Calculation of helium nuclei in quenched lattice QCD

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1. Introduction

Spectrum of Nuclei

success of Shell model since 1949: Jensen and Mayer

degrees of freedom of protons and neutrons

Spectrum of nucleon (proton and neutron)

degrees of freedom of quarks and gluons

success of non-perturbative calculation of QCD such as lattice QCD

Motivation :

Understand property and structure of nuclei from QCD

If we can study nuclei from QCD, we may be able to

1. reproduce spectrum of nuclei
2. predict property of nuclei hard to calculate or observe

such as neutron rich nuclei

multi-nucleon system from lattice QCD

1. ΛΛ system (S=−2, I=0)

    H dibaryon: $\Delta E_H \sim 80$ MeV '77 Jaffe

    '85 Mackenzie & Thacker : Quenched QCD
    unbound

    '88 Iwasaki *et al.* : Quenched QCD
    bound : binding energy = 500 − 700 MeV

    '99 Pochinsky *et al.* : Quenched QCD
    unbound : $E_{\Lambda\Lambda} - 2m_\Lambda > 110$ MeV

    '00 Wetzorke *et al.* : Quenched QCD
    hard to decide unbound or slightly bound

    '02 Wetzorke & Karsch : Quenched QCD
    unbound : through L dependence

    H dibaryon: unbound

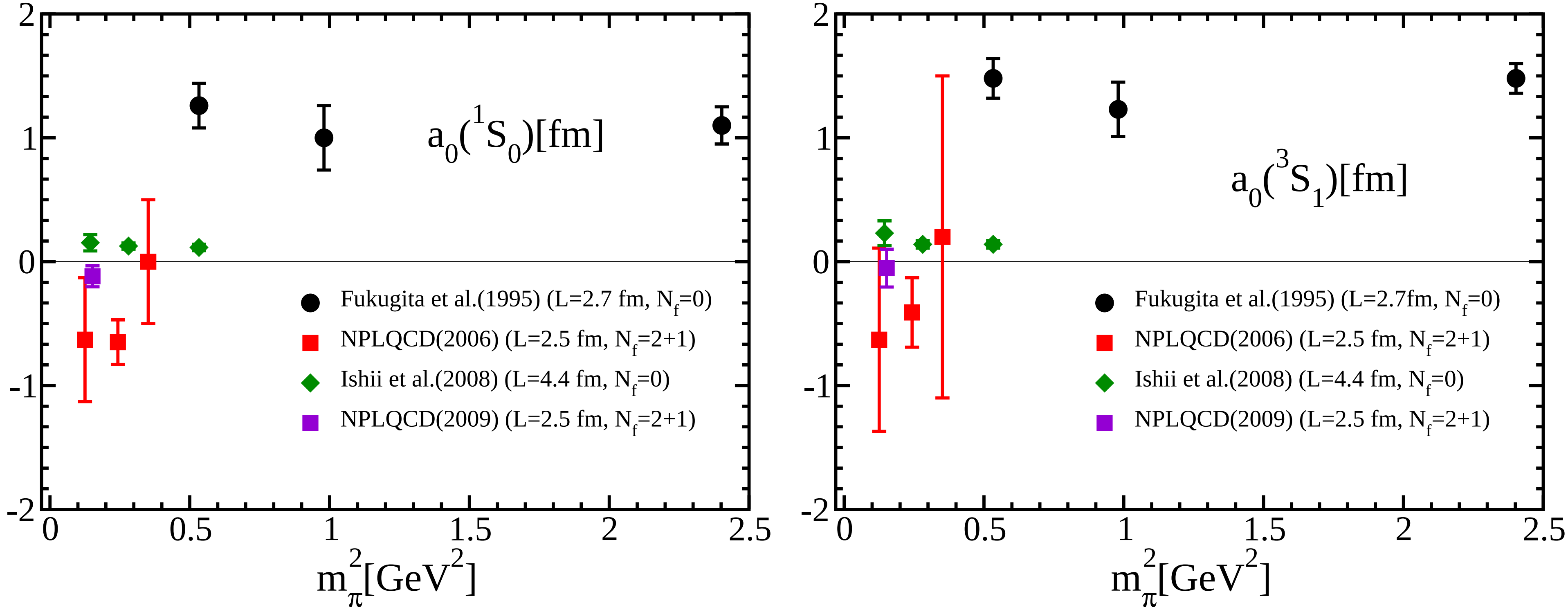
    '09 NPLQCD : $N_f = 2+1$ QCD
    $E_{\Lambda\Lambda} - 2m_\Lambda = -4.1(1.2)(1.4)$ MeV : require additional volumes

