Direct calculation of light nucleus from lattice QCD

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Refs: PRD81:111504(R)(2010); PRD84:054506(2011); PRD86:074514(2012)
PRD92:014501(2015); PoS(LATTICE 2015)081

First Tsukuba-CCS-RIKEN joint workshop
on microscopic theories of nuclear structure and dynamics
@ RIEKN, Dec. 12–13, 2016 and CCS, Dec. 14–16, 2016

Outline

- Introduction
- Calculation method of nucleus in lattice QCD
- Simulation parameters
- Results of light nuclei
  - NN channels
  - ^{4}He and ^{3}He channels
- Summary and future work

Introduction

$$\text{Binding force} \begin{cases} \text{protons and neutrons} \rightarrow \text{nuclei} \\ \text{quarks and gluons} \rightarrow \text{protons and neutrons} \end{cases}$$

both from fundamental strong interaction of quark and gluon

well known, but hard to prove

Spectrum of proton and neutron (nucleons)

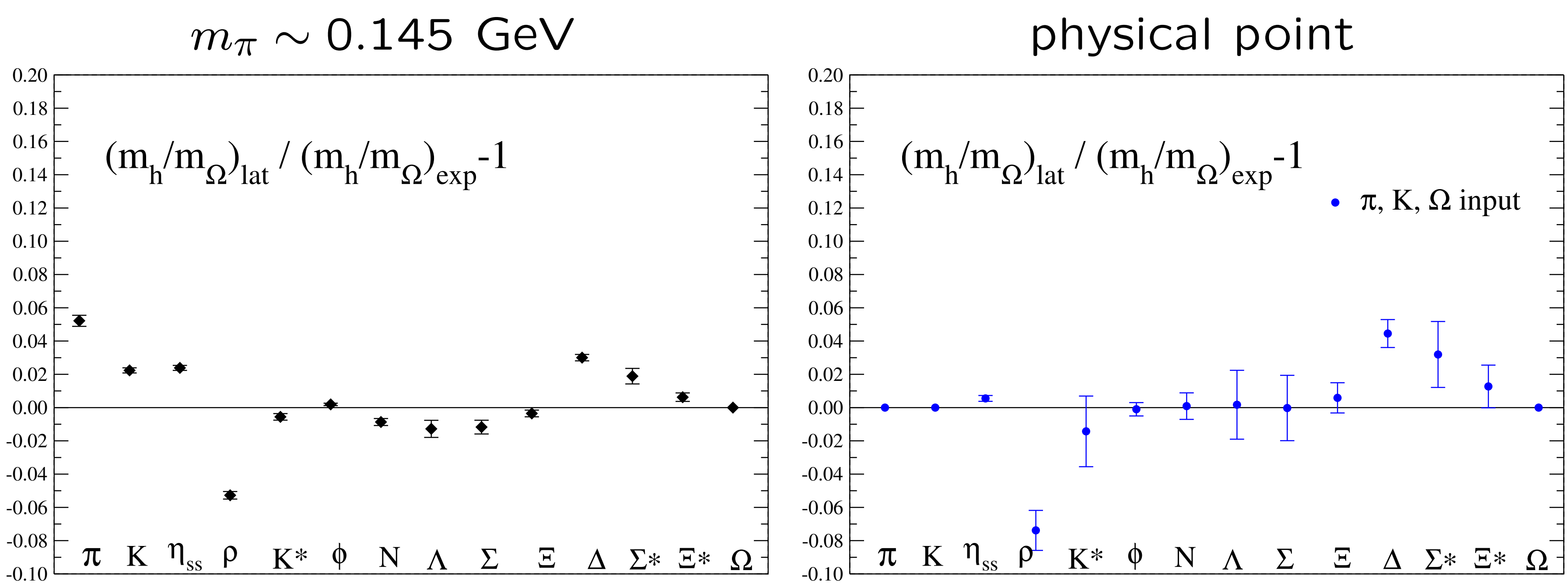
success of non-perturbative lattice QCD calculation

$$\overbrace{\text{quark and gluon} \rightarrow \text{proton and neutron}}^{\text{degrees of freedom of quarks and gluons}} \rightarrow \text{nucleus}$$

Hadron spectrum in $N_f = 2+1$ QCD

Lattice 2015, Ukita for PACS Collaboration PoS(LATTICE2015)075

$m_\pi \sim 0.145$ GeV on $L \sim 8$ fm at $a^{-1} = 2.33$ GeV (SPIRE Field 5)
using reweighting m_{ud}, m_s + extrapolation $\rightarrow$ physical m_π and m_K



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$$\bar{l}_3 = 2.87(62), \quad \bar{l}_4 = 4.38(33)$$

FLAG2013: $\bar{l}_3 = 3.05(99)$, $\bar{l}_4 = 4.02(28)$ at $\mu = m_\pi^{\mathrm{phys}}$

$$m_{ud}^{\overline{\mathrm{MS}}} = 3.142(26)(35)(28)\mathrm{MeV}, \quad m_s^{\overline{\mathrm{MS}}} = 88.59(61)(98)(79)\mathrm{MeV}$$

FLAG2013: $m_{ud}^{\overline{\mathrm{MS}}} = 3.42(6)(7)\mathrm{MeV}$, $m_s^{\overline{\mathrm{MS}}} = 93.8(1.5)(1.9)\mathrm{MeV}$

$$f_\pi = 131.79(80)(90)(1.25)\mathrm{MeV}, \quad f_K = 155.55(68)(1.06)(1.48)\mathrm{MeV}$$

FLAG2013: $f_\pi = 130.2(1.4)\mathrm{MeV}$, $f_K = 156.3(0.9)\mathrm{MeV}$

reasonably consistent

investigation of $a \to 0$ limit necessary

Introduction

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both from fundamental strong interaction of quark and gluon

well known, but hard to prove

Spectrum of proton and neutron (nucleons)

success of non-perturbative lattice QCD calculation

degrees of freedom of quarks and gluons

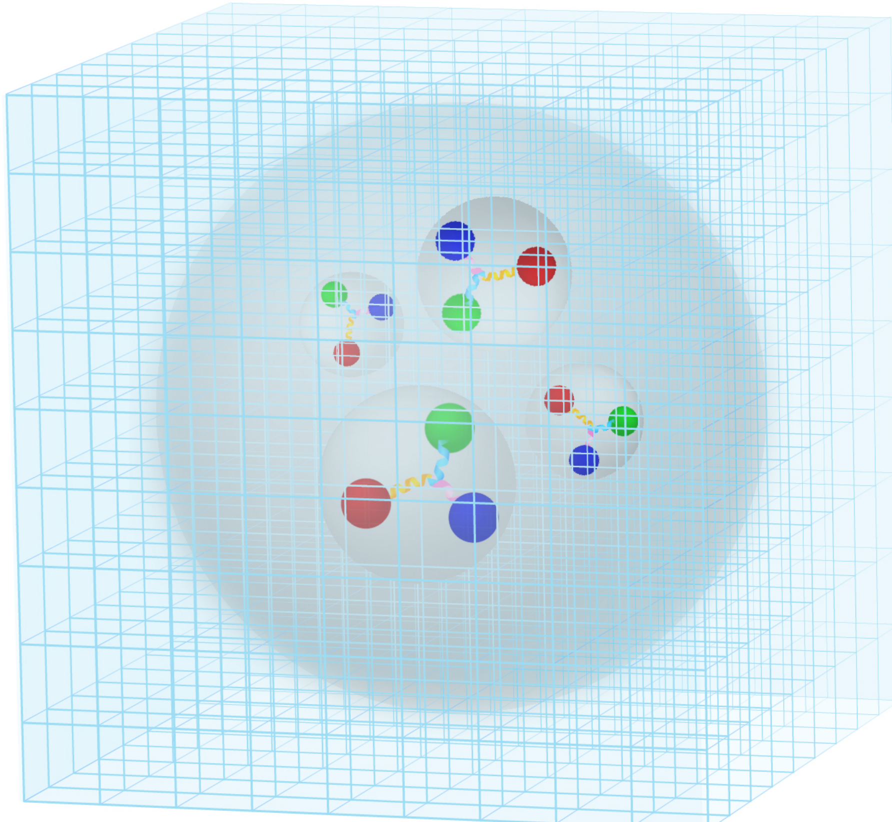
$$\underbrace{\overbrace{\text{quark and gluon} \rightarrow \text{proton and neutron}}\rightarrow \text{nucleus}}$$

