Lattice QCD on K computer

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Plan of Talk

§1. K computer and Strategic Field Program

§2. Introduction to Lattice QCD

§3. 1+1+1 Flavor QCD+QED Simulation

§4. Direct Construction of Light Nuclei

§5. Nuclear Force

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§1. K computer and Strategic Field Program

Overview of Project

- Development of 10 Pflops-class system in Kobe

  ⇒ named “K computer” by public competition
- Development of grand challenge applications in nano science and life science
- Buildup of a research center in computational science around the 10 Pflops-class system

  ⇒ Advanced Institute for Computational Science (AICS) at Kobe
- Project period (construction) is from Japanese FY 2006 to 2012
- RIKEN is responsible for the computer development

Note: independent of RIKEN-BNL-Colombia Collab.

Site for K computer

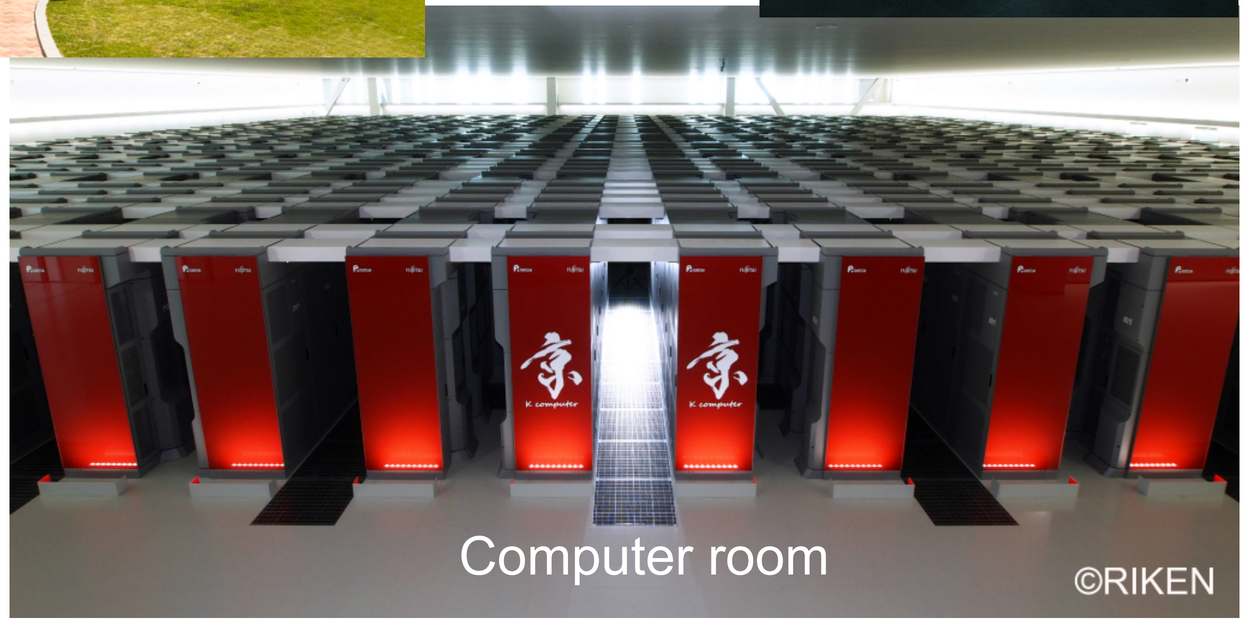
Osaka
Kyoto

Port Liner 'Monorail'

Some photo

Logo

K computer



Plan to host Lattice 2015 at Kobe

Strategic Field Program

For strategic use of K computer

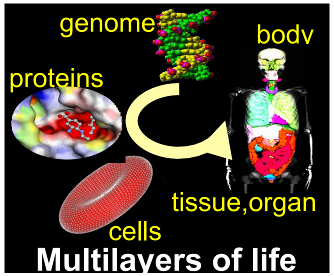
- Government selected 5 strategic fields in science and technology for importance from national view point
- For each field, Government also selected a core institute
- Each core institute is responsible for organizing research and supercomputer resources in the respective field and its community, for which they receive
  - priority allocation of K computer resources
    (～1% for lattice QCD)
  - funding to achieve the research goals

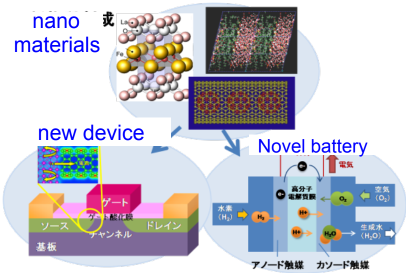
Strategic Fields and Core Institutes

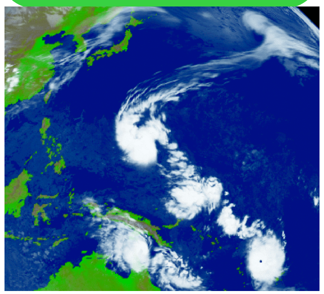
K computer

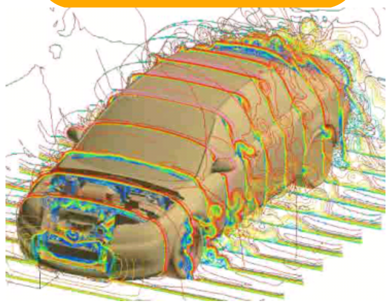
strategic field

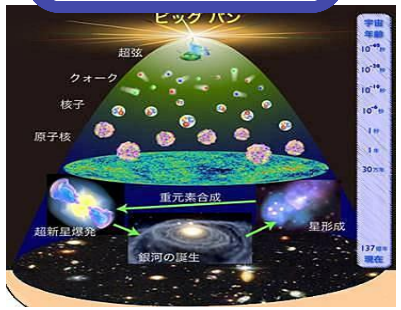
Life science & Medicine	New materials & Energy	Global change prediction	Next generation engineering	Matter & Universe