    Related talks : Inoue [Parallel 49, Fri], Sasaki [Parallel 49, Fri]

multi-nucleon system from lattice QCD

2. NN system $^3S_1$ and $^1S_0$

Deuteron: $^3S_1$ channel $\Delta E_d = 2.2$ MeV



'09 Ishii *et al.*: $N_f = 2 + 1$ QCD wave function $\rightarrow a_0 > 0$

multi-nucleon system from lattice QCD

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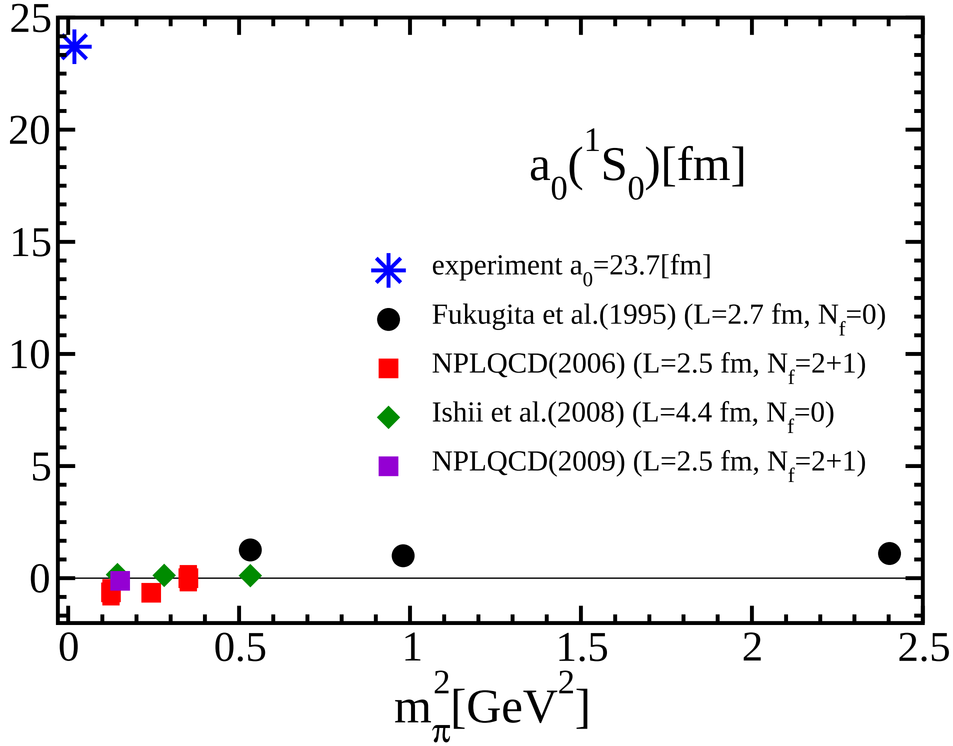

