Introduction to Lattice QCD

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Plan of Talk

§1. Introduction to Lattice QCD
§2. Hadron Spectrum
§3. Recent Algorithmic Improvements
§4. Nuclei in Lattice QCD
§5. Toward Post-Petascale
§6. Summary

§1. Introduction to Lattice QCD

Questions in history of mankind

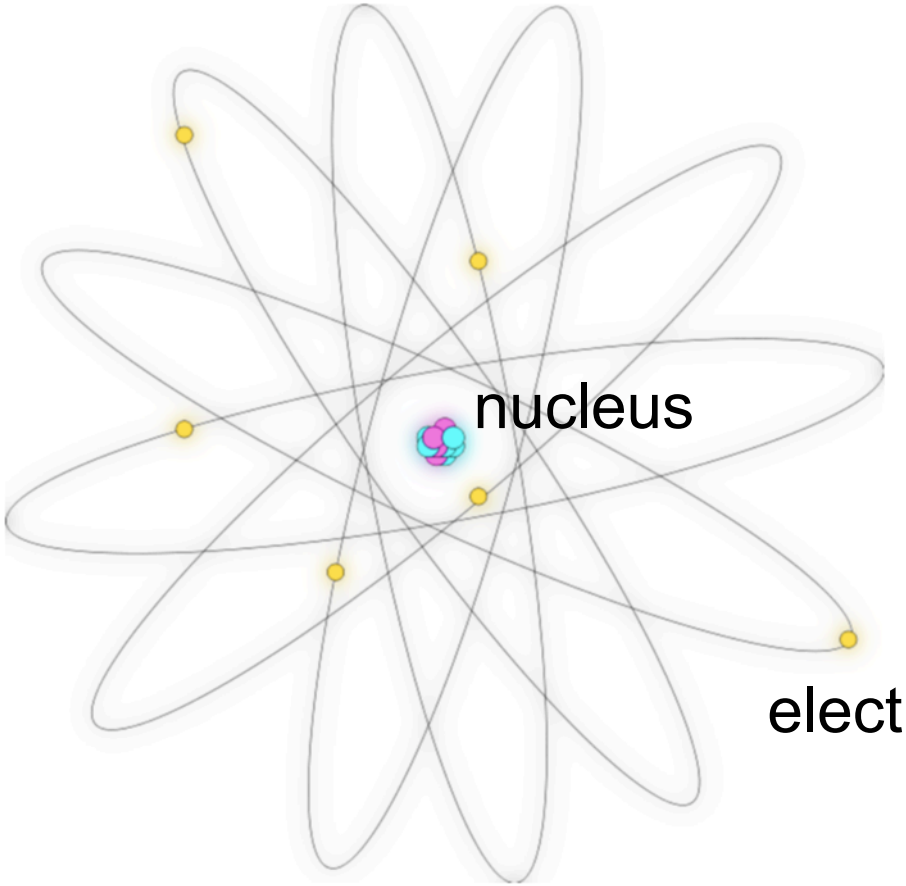
- What is the smallest component of matter?
- What is the most fundamental interaction?

