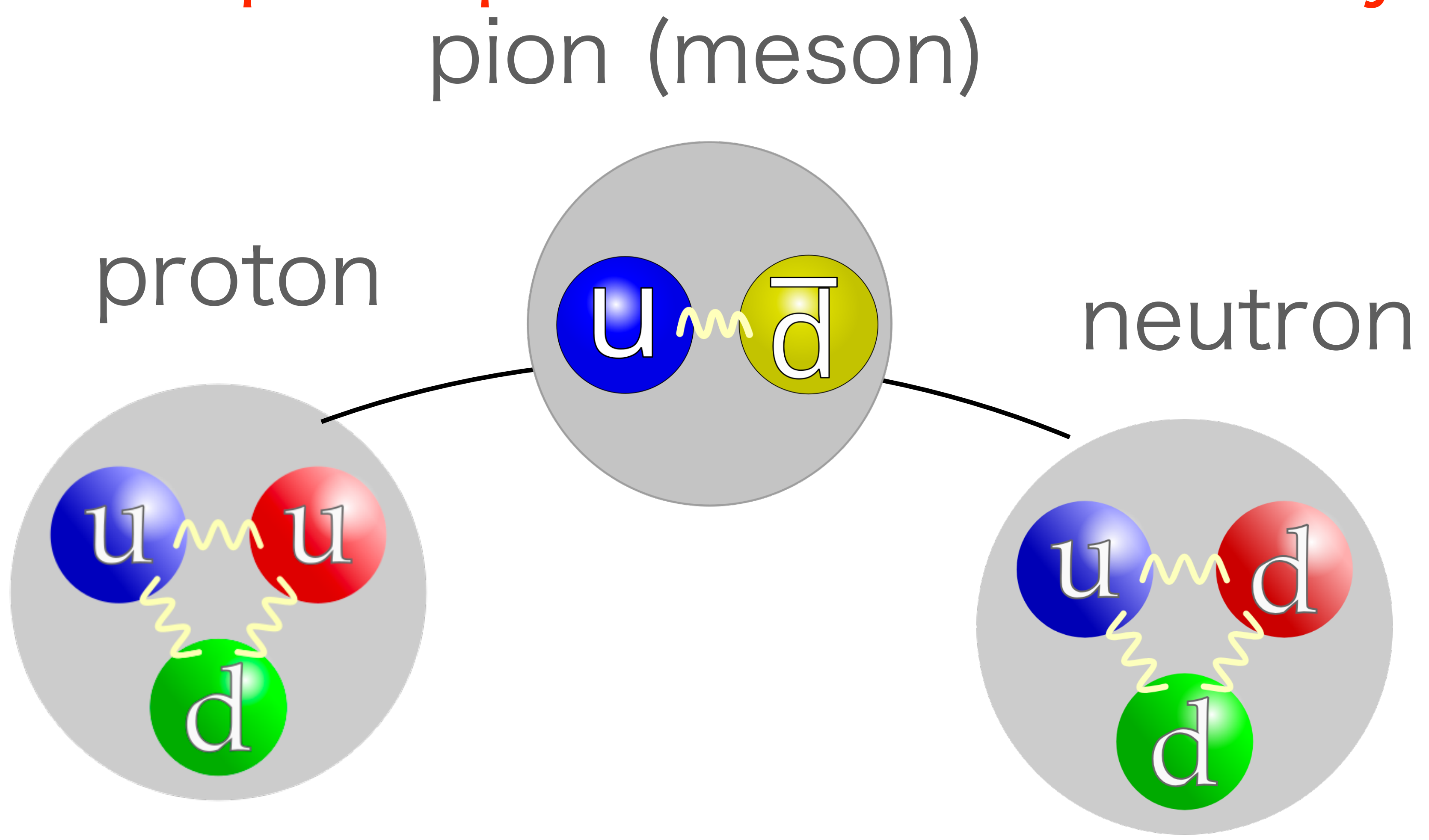
Proton, neutron and pion are composed of quarks

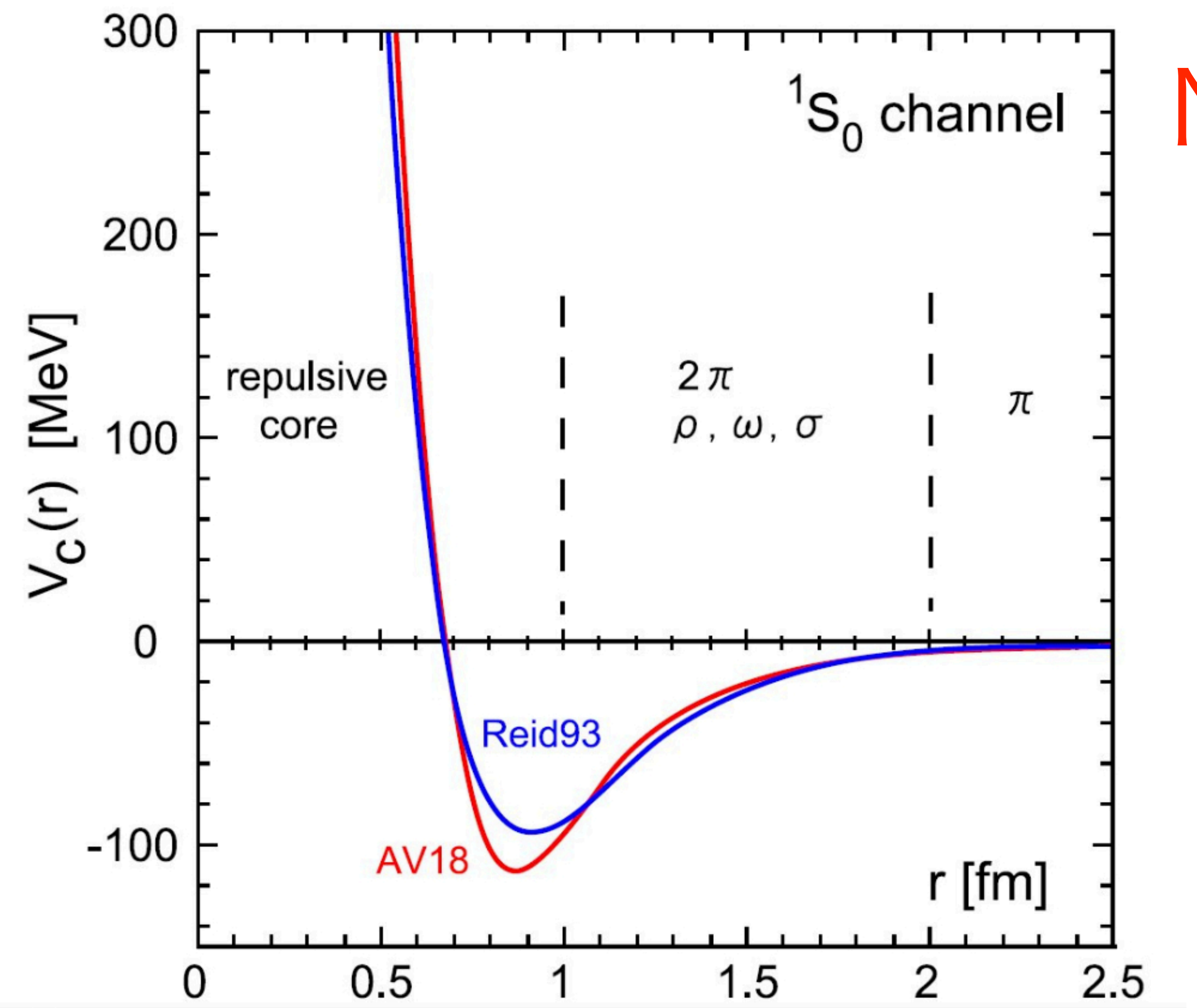
- Yukawa interaction is now described by further microscopic theory Quantum ChromoDynamics (QCD)

Yukawa interaction



Microscopical picture described by quarks





N-N potential obtained phenomenologically

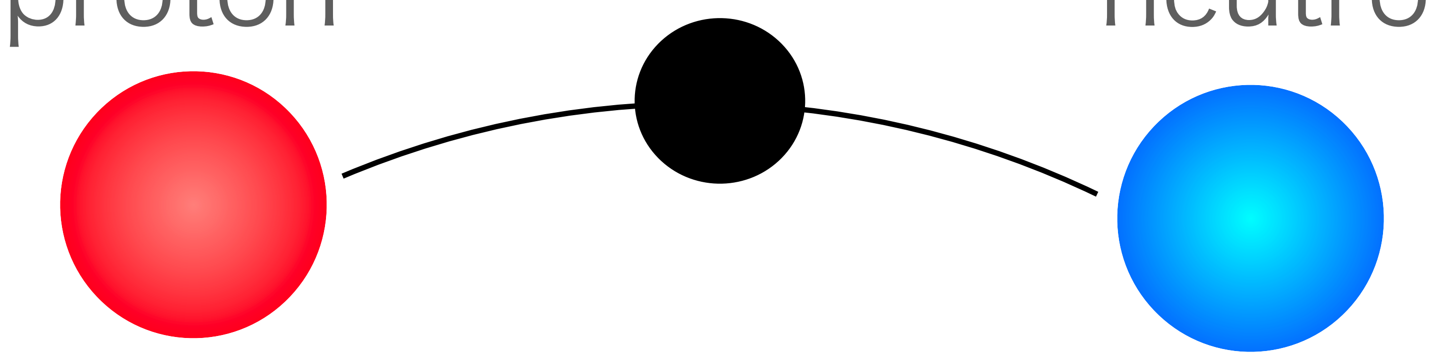
Proton, neutron and pion are composed of quarks

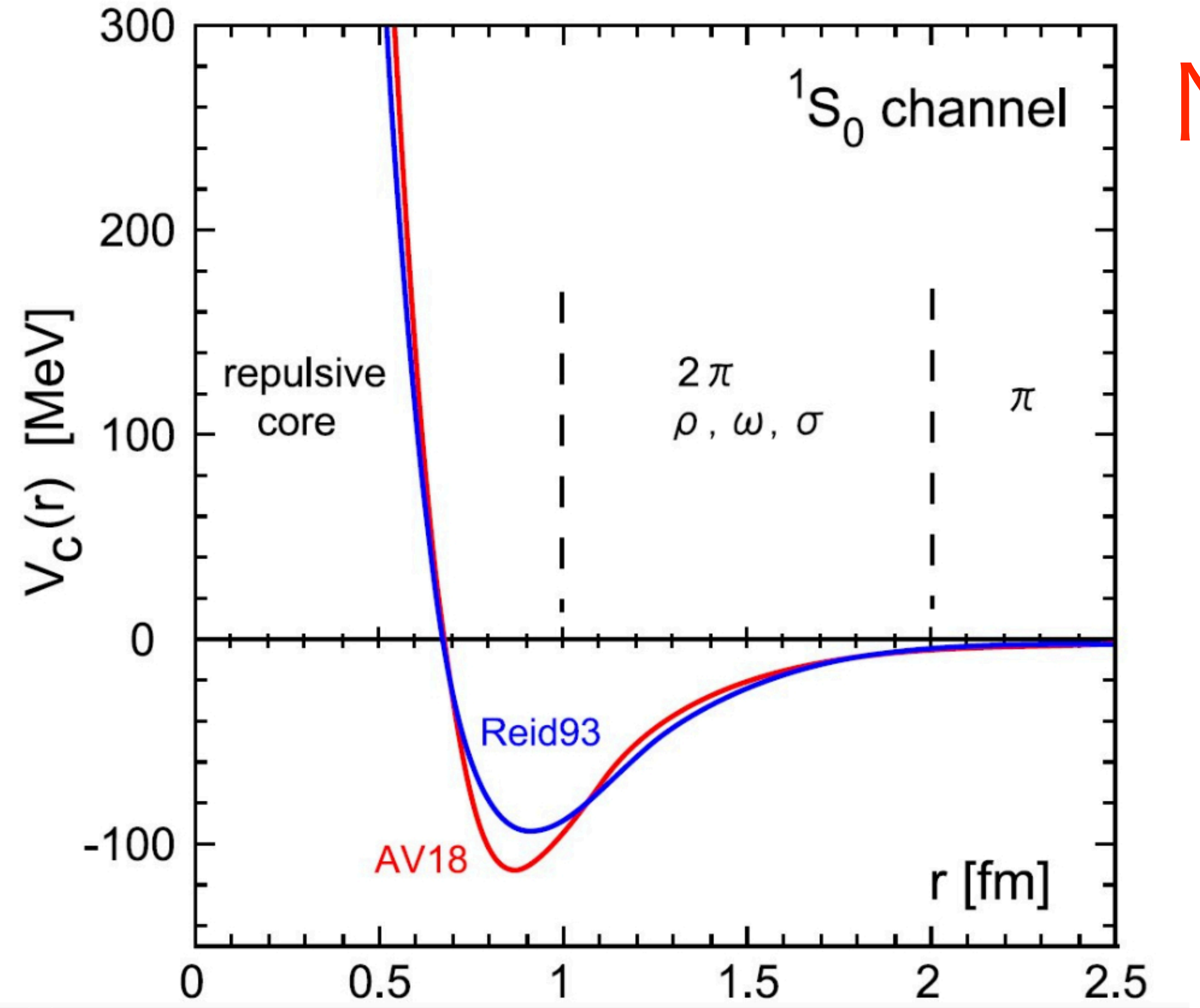
- Yukawa interaction is now described by further microscopic theory Quantum ChromoDynamics (QCD)

Yukawa interaction

pion (meson)

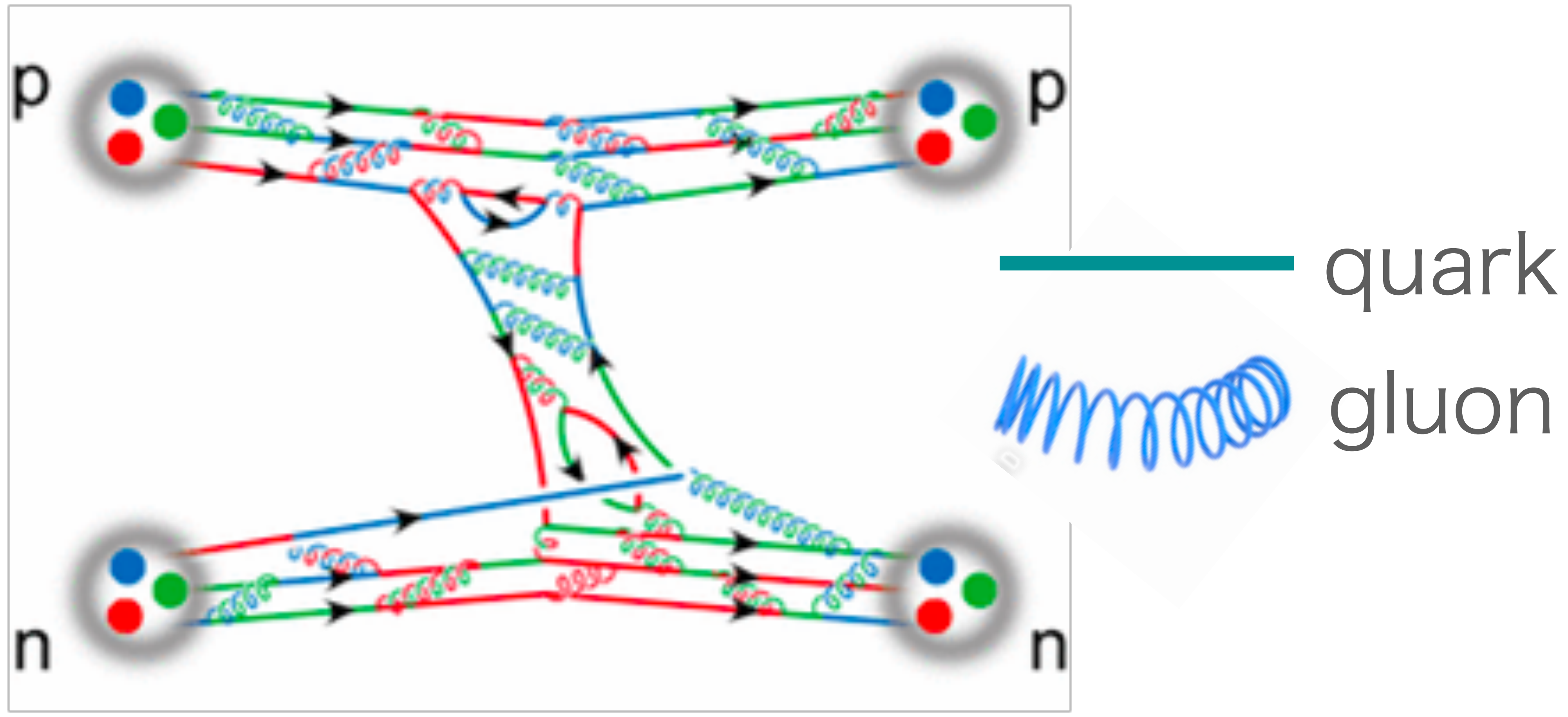
proton   neutron

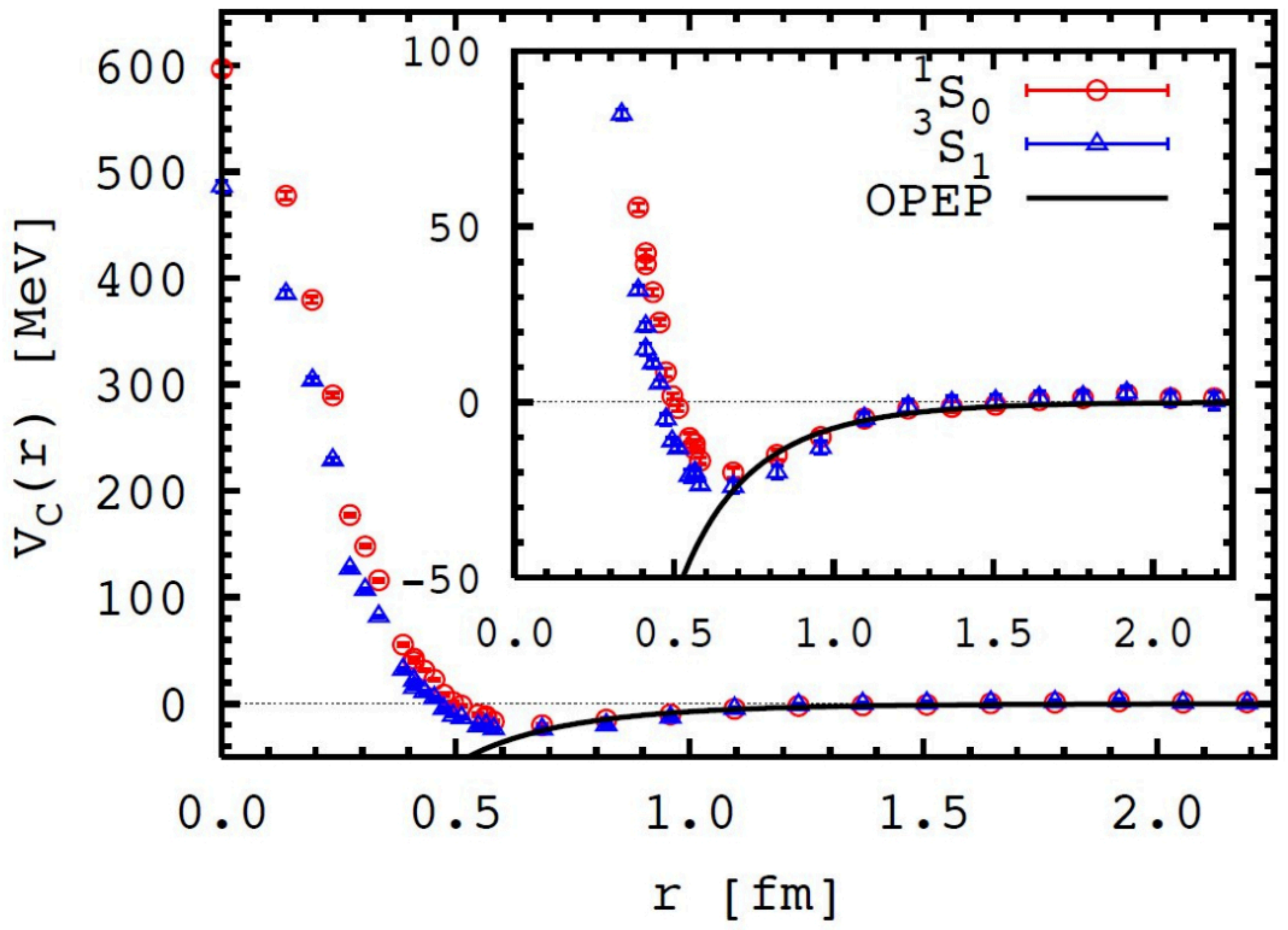




N-N potential obtained phenomenologically

Microscopical picture described by quarks





N-N potential obtained from QCD using Lattice simulation

(Lecture by T.Doi on Friday)

Contents (part 1 and part 2)

1. Introduction

2. Lattice gauge theory
   confinement and cont. lim. - analytical results -

3. Introduction to numerical calculation

4. Configuration generation

5. Hadron mass spectrum

6. Advanced topics for mass spectrum

7. Summary

2. Lattice gauge theory

QCD (quantum chromo dynamics)

May, 2023 @ U. of Minnesota

- QCD Lagrangian

$$\mathscr{L} = -\frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} + \bar{\psi}(i\gamma_\mu D_\mu + m)\psi,$$

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + gf^{abc}A^b_\mu A^c_\nu$$

$$D_\mu = \partial_\mu - igA^a_\mu T^a$$

A^a_μ : gluon, a=1…8

ψ : quark

- Gauge theory is given by this eq. form
cf.) Quantum electro-magnetic dynamics (QED)

A^a_μ : photon, a=1

ψ : electron

- Parameters of this theory

g : (bare) coupling

m : (bare) mass for each quark

Regularization of quantum field theories

- Quantum filed theory has infinite degrees of freedom (dof) at each point in spacetime

- But physical quantity is finite.
  Systematic method is needed to eliminate infinities from the calculations
  => renormalization / regularization

- perturbative renormalization, large-N expansion, ε expansion..