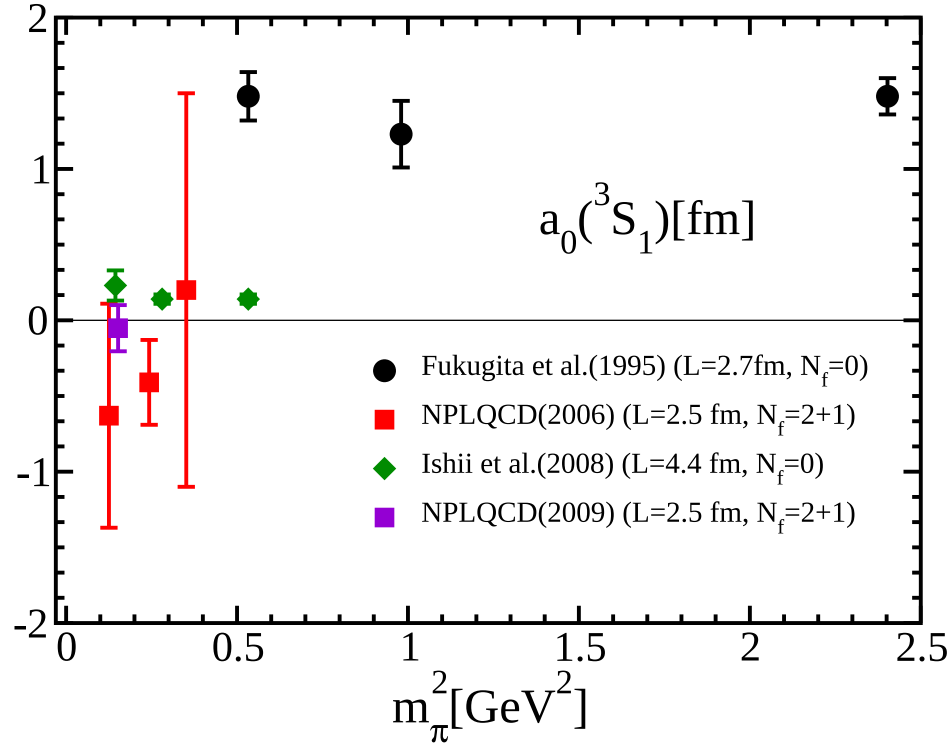

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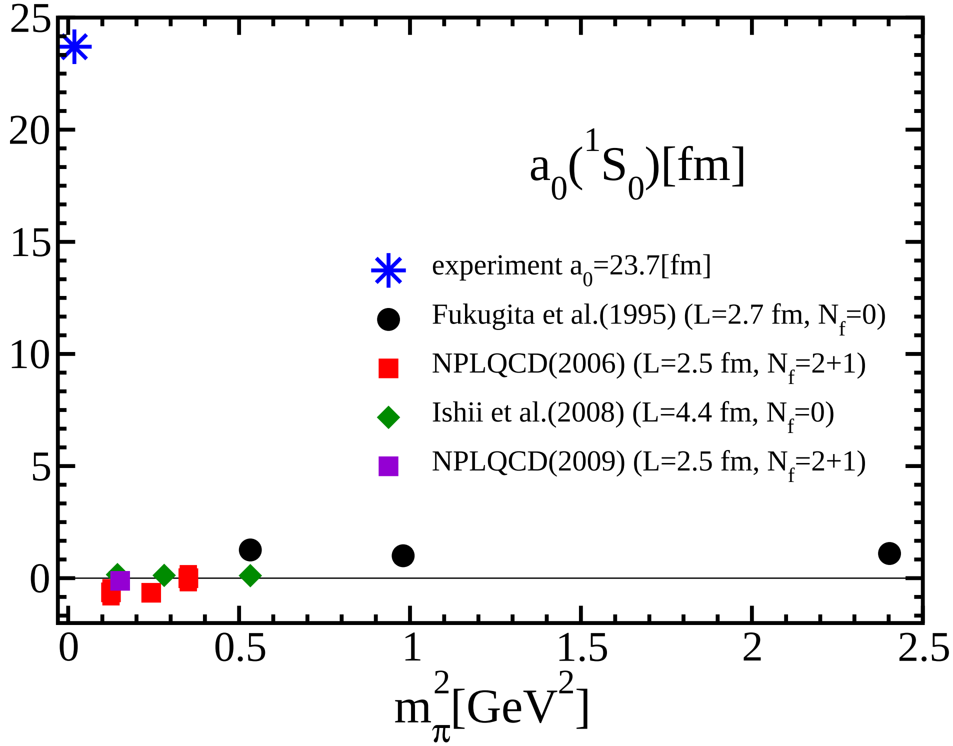
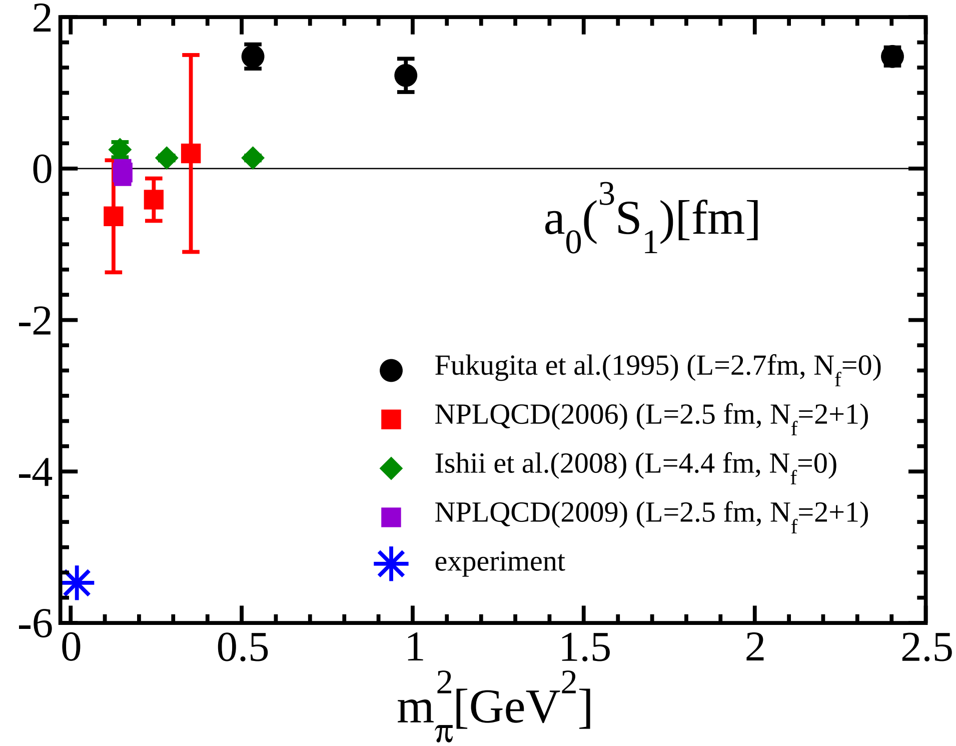