K computer

Do you know what diamond is made of？

10^{-8} cm

Carbon atom ^{12}C

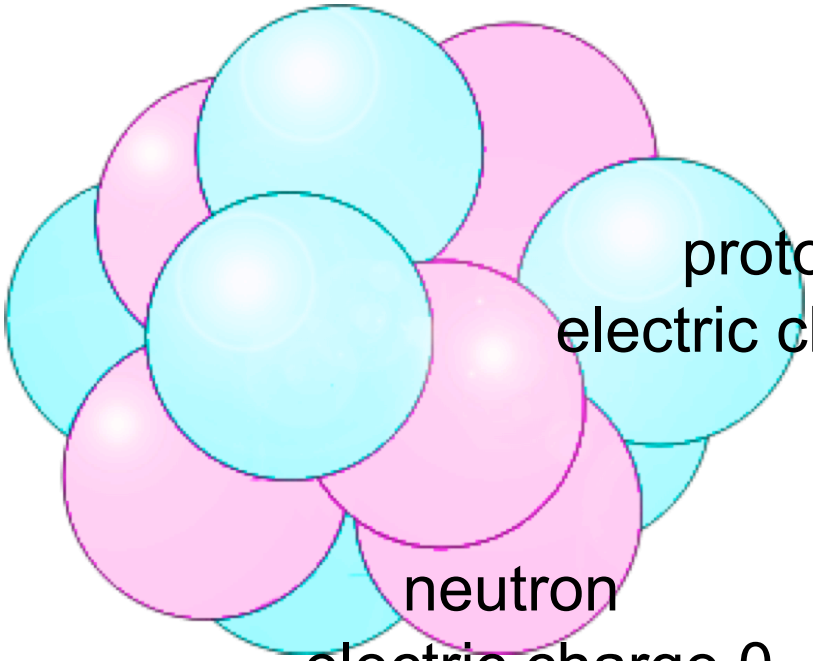


nucleus

electron

10^{-12} cm

Carbon nucleus

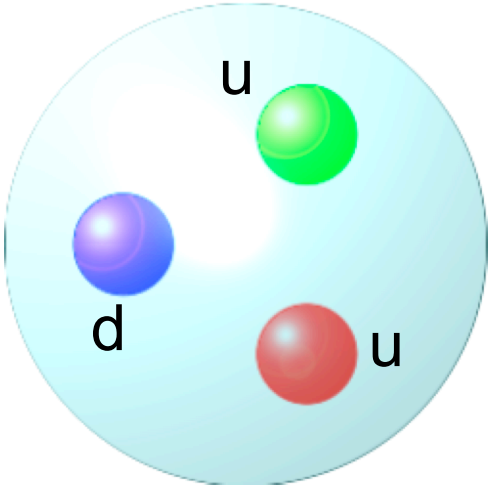


proton
electric charge +1

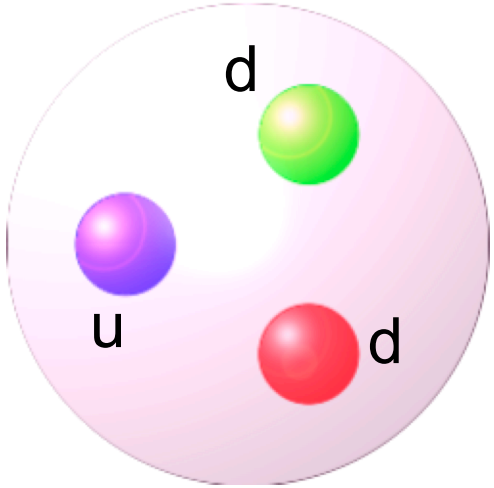
neutron
electric charge 0

10^{-13} cm

proton

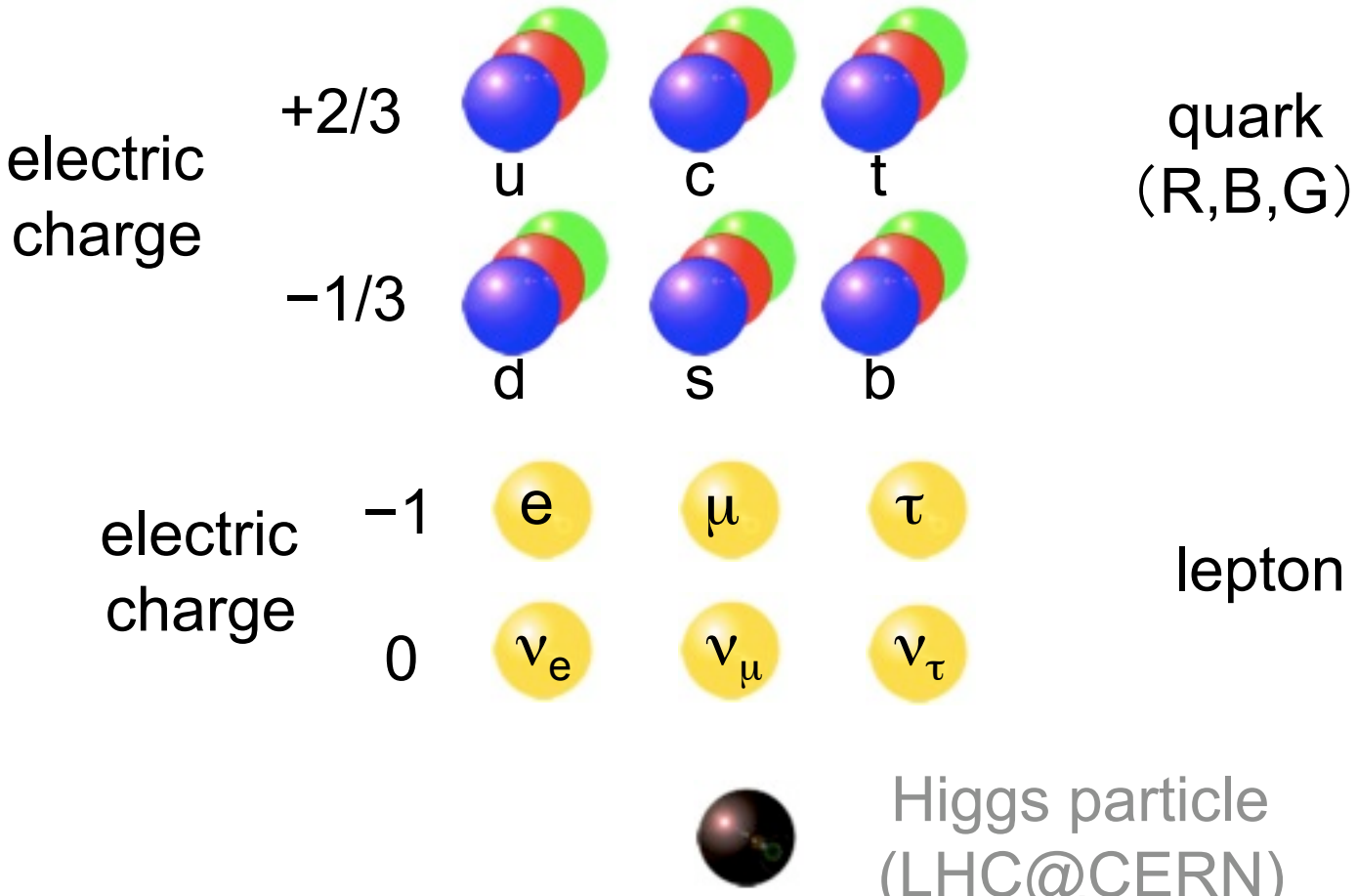


neutron



K computer

Elementary Particles Known to Date



Fundamental Interactions

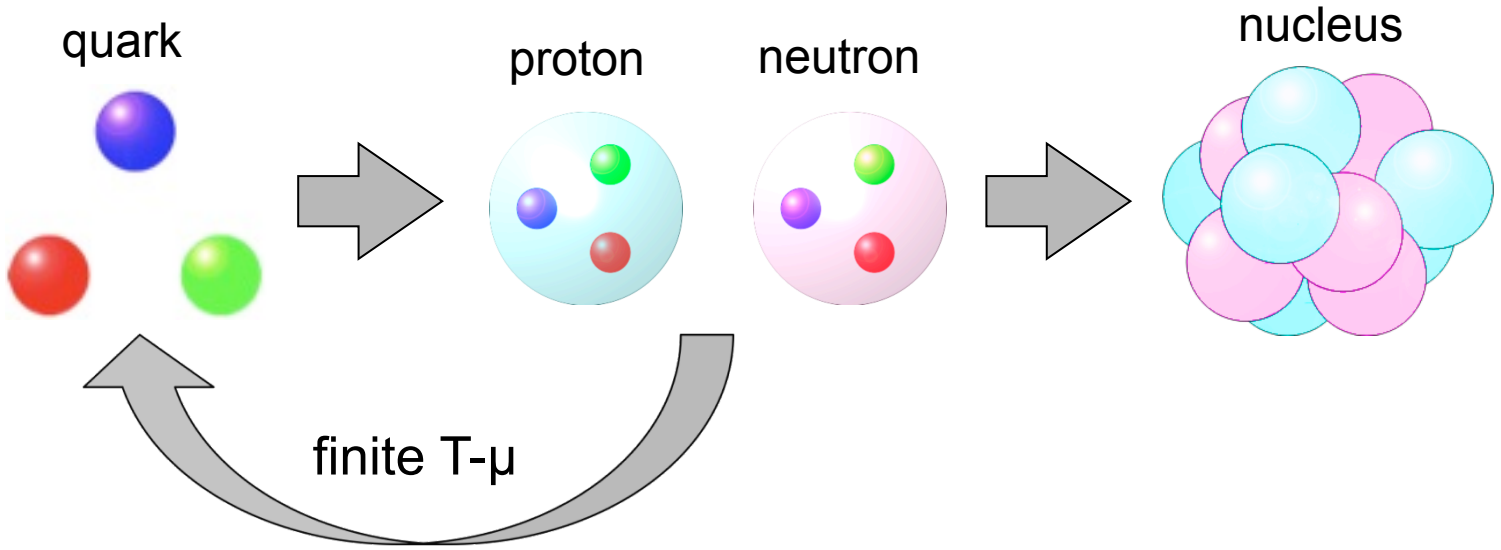
force	strength	gauge boson	theory
Strong	1	Gluon	QCD
EM	0.01	Photon	QED
Weak	0.00001	Weak Boson	Weinberg-Salam
Gravity	10^{-40}	Graviton	Superstring(?)