core institute

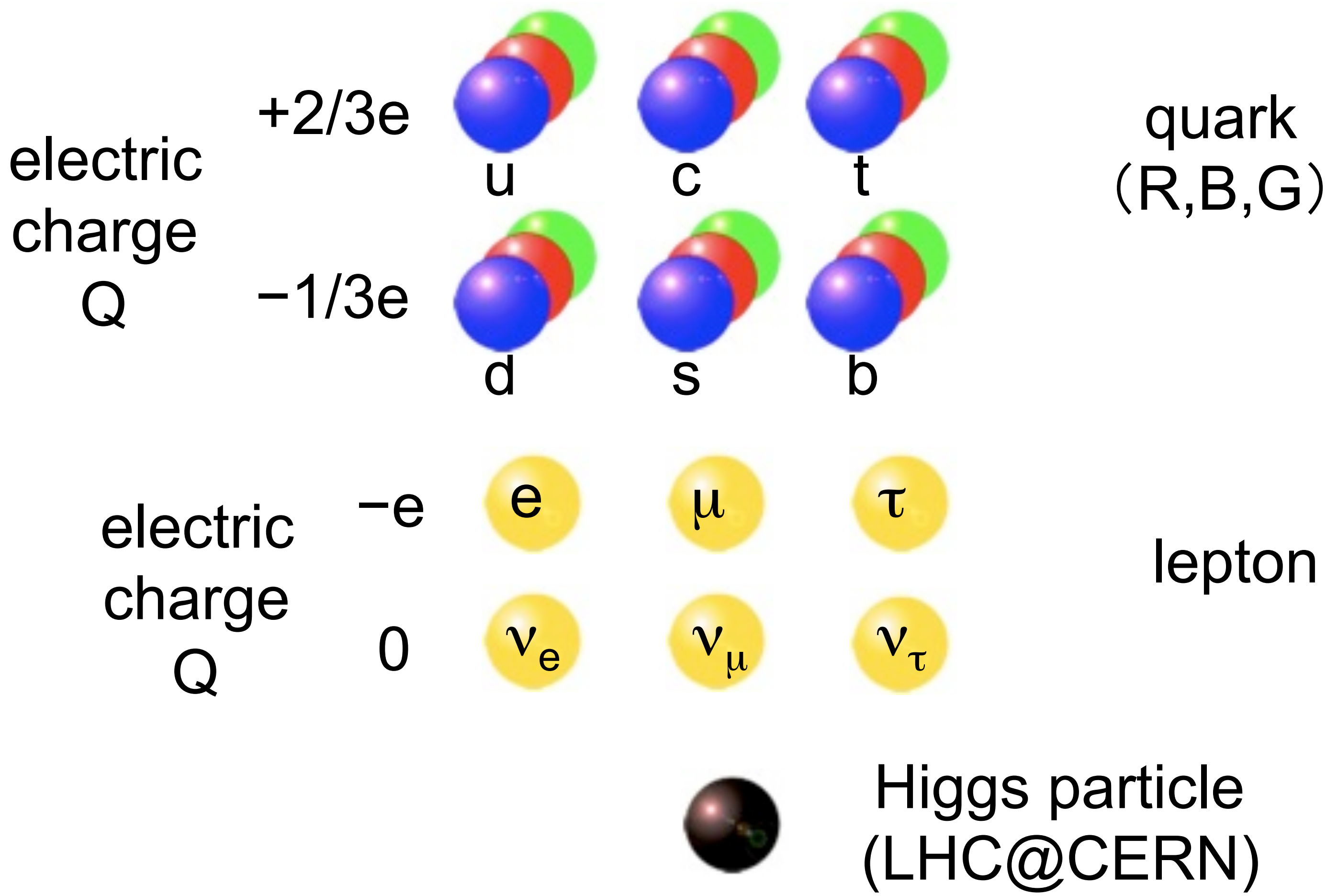
RIKEN	Institute for Solid State Physics U. Tokyo	Earth Simulator Center JAMSTEC	Institute for Industrial Science U. Tokyo	Center for Comp. Science U. Tsukuba
Life science Community	Materials science Community	Earth science Community	Engineering Community Industry	Basic science Community
Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources	Supercomputer resources

§2. Introduction to Lattice QCD

Questions in history of mankind

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

Elementary Particles Known to Date



Fundamental Interactions

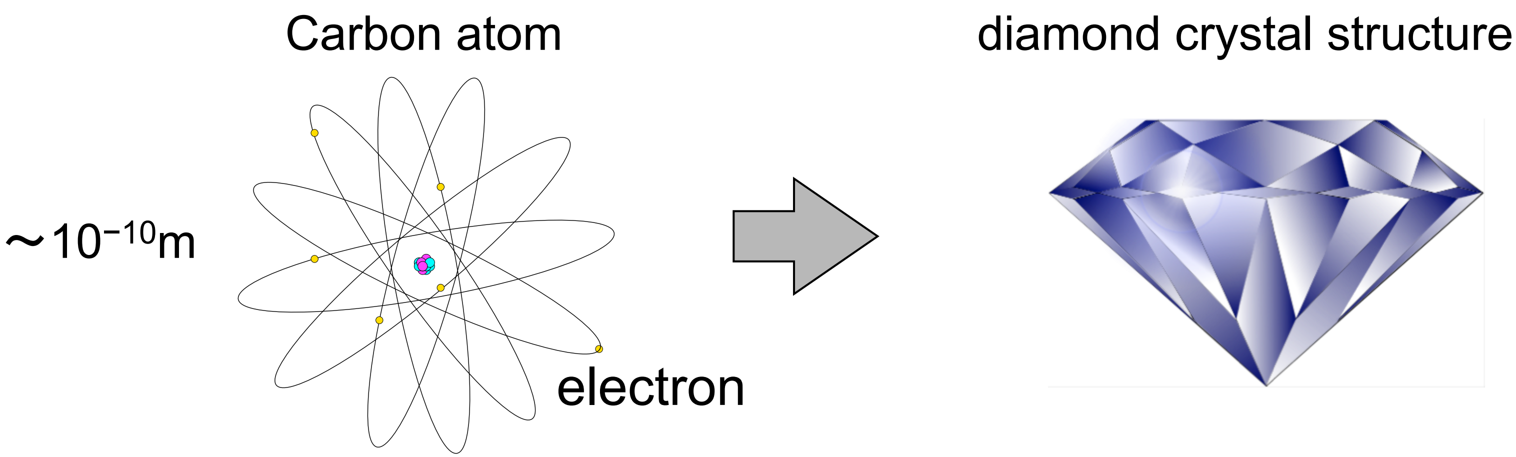
force	relative strength	gauge boson	quantum theory
Strong	1	Gluon	QCD
EM	0.01	Photon	QED
Weak	0.00001	Weak Boson	Weinberg-Salam
Gravity	10^{-40}	Graviton	Superstring(?)

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

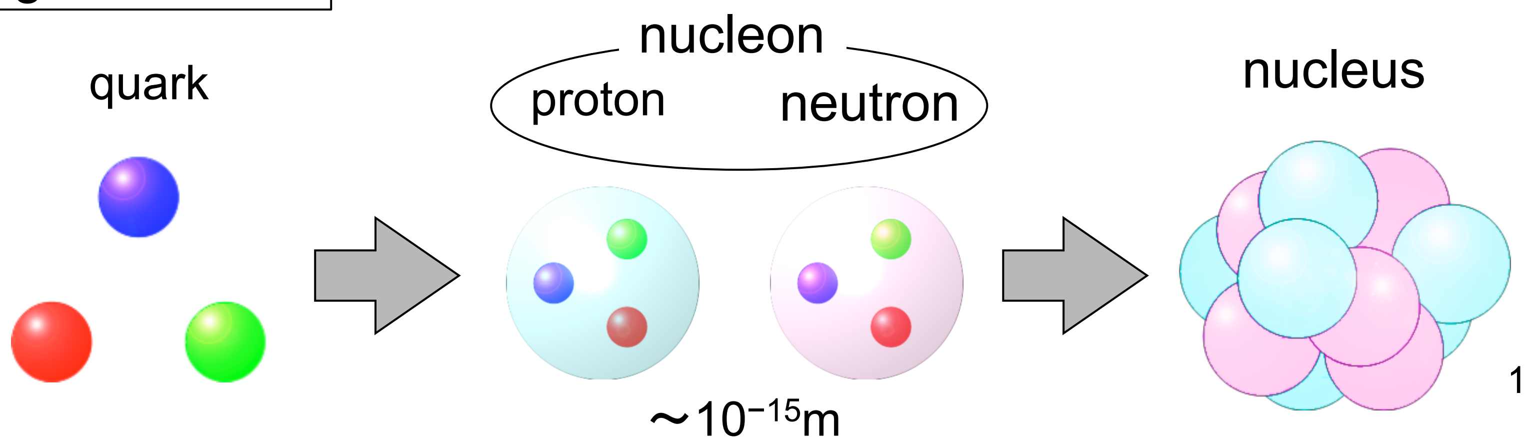
One of important applications on K computer