- Lattice regularization… Discretizing spacetime makes dof finite

K. Wilson, “Confinement of quarks”, Phys.Rev. D10 (1974)

Lattice regularization method

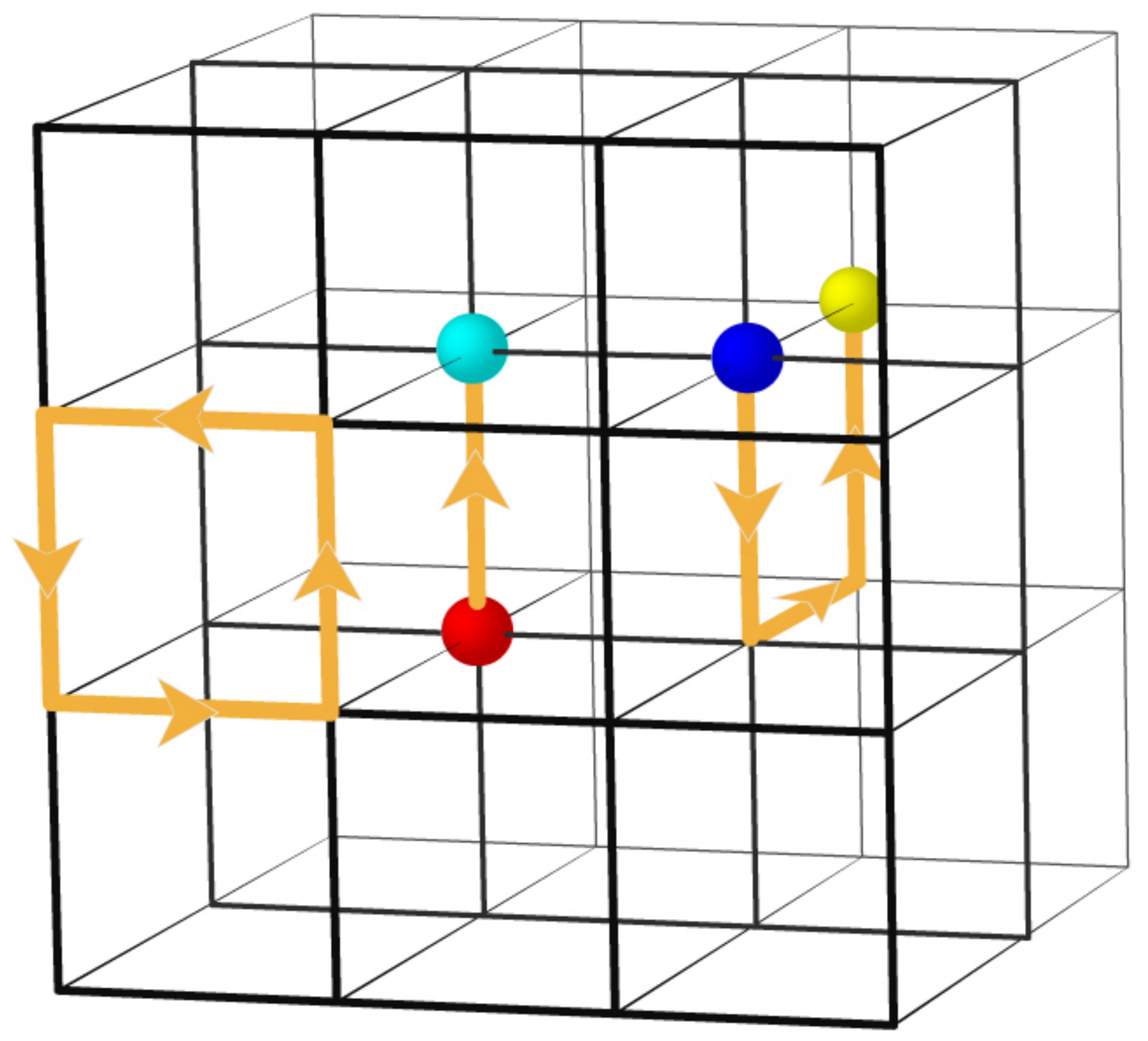
- Discretizing spacetime :

  lattice spacing a (UV cutoff) and finite volume $L = N_s a$ (IR cutoff)

  N_s : # of lattice site (for each space-time direction)

- Calculate $\langle \mathcal{O} \rangle$ on the lattice expressed by finite variables

  Exactly speaking, the result $\langle \mathcal{O} \rangle$ is the one for lattice model.



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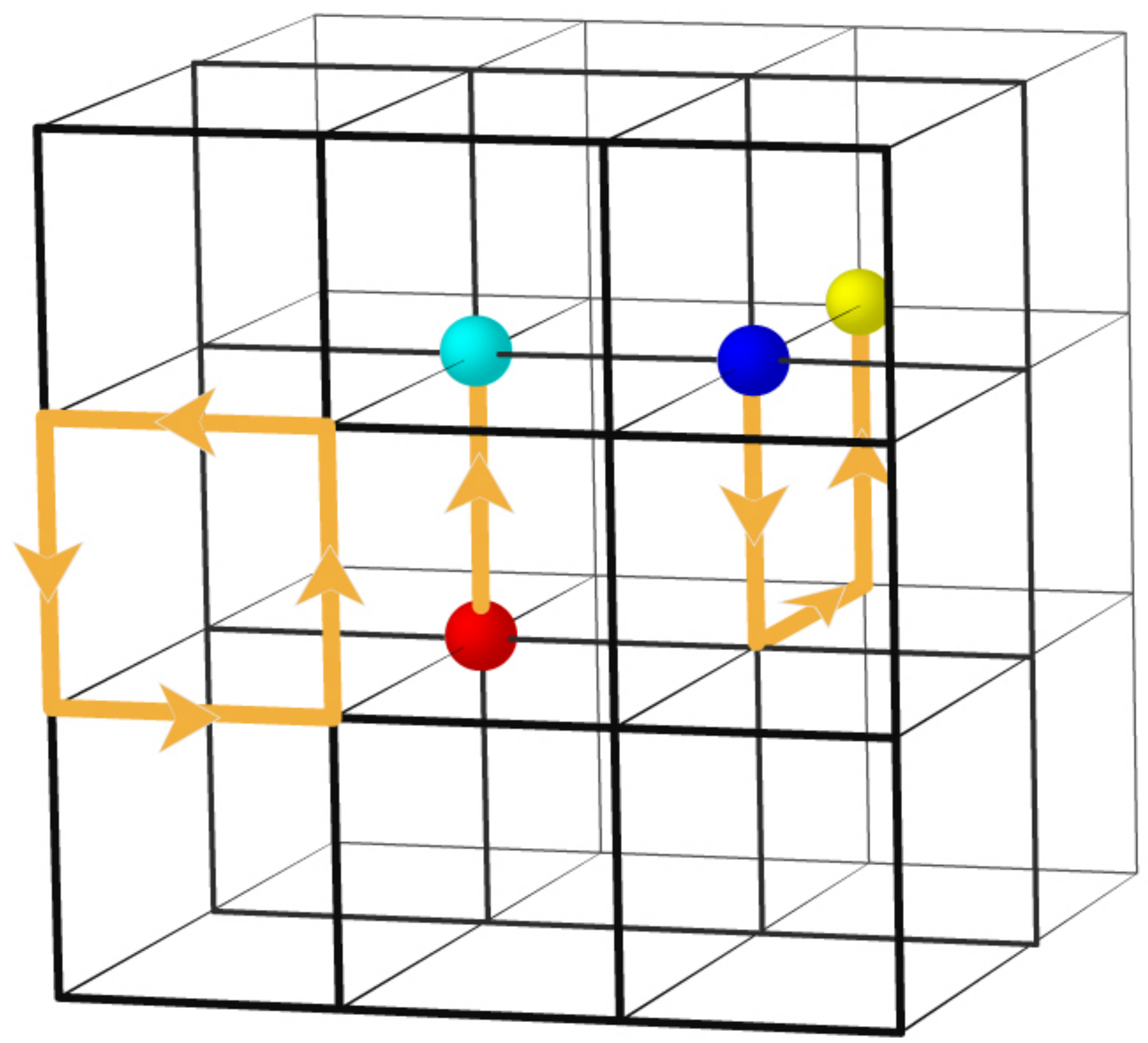
- The continuum limit $a \to 0$ (w/ fixed reference scale) and thermodynamic limit $L \to \infty$ will be taken to be back to continuum theory

Setup of lattice gauge theory

- Put the quarks on site and gluons on link

  the direction μ of A_μ^a correspond to the direction of the link



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- Note : Do not put A_μ^a itself on the link

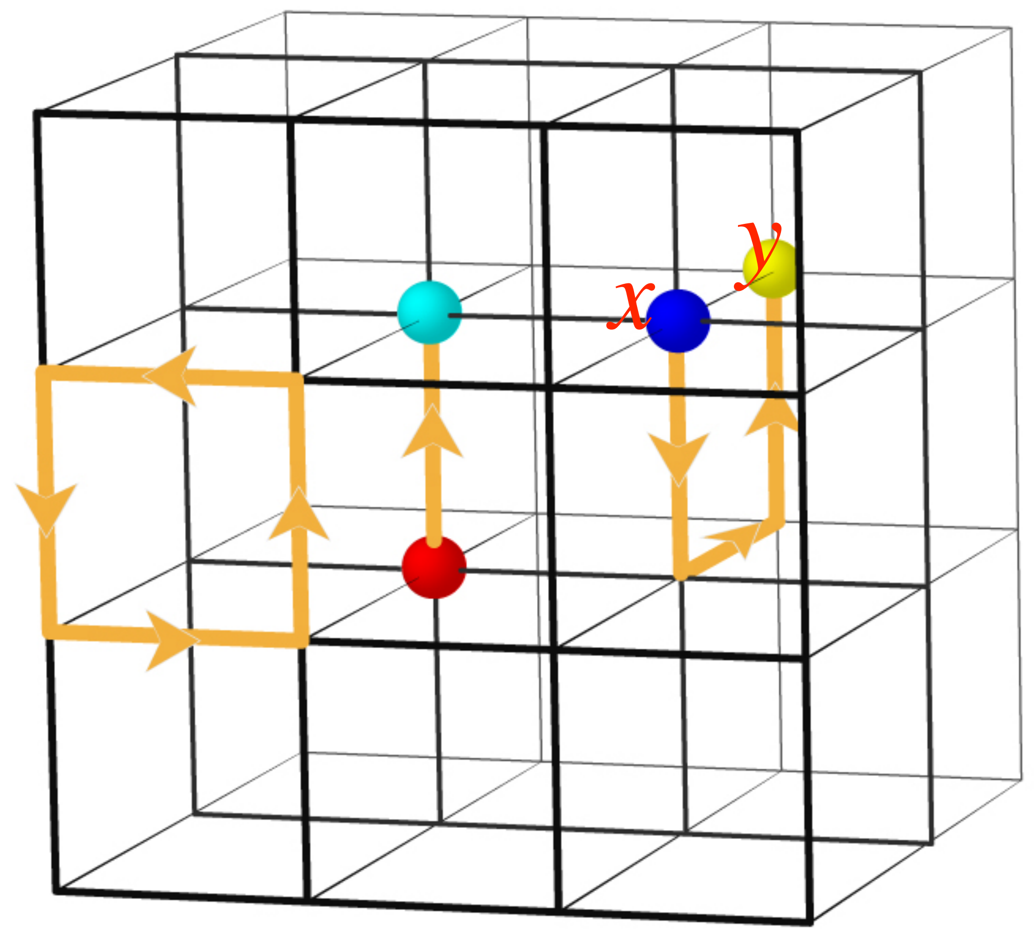
- link variable: $U_\mu = e^{iagA_\mu^a T^a}$; T^a SU(N) representation matrix

Link variable and gauge invariance

- gauge transformation : $\Omega(x) \in SU(3)$ local transformation

$$\psi'(x) = \Omega(x)\psi(x), \quad \bar{\psi}' = \bar{\psi}\Omega(x)^\dagger, \; A_\mu(x)' = \frac{1}{ig}\Omega(x)\partial_\mu\Omega(x)^\dagger + \Omega(x)A_\mu(x)\Omega(x)^\dagger$$

- QCD is invariance under this transformation at each space-time point independently



- Physical observable is gauge invariant

- Keeping the gauge invariance must be important

Link variable and gauge invariance

- gauge transformation : $\Omega(x) \in SU(3)$ local transformation

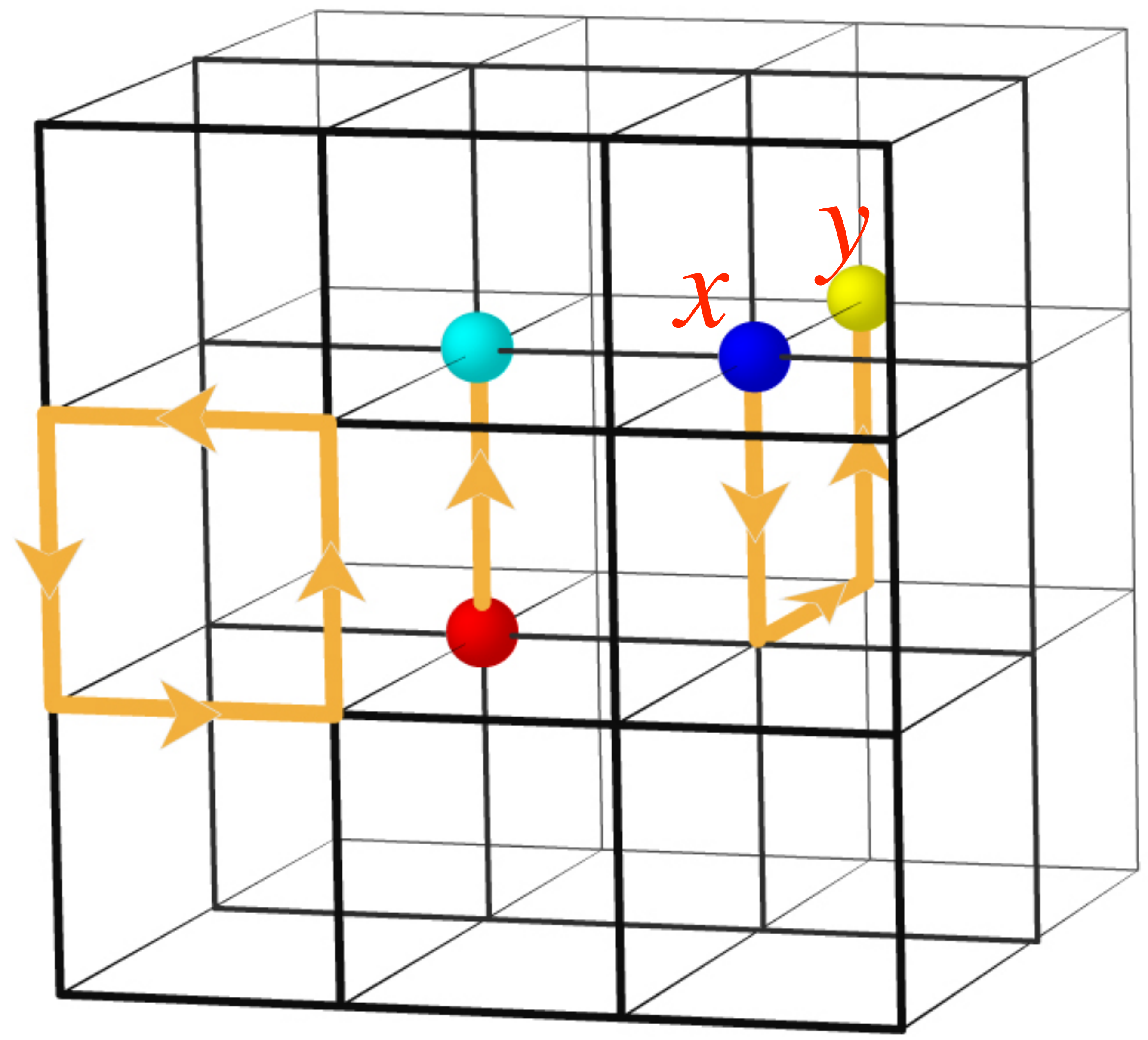
$$\psi'(x) = \Omega(x)\psi(x), \quad \bar{\psi}' = \bar{\psi}\Omega(x)^\dagger, \; A_\mu(x)' = \frac{1}{ig}\Omega(x)\partial_\mu\Omega(x)^\dagger + \Omega(x)A_\mu(x)\Omega(x)^\dagger$$

- Operators and its gauge invariance

$\bar{\psi}(x)\psi(x)$: gauge invariance ○

$\bar{\psi}(x)\psi(y), x \neq y$: gauge invariance ✕

$\bar{\psi}(x) \boxed{e^{i\int_y^x A_\mu dx_\mu}} \psi(y)$: gauge invariance ○

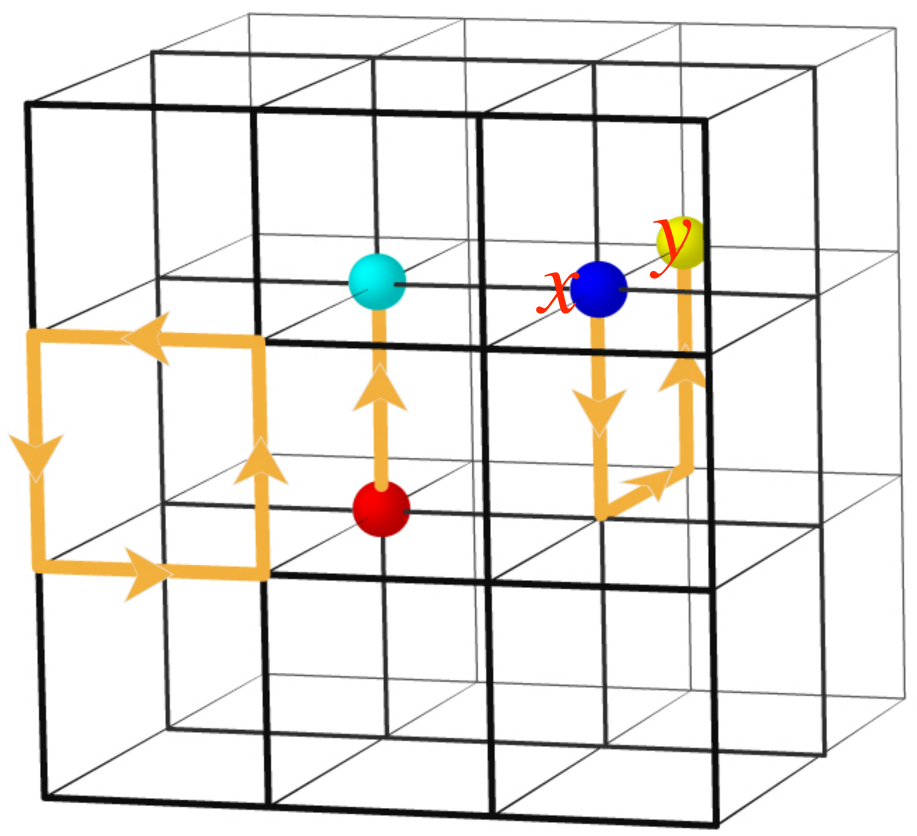


- Introducing the link variable, $U_\mu = e^{iagA_\mu^a T^a}$, makes it easier to see gauge invariance

Link variable and gauge invariance

- gauge transformation : $\Omega(x) \in \mathrm{SU}(3)$ local transformation

  for link variable : $U'_\mu(x) = \Omega(x)U_\mu(x)\Omega(x+\hat{\mu})^\dagger$



- Gauge invariant ops.