goal: quantitatively understand property of nucleus from QCD

So far not many studies for multi-baryon bound states

$\rightarrow$ Can we reproduce binding energy of light nuclei?

Ultimate goal of lattice QCD



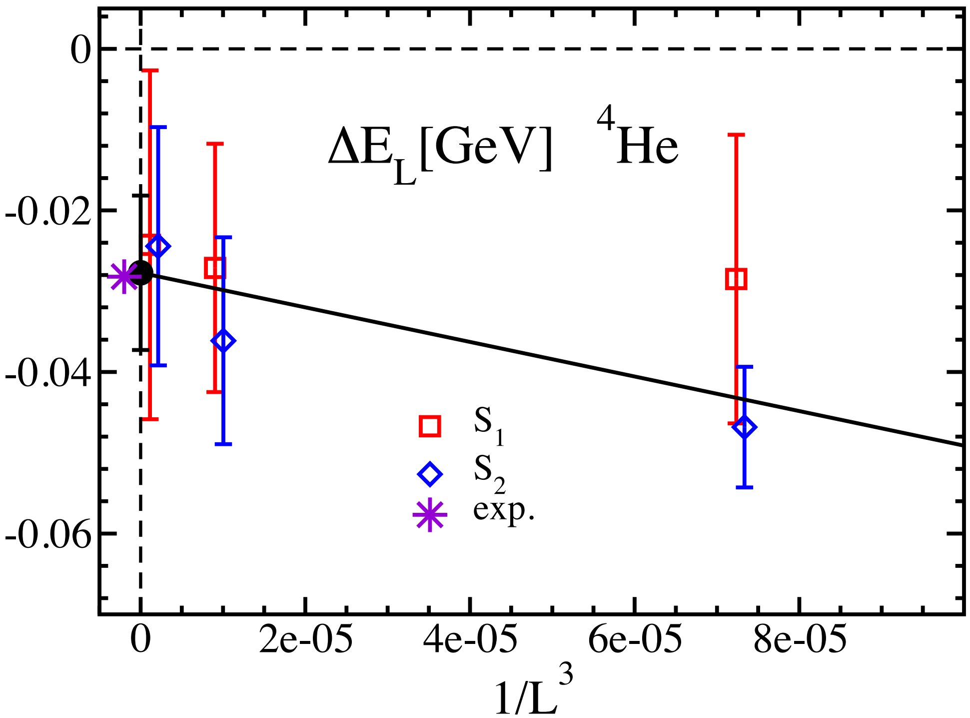
http://www.jicfus.jp/jp/promotion/pr/mj/2014-1/ ; figure from Irie-san

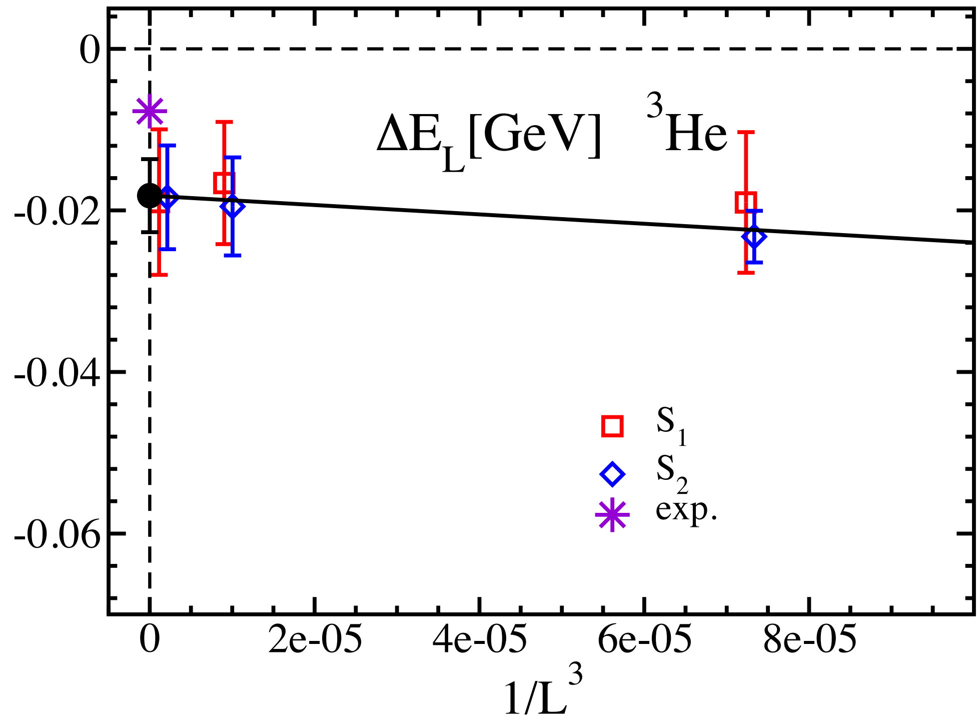
quantitatively understand property of nuclei from QCD

Exploratory study of three- and four-nucleon systems

PACS-CS Collaboration, PRD81:111504(R)(2010)

Identification of bound state from volume dependence of ΔE





$\Delta E_{^4\text{He}} = 27.7(7.8)(5.5)$ MeV $\qquad$ $\Delta E_{^3\text{He}} = 18.2(3.5)(2.9)$ MeV

1. Observe bound state in both channels
2. Same order of ΔE to experiment

Several systematic errors included, e.g., $N_f = 0$, $m_\pi = 0.8$ GeV

Multi-baryon bound state from lattice QCD

1. ^{4}He and ^{3}He
   - '10 PACS-CS $N_f = 0$ $m_\pi = 0.8$ GeV PRD81:111504(R)(2010)
   - '12 HALQCD $N_f = 3$ $m_\pi = 0.47$ GeV, $m_\pi > 1$ GeV ^{4}He
   - '12 NPLQCD $N_f = 3$ $m_\pi = 0.81$ GeV
   - '12 TY *et al.* $N_f = 2+1$ $m_\pi = 0.51$ GeV PRD86:074514(2012)
   - '15 TY *et al.* $N_f = 2+1$ $m_\pi = 0.30$ GeV PRD92:014501(2015)
2. H dibaryon in ΛΛ channel (S=−2, I=0)
   - '11, '12 NPLQCD $N_f = 2+1$ $m_\pi = 0.39$ GeV, $N_f = 3$ $m_\pi = 0.81$ GeV
   - '11, '12 HALQCD $N_f = 3$ $m_\pi = 0.47$–1.02 GeV
   - '11 Luo et al. $N_f = 0$ $m_\pi = 0.5$–1.3 GeV
   - '14, '15, '16 Mainz $N_f = 2$ $m_\pi = 0.45, 1.0$ GeV
3. NN
   - '11 PACS-CS $N_f = 0$ $m_\pi = 0.8$ GeV PRD84:054506(2011)
   - '12 NPLQCD $N_f = 2+1$ $m_\pi = 0.39$ GeV (Possibility)
   - '12 NPLQCD, '15 CalLat $N_f = 3$ $m_\pi = 0.81$ GeV
   - '12 TY *et al.* $N_f = 2+1$ $m_\pi = 0.51$ GeV PRD86:074514(2012)
   - '15 TY *et al.* $N_f = 2+1$ $m_\pi = 0.30$ GeV PRD92:014501(2015)
   - '15 NPLQCD $N_f = 2+1$ $m_\pi = 0.45$ GeV