Computational elementary particle physics has been led by lattice QCD over past 30 years

One of important applications on K computer

Strong Interaction

- Fundamental degree of freedom : quarks and gluons
- Confinement : quark can never be retrieved by itself
- Asymptotic freedom ： closer to each other, arbitrarily weaker
- Hierarchy : 3 quarks ⇒ proton･neutron ⇒ nuclear
- Finite temperature and finite density (finite T-μ) : phase transition



Aim of Lattice QCD

QCD Lagrangian

$$\mathcal{L} = \frac{1}{4} F_{\mu\nu} F_{\mu\nu} + \sum_{q=u,d,s,c,b,t} \bar{q} \left[\gamma_\mu (\partial_\mu - igA_\mu) + m_q \right] q$$

Only coupling const. g and quark masses m_q are free parameters

Why is numerical analysis necessary for strong interaction?

Too strong to investigate with perturbative analysis

Characteristic features (confinement etc.) are nonperturbative

Aiming at quantitative analyses on

- hierarchical structures made of quarks
- phase diagram and EOS under finite temperature/density

based on first principle (QCD Lagrangian) calculations

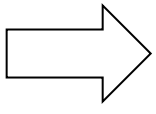
Numerical method (1)

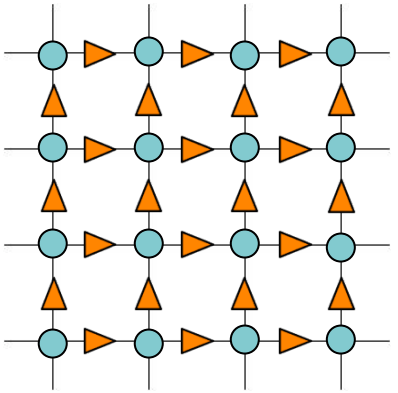
Path integral in 4-dim.（space 3-dim. + time 1-dim.）continuum theory

$$\langle \mathcal{O}[A_\mu, q, \bar{q}] \rangle = \frac{1}{Z} \int \mathcal{D}A_\mu \mathcal{D}q \mathcal{D}\bar{q}\, \mathcal{O}[A_\mu, q, \bar{q}]\ \exp\left\{ - \int d^4x \mathcal{L}[A_\mu, q, \bar{q}] \right\}$$

Similar to partition function in stat. mechanics ⇒ Monte Carlo method

Discretize 4-dim. space-time for finite degree of freedom ⇒ 4-dim. lattice





q(x) : quark field

$A_\mu(x)$: gauge field

q(n) : quark field

$U_\mu(n)$: SU(3) link variable

Numerical method (2)

K computer

Path integral on 4-dim. lattice

$$\langle \mathcal{O}[U_\mu, q, \bar{q}] \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_\mu dq d\bar{q}\ \mathcal{O}[U_\mu, q, \bar{q}]\ \exp\left\{ -\sum_n \mathcal{L}_{\rm latt}[U_\mu, q, \bar{q}] \right\}$$

Quark fields are Grassmann (anticommuting) numbers

⇒ analytically integratied

$$\langle \bar{\mathcal{O}}[U_\mu] \rangle = \frac{1}{Z} \int \prod_{n,\mu} dU_\mu\ \bar{\mathcal{O}}[U_\mu]\ \exp\left\{ -S^{\rm eff}_{\rm latt}[U_\mu] \right\}$$

Average over the configurations gives expectation value

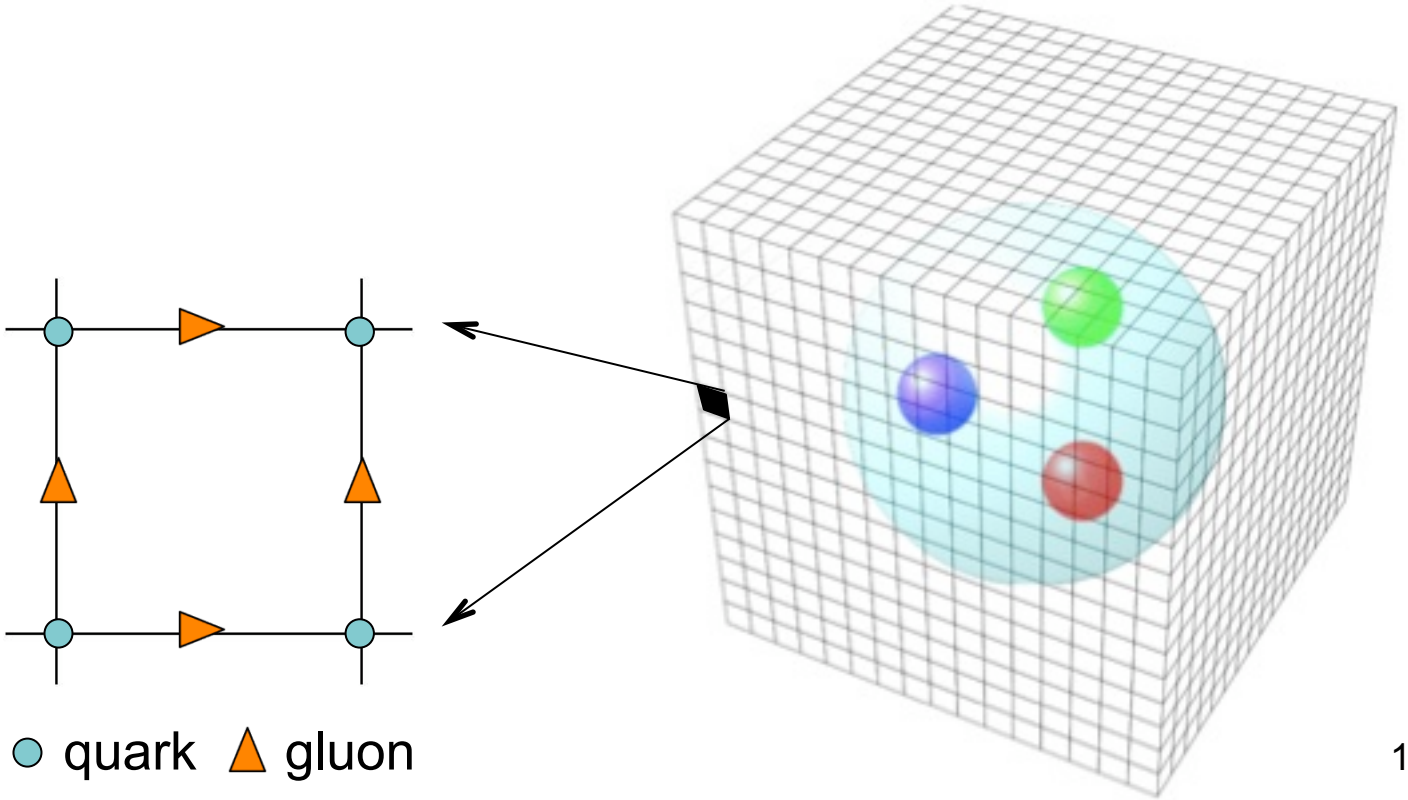
$$\langle \bar{\mathcal{O}}[U_\mu] \rangle = \frac{1}{N} \sum_{i=1}^{N} \bar{\mathcal{O}}[U_\mu^{(i)}] + O\left(\frac{1}{\sqrt{N}} \right)$$

statistical error

Physical Parameters

Few parameters

- 4-dim. volume: V=NX・NY・NZ・NT
- lattice spacing: a (as a function of coupling const. g)
- quark masses: m_q (q=u,d,s,c,b,t)