Particles and Interactions

Chemical bond with EM interaction



Strong interaction

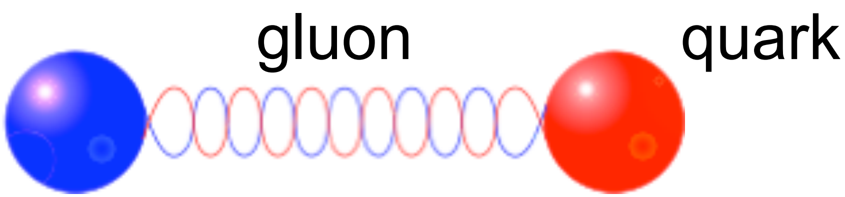


Aim of Lattice QCD

QCD Lagrangian ＝ first principle

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

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



Too strong to investigate with perturbative analysis

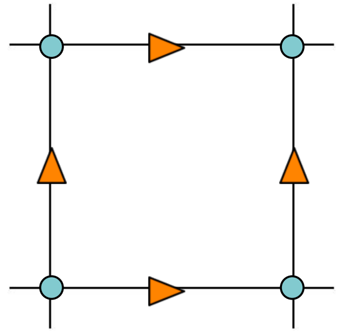
⇒ nonperturbative analysis with numerical method based on first principle

Numerical method

Numerical integration with Monte Carlo method

on discretized 4-dim. space-time lattice

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



quark gluon

Average over the values evaluated on configurations

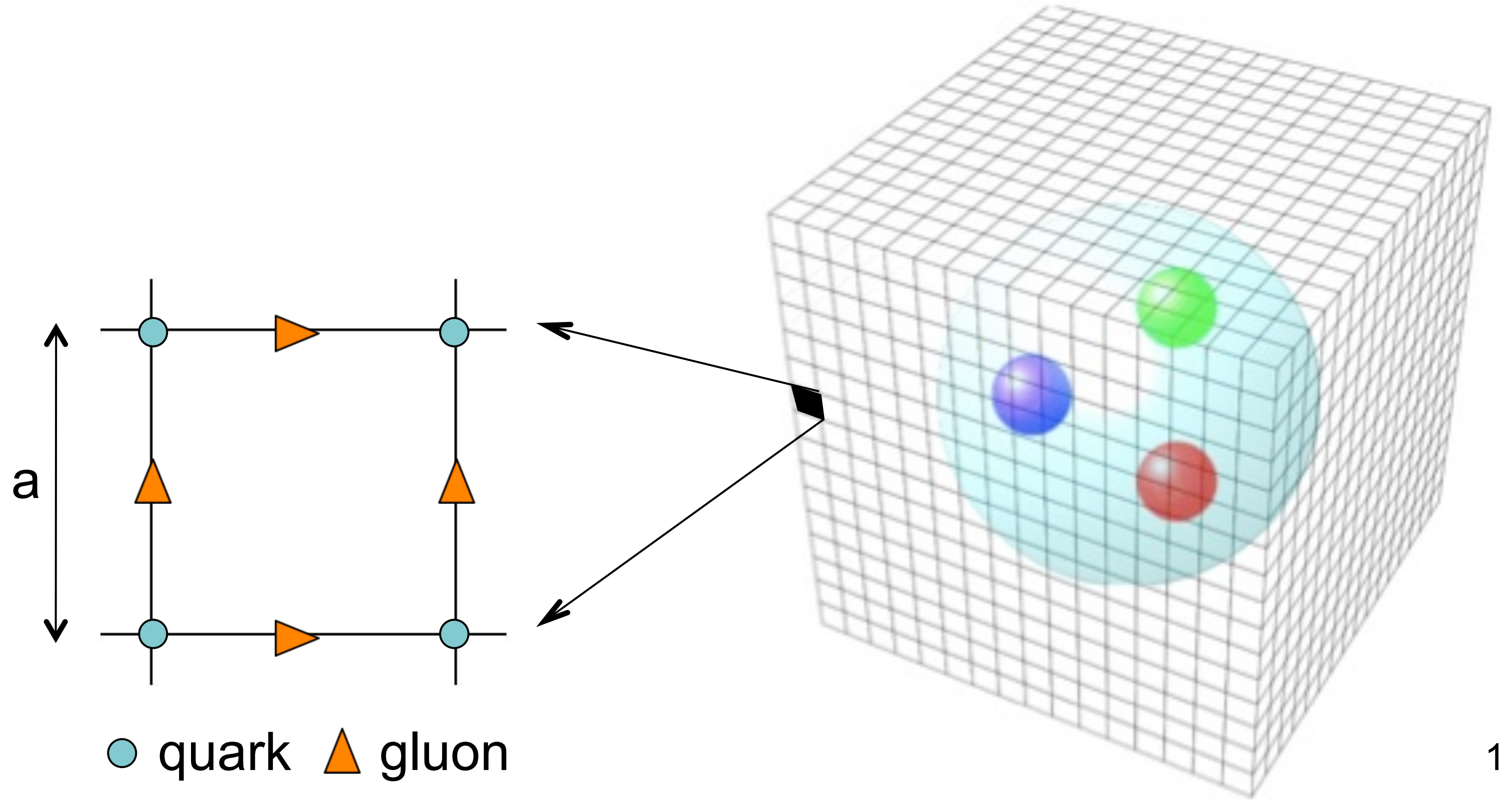
$$\langle \mathcal{O}[A_\mu, q, \bar{q}] \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}[A_\mu^{(i)}, q^{(i)}, \bar{q}^{(i)}] + O\left(\frac{1}{\sqrt{N}}\right)$$

statistical error

Physical Parameters

Small number of parameters

- 4-dim. volume: $V = NX \cdot NY \cdot NZ \cdot NT$
- lattice spacing: a (as a function of coupling const. g)
- quark masses: m_q (q=u,d,s,…)



Hadron Masses

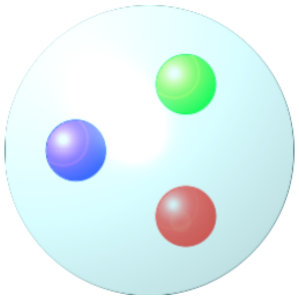
Confinement : quark can never be retrieved by itself

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 Mass Calculation

Fundamental quantities both in physical and technical senses

physical side

physical input ⇒ $m_u, m_d, m_s, \dots$ ⇒ reproduce all the hadron spectrum?

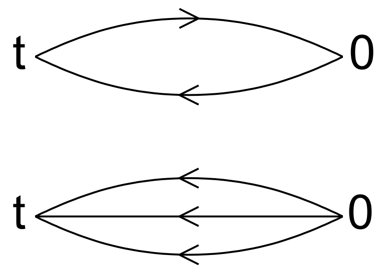
(ex. m_π, m_K, m_Ω) validity of QCD / determination of m_q

technical side

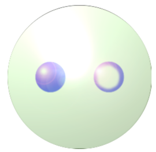
hadron correlators in terms of quark fields

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

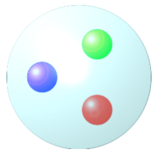
quark line diagrams
from Wick contractions