  (1)All closed loop of links are gauge invariant

  (ex) Plaquette: $\mathrm{tr}[U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x)]$

  (2) quark-antiquark connected by link products between them

- Note: The Elitzur's theorem

  only gauge-inv. operators can have non-vanishing expectation values

  Lattice calc. respects to the invariance, then it is hold naturally

Numerical advantage of introducing link variables

- Gauge field takes value of $-\infty \leq A_\mu^a \leq \infty$

  Link variable is a compact reps.: $\| U_\mu = e^{iagA_\mu^a T^a} \| \leq 1$

- Numerically, it's important.

  If we use $-\infty \leq A_\mu^a \leq \infty$, keeping the calculation accuracy is hard

confinement and cont. lim.
- analytical results-

Outline of discussions

- Introduce a lattice model
- The lattice model in cont. lim. converges to Yang-Mills theory (QCD)
- In $g \to \infty$, the lattice model shows the confinement of probe quarks
- In $g \to 0$, we can analyze it using lattice perturbation
- Using non-pertubative analysis (=numerical simulation), we can see that the lattice model connects $g \to \infty$ and $g \to 0$ correctly
- So, we can calc. physical quantity of QCD from the nonperturbative simulation of the lattice model

Yang-Mills theory and lattice models

- (Euclidean) Yang-Mills action in the continuum limit : $S_{YM} = -\frac{1}{4}\int d^4x F^a_{\mu\nu}F^a_{\mu\nu}(x)$

- A lattice action : $S_G = \frac{1}{g^2}\sum_n \sum_{\mu\neq\nu} \mathrm{tr}[U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}]$ (plaquette gauge action)

- (calc.) Expand the link variable, $U_{n,\mu} = e^{iagA^a_\mu(n+\hat{\mu}/2)T^a}$, in small a.

  Here, a denotes lattice spacing (mass-dim. = -1), agA^a_μ is dimension-less

  $$\mathrm{tr}[U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}] = \mathrm{tr}\left[1 + ia^2 gF_{\mu\nu} + (*)a^3 + \boxed{\frac{a^4g^2}{2}F^2_{\mu\nu}} + O(a^5)\right]$$

  2nd and 3rd terms = 0 because of $\mathrm{tr}T^a = 0$, $O(a^5)$ becomes zero in $a \to 0$

  only $\mathrm{tr}[F^2_{\mu\nu}]$ remains in the continuum limit

- Cf.) $O(a^5)$ term can vanish by adding some higher mass dim. term

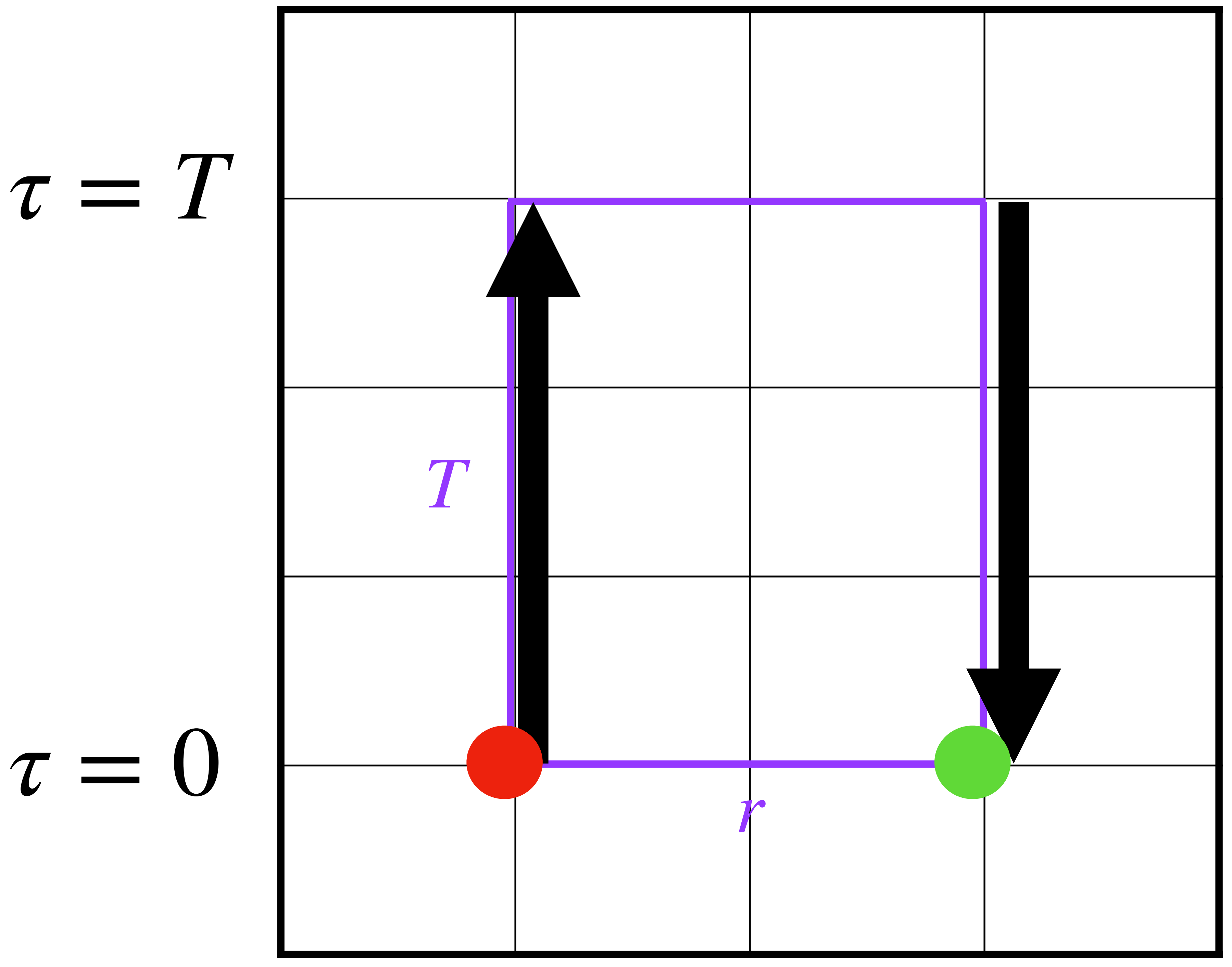
  Improved action (Symanzik action/ Iwasaki gauge action....)

  Any lattice action is fine if it goes to the Yang-Mills action in the continuum limit

Wilson loop : probe quark anti-quark potential

Wilson loop on the lattice

$$W(C) = \mathrm{tr}\left[\prod_{i\in C} U_i\right]$$



probe quark

probe anti-quark

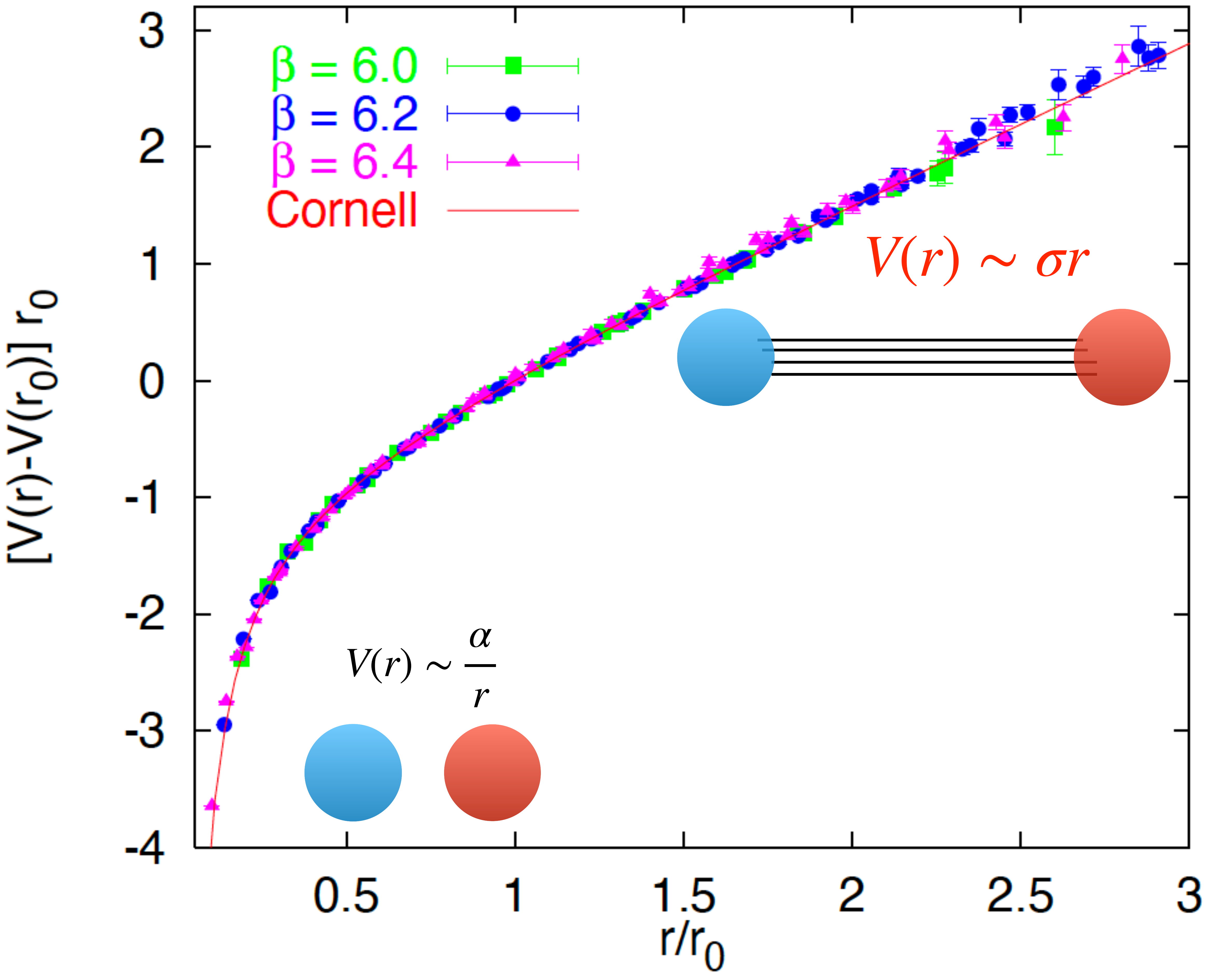
- $\langle W(C)\rangle \approx e^{-TV(r)}$ in $T \to \infty$

- The path describes...
  at $\tau = 0$, q and $\bar{q}$ are pair-created
  (immediately separate distance r)
  at $\tau = T$, the pair-annihilation occurs

- $V(r)$ corresponds to probe q and $\bar{q}$
  potential w/ distance r

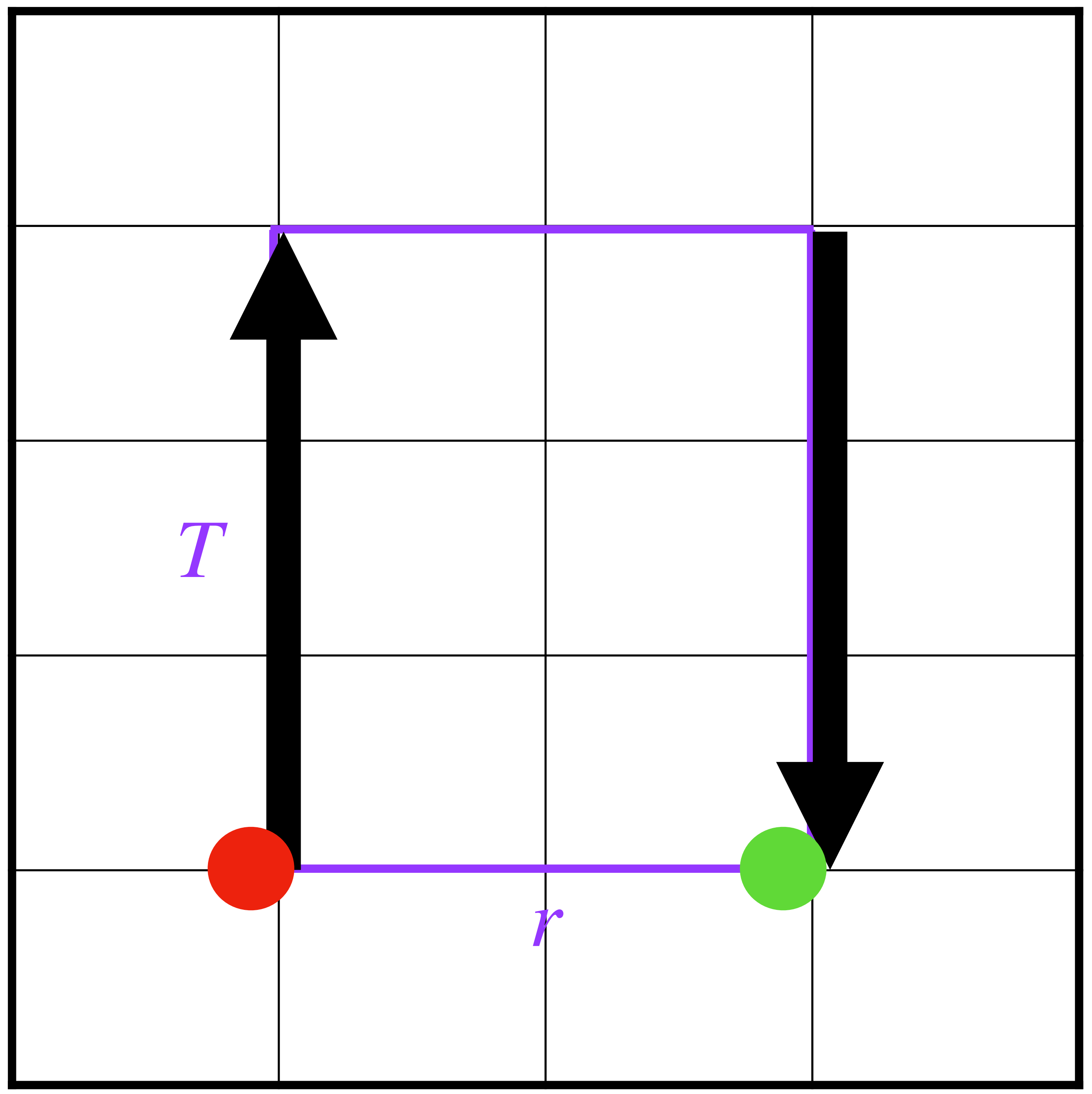
Lattice results of potential for probe quarks

G.Bali, Phys.Rept.343:1 (2000)



Wilson loop on the lattice

$$W(C) = \mathrm{tr}\left[\prod_{i \in C} U_i\right]$$



probe quark probe anti-quark

Integration rules of link variables (SU(N) group)

- Now, we want to calculate $\langle W(r\times T)\rangle = \int dU W(r\times T) e^{-S_G}$ analytically in some coupling limits.

- To do that, we need a integration rules of SU(N) group variables:

normalization: $\int dU 1 = 1, \quad \int dU U_{ab} = 0$

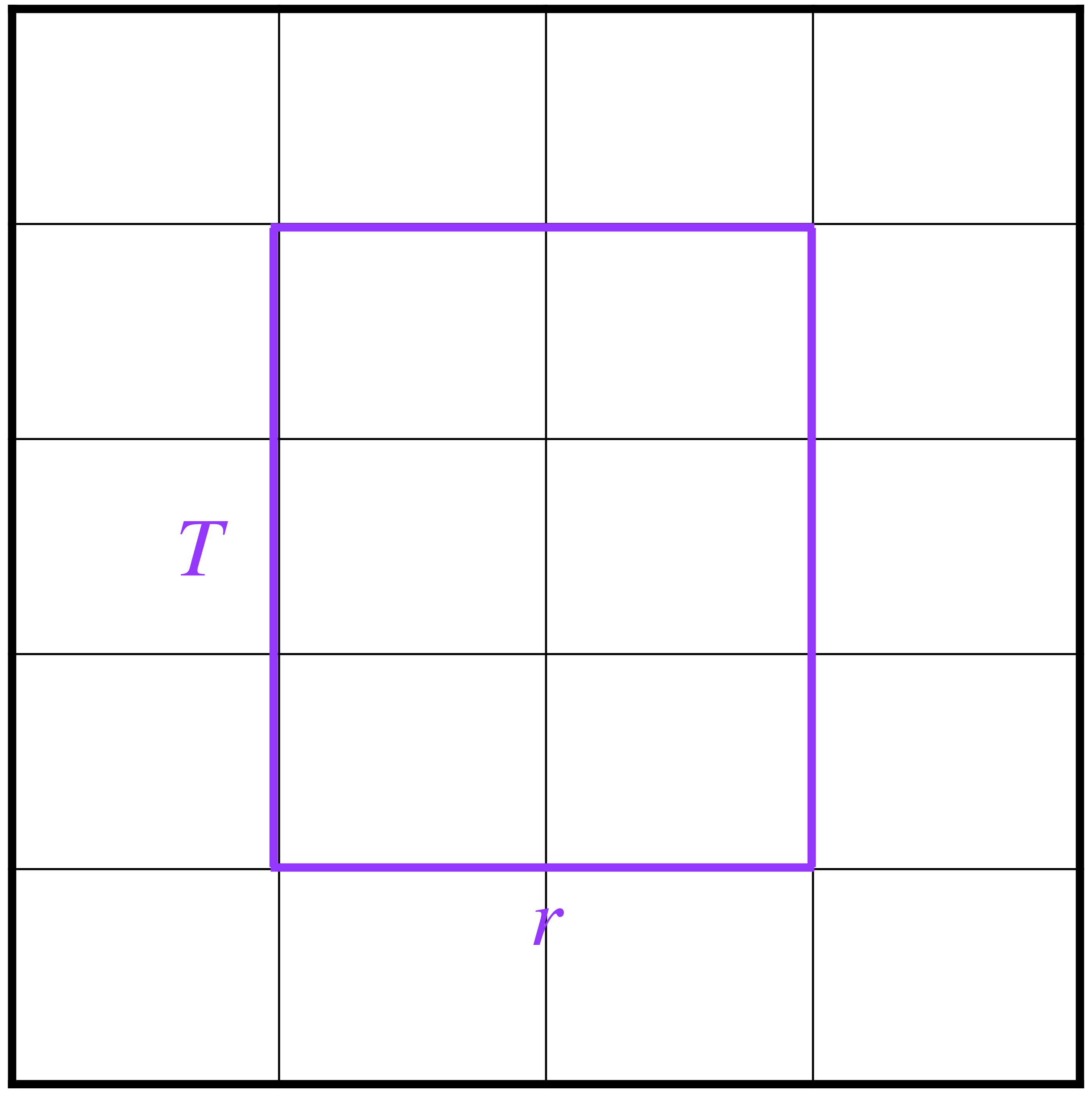
$\int dU U_{ab} U^\dagger_{kl} = \frac{1}{N}\delta_{al}\delta_{bk}$ (propagator) Only if $U_\mu(n)U^\dagger_\mu(n)$ can take non-vanishing value

(not take a sum of indices)

$\int dU U_{a_1b_1}U_{a_2b_2}\cdots U_{a_Nb_N} = \frac{1}{N!}\epsilon_{a_1a_2\cdots a_N}\epsilon_{b_1b_2\cdots b_N}$ (vertex contraction)