Major Systematic Errors

- Finite volume effects
  ⇒ larger V=NX・NY・NZ・NT

- Finite lattice spacing effects
  ⇒ smaller a

- Quenched approximation (neglect quark vacuum polarization)
  ⇒ 2+1 (m_u=m_d≠m_s) flavor simulation

- Chiral extrapolation with heavier quark masses
  ⇒ simulations at physical quark masses (physical point)

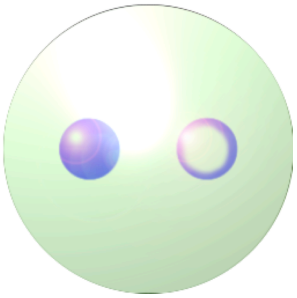
Need heavier computational cost to diminish the systematic errors

cost ∝ (physical vol.)$^{1.25}$・(lattice spacing)$^{-6\sim-7}$・(quark mass)$^{-2\sim-3}$

§2. Hadron Spectrum

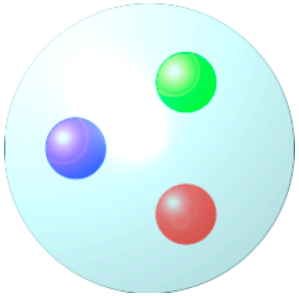
Hadron

Meson (quark and anti-quark)



π, K, K*, ρ, ω, η, φ, a, b, f, D, B, ...

Baryon (3 quarks)



p, n, Δ, Λ, Σ, Σ*, Ξ, Ξ*, Ω, Λc, Ξc, Λc, ...

Hadron Spectrum Calculation

K computer

Fundamental quantities both in physical and technical senses

physical side

physical input ⇒ m_u,m_d,m_s,… ⇒ reproduce hadron spectrum?

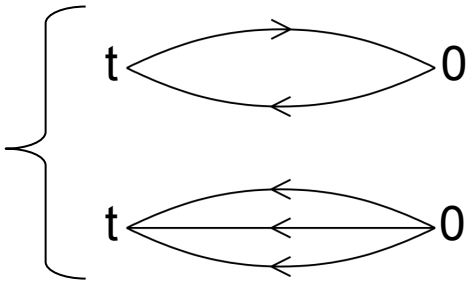
(ex. m_π, m_K, m_Ω) validity of QCD / determination of m_q

technical side

hadron correlators in terms of quark fields

$$\langle \mathcal{O}_h(t)\mathcal{O}_h^\dagger(0)\rangle \overset{t\gg 0}{\approx} C\exp\left(-m_h t\right)$$ ⇒ extract m_h by fit

quark diagrams from Wick contractions



meson

baryon

Brief History

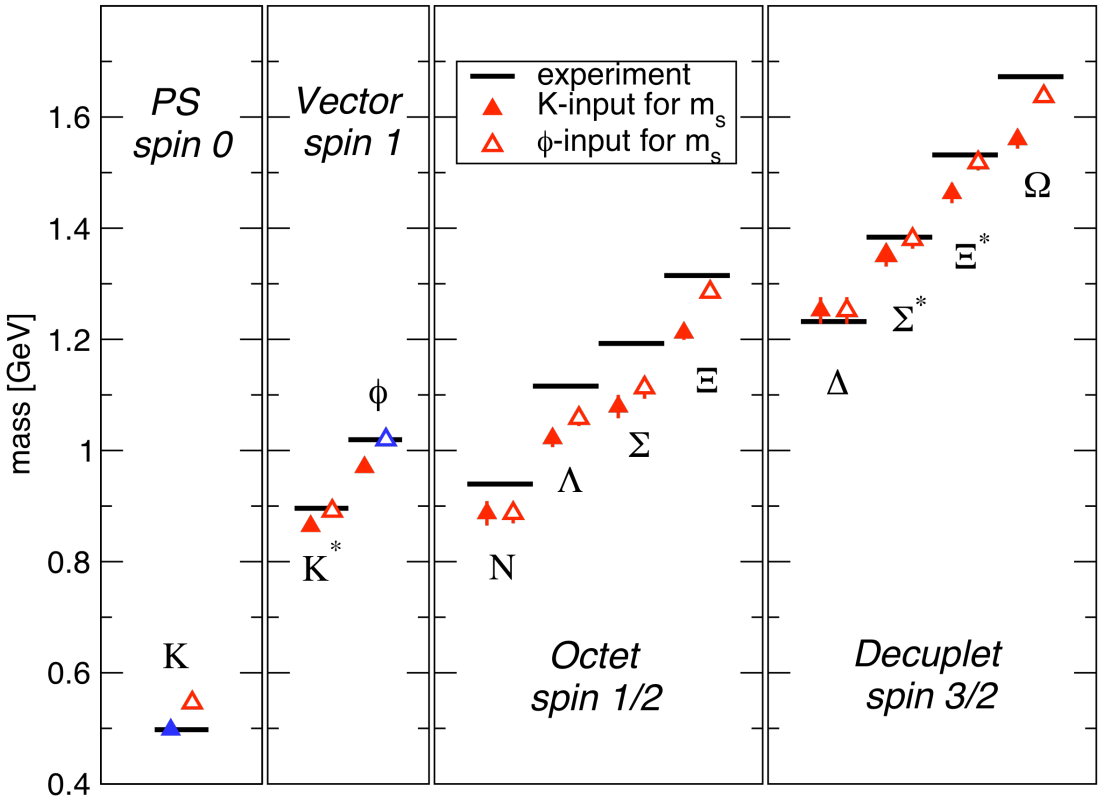
1981 first calculation of hadron masses in quenched approx.
Hamber-Parisi
demonstrate the possibility of first principle calculations

1996～2000 precision measurement in quenched approx.
CP-PACS
clear deviation from the experiment

2000～ initiate 2+1 flavor QCD simulations
CP-PACS/JLQCD, MILC, …
incorporate u,d,s vacuum polarization effects
reduce ud quark mass toward physical value