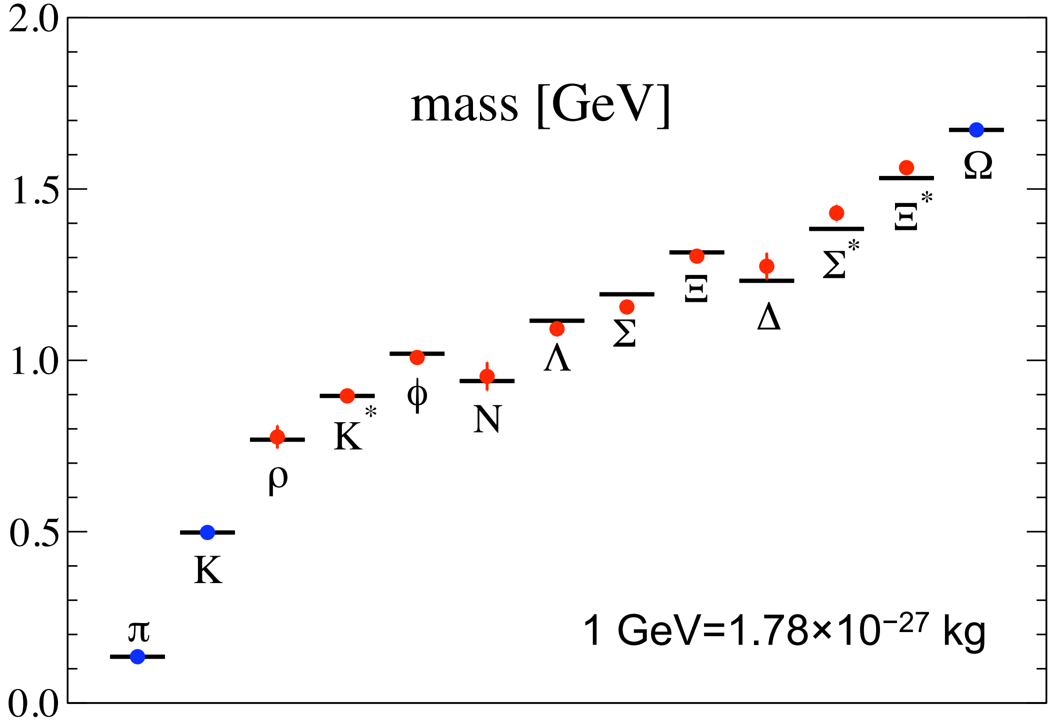
meson



baryon



Hadron masses in 2+1 Flavor QCD



PACS-CS 09

physical input
m_π, m_K, m_Ω

⇩

m_u=m_d, m_s, a

Isospin symmetry breaking effects

$K^0(d\bar{s})$ 497.6MeV	1%
$K^+(u\bar{s})$ 493.7MeV	

consistent within 2～3% error bars

similar results are obtained by other groups

§3. 1+1+1フレーバーQCD+QED

PACS-CS 12

Isospin symmetry breaking

- EM interaction

  $Q_u=+2/3e$, $Q_d=Q_s=-1/3e$, $e=\sqrt{4\pi/137}$

- u-d quark mass difference

  $m_u=m_d\neq m_s$ (2+1フレーバー) ⇒ $m_u\neq m_d\neq m_s$ (1+1+1フレーバー)

Physical input:

$m_{\pi+}$(ud), m_{K0}(ds), m_{K+}(us), $m_{\Omega-}$(sss)

Output:

m_u, m_d, m_s, lattice spacing, …

2+1 flavor QCD generation around the physical point	$\xrightarrow{\text{reweighting method}}$	1+1+1flavor QCD+QED on the physical point

Reweighting Method

Simulation parameter : m
Target parameter : m'

$$\langle \mathcal{O}[m] \rangle_m \Rightarrow \langle \mathcal{O}[m'] \rangle_{m'}$$

$$\begin{aligned}
\langle \mathcal{O}[m'] \rangle_{m'} &= \frac{\int \mathcal{D}U \mathcal{O}[m'] \mathrm{e}^{-S[m']}}{\int \mathcal{D}U \mathrm{e}^{-S[m']}} \\
&= \frac{\int \mathcal{D}U \mathcal{O}[m'] \mathrm{e}^{-S[m]-(S[m']-S[m])}}{\int \mathcal{D}U \mathrm{e}^{-S[m]-(S[m']-S[m])}} \\
&= \frac{\int \mathcal{D}U \mathcal{O}[m'] \mathrm{e}^{-S[m]-\Delta[m',m]}}{\int \mathcal{D}U \mathrm{e}^{-S[m]-\Delta[m',m]}} \\
&= \frac{\left\langle \mathcal{O}[m'] \mathrm{e}^{-\Delta[m',m]} \right\rangle_m}{\left\langle \mathrm{e}^{-\Delta[m',m]} \right\rangle_m}
\end{aligned}$$

Expectation value at target parameter m' can be obtained with the use of configurations generated at parameter m(≠m')
※ works better as the difference of m and m' diminishes

K^0-K^+ mass difference

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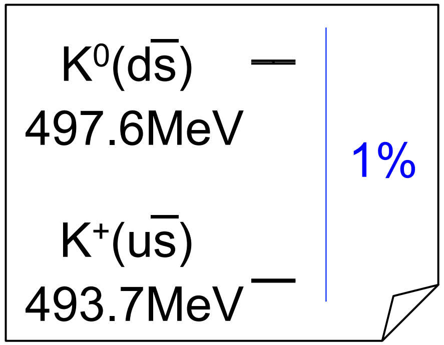
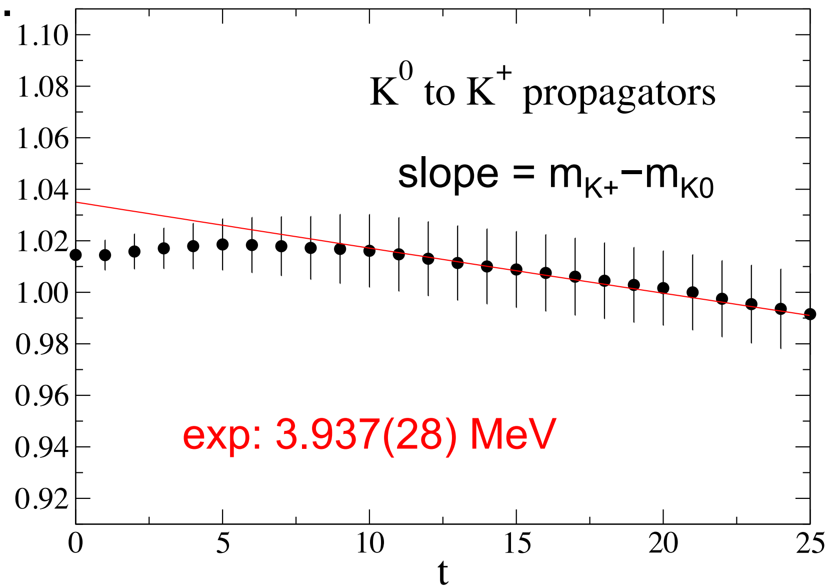
EM interaction + u-d quark mass diff.
⇒ diff. of $m_{K0}(ds)$ and $m_{K+}(us)$



lattice size=$32^3\times64$, a ∼ 0.1 fm



$$\frac{\langle K^0(t)K^0(0)\rangle}{\langle K^+(t)K^+(0)\rangle} \simeq Z\left(1-\underbrace{(m_{K^0}-m_{K^+})t}_{\text{much smaller than 1}}\right)$$

Fit result 4.54(1.09) MeV is consistent with exp. value 3.937(28) MeV within error bars

Quark masses

PACS-CS 12

Physical input:

$m_{\pi+}$(ud)=139.7(15.5) [MeV] exp: 139.6 [MeV]

m_{K0}(ds)=497.6(8.1) [MeV] exp: 497.6 [MeV]

m_{K+}(us)=492.4(8.1) [MeV] exp: 493.7 [MeV]

m_{Ω}(sss)は実験値に固定 exp: 1672.5 [MeV]

Quark masses (MSbar scheme at μ=2 GeV):

m_u=2.57(26)(07) [MeV]

m_d=3.68(29)(10) [MeV]

m_s=83.60(58)(2.23) [MeV]