$\int dU U_{ab}U_{cd}U^\dagger_{ij}U^\dagger_{kl} = \frac{1}{N^2-1}[\delta_{aj}\delta_{aj}\delta_{aj}\delta_{aj} + \cdots]$ (combination of contraction)

Strong coupling expansion



- Let us consider $\langle W(r \times T)\rangle = \int dU W(r \times T) e^{-S_G}$, where

$$W(r \times T) = \mathrm{tr}\left[\prod_i U_{n,1}U_{n+\hat{1},1}\cdots U_{n+r\hat{1},1}U_{n+r\hat{1},4}U_{n+r\hat{1}+\hat{4},4}\cdots U^\dagger_{n,4}\right] = \mathrm{tr}U_{n,1}\hat{W}U_{n,4^\dagger}$$

and plaquette gauge action: $S_G = \frac{1}{g^2}\sum_n \sum_{\mu \neq \nu} \mathrm{tr}[U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}]$

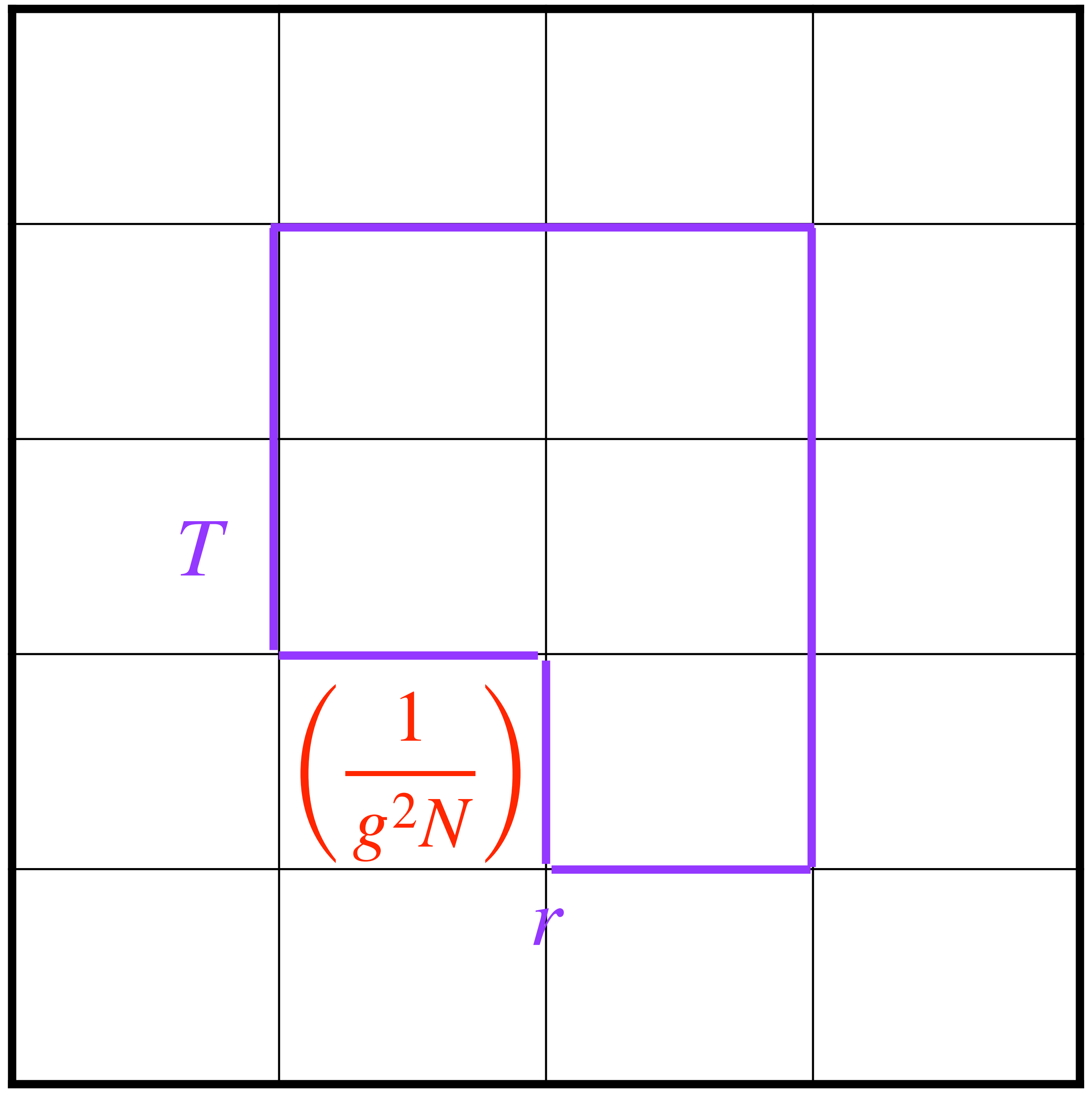
- In large g, the action is expanded as

$$e^{-S_G} = \prod_{n,\mu\neq\nu}\left[1 - \frac{1}{g^2}\mathrm{tr}[U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu} + \cdots]\right]$$

- At site n, only if $\int dU_{n,1}dU_{n,4}U_{n,1}U^\dagger_{n,1}U_{n,4}U^\dagger_{n,4}$ combination exists, the integral has non-zero value.

If $U^\dagger_{n,1}U_{n,4}$ comes from the plaquette action at site n: $\frac{1}{g^2}\mathrm{tr}[U_{n,4}U_{n+\hat{4},1}U^\dagger_{n+\hat{1},4}U^\dagger_{n,1}]$

Strong coupling expansion



- The result of $\int dU_{n,1}dU_{n,4}$ integral gives

$$\frac{1}{g^2N}\text{tr}U_{n+\hat{4},1}U^\dagger_{n+\hat{1},4}\hat{W}$$

- Iteratively, we perform all U integral and get

$$\langle W(r\times T)\rangle = \left(\frac{1}{g^2N}\right)^{rT-1}\langle W(1\times 1)\rangle = N\left(\frac{1}{g^2N}\right)^{rT}$$

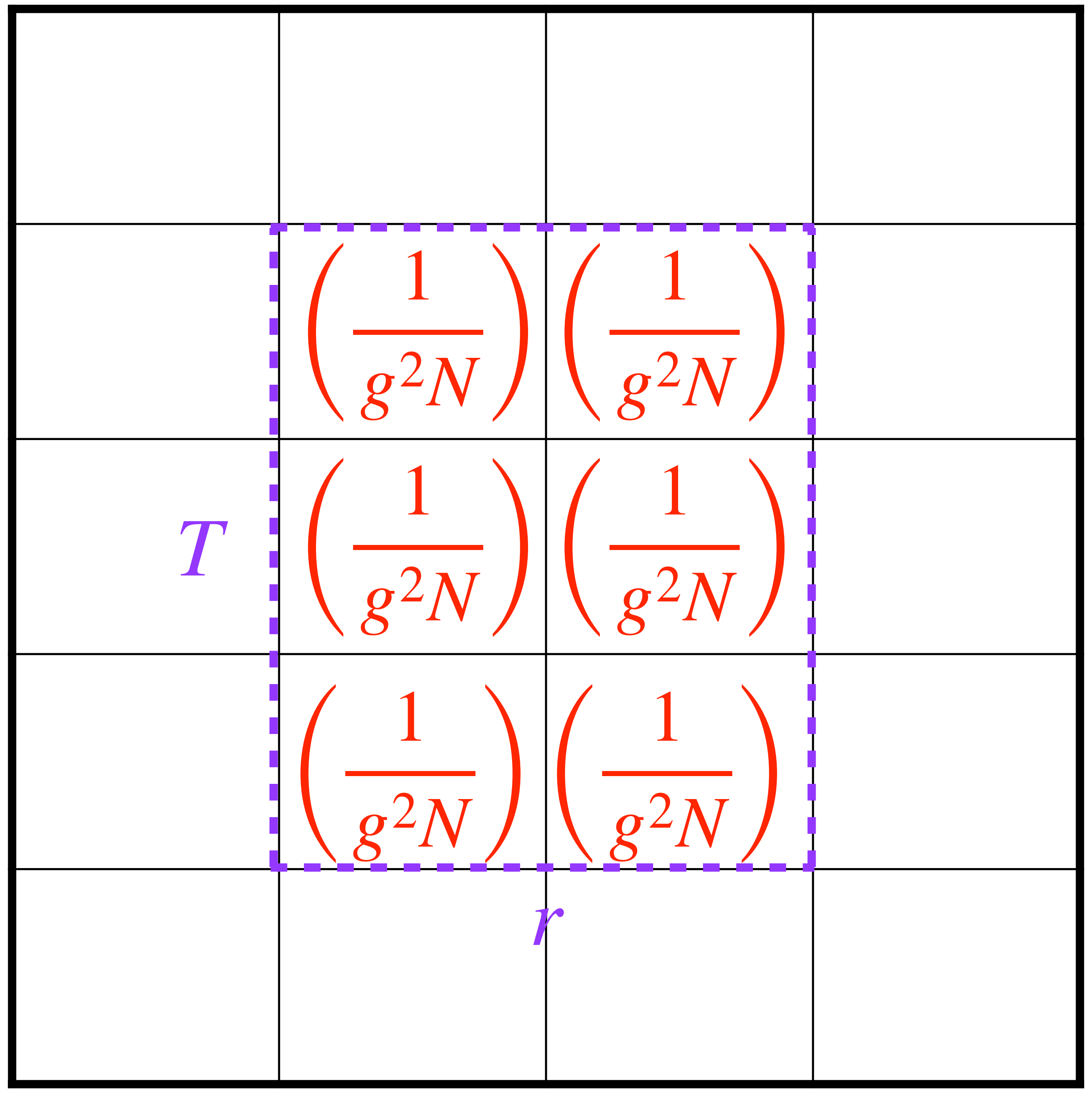
$$= Ne^{-rT\log(g^2N)}$$

Namely, the potential $V(r) = r\log(g^2N)$ shows a linear fn. of r

- In large g, the confinement occurs and its string tension is

$$\sigma = \frac{1}{a^2}\log(g^2N)$$

Strong coupling expansion for the plaquette



- Plaquette (energy density) is 1x1 Wilson loop

$$\langle W(r \times T)\rangle = N\left(\frac{1}{g^2N}\right) = \frac{\beta}{6},\ \beta \equiv 2N/g^2$$

- Here, we drop the normalization of trace (1/3 for SU(3)) and the leading term of 1

$$S_G = \frac{1}{g^2}\sum_n \sum_{\mu\neq\nu} \mathrm{tr}[U_{n,\mu}U_{n+\hat{\mu},\nu}U^\dagger_{n+\hat{\nu},\mu}U^\dagger_{n,\nu}] = \frac{1}{g^2}\sum_{\square}\mathrm{tr}(1-\frac{1}{3}\Re\mathrm{Tr}U_{\square})$$

- In the strong coupling regime,

$$\langle P\rangle = 1 - \frac{\beta}{18} + \cdots$$

Weak coupling expansion

- The partition fn. $Z = \int [dU] e^{-S_G}$

$$S_G = \frac{1}{g^2} \sum_n \sum_{\mu \neq \nu} \mathrm{tr}[U_{n,\mu} U_{n+\hat{\mu},\nu} U^\dagger_{n+\hat{\nu},\mu} U^\dagger_{n,\nu}] = \frac{1}{g^2} \sum_{\Box} \mathrm{tr}(1 - \frac{1}{3} \Re \mathrm{Tr} U_{\Box})$$

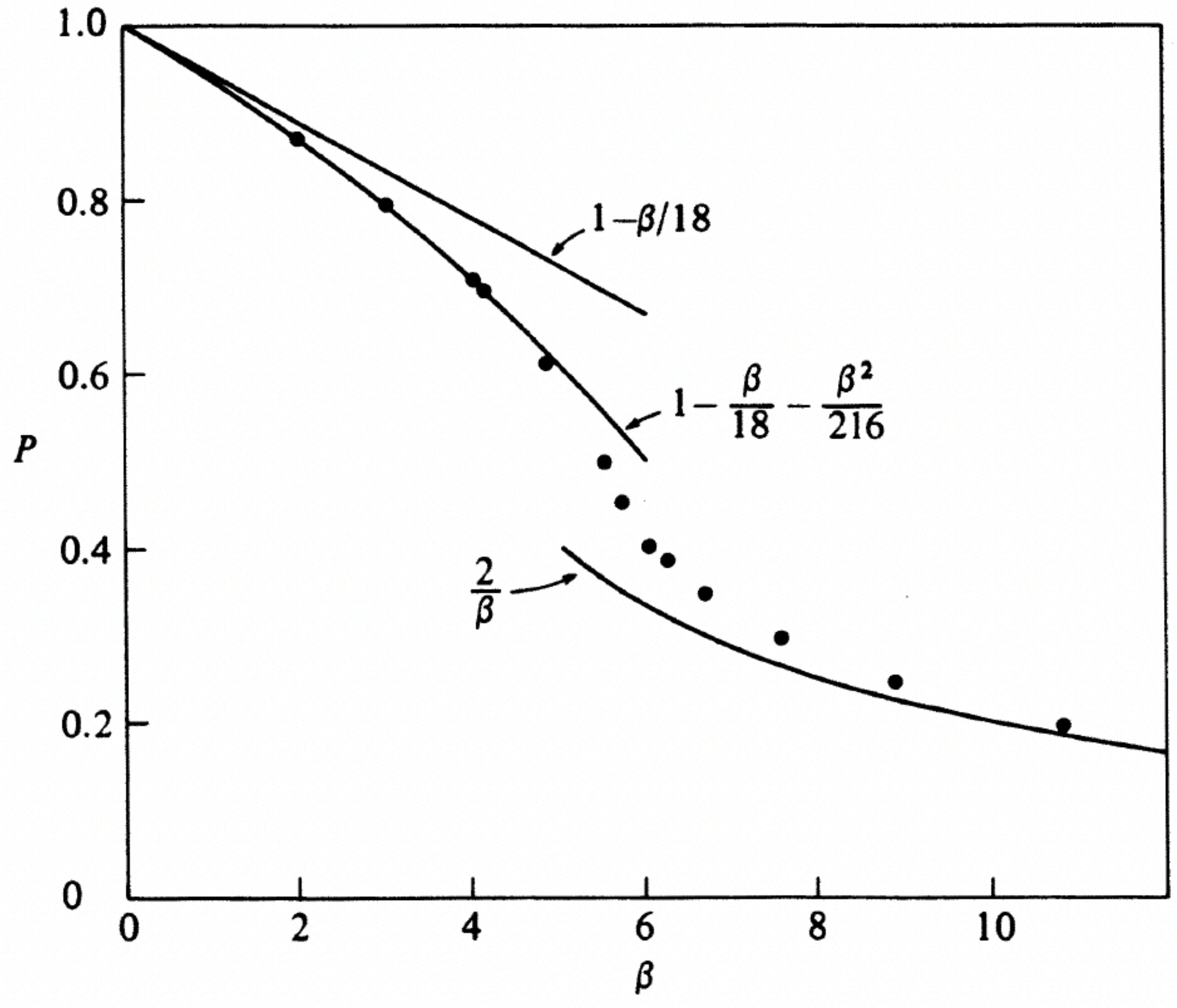
$U_{\Box}$ is plaquette op.

- In small g, $U_{\Box} \approx 1$ is dominated

- The perturbation theory around this saddle point gives $\langle P \rangle = \frac{2}{\beta} + \cdots$

cf.) M.Creutz's textbook, (open access) chapter 11

Is lattice theory valid in all coupling regime?



M.Creutz, Textbook

- The results obtained by some expansion are not valid for all coupling regime
- Middle coupling regime is difficult to analysis
- Lattice numerical results connect both coupling regimes smoothly
- Looks valid for all coupling regime

String tension (of the lattice theory)

Monte Carlo, SU(2) gauge, 10^4 lattice
M.Creutz, PRD21 (1980) 2308

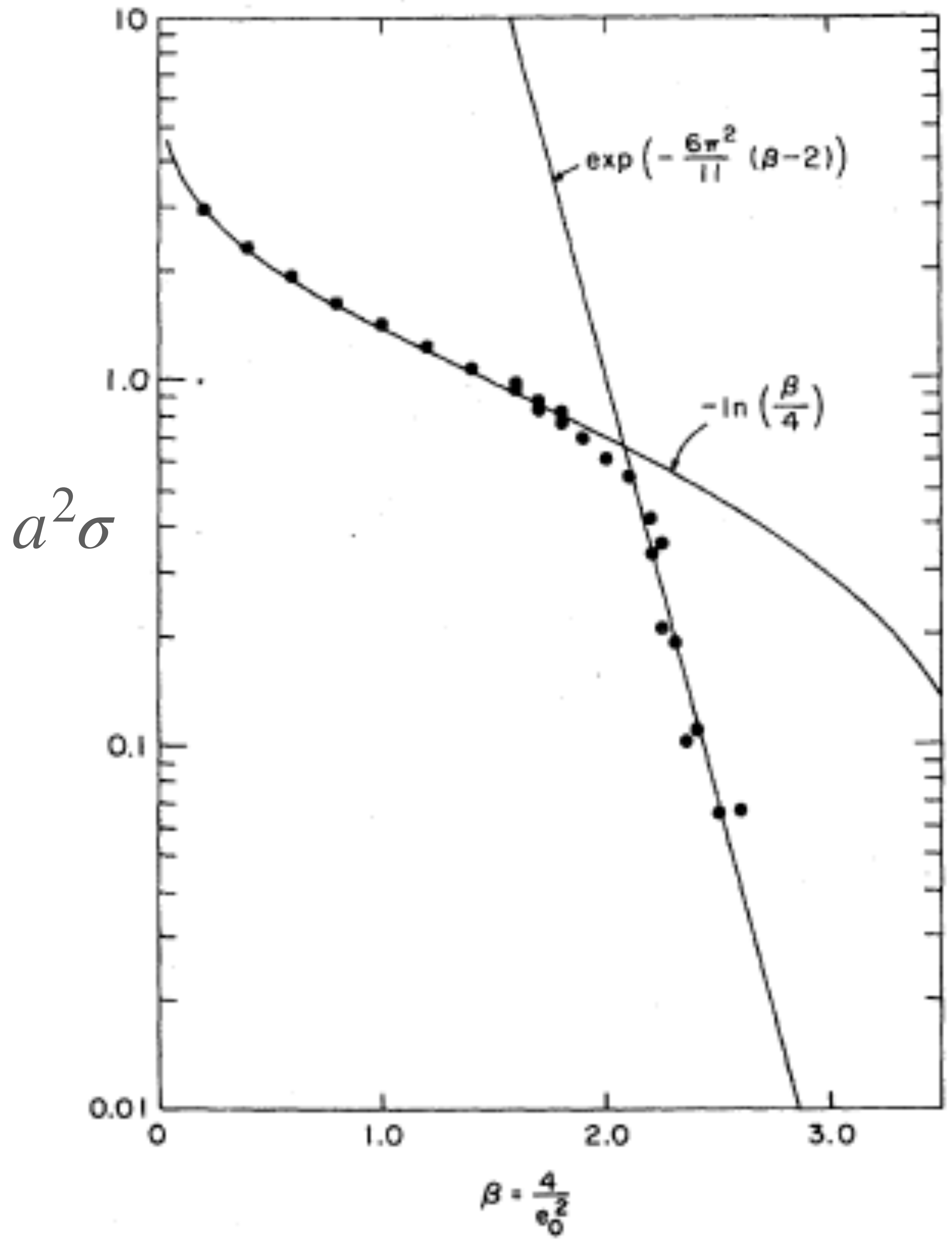


FIG. 6. The cutoff squared times the string tension as a function of β. The solid lines are the strong- and weak-coupling limits.