Other states: ΞΞ, '12 NPLQCD; spin-2 $N\Omega$, ^{16}O and ^{40}Ca, '14 HALQCD, $\cdots$

Calculation method of multi-nucleon bound state

Traditional method: example ^{4}He channel

$$\langle 0|O_{^4\text{He}}(t)\overline{O}_{^4\text{He}}(0)|0\rangle = \sum_n \langle 0|O_{^4\text{He}}|n\rangle\langle n|\overline{O}_{^4\text{He}}|0\rangle e^{-E_n t} \xrightarrow[t\gg 1]{} A_0\, e^{-E_0 t}$$

Difficulties for multi-nucleon calculation

1. Statistical error

Statistical error $\propto \exp\left(N_N \left[m_N - \frac{3}{2}m_\pi\right] t\right)$

$\rightarrow$ heavy quark $m_\pi = 0.8$–0.3 GeV + large # of measurements

2. Calculation cost PACS-CS PRD81:111504(R)(2010)

Wick contraction for ^{4}He $= p^2 n^2 = (udu)^2(dud)^2$: 518400 $\rightarrow$ 1107

$\rightarrow$ reduction using $p(n) \leftrightarrow p(n)$ $p \leftrightarrow n$, $u(d) \leftrightarrow u(d)$ in $p(n)$

+ block of 3 quark props(parallel) and contraction(workstation)

'12 Doi and Endres; Detmold and Orginos; '13 Günther et al.; '15 Nemura

3. Identification of bound state on finite volume

attractive scattering state $\Delta E_L = E_0 - N_N m_N = O(L^{-3}) < 0$

'86,'91 Lüscher, '07 Beane *et al.*

$\rightarrow$ Volume dependence of $\Delta E_L \rightarrow \Delta E_\infty \neq 0 \rightarrow$ bound state

Spectral weight: '04 Mathur *et al.*, Anti-PBC '05 Ishii *et al.*

Calculation method of multi-nucleon bound state

Traditional method in lattice QCD (NN channel)

nucleon correlation function

$$C_N(t) \;=\; \langle 0|N(t)\overline{N}(0)|0\rangle = \sum_n \langle 0|N|n\rangle\langle n|\overline{N}|0\rangle e^{-E_n^N t} \xrightarrow[t\geq t_N\gg 1]{} A_0^N\, e^{-m_N t}$$

NN correlation function

$$C_{NN}(t) \;=\; \langle 0|O_{NN}(t)\overline{O}_{NN}(0)|0\rangle = \sum_n \langle 0|O_{NN}|n\rangle\langle n|\overline{O}_{NN}|0\rangle e^{-E_n t} \xrightarrow[t\geq t_{NN}\gg 1]{} A_0\, e^{-E_{NN} t}$$

Ratio of correlation functions

$$R(t) = \frac{C_{NN}(t)}{(C_N(t))^2} \xrightarrow[t\geq t_R\gg 1]{} A_0'\, e^{-\Delta E t}, \qquad \Delta E = E_{NN} - 2m_N$$

$\boxed{\text{Important condition: } t_R \geq t_N, t_{NN}}$

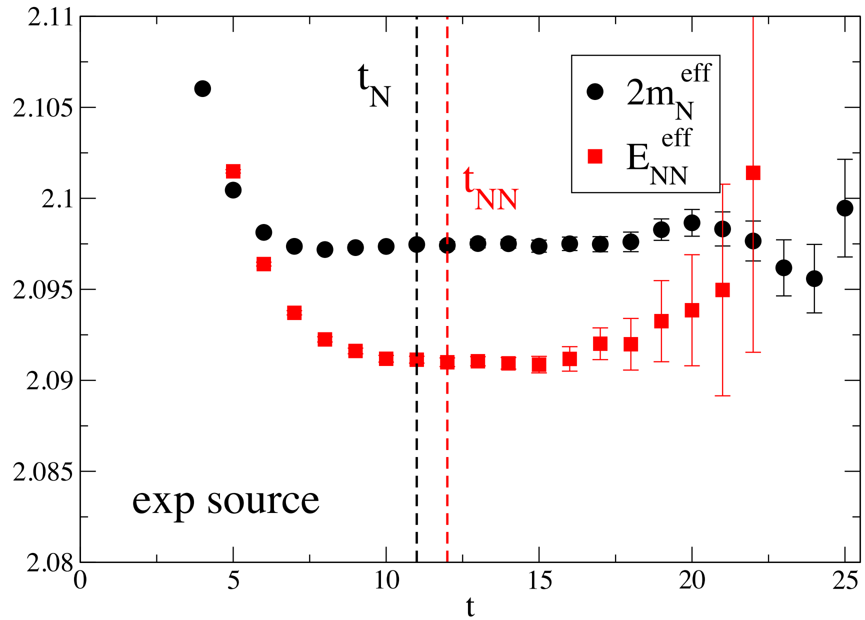
$C_N(t)$ and $C_{NN}(t)$ are written by each ground state in $t \geq t_R$

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $N_f = 0$

Preliminary result: $L^3 \times T = 20^3 \times 64$ $N_f = 0$ $m_\pi = 0.8$ GeV, $N_{\text{meas}} \sim 1.1 \times 10^7$