Hadron Spectrum in Quenched QCD

physical input m_π, m_K or m_ϕ, m_ρ ⇒ m_u=m_d, m_s, a

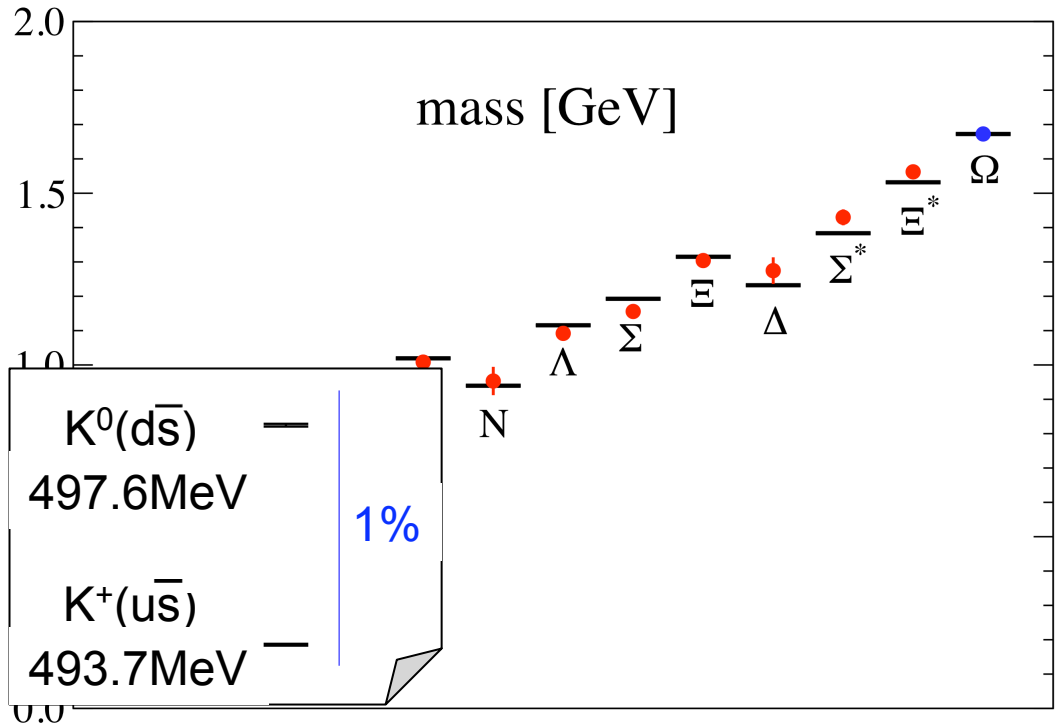


CP-PACS 00

~10% deviation from experimental values

Hadron Spectrum in 2+1 Flavor QCD

physical input m_π, m_K, m_Ω ⇒ m_u=m_d, m_s, a



PACS-CS 09

consistent within 2～3% error bars

2+1(m_u=m_d≠m_s) ⇒ 1+1+1(m_u≠m_d≠m_s) with QED

§3. Recent Algorithmic Improvements

Gauge configuration generation with Hybrid Monte Carlo method

(a variant of Molecular Dynamics)

$$\langle \bar{\mathcal{O}}[U_\mu] \rangle = \frac{1}{Z} \int \prod_{n,\mu} dP_\mu dU_\mu \; \bar{\mathcal{O}}[U_\mu] \; \exp\left(-\mathcal{H}_{\mathrm{HMC}}[P_\mu, U_\mu]\right)$$

Time consuming part

Solution of linear eqs. are require in each MD step

$$\begin{aligned} \frac{d}{d\tau} P_\mu(n,\tau) &= -\frac{\delta \mathcal{H}_{\mathrm{HMC}}}{\delta U_\mu(n,\tau)} \\ &= F_\mu(n,\tau) \quad \Rightarrow \quad x = (D[U_\mu])^{-1} b \end{aligned}$$

Solver Improvement on Cluster Machine

Bottle neck

memory bandwidth

Byte/Flop ≈ 2.1 in MatVec Dx

Advantage in 32bit arithmetic are effective use of

(1) memory and network bandwidth

(2) cache size

Maximum use of 32bit arithmetic with the solution kept in 64bit

1: x:initial guess	(64bit)	iterative refinement
2: $r = b - Dx$	(64bit)	
3: convert $r_{32} := r$	(64bit $\rightarrow$ 32bit)	
4: solve $\delta x_{32} = D^{-1} r_{32}$	(32bit)	preconditioning δx=Mr
5: convert $\delta x := \delta x_{32}$	(32bit $\rightarrow$ 64bit)	
6: $r = r - D\delta x$	(64bit)	
7: $x = x + \delta x$	(64bit)	the relation $r = b - Dx$ is kept in 64bit
8: if $\|r\|$ is small end else goto 3		