Sizable finite size effects are expected in QCD+QED simulation

π meson mass(140MeV)@QCD ⇔ photon(massless)@QED

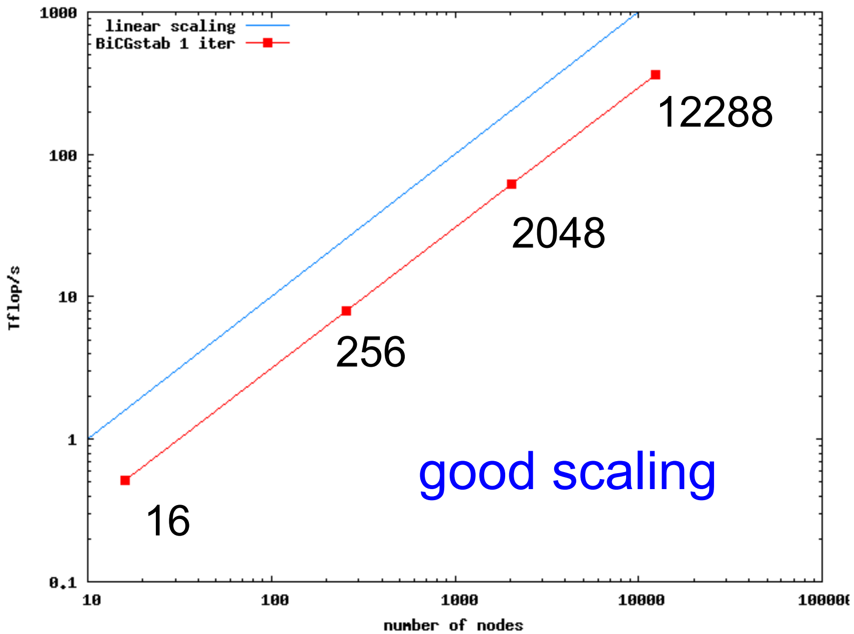
⇒ Simulation with larger lattice size 96^4 on K computer

Also useful for calculation of light nuclei and nuclear force

Performance on K computer

- Kernel (MatVec) performance: >50%
- Solver performance: ～26%
- Weak scaling test
  - $6^3 \times 12$/node fixed
  - 16 nodes ($V=12^3 \times 24$) ⇒ 12288 nodes ($V=48 \times 72 \times 96^2$)

B/F=0.5 on K computer

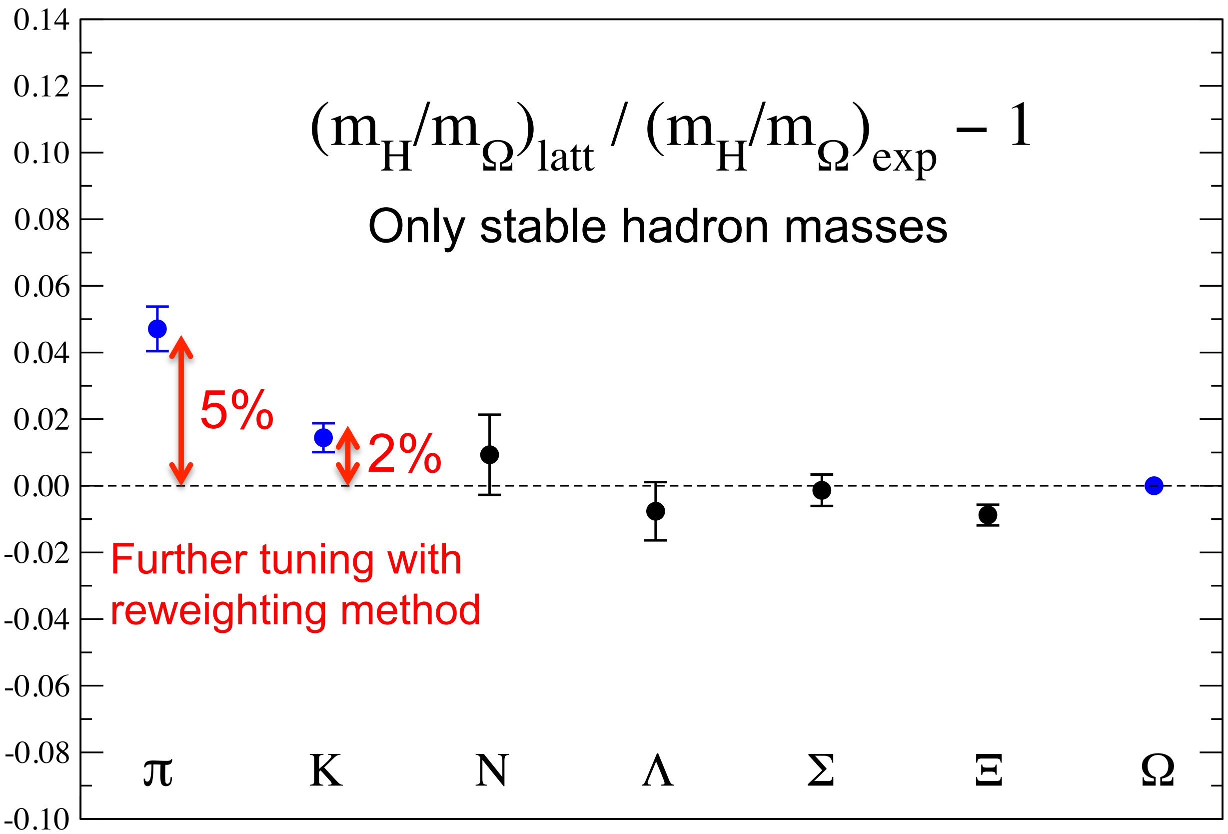


#node	scalability
16 ⇒ 256	98%
256 ⇒ 2048	98%
2048 ⇒ 12288	96%

Production run started in fall of 2012

Current status

- Configuration generation with DDHMC
  - 2+1 flavor (m_u=m_d≠m_s) QCD
  - stout-smeared Wilson-clover with NP C_{SW}
  - lattice size=96^4, lattice spacing∼0.1fm



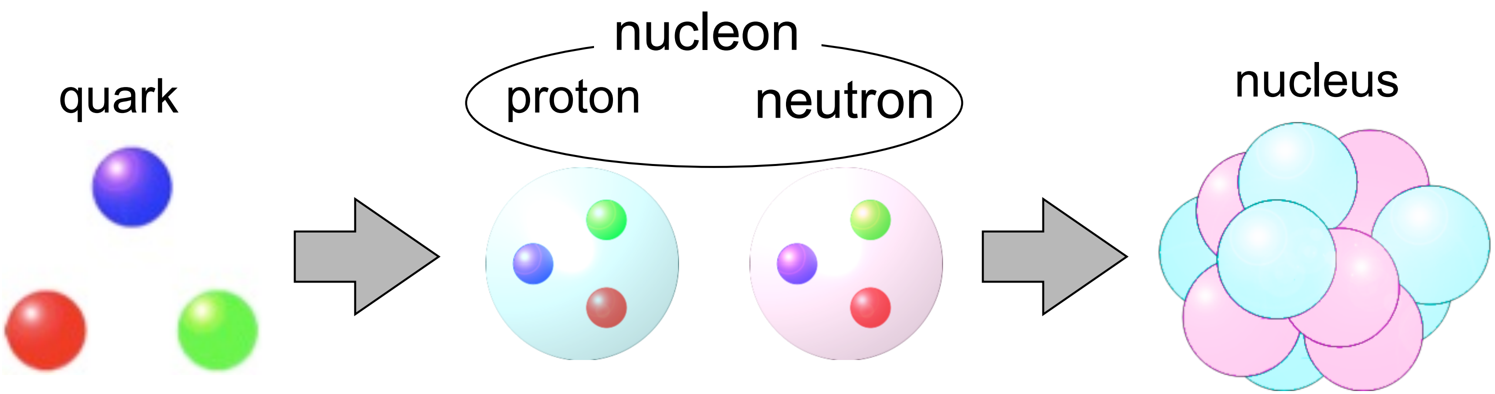
preliminary

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

§4. Construction of Nuclei

We are now achieving a precision measurement of hadron masses

Next step is a challenge for multi-scale physics



Exploratory study for ^{4}He and ^{3}He nuclei   Yamazaki-YK-Ukawa 10,12

$$\langle \mathcal{O}_{^4\mathrm{He}}(t)\mathcal{O}^\dagger_{^4\mathrm{He}}(0)\rangle \stackrel{t\gg 0}{\approx} C\exp\left(-m_{^4\mathrm{He}}t\right)$$