Effective mass : $m^{\text{eff}} = \log(C(t)/C(t+1)) \xrightarrow[t \gg 1]{} m$

Effective mass in $^3S_1$ channel



vertical dashed line : plateau starts t_N or t_{NN}

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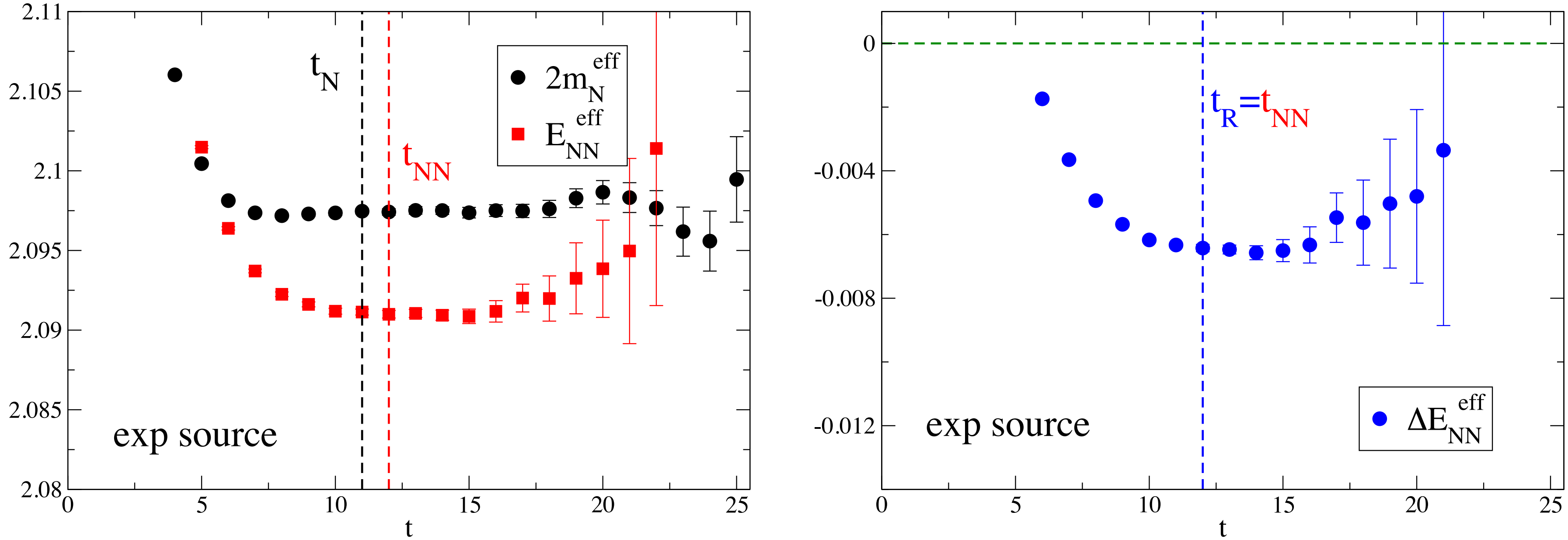
Effective mass in $^3S_1$ channel

$$\Delta E_{NN}^{\text{eff}} = \log(R(t)/R(t+1)) \xrightarrow[t \geq t_R]{} E_{NN} - 2m_N$$



vertical dashed line : plateau starts t_N or t_{NN} or t_R

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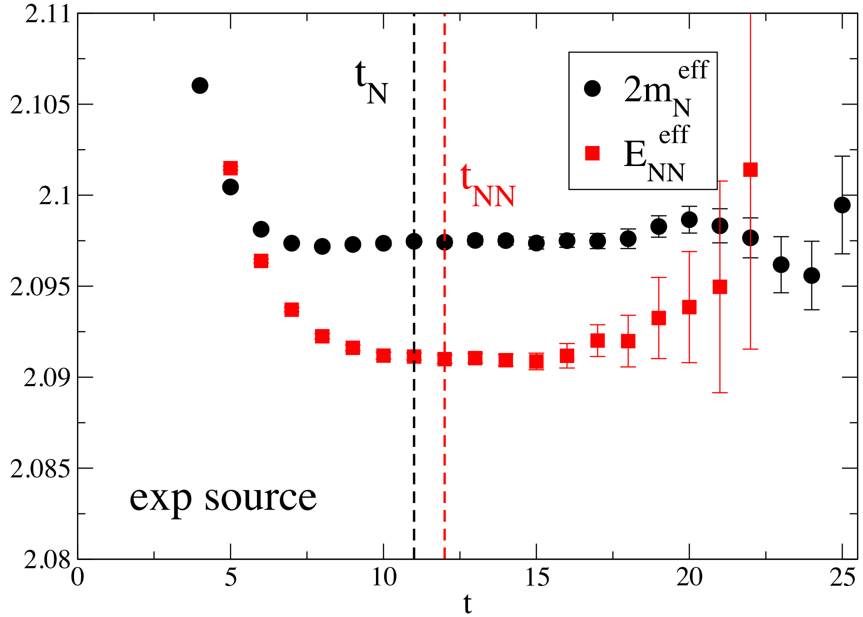
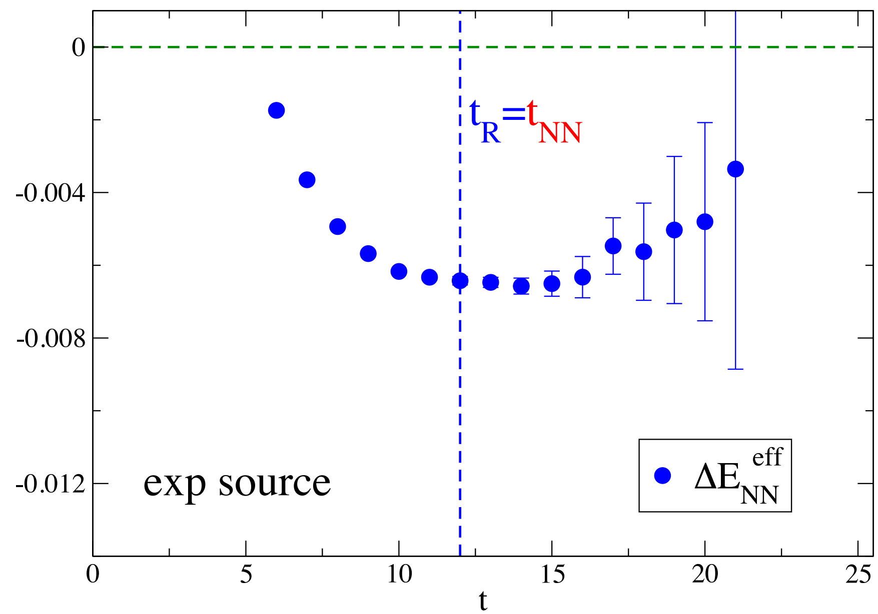