- Again the Lattice numerical result connect both coupling regimes smoothly
- In strong coupling, it corresponds to the confinement area law
- In weak coupling, the perturbative theory is valid
- After calculate $\langle \mathcal{O} \rangle$ in strong coupling regime, then taking a weak coupling limit looks possible!!
  (From lattice model calculation, we can obtain $\langle \mathcal{O} \rangle$ of QCD in the continuum spacetime)

More about the continuum limit

- In non-abelian gauge theory, the beta fn. of coupling const.

$$\beta(g) = \mu \frac{dg}{d\mu} = -b_0 g^3 - b_1 g^5 + \cdots \qquad \text{(asymptotic free)}$$

- At UV cutoff ($\mu = 1/a$), $g = g_0$: (lattice) bare coupling constant

  At an IR scale $\mu = \Lambda$ (Lambda scale), $g = \infty$

$$\int_{1/a}^{\Lambda} \frac{d\mu}{\mu} = -\frac{1}{2b_0} \int_{g_0^2}^{\infty} \frac{dg^2}{g^4(1 + \frac{b_1}{b_0} g^2)} \Rightarrow \Lambda a = (b_0 g_0^2)^{-b_1/(2b_0^2)} e^{-1/(2b_0 g_0^2)}$$

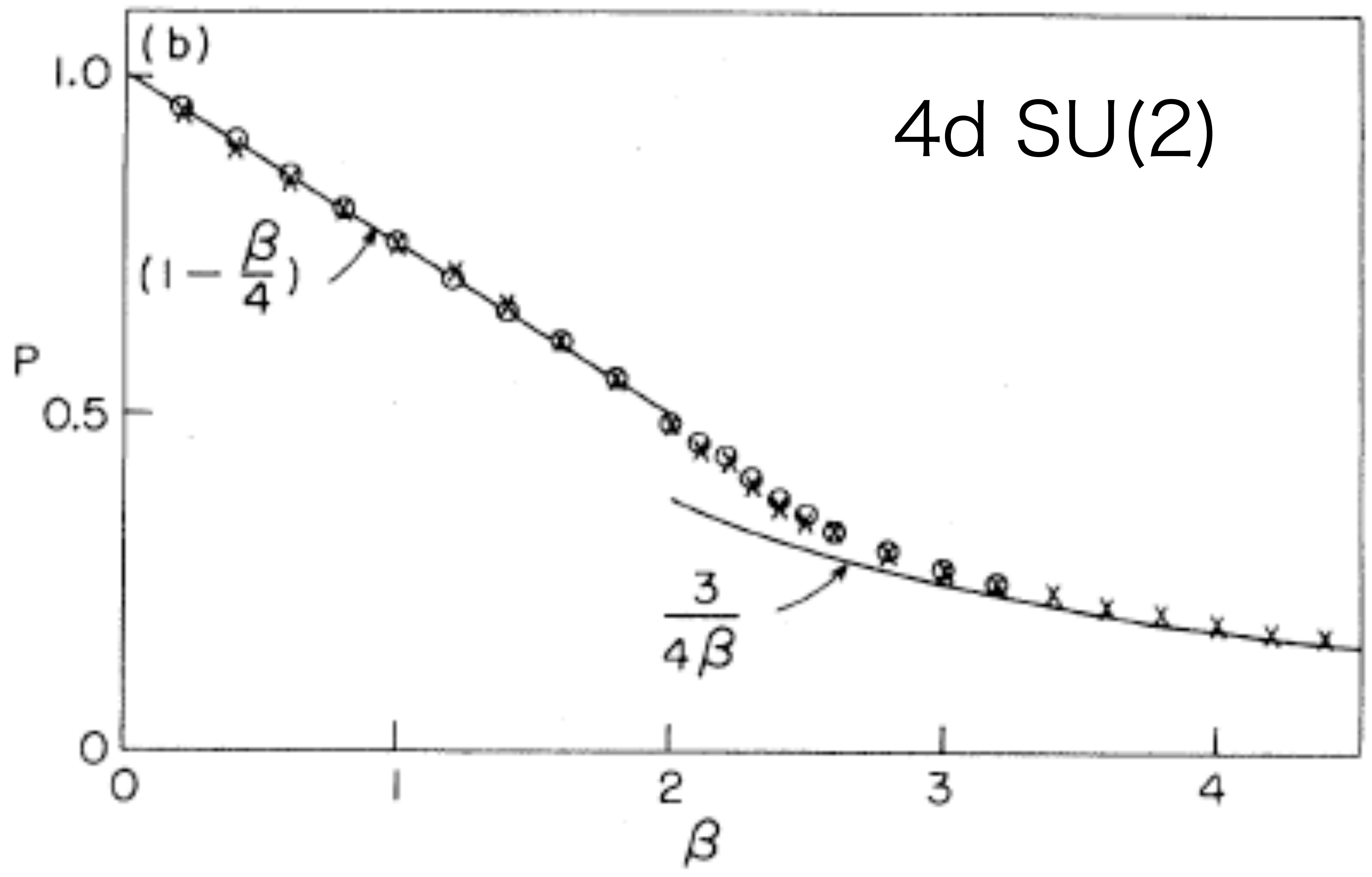
- continuum limit ($a \to 0$) corresponds to the weak coupling limit ($g_0^2 \to 0$)

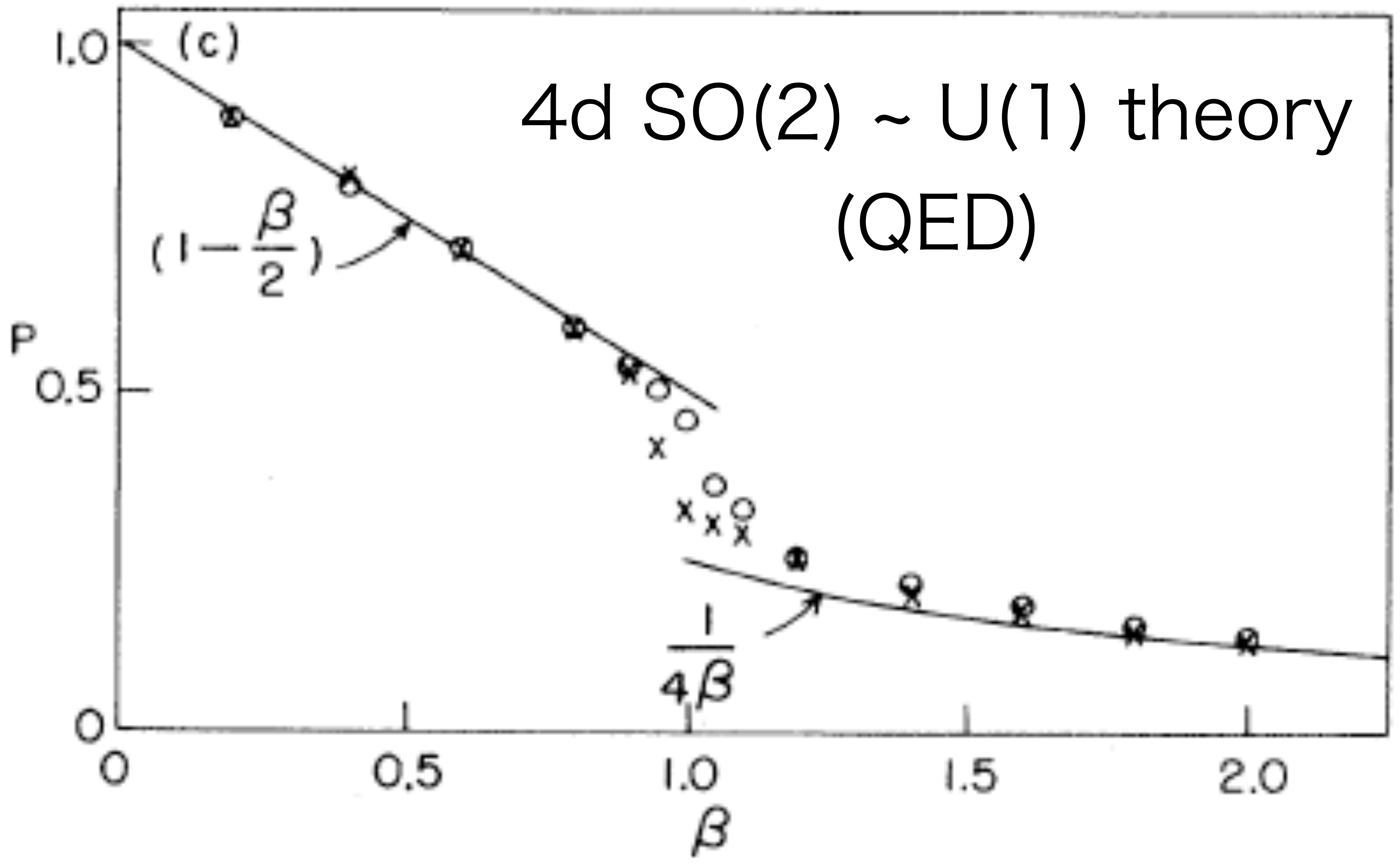
- If there is no phase transition from $g_0^2 = 0$ to $g_0^2 = \infty$, then the confinement occurs even in the continuum theory

- Otherwise (there is phase transition), the lattice model cannot connect to the continuum theory. We cannot say anything about the continuum theory

4d U(1), 5d SU(2) cases

Michael Creutz (1979)

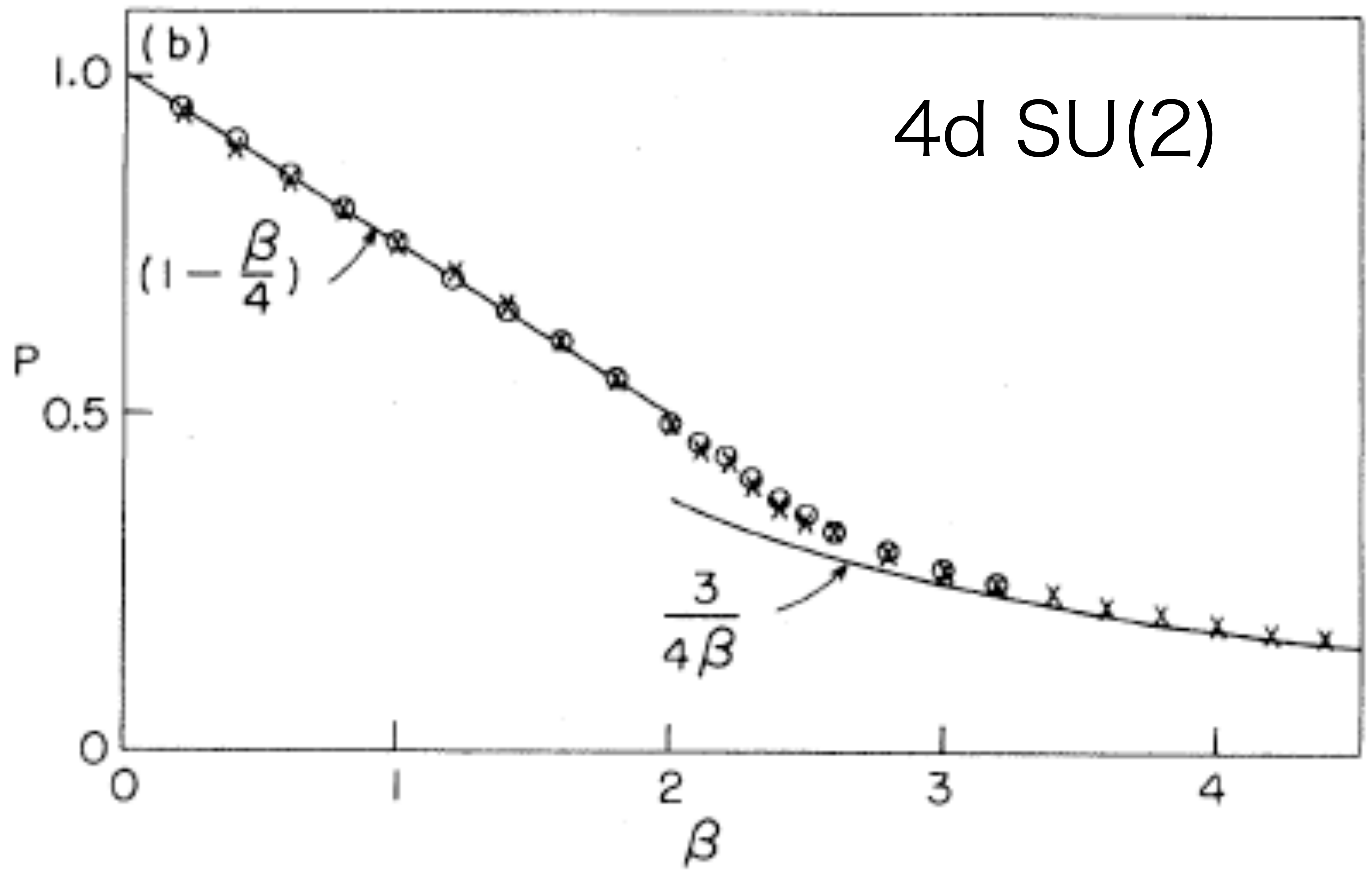


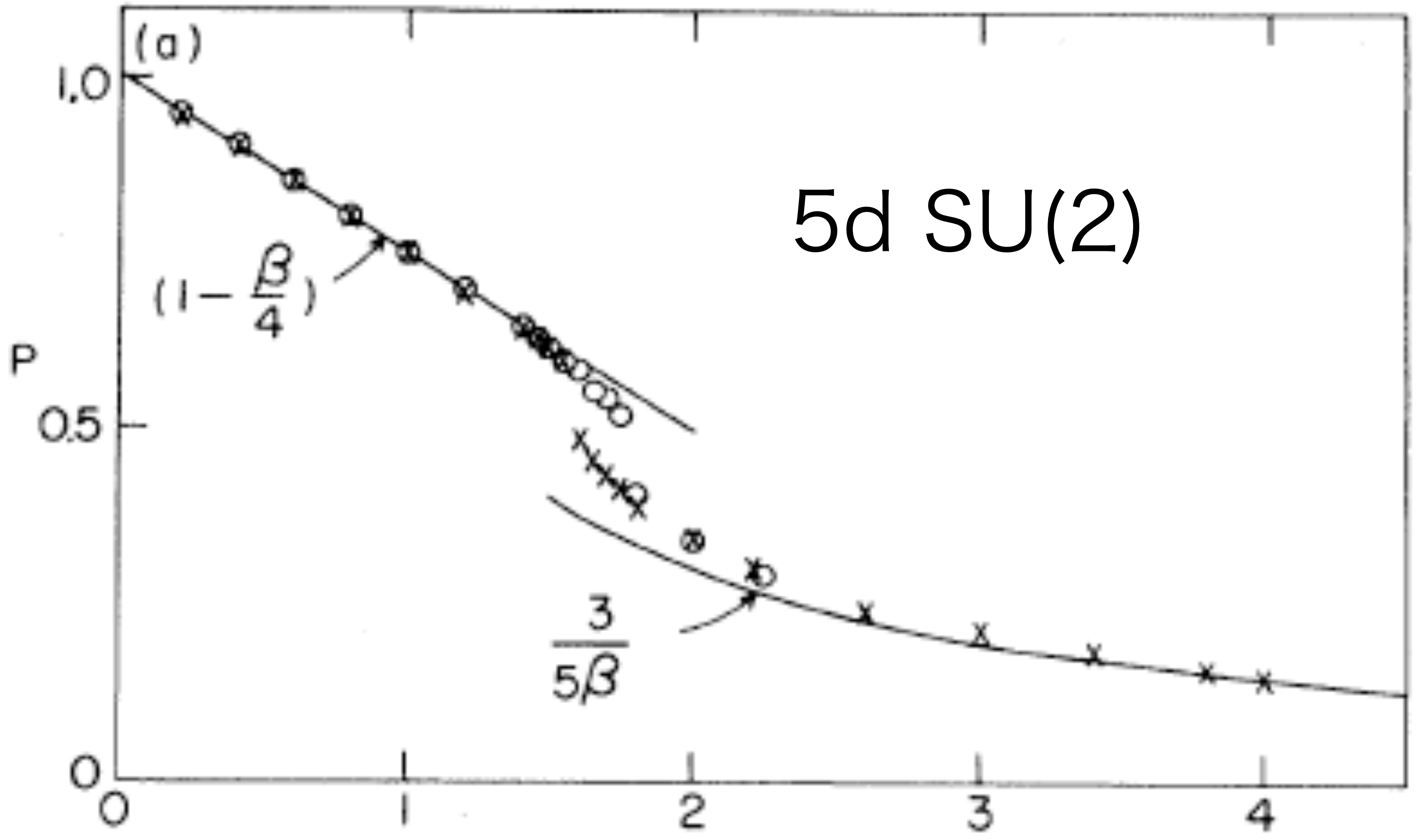


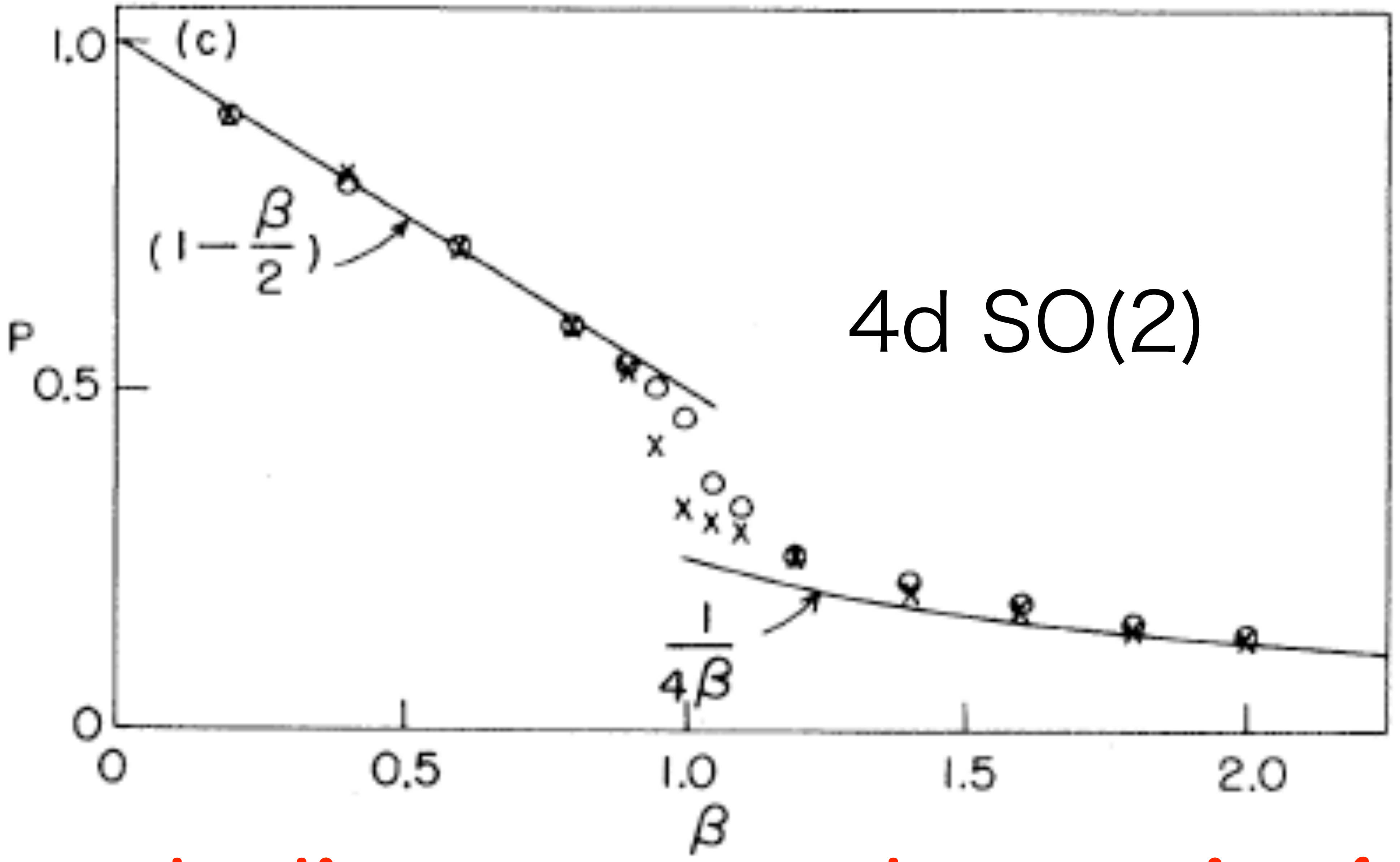
plaquette in 4d SU(2) smoothly connects between weak and strong coupling region
But, there is1st order phase transition 4d SO(2)~U(1), which has a Landau pole.
The ill-defined theory as a quantum field theory (nonperturbative sense),
we cannot take a continuum limit at least from the plaquette gauge action.

4d U(1), 5d SU(2) cases

Michael Creutz (1979)







The 1st order phase transition emerges in 5d SU(2) as like 4d U(1) theory.