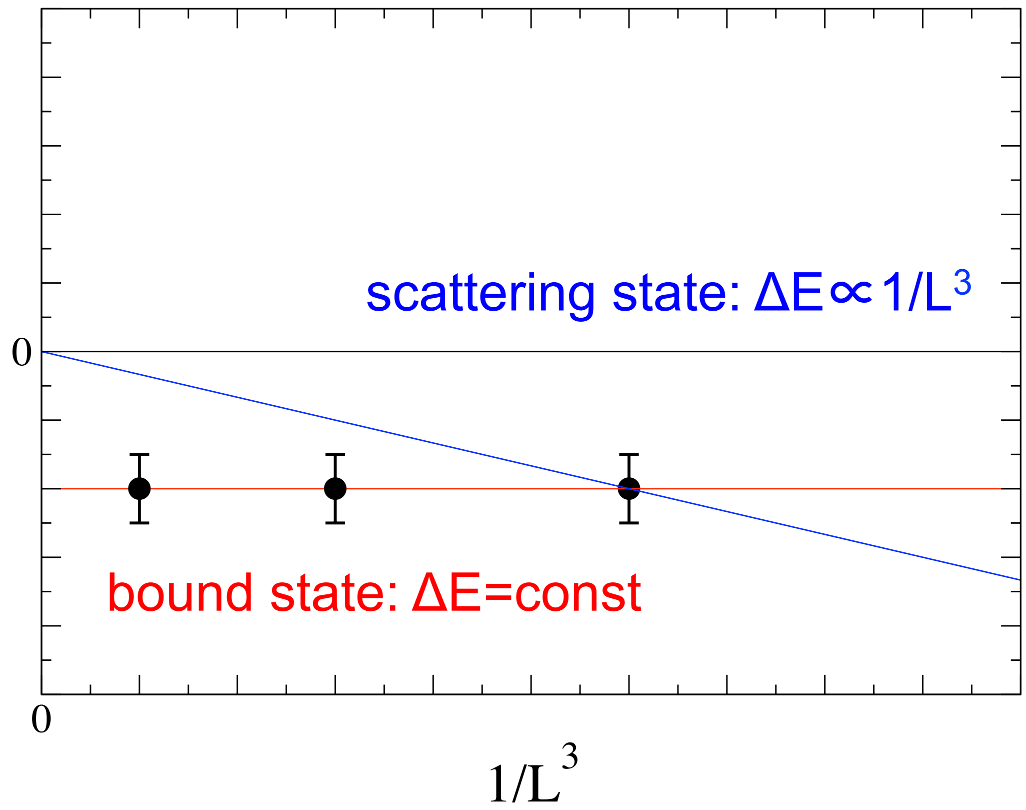
^{4}He: 2 proton+2 neutron ⇒ 12 quark propagators

^{3}He: 2 proton+1 neutron ⇒ 9 quark propagators

Identification of Bound State in a Finite Box

$\Delta E<0$ both for bound state and attractive scattering state in L^3 box

ex. ^{4}He case: $\Delta E_{^4\mathrm{He}} = m_{^4\mathrm{He}} - 4m_N$

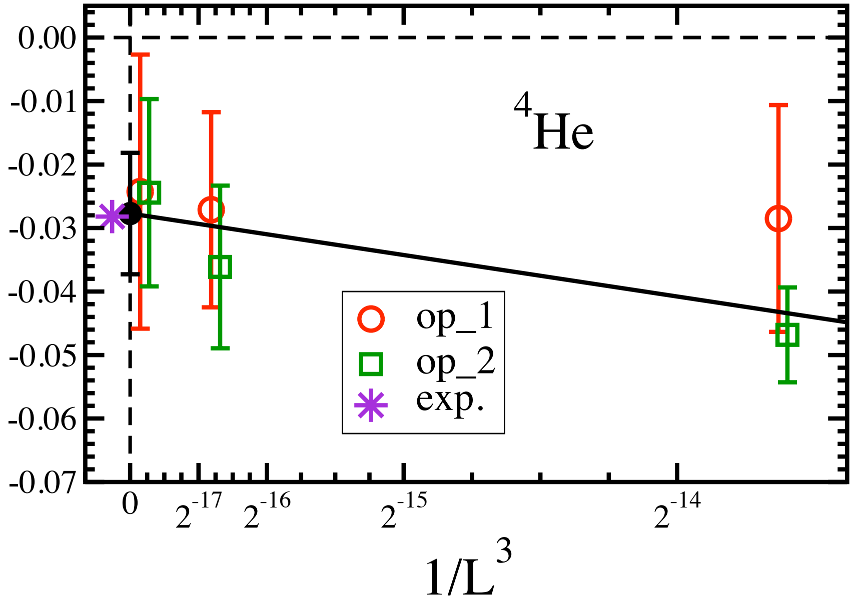


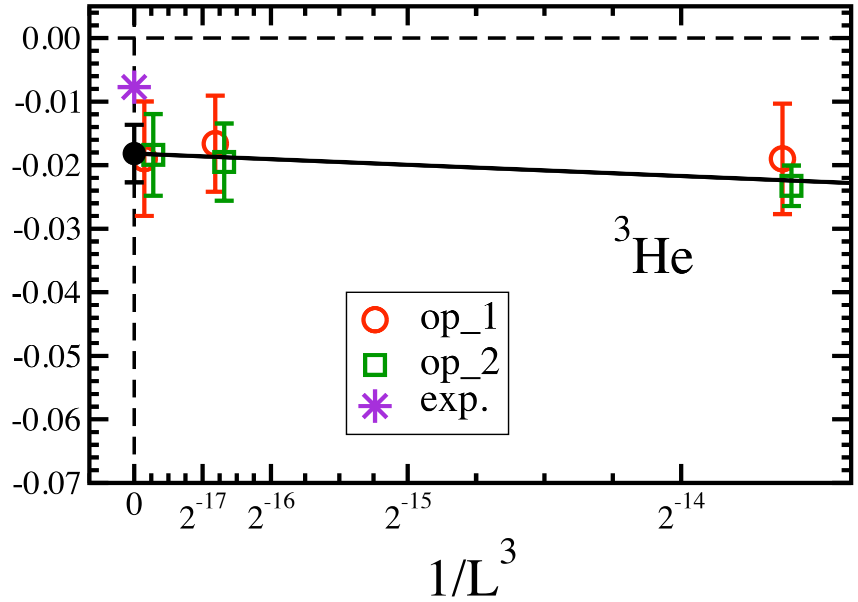
Mandatory to check volume dependence of ΔE