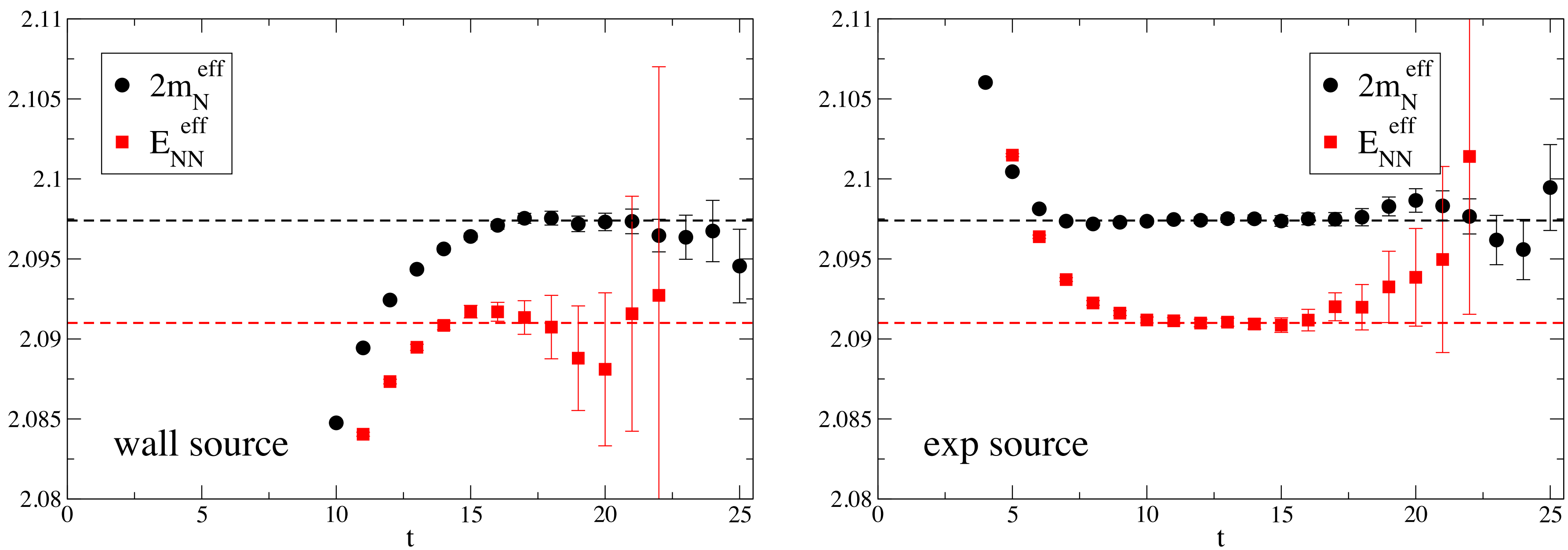


claim: different results from exp source and wall source '16 HALQCD

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $N_f = 0$

Preliminary result: $L^3 \times T = 20^3 \times 64$ $N_f = 0$ $m_\pi = 0.8$ GeV, $N_{\text{meas}} \gtrsim 1.1 \times 10^7$

Effective mass in $^3S_1$ channel



wall source needs longer t for plateau $\leftarrow$ harder to calculate due to noise

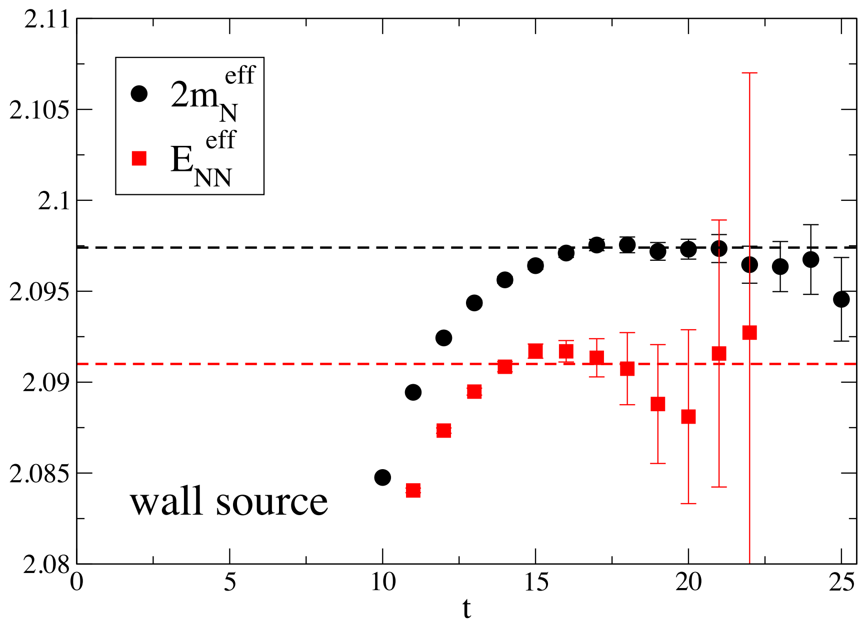
consistent results in plateau region

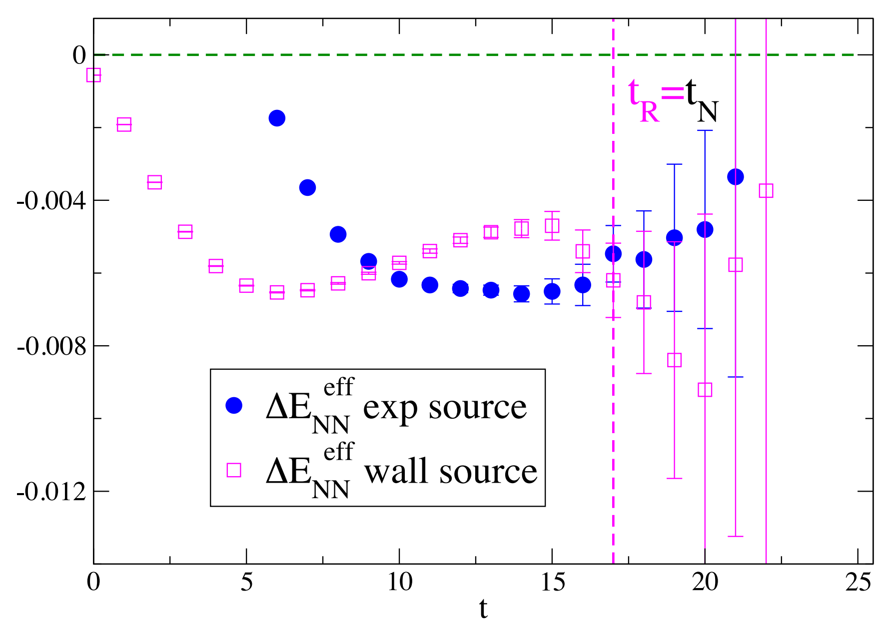
$R(t) = C_{NN}(t)/(C_N(t))^2$ in $N_f = 0$

Preliminary result: $L^3 \times T = 20^3 \times 64$ $N_f = 0$ $m_\pi = 0.8$ GeV, $N_{\text{meas}} \gtrsim 1.1 \times 10^7$

Effective mass in $^3\text{S}_1$ channel

$$\Delta E_{NN}^{\text{eff}} = \log(R(t)/R(t+1)) \xrightarrow[t \geq t_R]{} E_{NN} - 2m_N$$





$\Delta E_{NN}^{\text{eff}}$ of wall source : nontrivial structure (also observed in other volumes)

consistent result with exp source in $t \geq t_R$

exp source : easier to calculate ΔE_{NN} $\rightarrow$ used in our calculation

Simulation parameters

$N_f = 2{+}1$ QCD $\beta = 1.90$, $a^{-1} = 2.194$ GeV with $m_\Omega = 1.6725$ GeV, '10 PACS-CS

Iwasaki gauge + non-perturbative $O(a)$-improved Wilson fermion actions

$m_\pi = 0.51$ GeV and $m_N = 1.32$ GeV PRD86:074514(2012)

$m_\pi = 0.30$ GeV and $m_N = 1.05$ GeV PRD92:014501(2015)

$m_s \sim$ physical strange quark mass

^{4}He, ^{3}He, NN(^{3}S$_1$ and ^{1}S$_0$)

		$m_\pi = 0.5$ GeV		$m_\pi = 0.3$ GeV		R
L	L [fm]	N_{conf}	N_{meas}	N_{conf}	N_{meas}	
32	2.9	200	192			
40	3.6	200	192			
48	4.3	200	192	400	1152	12
64	5.8	190	256	160	1536	5

$R = (N_{\text{conf}} \cdot N_{\text{meas}})_{0.3\text{GeV}} / (N_{\text{conf}} \cdot N_{\text{meas}})_{0.5\text{GeV}}$