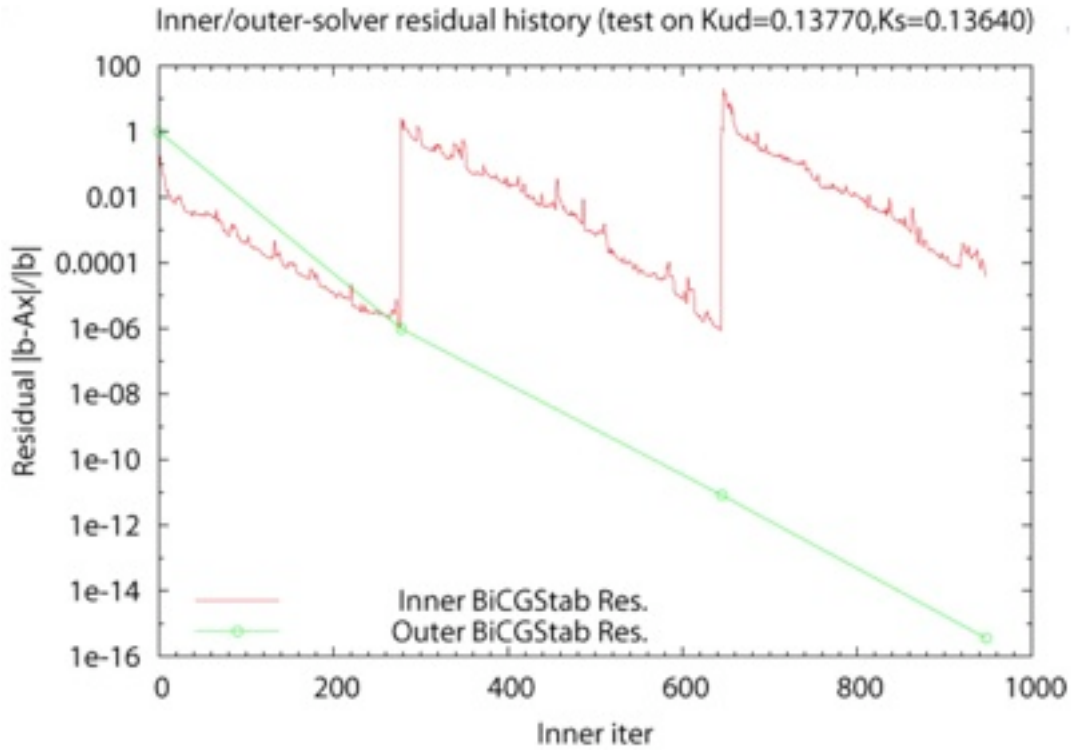
Mixed precision nested BiCGStab

Based on $DMy = b$, $x = My$

1: x:initial guess, $M \approx D^{-1}$:32bit-preconditioner
2: $r = b - Dx$, $\tilde{r} = r$, $\rho_0 = |r|^2$, $p = r$
3: loop
4: $\nu = Mp$, $q = D\nu$, $\alpha = \rho_0 / \langle \tilde{r} | q \rangle$
5: $r = r - \alpha q$, $x = x + \alpha \nu$, if $|r|$ is small exit
6: $\nu = Mr$, $t = D\nu$, $\omega = \langle t | r \rangle / \langle t | t \rangle$
7: $r = r - \omega t$, $x = x + \omega \nu$, if $|r|$ is small exit
8: $\rho_1 = \langle \tilde{r} | r \rangle$, $\beta = (\alpha / \omega)(\rho_1 / \rho_0)$, $\rho_0 = \rho_1$
9: $p = r + \beta(p - \omega q)$
10: end loop

Almost all the computational cost is spent by 32bit arithmetic

Residual vs. Iteration



Converged after 1.5 outer iteration

Time is reduced by a factor 2 on Intel 64 with SSE3 and link reconstruction technique（though, iteration number is increased）

⇒ need algorithmic improvements based on architecture

Improvement of Molecular Dynamics

Domain-Decomposed Hybrid Monte Carlo (DDHMC) Lüscher 03

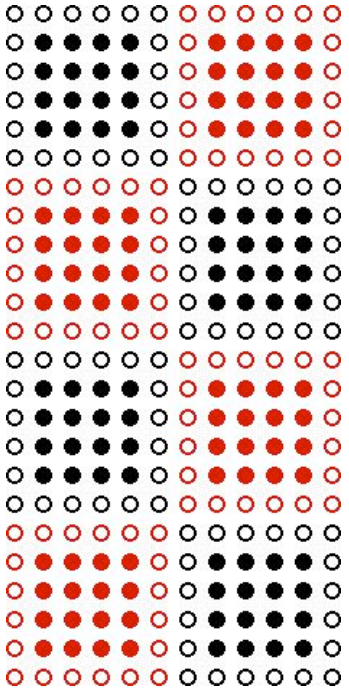
4-dim. lattice is decomposed into small blocks

⇒ introduction of hierarchy

$$\frac{d}{d\tau}P_\mu(n,\tau) = -\frac{\delta\mathcal{H}_{\rm HMC}}{\delta U_\mu(n,\tau)} = F_\mu^{\rm UV}(n,\tau) + F_\mu^{\rm IR}(n,\tau) + \cdots$$

domain (single core)

whole lattice (many nodes)



$F_\mu^{\rm UV}$: $x = (D_{\rm UV}[U_\mu])^{-1} b$ within domain

⇒ small condition number w/o communication

$F_\mu^{\rm IR}$: $x = (D_{\rm IR}[U_\mu])^{-1} b$ on whole lattice

⇒ large condition number w/ communication

Multiple Time Step MD Integrator

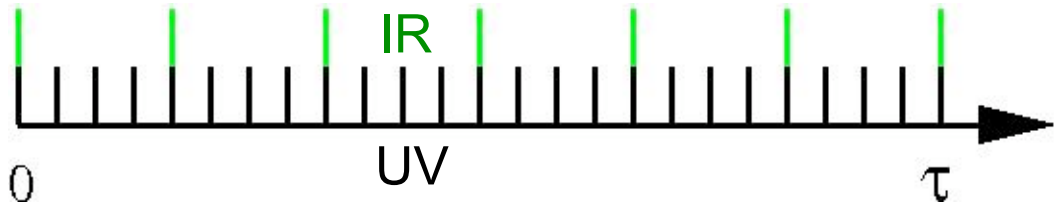
Sexton-Weingarten 92

Adjust step size according to the magnitude of force

$$\delta\tau^{\mathrm{UV}}||F_\mu^{\mathrm{UV}}|| \approx \delta\tau^{\mathrm{IR}}||F_\mu^{\mathrm{IR}}||$$

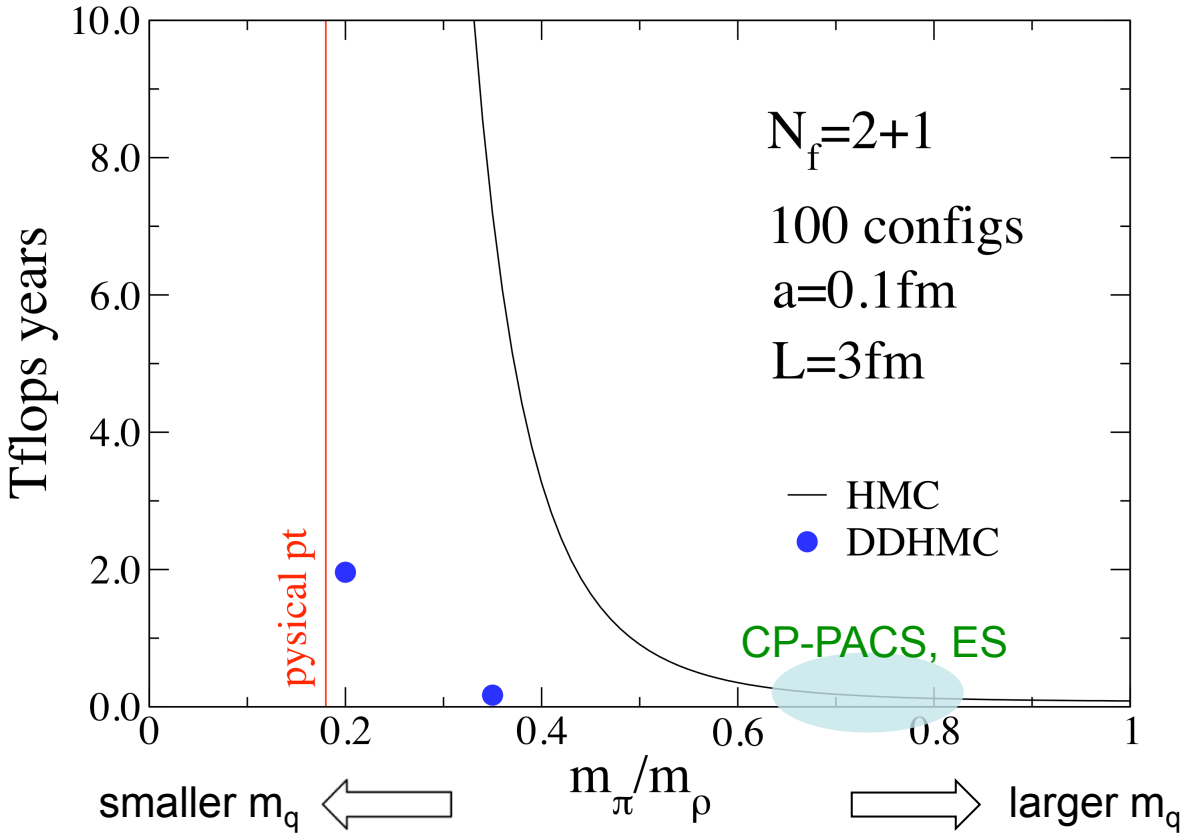
For example

$$||F_\mu^{\mathrm{UV}}|| \ : \ ||F_\mu^{\mathrm{IR}}|| = 4 \ : \ 1 \quad \Rightarrow \quad \delta\tau^{\mathrm{UV}} \ : \ \delta\tau^{\mathrm{IR}} = 1 \ : \ 4$$