It suggests the critical dim. of non-abelian gauge theory is 4 ?

From Yang-Mills to QCD w/ dynamical fermion

- QCD Lagrangian: $\mathscr{L} = -\frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} + \bar{\psi}(i\gamma_\mu D_\mu + m)\psi$

  We want to know $\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi \mathcal{O} e^{-S[\phi]}$

- Difficult to deal with the fermion dof. (Grassmann number) on computers

- In the partition fn. : $Z = \int \mathscr{D}A_\mu \mathscr{D}\bar{\psi}\mathscr{D}\psi \exp[-S_G(A_\mu) + \int d^4x \bar{\psi}(i\gamma_\mu D_\mu(A_\mu) + m)\psi(x)]$

  Perform the Gaussian integral of ψ and $\bar{\psi}$

  $Z = \int \mathscr{D}A_\mu \sqrt{\det[i\gamma_\mu D_\mu(A_\mu) + m]} \exp[-S_G(A_\mu)]$ written only by gauge fields!

Short summary, so far

- Lattice regularization is gauge invariant one.
  It is only known the gauge invariant and nonperturbative formula.

- Quark confinement can be shown using the strong coupling expansion analytically

- In weak coupling regime, the lattice action converges to QCD action

- Lattice numerical results correctly reproduce both weak and strong coupling expansions, and smoothly connect them

- From lattice model calculation, we can obtain $\langle \mathcal{O} \rangle$ of actual QCD

3. Introduction to numerical calculation

Lattice QCD and supercomputer usage

- Interesting dynamics of QCD
  confinement
  chiral symmetry breaking
  hadron spectrum
  instanton effect
  hadron scattering/potential
  thermodynamic quantities

- 40% of supercomputer resources are used!
  (In Fugaku case, around 25%)

Slide of Lena Funcke @ Lattice2022

Supercomputer usage for different fields (INCITE 2019)

→ **Lattice QCD: ~ 40%**

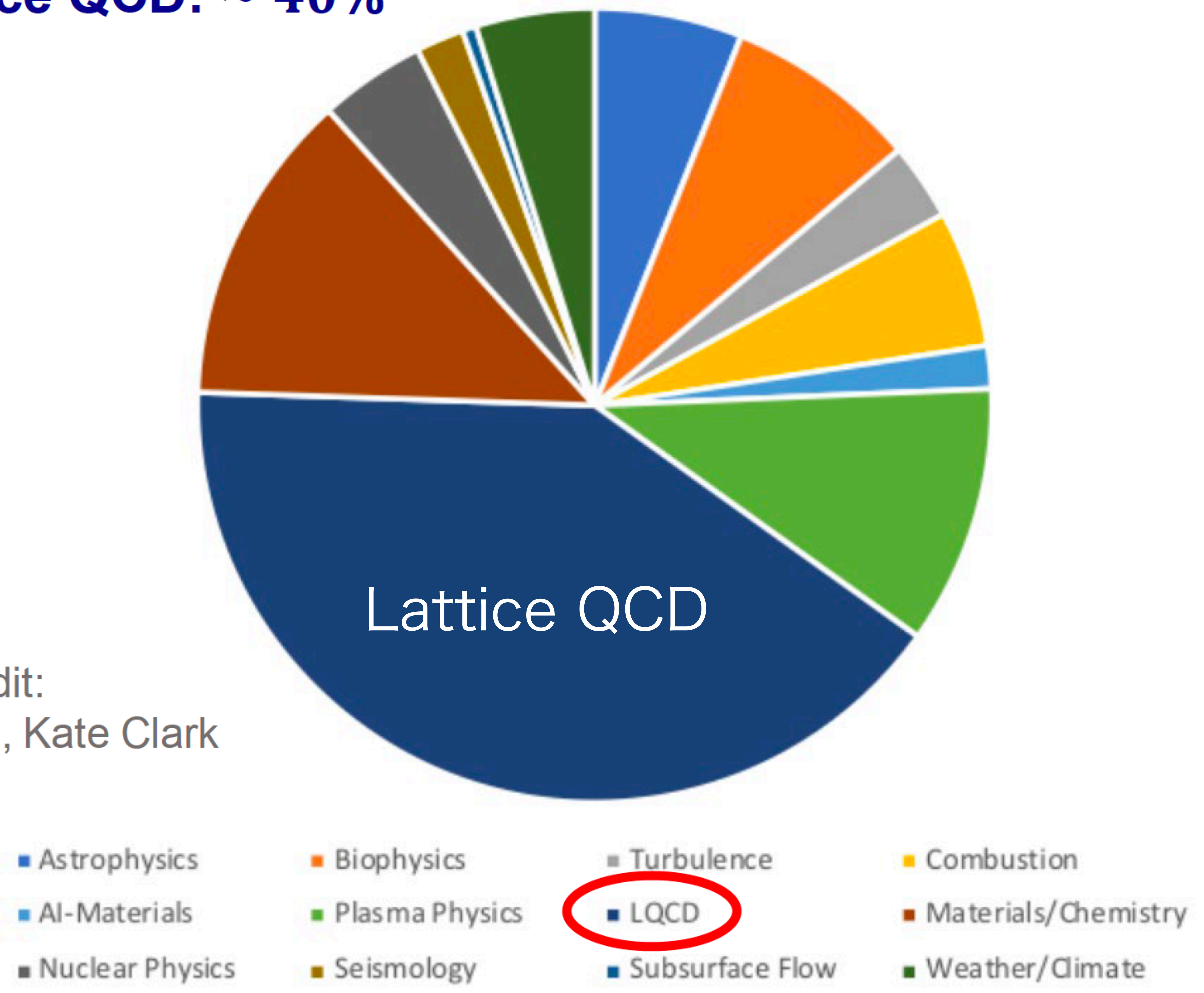


Figure credit:
Jack Wells, Kate Clark

Supercomputer Fugaku @ RIKEN in Kobe

Fugaku = 富岳 = Mt. Fuji

- first place in four global supercomputer rankings for 2 years
  「TOP500」「HPCG」「HPL-AI」「Graph500」

- performance：400 PFlops
  4×10^{17} times floating-point operations per second
  Total memory：
  4.85PiB(ペビバイト, 1PiB=2^{50}B)

In this lecture, I sometimes assume a recent work on HAL QCD collaboration (arXiv:2406.16665), which has been done by Fugaku.

Calculation strategy of Lattice QCD

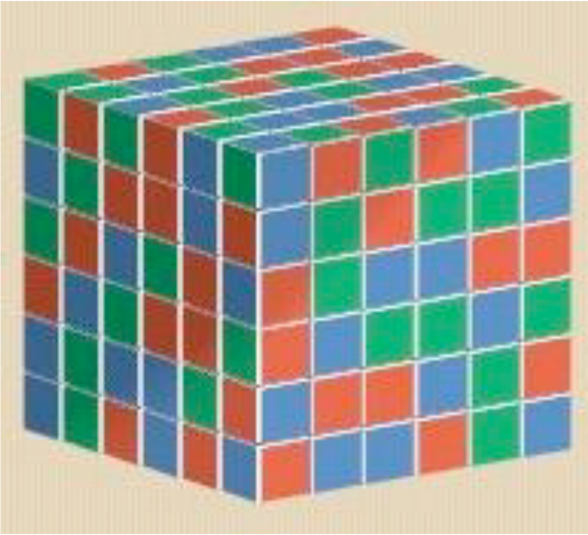
- We want to calculate the value: $\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \mathcal{O} e^{-S[\phi]}$
- Main message here:
  Not perform an actual integration!!
  Estimate the value of $\langle \mathcal{O} \rangle$!
- For instance, the work on HAL QCD paper, we perform the calculation corresponding to "6×10^9 dof of integral" @ Fugaku supercomputer

Calculation strategy of Lattice QCD

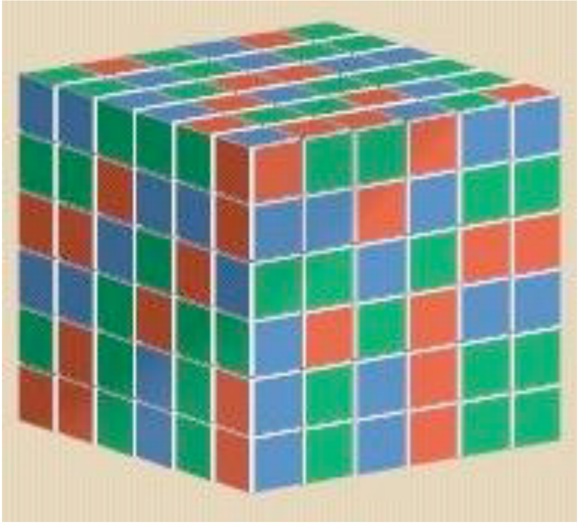
- We want to calculate the value: $\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi \mathcal{O} e^{-S[\phi]}$

- Step1 : Generate configuration samples

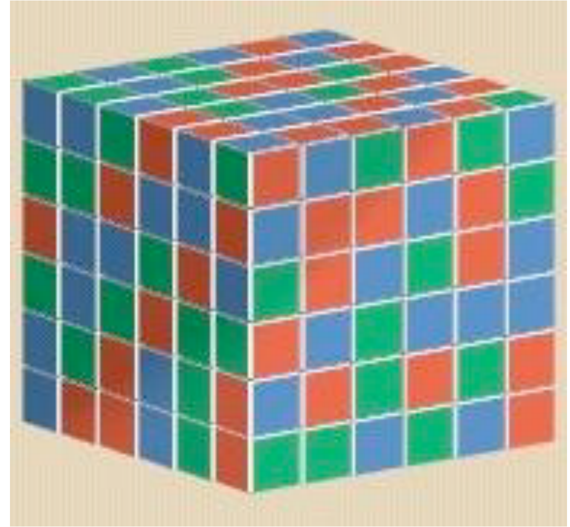
- Step2 : Measure the value of observable for each conf.



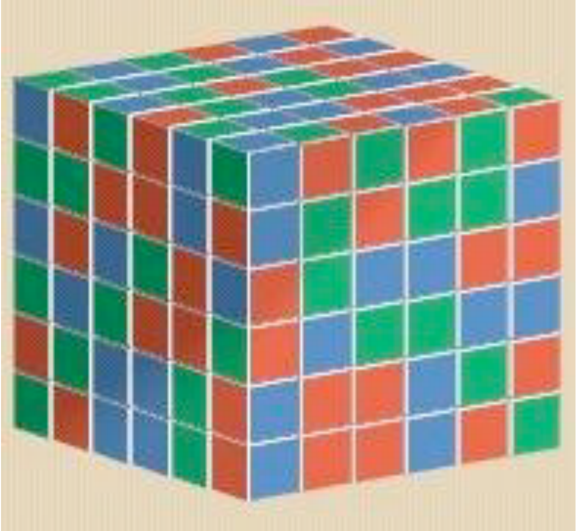
$\mathcal{O}_1$



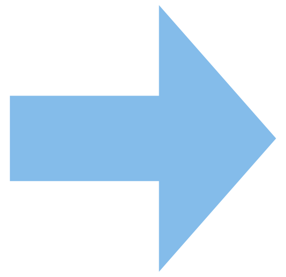
$\mathcal{O}_2$

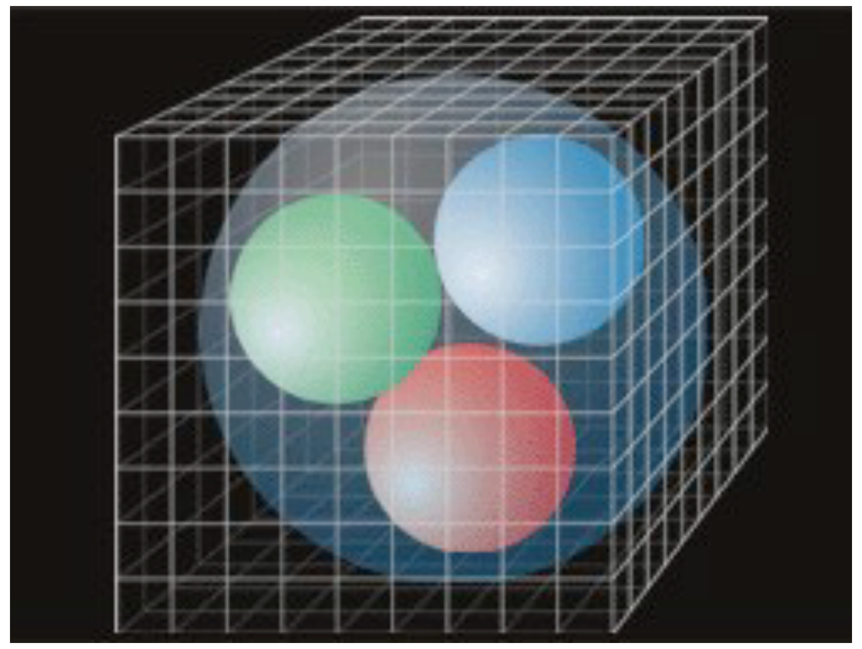


$\mathcal{O}_3$



$\mathcal{O}_N$





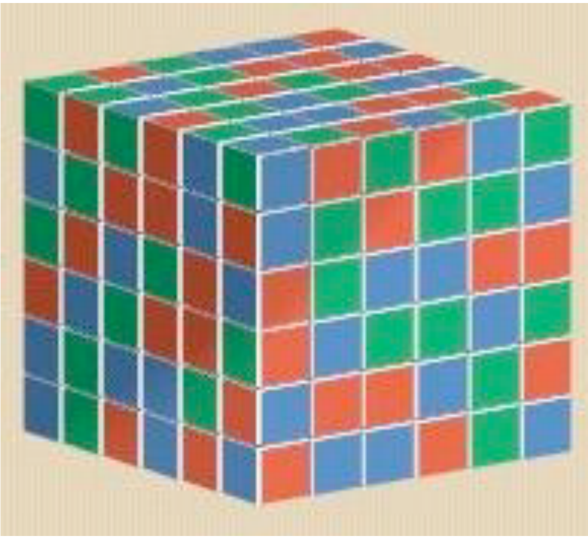
$$\langle O \rangle = \lim_{N\to\infty} \frac{1}{N}\sum_i^N O_i$$

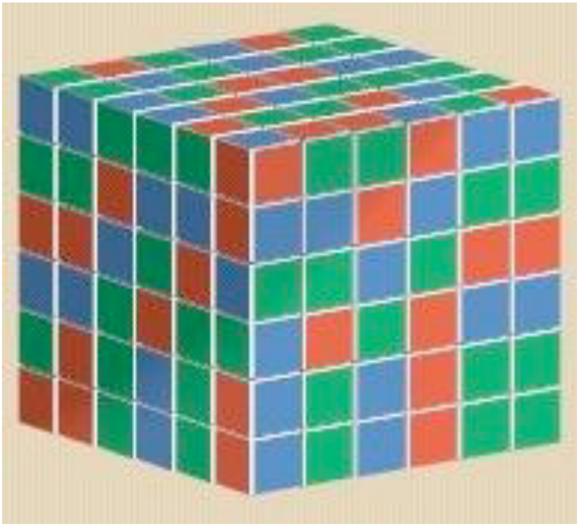
Calculation strategy of Lattice QCD

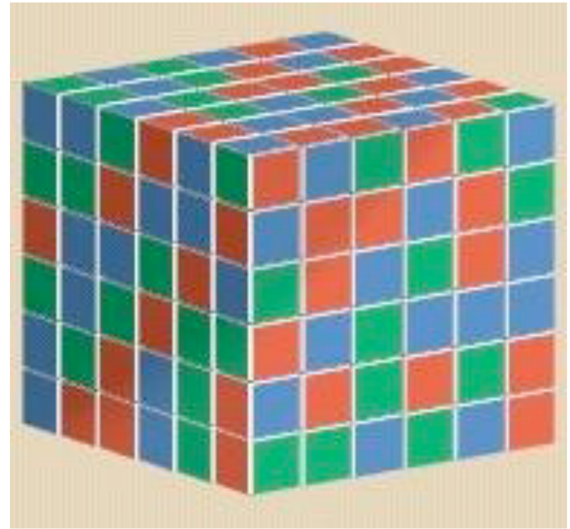
- We want to calculate the value: $\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \mathcal{O} e^{-S[\phi]}$

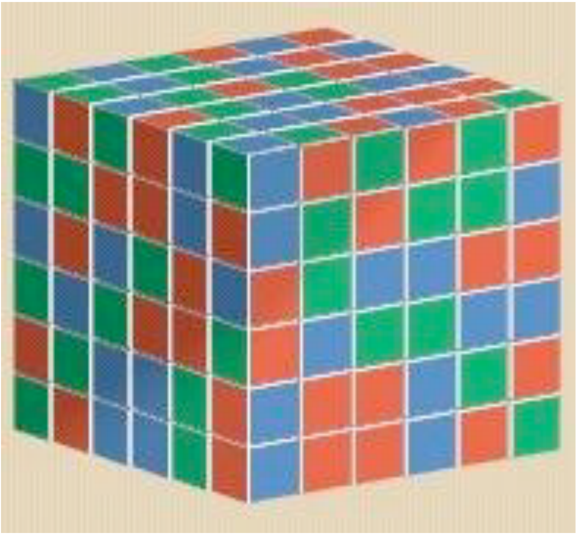
- Step1：Generate configuration samples
  High calculation cost. On HAL QCD paper, we need 1.5 years in total. We store the ensembles. In some cases, the ensembles are shared globally.