Exponential smeared source and point sink (N with $p = 0$) operators

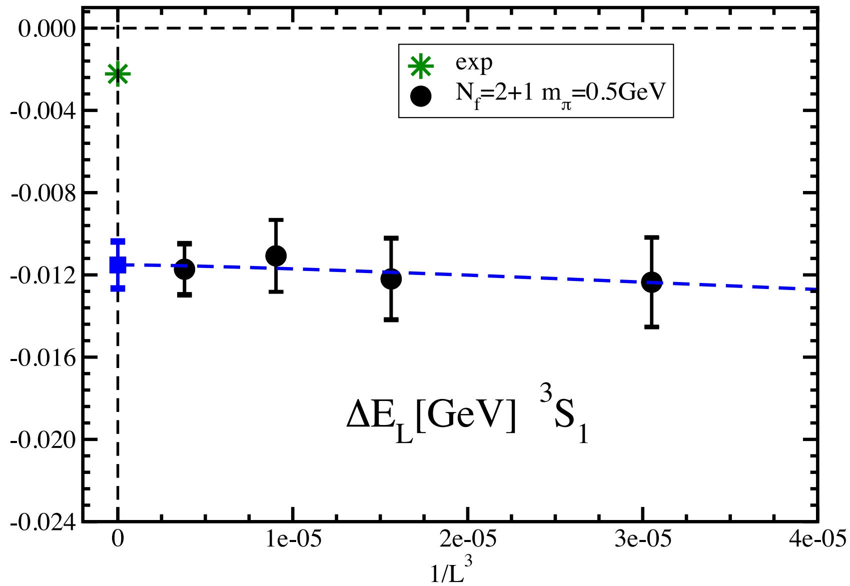
Computational resources

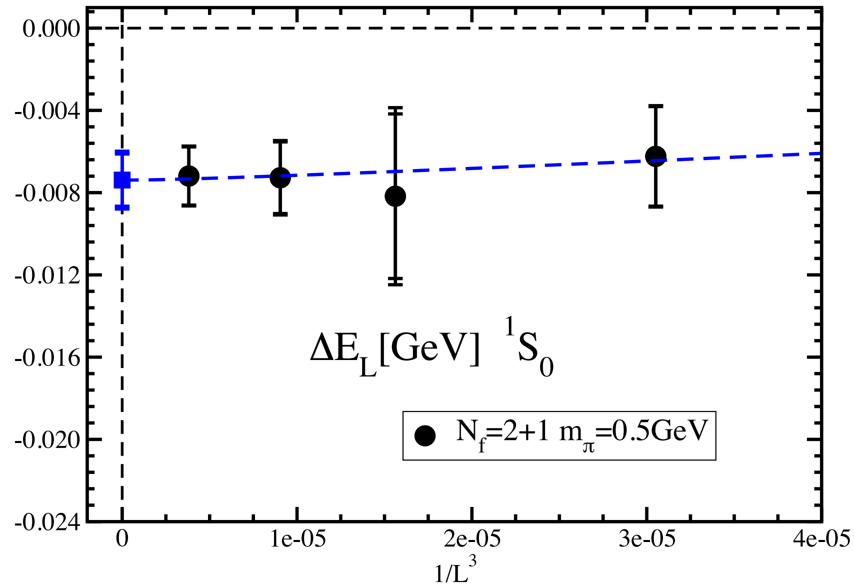
PACS-CS, T2K-Tsukuba, HA-PACS, COMA at Univ. of Tsukuba

T2K-Tokyo and FX10 at Univ. of Tokyo, and K at AICS

Result: NN channels $\Delta E_{NN} = E_{NN} - 2m_N$

Effective energy shift $\Delta E_{NN}^{\mathrm{eff}}$ in $m_\pi = 0.5$ GeV



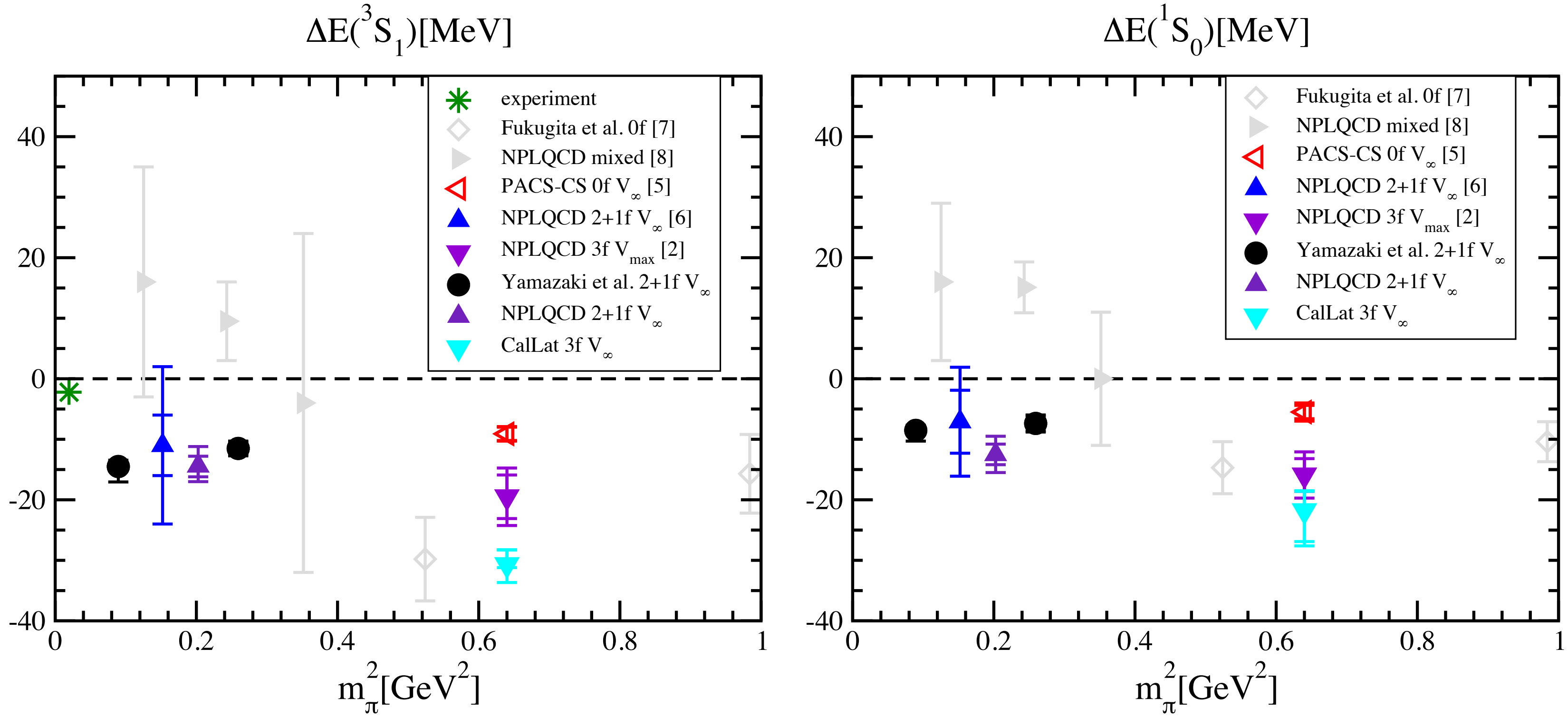


$L^3 \to \infty$ extrapolation based on Lüscher's finite volume formula

$$\Delta E_L = -\frac{\gamma^2}{m_N}\left\{1 + \frac{C_\gamma}{\gamma L}\sum_{\vec{n}}{}' \frac{\exp(-\gamma L\sqrt{\vec{n}^2})}{\sqrt{\vec{n}^2}}\right\}, \quad \Delta E_{NN} = \frac{\gamma^2}{m_N}$$