Less frequent calculation of F_μ^{IR} ⇒ save computational cost

Cost Reduction due to DDHMC

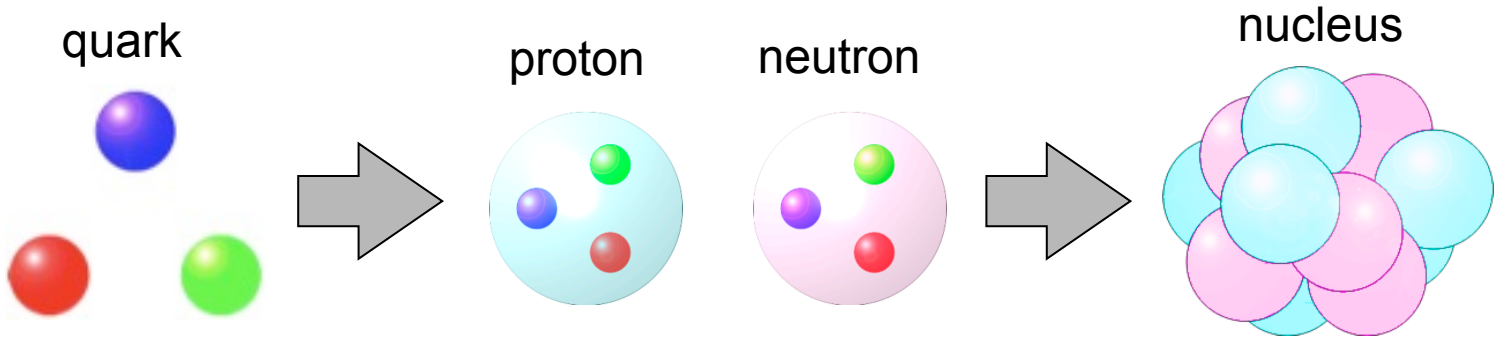


⇒ Physical point simulation is now possible

§4. Nuclei on the Lattice

Now precision measurement of hadron masses is achieved

Next step is a challenge for multi-scale physics



Exploratory study for ^{4}He and ^{3}He nuclei Yamazaki-YK-Ukawa 10

large binding energy $\Delta E_{^4\mathrm{He}}$=28.3 MeV

^{4}He has double magic numbers (Z=2,N=2)

Difficulties in multi-nucleon system

(1) No. of Wick contractions

(2) how to distinguish bound state from scattering state?

Wick Contractions

He nucleus correlator in terms of quark fields

$$\langle \mathcal{O}_{^4\mathrm{He}}(t)\mathcal{O}^{\dagger}_{^4\mathrm{He}}(0)\rangle \overset{t\gg 0}{\approx} C\exp\left(-m_{^4\mathrm{He}}t\right) \qquad \Delta E_{^4\mathrm{He}} = E_{^4\mathrm{He}} - 4E_N$$

^{4}He operator consists of two protons (udu) and two neutrons (dud)