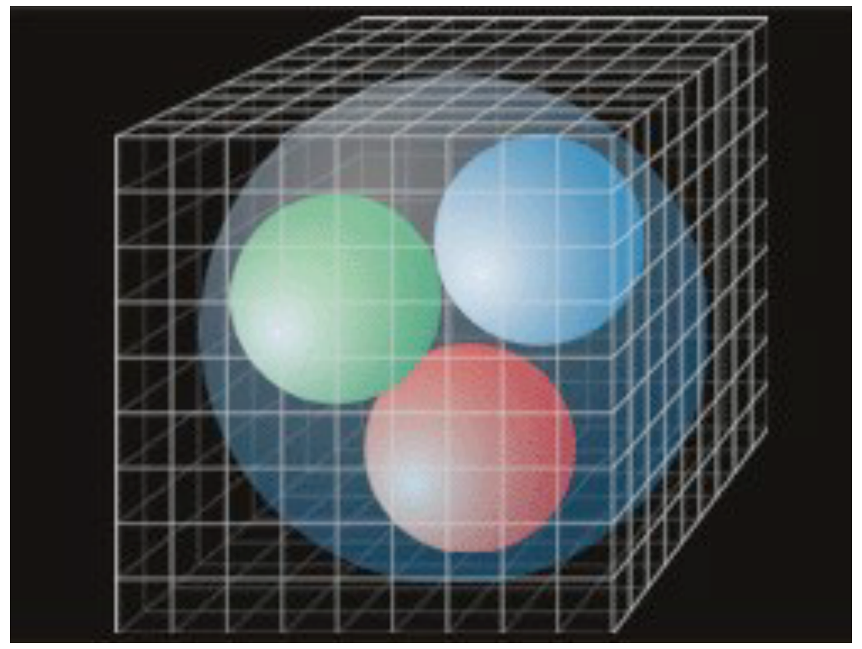
- Step2：Measure the value of observable for each conf.
  Cost depends on quantities. In nuclear force calculations, it needs much more time than Step1


$\mathcal{O}_1$


$\mathcal{O}_2$


$\mathcal{O}_3$


$\mathcal{O}_N$



$$\langle O \rangle = \lim_{N\to\infty} \frac{1}{N} \sum_i^N O_i$$

4. Configuration generation

Methodology of configuration generation

4-1. What is Monte Carlo method

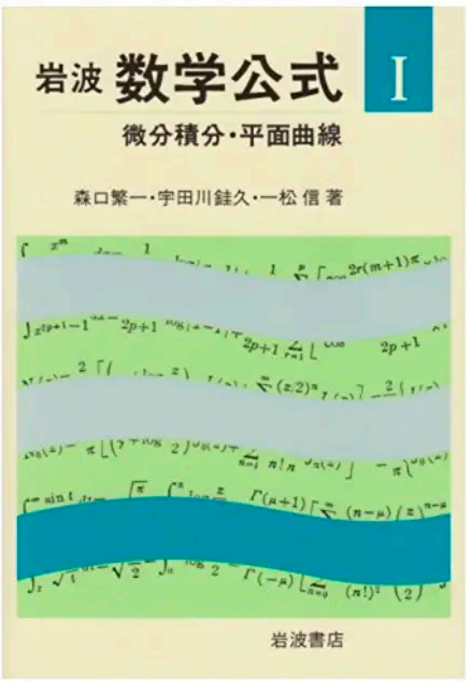
4-2. Importance sampling method

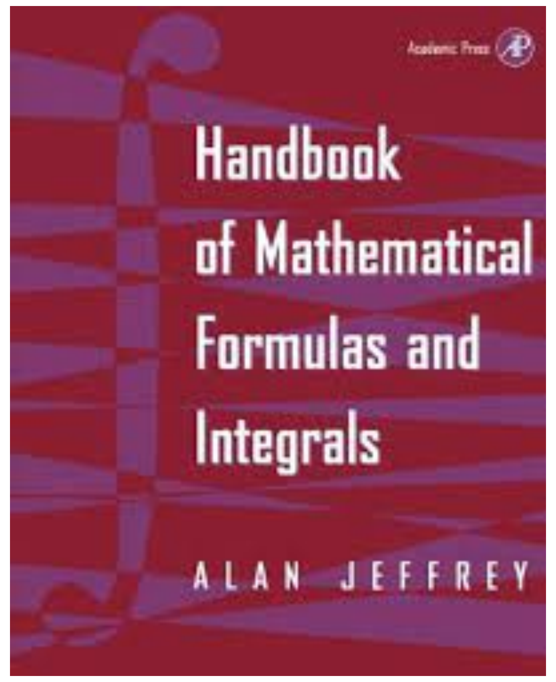
4-3. Algorithms and open codes

4-1. What is Monte Carlo method

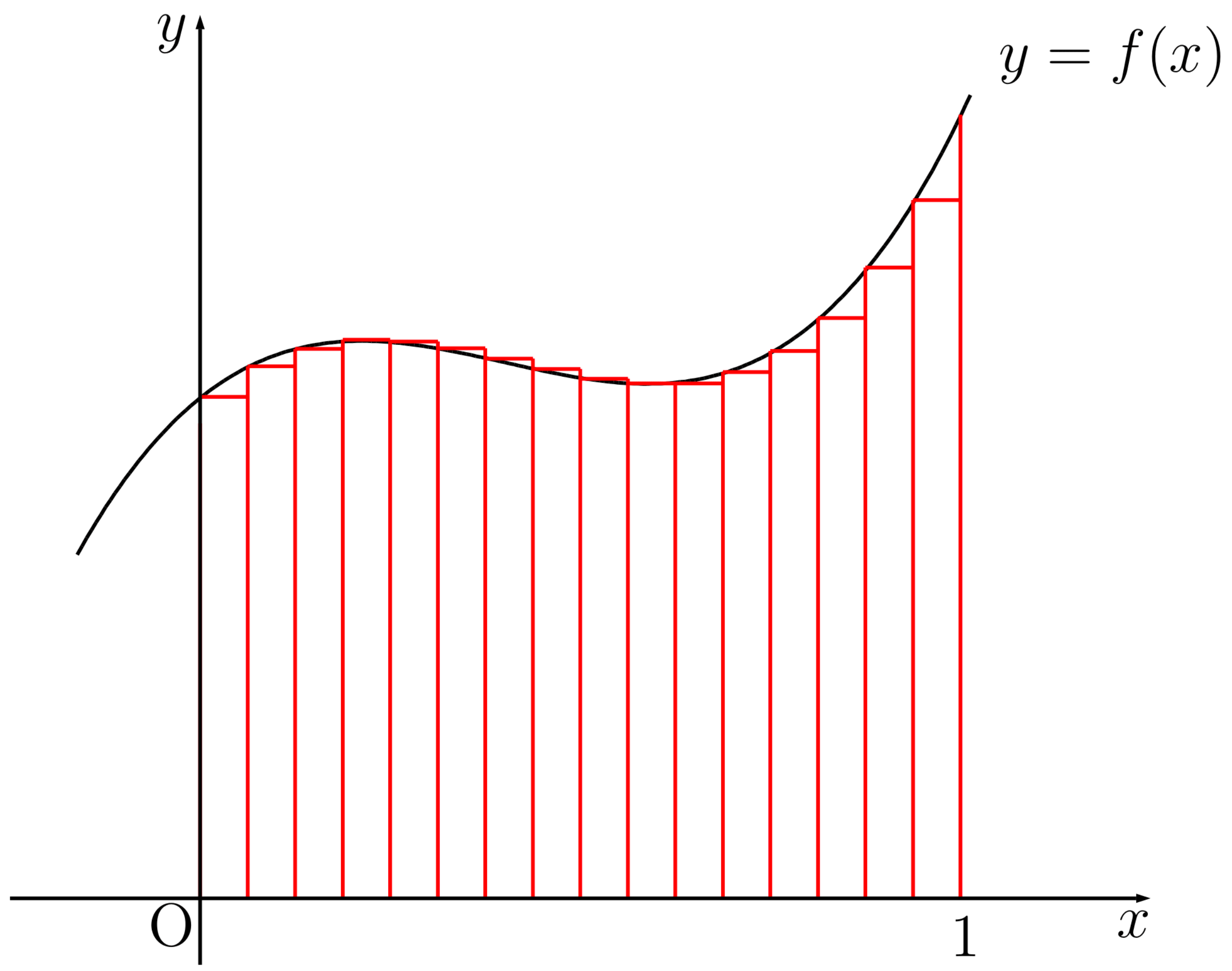
How to calculate integral

- See a library of integral formulas for typical fns. and apply them as needed





- Numerical integration approximated by rectangular



- Monte Carlo method
  (A method that humans cannot do)

Monte Carlo method of integration

Wikipedia

- Consider the area of quarter circle w/ radius 1

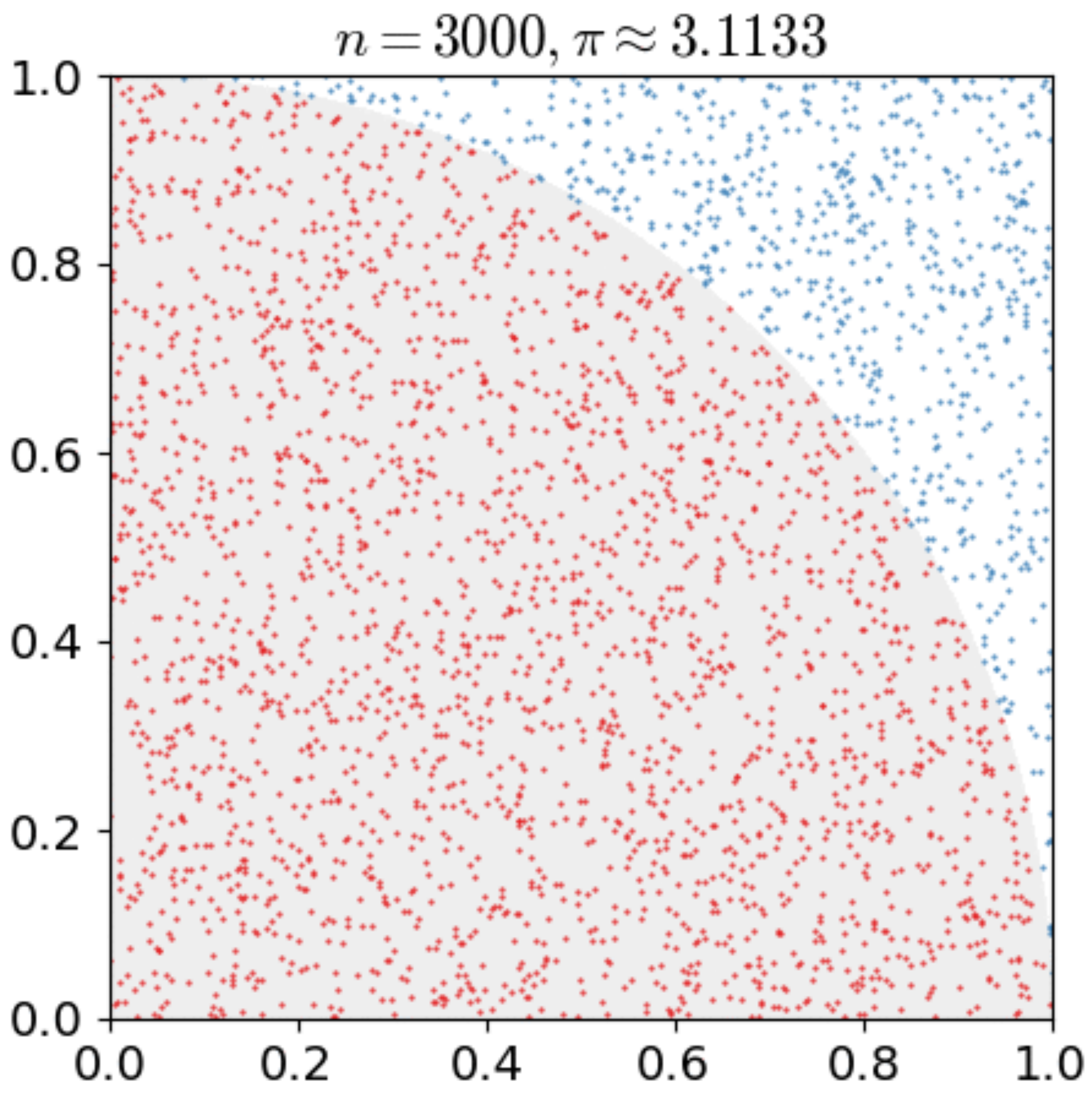
$$S = \int_0^1 \sqrt{1 - x^2}dx = \frac{\pi}{4}$$

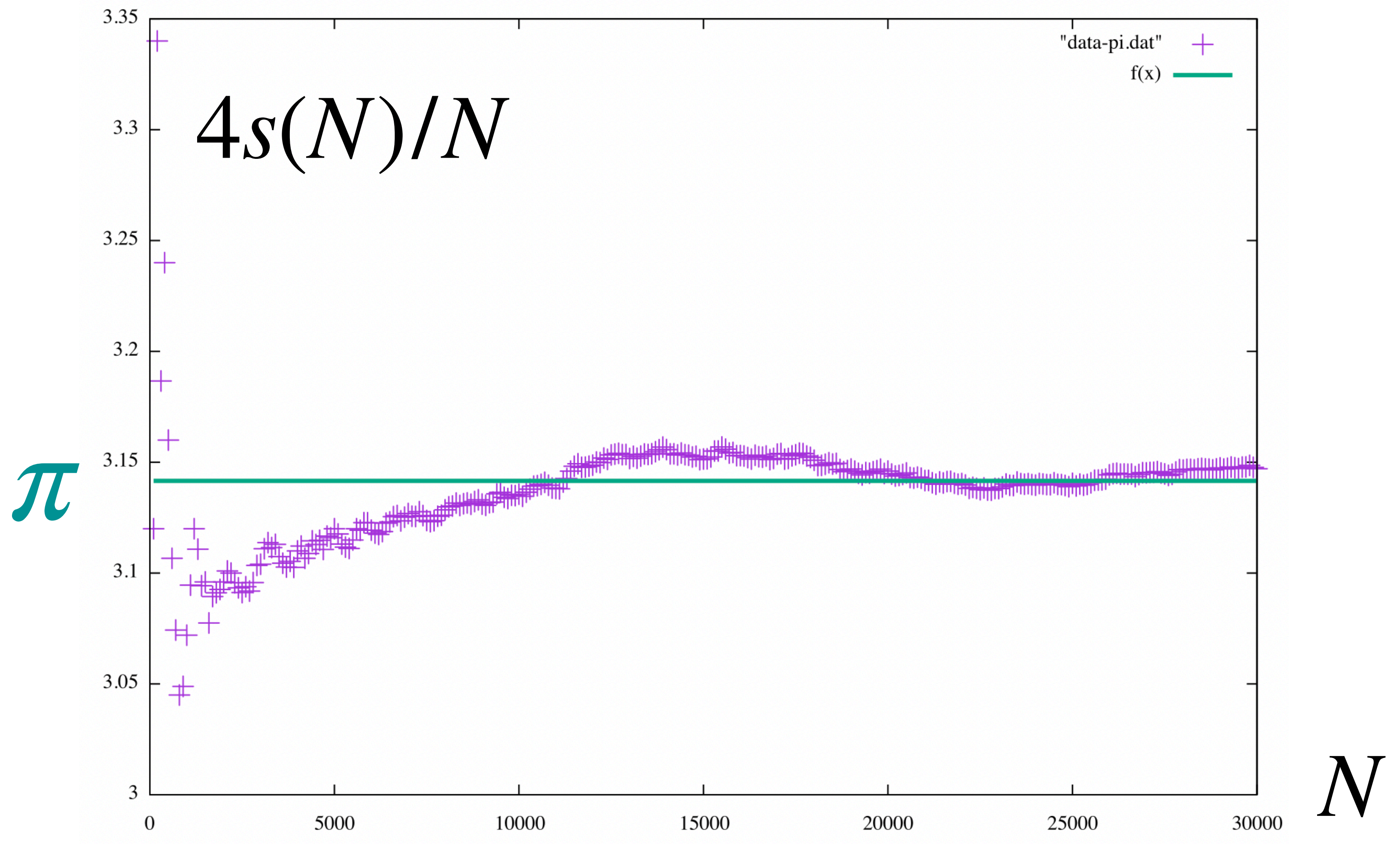
(1) Generate two uniform random numbers
w/ interval [0:1]

(2) Put a dot at (x_i, y_i)=(1st #, 2nd #)

(3) Repeat N-times, and count the data point ($s(N)$)
satisfying $x_i^2 + y_i^2 \leq 1$

(4) Area of quarter circle : $S = \lim_{N\to\infty} s(N)/N$





Monte Carlo method of integration

Wikipedia

- Estimate the integral

$$\int f(x)dx$$

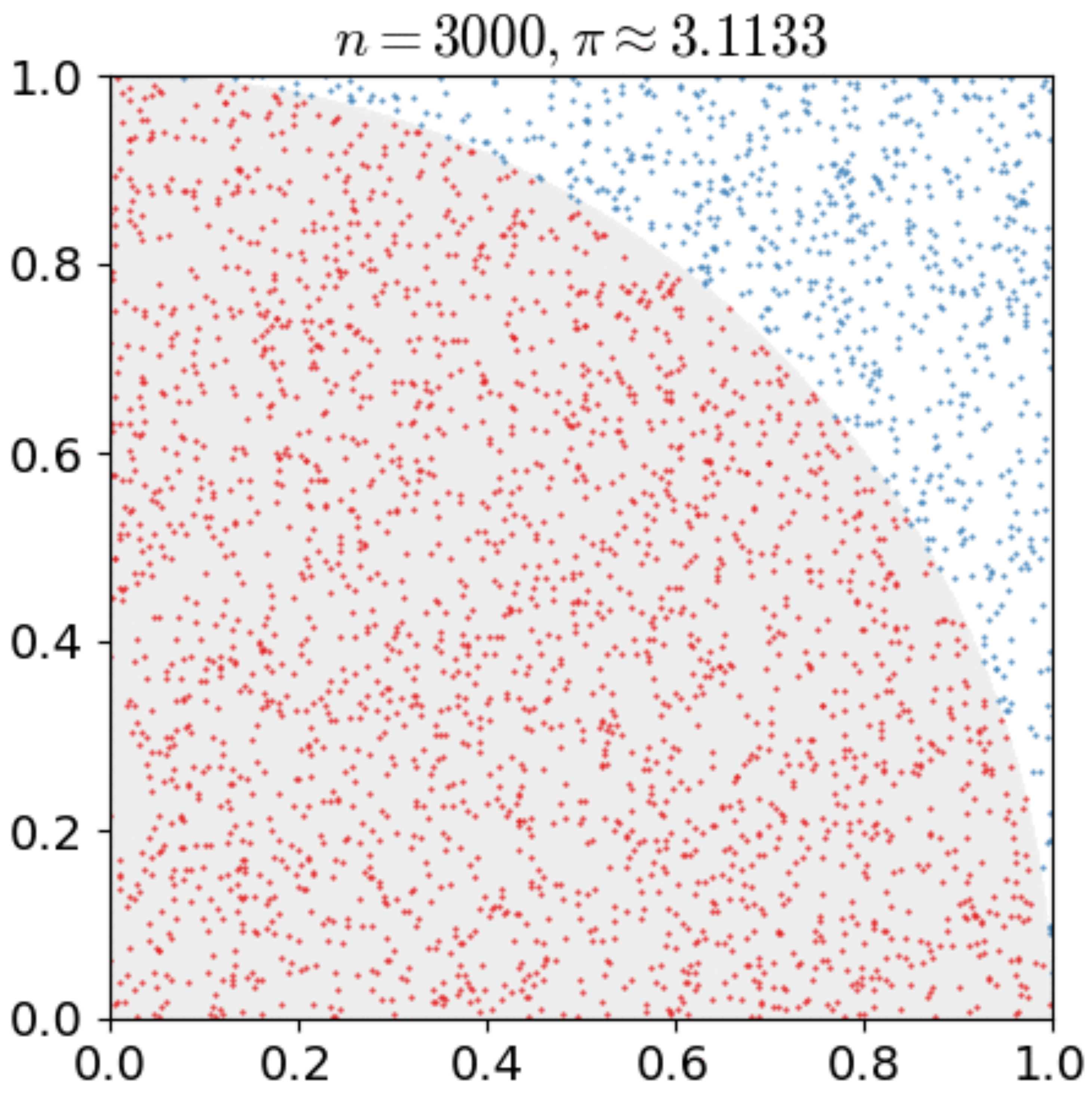
- (1) Generate random number (X_i)

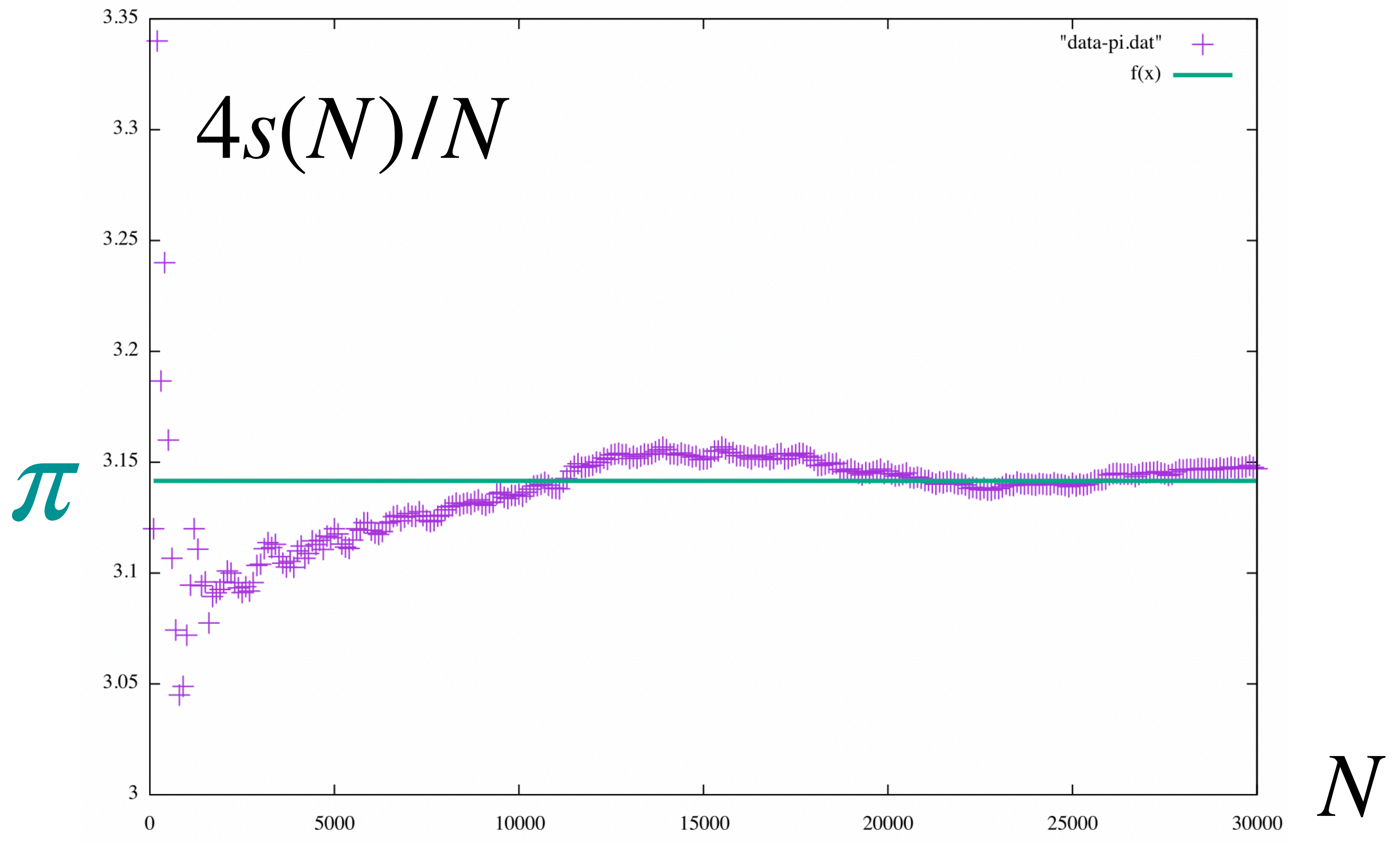
  (2) Using X_i, calculate f(X_i)

  (3) take an average $\frac{1}{N}\sum_i$ f(X_i)

  (4) the expectation value is given by

$$\langle f \rangle = \frac{1}{N}\sum_i f(X_i) + \mathcal{O}\left(\frac{1}{\sqrt{N}}\right)$$, so take $N \to \infty$!