'04 Beane *et al.*, '06 Sasaki & TY

Result: NN channels (direct calculation) $\Delta E_{NN} = E_{NN} - 2m_N$



gray data: single volume calculation

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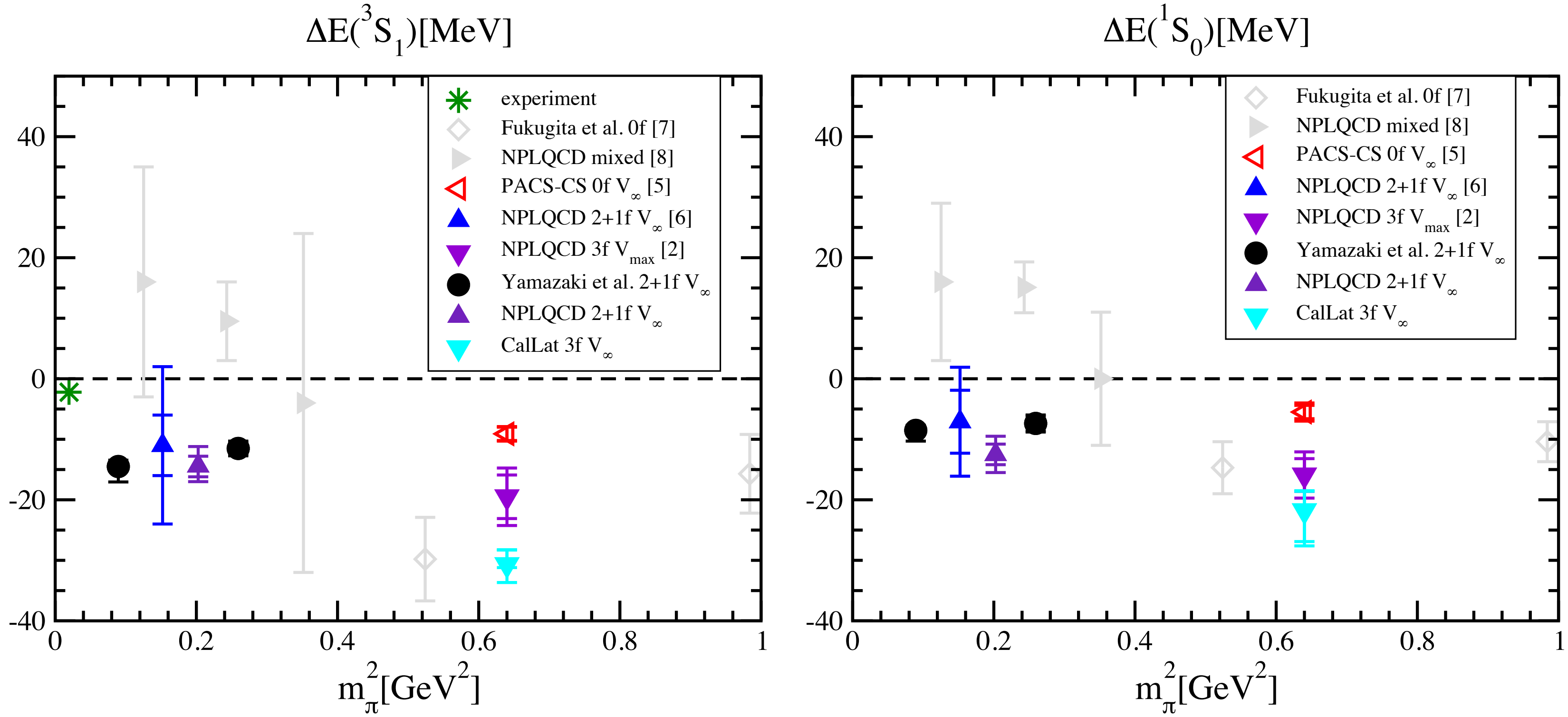
'04 Beane *et al.*, '06 Sasaki & TY

existence of bound states in $^3S_1$ and $^1S_0$

inconsistent with experiment due to larger m_π(?)

Investigation of m_π dependence $\to$ $m_\pi \sim 0.145$ GeV on $L \sim 8$ fm

Result: NN channels (direct calculation) $\Delta E_{NN} = E_{NN} - 2m_N$



gray data: single volume calculation

Investigations of m_π dependence $\to$ $m_\pi \sim 0.145$ GeV on $L \sim 8$ fm

Large finite volume effect expected even on $L \sim 8$ fm

'86 Lüscher, '04 Beane *et al.*, '14 Briceño *et al.*

^{3}S$_1$: $\Delta E_{\rm exp} = 2.2$ MeV

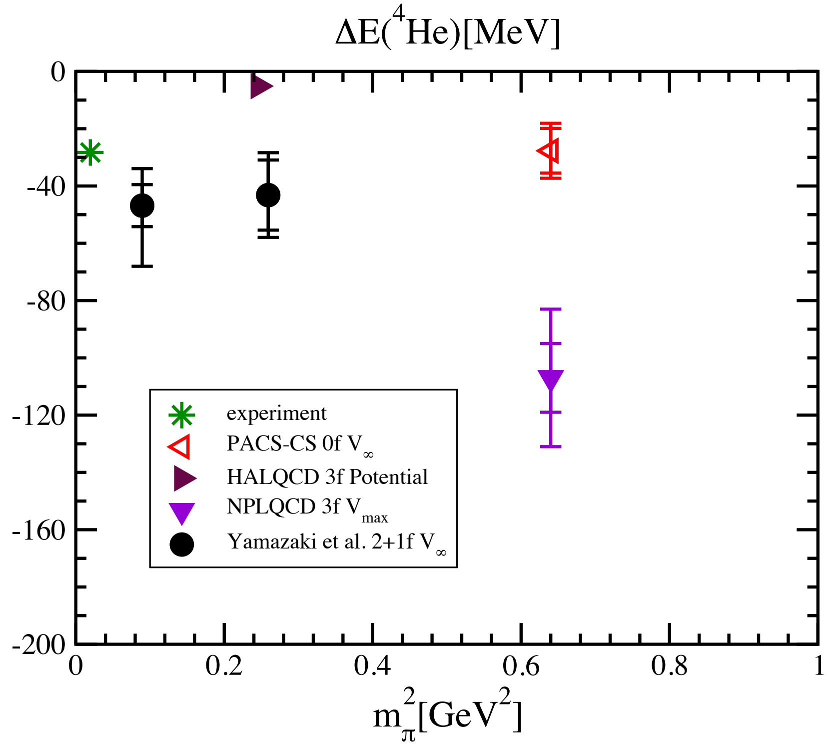
$$\Delta E_L = -\left(\Delta E_{\rm exp} + \mathcal{O}(\exp(-L\sqrt{m_N \Delta E_{\rm exp}}))\right) \lesssim -4 \text{ MeV}$$