Exploratory Study in Quenched QCD

Yamazaki-YK-Ukawa 10

m_π=0.8 GeV, m_N=1.6 GeV in quenched QCD
(Real world: m_N=0.94 GeV)





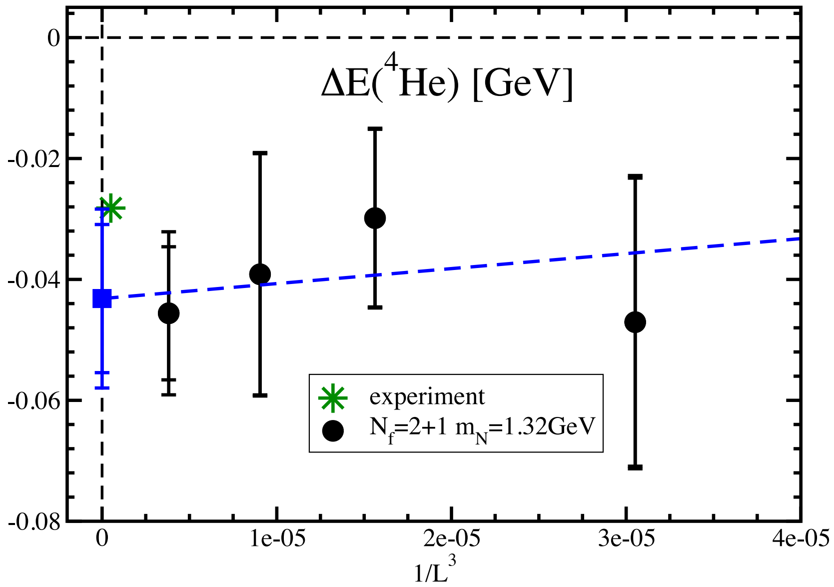
First successful construction of helium nuclei
⇒ 2+1 flavor QCD with lighter quark masses

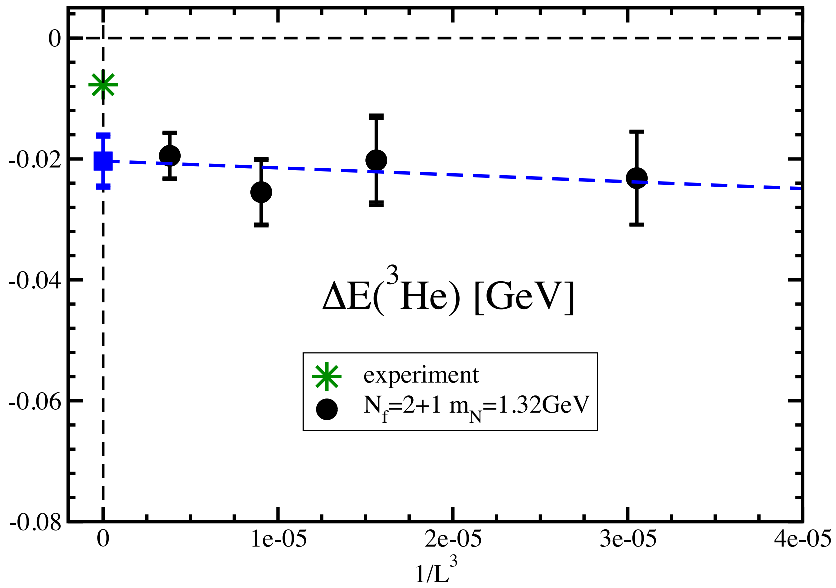
Light Nuclei in 2+1 Flavor QCD (1)

Yamazaki-YK-Ukawa 12

2+1フレーバーQCD, m_π＝0.5 GeV, m_N=1.32 GeV on HA-PACS

	4He	3He	NN(3S1)	NN(1S0)
Binding energy [MeV]	43(12)(8)	20.3(4.0)(2.0)	11.5(1.1)(0.6)	7.4(1.3)(0.6)
Exp. value [MeV]	28.3	7.72	2.22	0





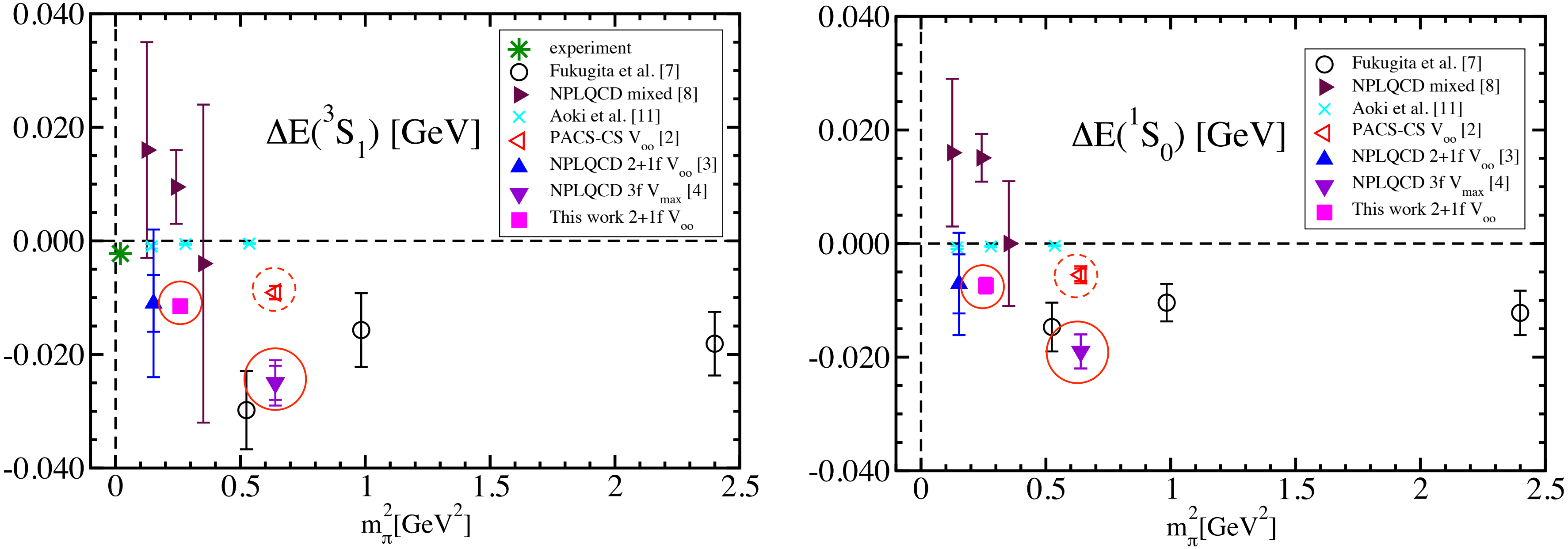
Successful construction of helium nuclei in 2+1 flavor QCD

Light Nuclei in 2+1 Flavor QCD(2)