Advantages of the Monte Carlo method

- Faster algorithm even for the d.o.f. increases

  multiple integral

  $$I = \int_0^1 dx_1 \int_0^1 dx_2 \cdots \int_0^1 dx_n f(x_1, \cdots, x_n)$$

  Numerical integration (区分求積法)
  suffer from "The curse of dimensionality"
  (exp. increasing of complexity)

  Using a set (N) of uniform random numbers w/ [0:1] for integral variables $x_1, \cdots, x_n$

  $(X_{i,j},\ i = 1,\cdots,n,\ j = 1,\cdots,N)$, we can estimate of I as

  $$I = \lim_{N\to\infty} \frac{1}{N} \sum_j f(X_{1,j}, \cdots, X_{n,j})$$

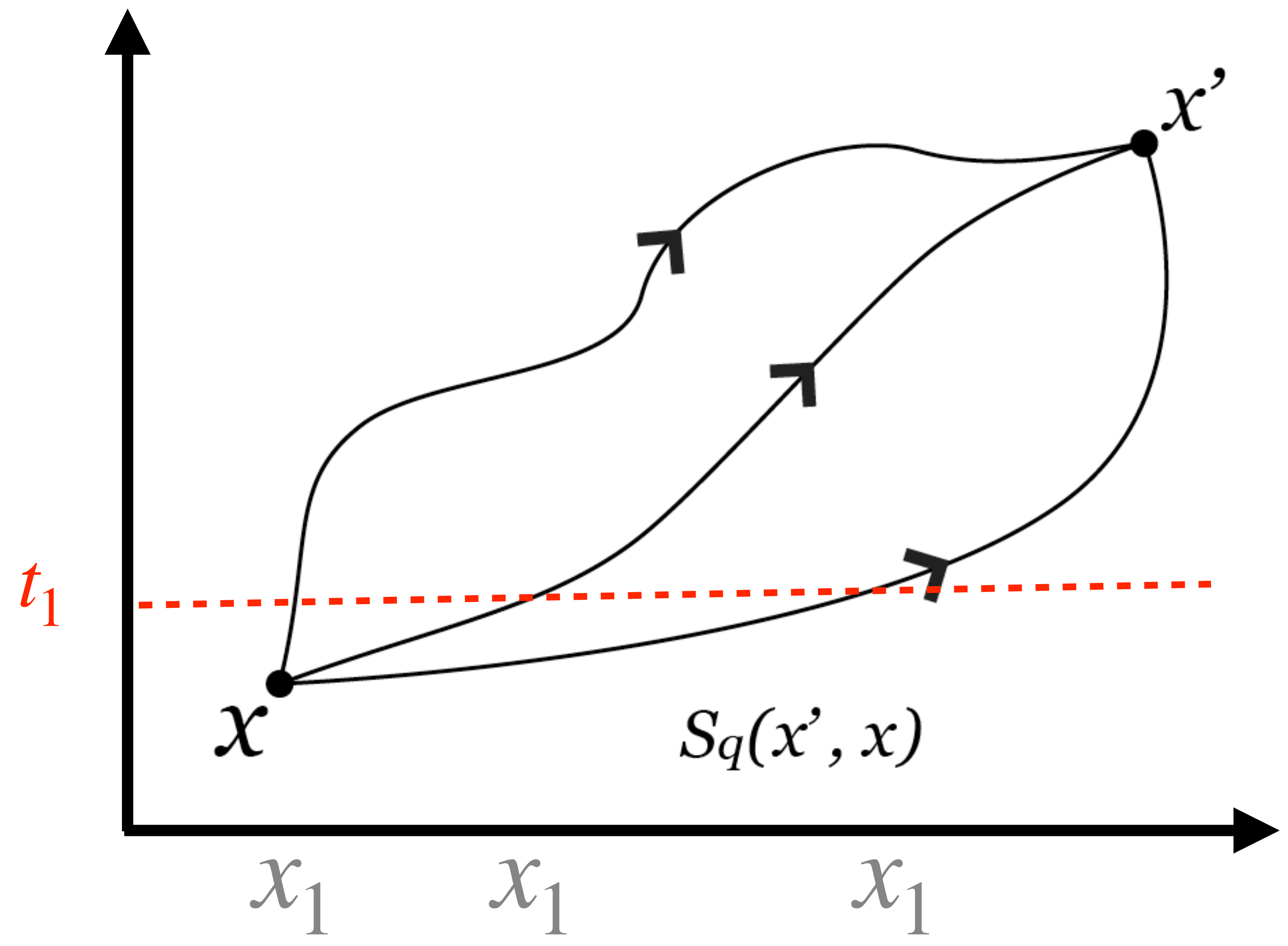
  Error from the true value is independent of dimensionality (n). It scales as $\mathcal{O}(1/\sqrt{N})$

- If you can generate uniform random numbers at fast, simply calculate the average value of the function f using the random numbers!

4-2. Importance sampling method

Configuration generation

- Now, we know that the Monte Carlo method must be useful.
  But using uniform number is not effective for physical system. We improve it.



- Our target: $\langle \mathcal{O} \rangle = \frac{1}{Z}\int D\phi \mathcal{O} e^{-S[\phi]}$ for QCD observables and QCD action

- Simple ex.) Path integral of propagation x to x' in quantum mechanics

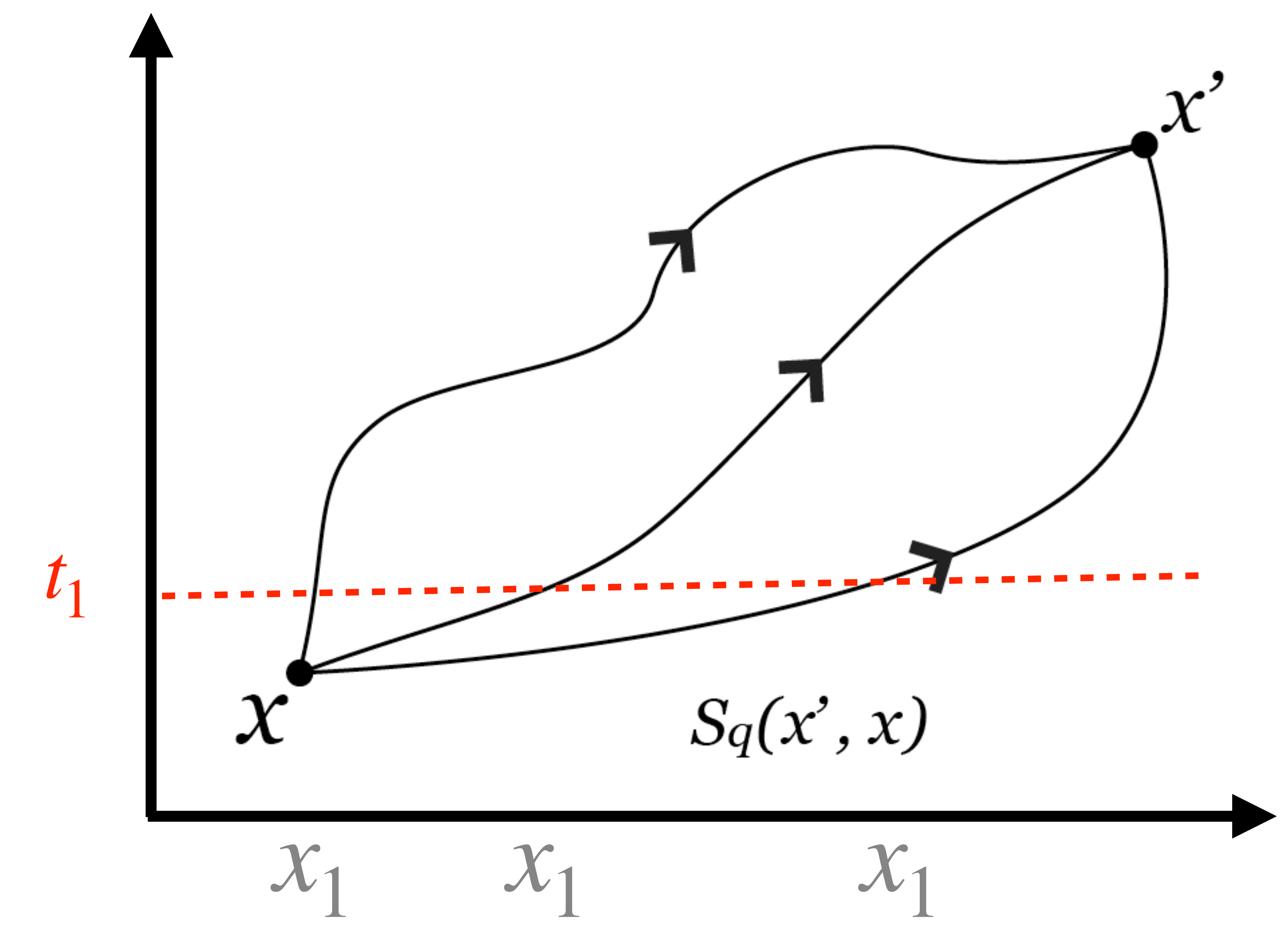
$$\langle x'(t) | x(0) \rangle = \int dx_1 dx_2 \cdots dx_N \langle x' | e^{-iH\Delta t} | x_N \rangle \cdots \langle x_2 | e^{-iH\Delta t} | x_1 \rangle \langle x_1 | e^{-iH\Delta t} | x \rangle$$

Monte Carlo methods in quantum theory

- To obtain

$$\langle x'(t)\,|\,x(0)\rangle = \int dx_1 dx_2 \cdots dx_N \langle x'\,|\,e^{-iH\Delta t}\,|\,x_N\rangle \cdots \langle x_1\,|\,e^{-iH\Delta t}\,|\,x\rangle$$

  we take a sum of all path contributions



- Easier paths and less-frequented paths depending on the potential

- Monte Carlo method using uniform random numbers is not effective, then change to importance sampling method (effectively collect easier paths)

Importance sampling method

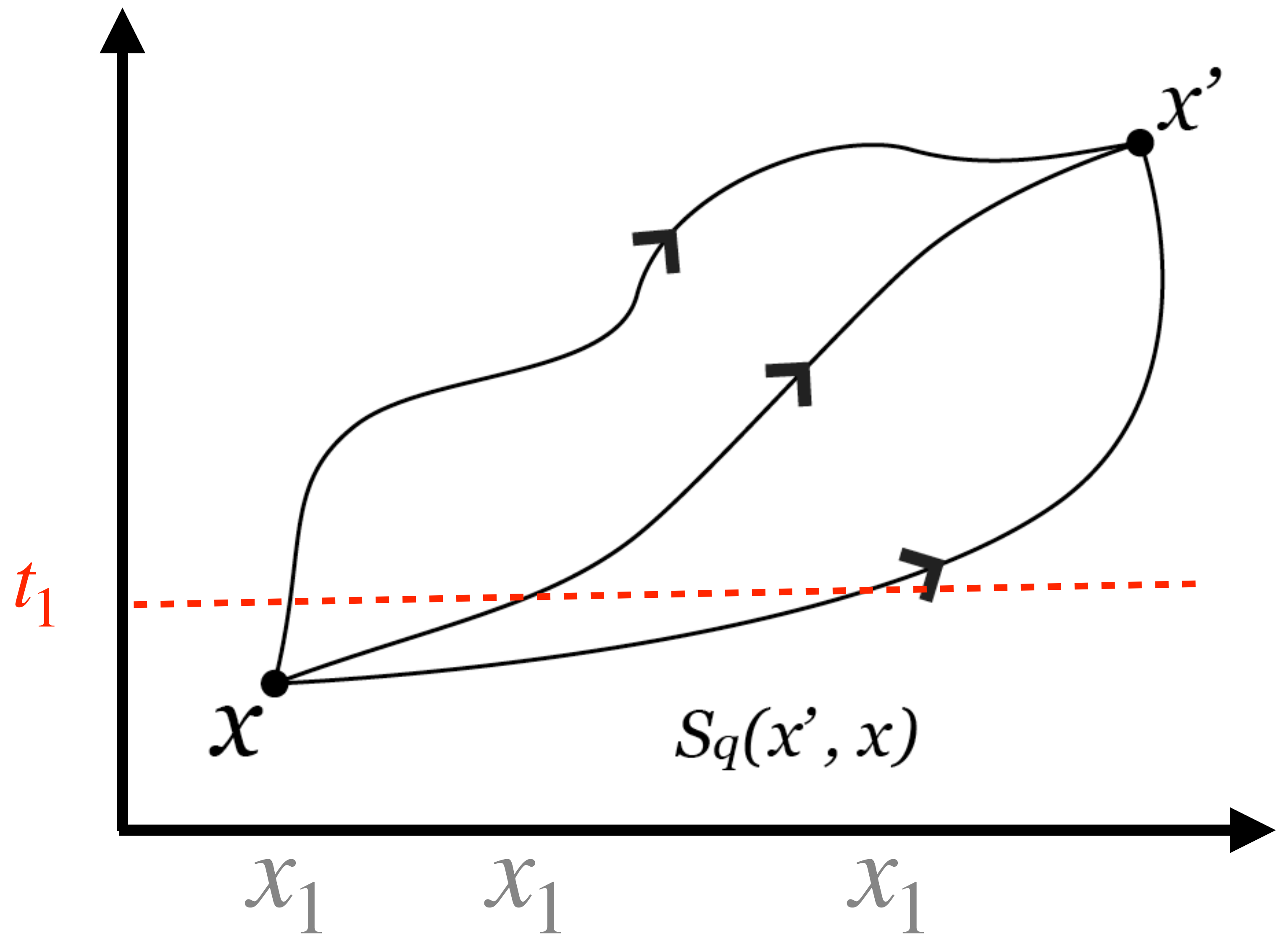
- Hamiltonian (density) to Lagrangian density

  $H(x, p) \rightarrow L(x, \dot{x})$

  Euclideanization ($it = \tau$: imaginary-time)

  $S = \int dt d\vec{x} L(x, \dot{x})$ -> $S_E = \int d\tau d\vec{x} L(x, \dot{x})$,

  The time evolution is written by $e^{iH\Delta t} \rightarrow e^{iL\Delta t}$ and then $e^{iS} \rightarrow e^{-S_E}$



- In ex. for quantum mechanics,

  $\langle x'(t) | x(0) \rangle = \int dx_1 dx_2 \cdots dx_N \langle x' | e^{-iH\Delta t} | x_N \rangle \cdots \langle x_2 | e^{-iH\Delta t} | x_1 \rangle \langle x_1 | e^{-iH\Delta t} | x \rangle$ => $\langle x'(t) x(0) \rangle = \int dx_1 \cdots dx_N x'(t) x(0) e^{-S_q(x', x)}$

  $S_q(x', x)$ is the action for the path q

Importance sampling method

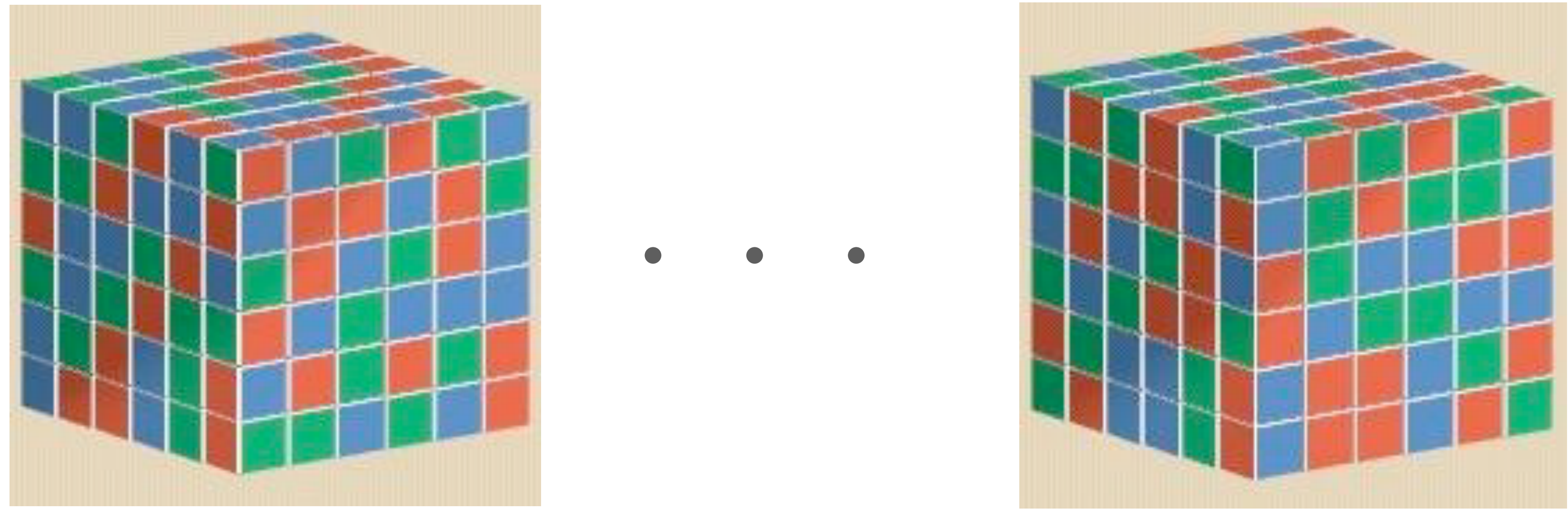
- Generate integral variable x_n w/ the Boltzmann weight $e^{-S_q(x',x)}$ from random numbers instead of uniform random numbers.

  For small $S_q(x', x)$, $e^{-S_q(x',x)}$ takes large value.

  => Gives a significant contribution to the integral

  => Such configuration x are frequently generated

- For QCD, $S_q(x', x) \to S_E[\phi]$: Euclidean QCD action and generate gluon configuration ϕ from random numbers



4-3. Algorithms

How to generate configuration numerically?

- Pseudo-Heat bath method… obtain SU(2) matrix from random numbers
  SU(3) matrix is constructed by combination of SU(2) matrices
  Most efficient for Yang-Mills theory
  (consider quarks are heavy and decoupled, so-called quenched QCD)

- Hybrid Monte Carlo (HMC) algorithm
  for QCD w/ even-number quarks (Nf=2 QCD)
  …Molecular dynamics methods and the Metropolis Test
  Solve (discrete) time evolution step for gluons and quarks, but energy is not conserved in finite increments. Metropolis to the correct probability distribution.

- Rational Hybrid Monte Carlo for odd-number of quark system (Nf=2+1 QCD)
  …Dealing with quark action $(\det DD^\dagger)^{N_f/2}$ using a rational approximation.

Open code for QCD simulation

- MILC code (C++): USQCD
- Bridge++ (C++) : Japanese people (leader: H.Matsufuru in KEK)
  General purpose code
  (HMC for several fermion, measurements, SU(2) gauge theory)
- Lattice tool kit (fortran) : A. Nakamura
  For improved Wilson fermion, MPI, simple
- LatticeQCD.jl (Julia) : A. Tomiya
- Highly tuned fortran actually used in supercomputers such as Fugaku