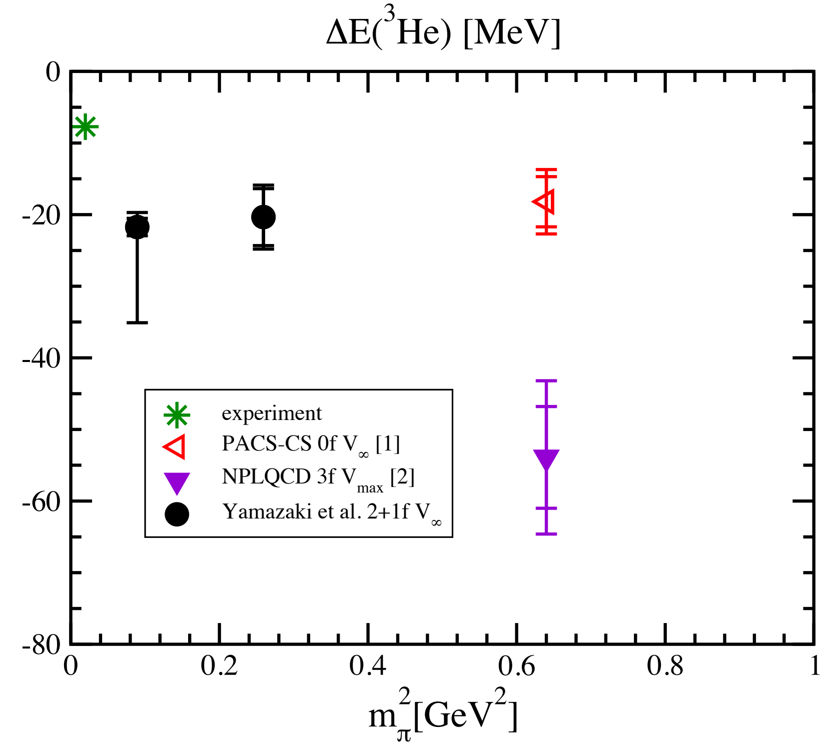
^{1}S$_0$: $a_0^{\rm exp} = 23.7$ fm

$$\Delta E_L = -\frac{4\pi a_0^{\rm exp}}{m_N L^3} + \mathcal{O}(1/L^4) \lesssim -2 \text{ MeV}$$

Result: ^{4}He and ^{3}He channels

$$\Delta E(^4\text{He}) = E_{^4\text{He}} - 4m_N \qquad \Delta E(^3\text{He}) = E_{^3\text{He}} - 3m_N$$





Light nuclei likely formed in 0.3 GeV $\leq m_\pi \leq$ 0.8 GeV

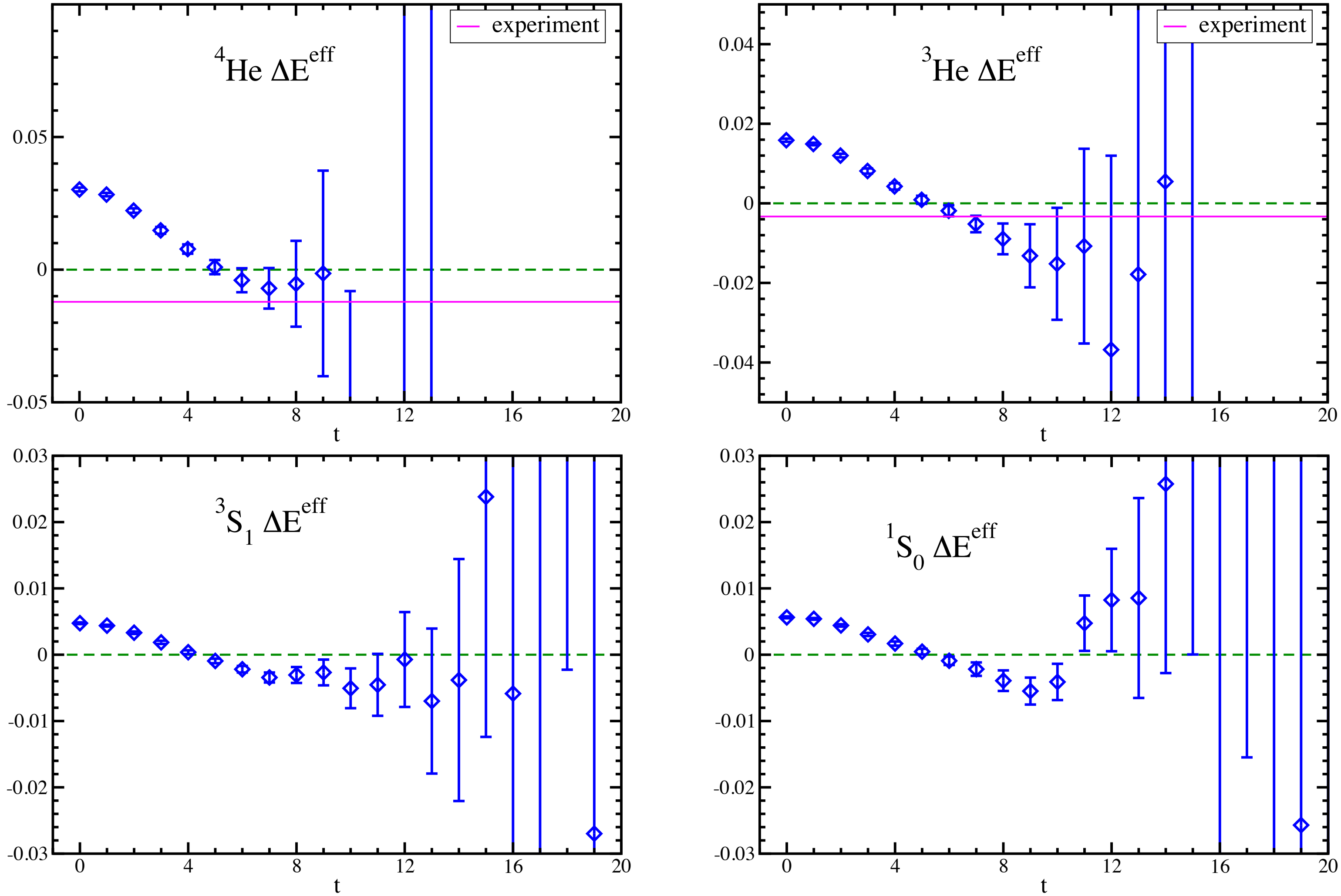
Same order of ΔE to experiments $\to$ relatively easier than NN

large $|\Delta E|$ makes less V dependence at physical m_π

touchstone of quantitative understanding of nuclei from lattice QCD

Investigations of m_π dependence $\to$ $m_\pi \sim$ 0.145 GeV on $L \sim$ 8 fm

Preliminary results of effective ΔE at $m_\pi \sim 0.145$ GeV on $L \sim 8$ fm



need more statistics to obtain clear signal

Computational resources (HPCI System Research Project: hp160124)

HA-PACS, COMA @Univ. of Tsukuba, K @AICS, FX100 @RIKEN

Summary

Direct calculation of light nucleus $NN(^3\mathrm{S}_1,\ ^1\mathrm{S}_0)$, ^{3}He, ^{4}He

$N_f = 0$ QCD $m_\pi = 0.8$ GeV

Wall source gives consistent result with exp source, but not suitable for direct calculation

- hard to obtain clear signal in plateau region
- $\Delta E_{NN}^{\mathrm{eff}}$: non monotonic structure in small t region

more sophisticated method (GEVP) necessary for more reliable result

$N_f = 2+1$ QCD $m_\pi = 0.5, 0.3$ GeV

bound state in ^{4}He, ^{3}He, $^3\mathrm{S}_1$ and $^1\mathrm{S}_0$

- ΔE larger than experiment and small m_π dependence
- Bound state in $^1\mathrm{S}_0$ not observed in experiment, but similar to

$N_f = 3$ $m_\pi = 0.8$ GeV by NPLQCD and CalLat; $N_f = 2+1$ $m_\pi = 0.45$ GeV by NPLQCD

Need further investigations of systematic errors

e.g. large m_π, finite lattice spacing, excited state

$N_f = 2+1$ $m_\pi \sim 0.145$ GeV on $L \sim 8$ fm