Yamazaki-YK-Ukawa 12

Both $^3S_1$ and $^1S_0$ channels are bound at heavy quark region

$\Delta E_{NN}=m_{NN}-2m_N$



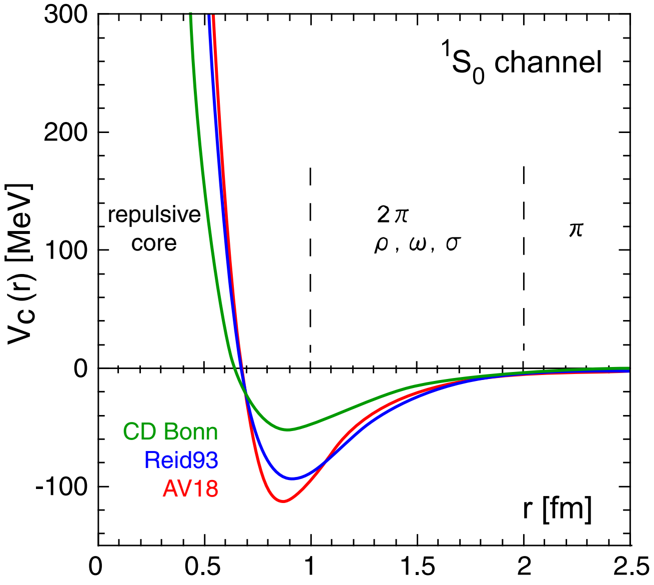
$|\Delta E(^3S_1)| > |\Delta E(^1S_0)|$ is observed

Important to check quark mass dependence

Target on K computer: construction of nuclei at the physical point

§5. Nuclear Force

Phenomenological model

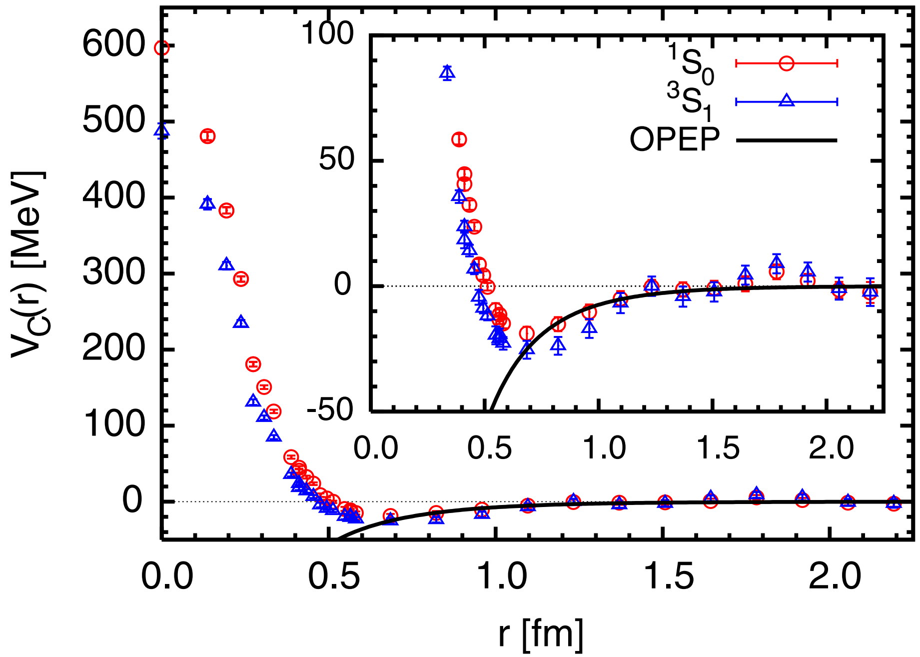


Ishii-Aoki-Hatsuda 07

based on equal-time BS amplitude

$$\varphi_E(\mathbf{r}) = \langle 0|N(\mathbf{x}+\mathbf{r},0)N(\mathbf{x},0)|6q,E\rangle$$

Quenched QCD, m_N=1.34GeV



$$V_C(r) = E + \frac{1}{2\mu}\frac{\vec{\nabla}^2\phi(r)}{\phi(r)}$$

BS wave function with lattice QCD ⇒ NN Potential

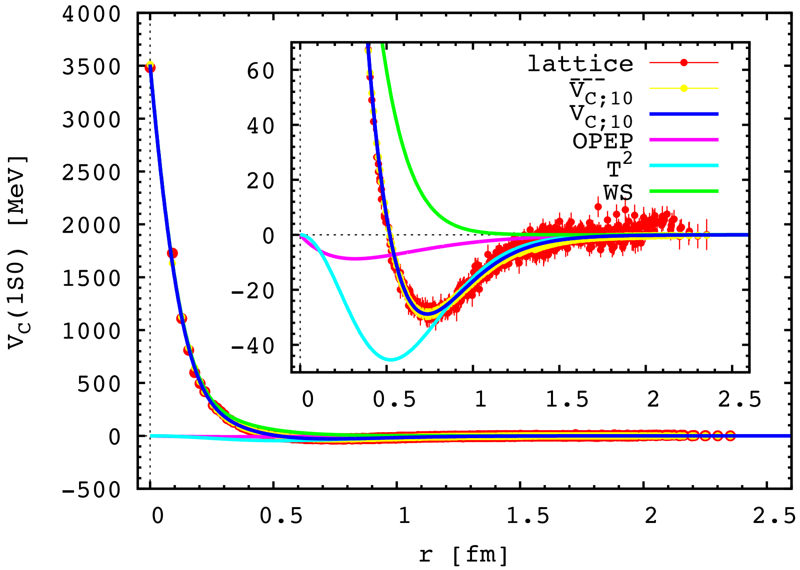
Possible Applications

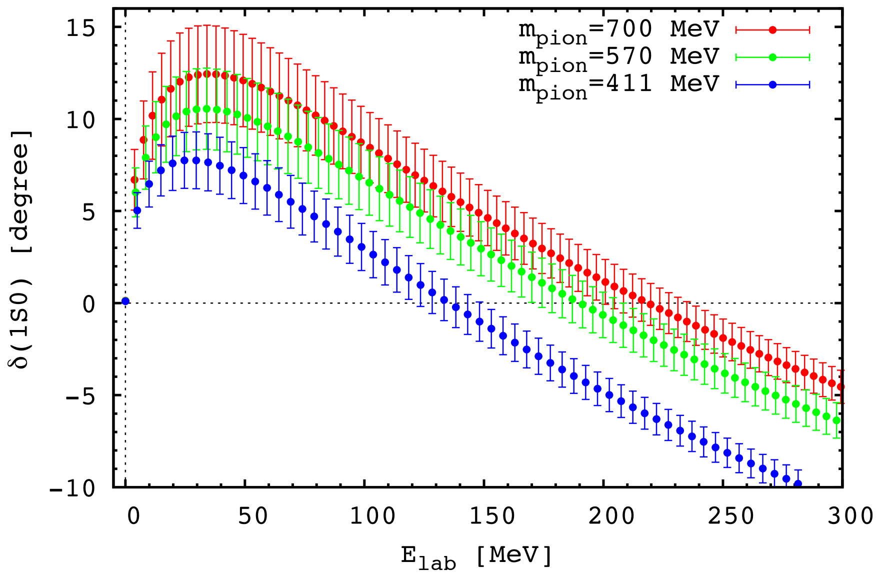
- Determination of nuclear force at the physical point
  Center force, tensor force, LS force, …
- Determination of hyperon force at the physical point
  various channels with the strangeness $S=-1, -2, -3, -4$
- 3 body force
  repulsive force at the short distance?
- Studies of exotic hadrons
  representative case is H-dibaryon

Preparatory Studies

HAL QCD 12

2+1 flavor QCD, lattice size=$32^3\times64$, m_π＝0.70, 0.57, 0.41 GeV





Attractive phase shift, though the magnitude is just 10% of exp. value
(no bound state ⇒ inconsistency against the direct method)
Phase shift becomes smaller, as quark mass decreases
⇒ need direct comparison with exp. values at the physical point

§6. Summary

Lattice QCD on K computer

<u>scientific target</u>

- 1+1+1 flavor QCD+QED at the physical point
- Investigation of resonances
- Direct construction of light nuclei
- Determination of baryon-baryon potentials
- Other physical quantities …