Beam 67

⇒ No. of Wick contraction: $N_u!\times N_d! = (2N_p+N_n)!\times(2N_n+N_p)!$

^{4}He: 6!×6!=518400

^{3}He: 5!×4!=2880

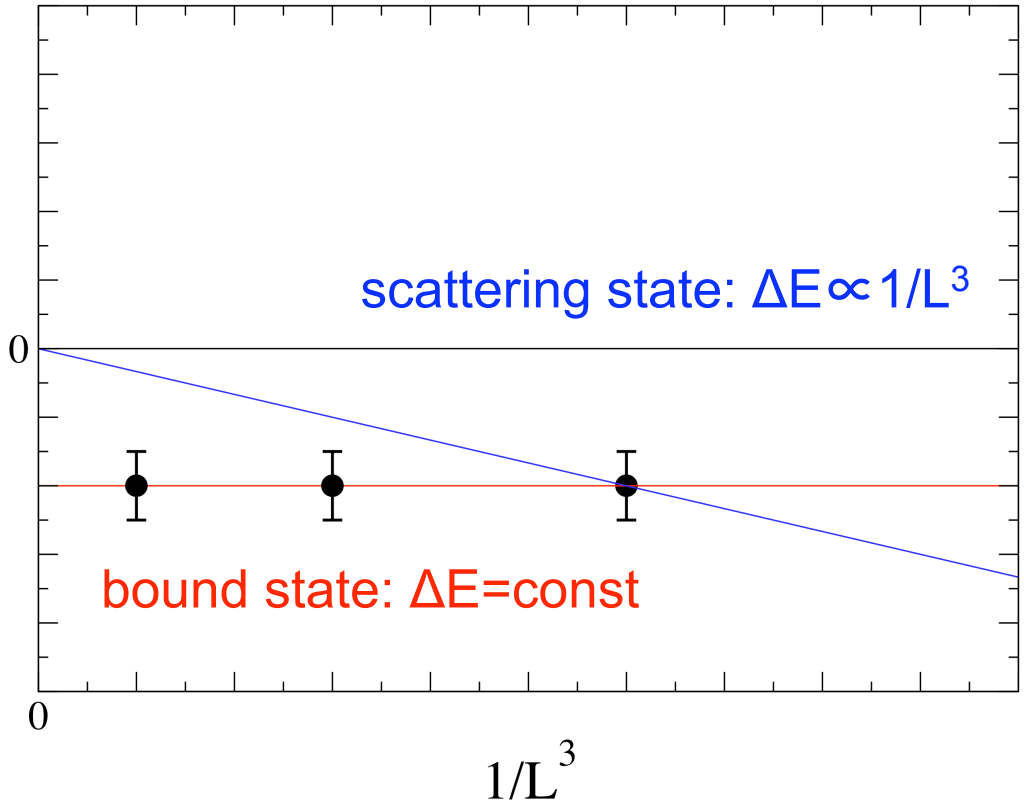
cf. N-N: 3! ×3!=36

^{12}C: 18!×18!∼4×10^{31}

independent quark diagrams are reduced by imposing $m_u=m_d$

Identification of Bound State in a Finite Box

$\Delta E<0$ both for bound state and attractive scattering state

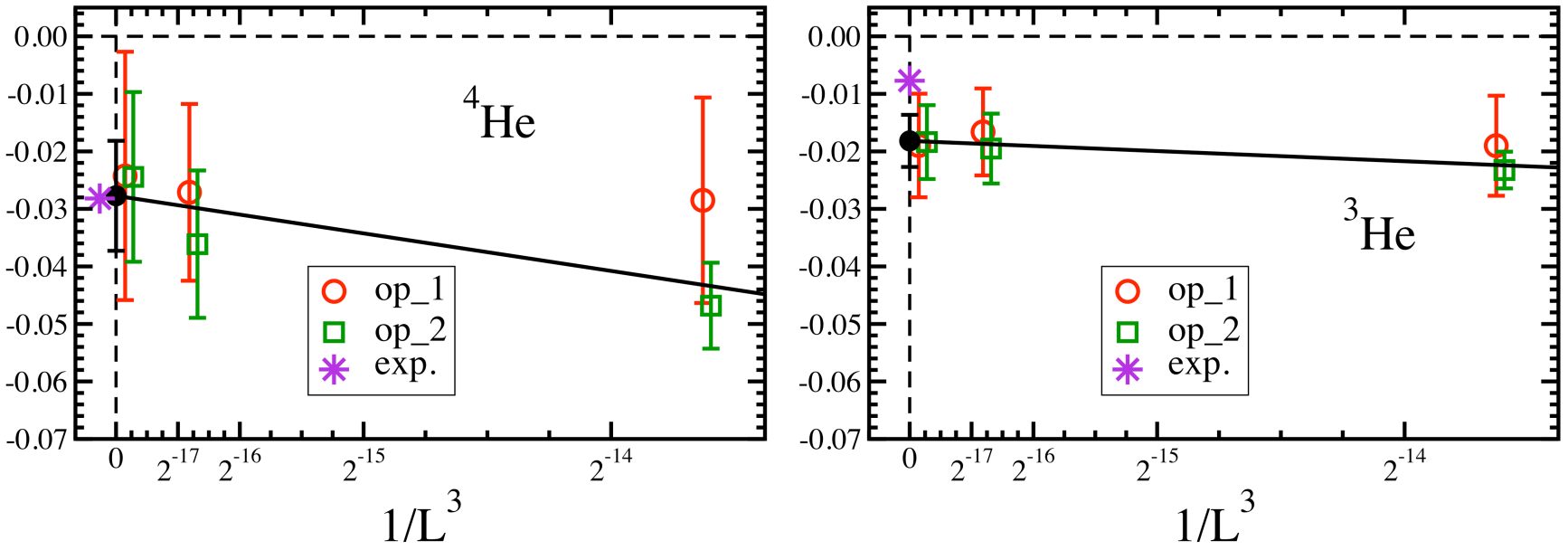


mandatory to check volume dependence of ΔE

Volume Dependence of ΔE_{4He}

Yamazaki-YK-Ukawa 10

Exploratory study with m_N=1.6 GeV in quenched QCD



same order to experimental values

§5. Toward Post-Petascale

Lattice QCD with Petascale computing

- scientific target:
  - 1+1+1 flavor QCD+QED simulation
    - direct construction of nuclei
- technical points:
  - mixed precision
  - reduction of communication

comparison with exp.
⇩
understand the nature

Toward Post-Petascale

- scientific target:
  - finite temperature and finite density
- technical points
  - may need further algorithmic improvements for diminishing B/F and hierarchical parallel architecture

exp. is impossible
⇩
prediction

Finite Temperature and Finite Density

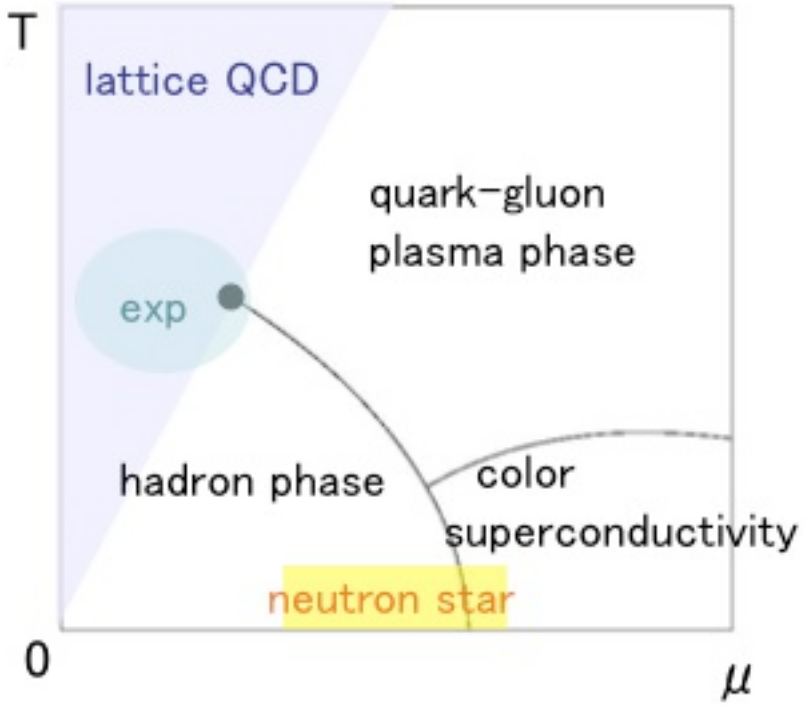
finite T-μ simulation

⇓

information of early universe and
inside of neutron star

an important research subject
with post-peta to exascale computing

expected phase diagram



Sign Problem

Introduction of chemical potential μ ⇒ complex phase

$$\langle \mathcal{O}[U_\rho] \rangle = \frac{1}{Z} \int \prod_{n,\rho} dU_\rho \, \mathcal{O}[U_\rho] \, \exp\{-S_0[U_\rho] + i\theta_\mu[U_\rho]\}$$
$$= \frac{\langle \mathcal{O}[U_\rho] \, \mathrm{e}^{i\theta_\mu[U_\rho]} \rangle_0}{\langle \mathrm{e}^{i\theta_\mu[U_\rho]} \rangle_0}$$

large fluctuation of phase ⇒ hardly obtain the average

Current popular approach: Taylor expansion in terms of μ/T
⇒ restricted region in T-μ plain
(previous slide)

We are developing a new algorithm to explore in the region of low temperature and high density

§6. Summary

Lattice QCD with petascale computing and beyond

<u>scientific target</u>

turning point from understanding the nature to prediction

<u>technical points</u>

further algorithmic improvements for

diminishing B/F and hierarchical parallel architecture