'09 Ishii *et al.*: $N_f = 2+1$ QCD wave function $\rightarrow a_0 > 0$

Deuteron: unbound due to $m_\pi \gtrsim 0.3$ GeV

NN potential : Murano [Parallel 38, Thu.]

multi-nucleon system from lattice QCD

3. NNN system

Triton: $J^P = \frac{1}{2}^+$ $I = \frac{1}{2}$ $\Delta E_{\mathrm{Triton}} = 8.5$ MeV

'09 NPLQCD : $N_f = 2+1$ QCD $m_\pi = 0.39$ GeV $L = 2.5$ fm

$\Xi^0\Xi^0 n$ and pnn channels

$$E_{pnn} - 3m_N \gtrsim 0$$

Triton: likely unbound

Three-nucleon force : Doi [Parallel 49, Fri.]

multi-nucleon system from lattice QCD

1. $\Lambda\Lambda$ system (Quenched QCD)

   '85 Mackenzie & Thacker
   '88 Iwasaki *et al.*
   '99 Pochinsky *et al.*
   '00 Wetzorke *et al.*
   '02 Wetzorke & Karsch

   H dibaryon: unbound

2. NN system $^3\mathrm{S}_1$ and $^1\mathrm{S}_0$

   '95 Fukugita *et al.* : Quenched QCD
   '06 NPLQCD : $N_f = 2+1$ QCD
   '08 Ishii *et al.* : Quenched and $N_f = 2+1$ QCD
   '09 NPLQCD : $N_f = 2+1$ QCD

   Deuteron: unbound due to $m_\pi \gtrsim 0.3$ GeV

3. NNN system

   '09 NPLQCD : $N_f = 2+1$ QCD

   Triton: likely unbound

Helium nucleus: larger binding energy, $\Delta E_{\mathrm{He}} = 28.3$ MeV

He : double magic numbers $Z = 2, N = 2$

In this work : Exploratory study for He and ^{3}He nuclei

Outline

1. ~~Introduction~~

2. Problems of multi-nucleon bound state

3. Simulation parameters

4. Results for He and ^{3}He

5. Summary

2. Problems of multi-nucleon bound state

1. Statistical error

$$\begin{array}{ccc} m_\pi & \to & \text{small} \\ \#\ \text{nucleon} & \to & \text{large} \end{array} \Rightarrow \frac{\text{noise}}{\text{signal}} \to \text{large}$$

   Avoid large statistical fluctuation

   unphysically heavy quark mass + $O(10^3)$ measurements

   $m_\pi = 0.8$ GeV and $m_N = 1.62$ GeV

   Need new method at lighter m_π

   Orginos [Parallel 22, Tue.], Foley, Wong, Juge [Parallel 34, Tue.]

2. Calculation cost

3. Identification of bound state in finite volume

Calculation cost

$C_{\text{He}}(t) = \langle 0|\text{He}(t)\overline{\text{He}}(0)|0\rangle$ with $\text{He} = p^2 n^2 = [udu]^2[dud]^2$

Number of Wick contraction $N_u! \times N_d! = (2N_p + N_n)! \times (2N_n + N_p)!$

contain identical contractions

$$\begin{aligned} \text{He:} &\quad 6! \times 6! = 518400 \\ {}^3\text{He:} &\quad 5! \times 4! = 2880 \end{aligned}$$

Reduction of contractions

Symmetries

$p \leftrightarrow p$, $n \leftrightarrow n$ in He operator

Isospin all $p \leftrightarrow$ all n

Calculate two contractions simultaneously

$u \leftrightarrow u$ in p or $d \leftrightarrow d$ in n

Calculation cost (cont'd)

$C_{\mathrm{He}}(t) = \langle 0|\mathrm{He}(t)\overline{\mathrm{He}}(0)|0\rangle$ with $\mathrm{He} = p^2n^2 = [udu]^2[dud]^2$

Number of Wick contraction $N_u! \times N_d! = (2N_p + N_n)! \times (2N_n + N_p)!$
contain identical contractions

He:	$6! \times 6! = 518400$	$\longrightarrow$	1107
^{3}He:	$5! \times 4! = 2880$	$\longrightarrow$	93

Further reduction: avoid same calculations of dirac and color indices

Block of three quark propagators B_3
zero momentum nucleon operator in sink time slice

Blocks of two B_3
1, 2, 3 dirac contractions carried out

Multi-meson systems : Detmold [Parallel 34, Tue.] arXiv:1001.2768
Recursion relations: $R_{n+1} = \langle R_n\rangle \cdot R_1 - nR_n \cdot R_1$
multi-meson with multi-species: n-π's + m-K's system, etc.

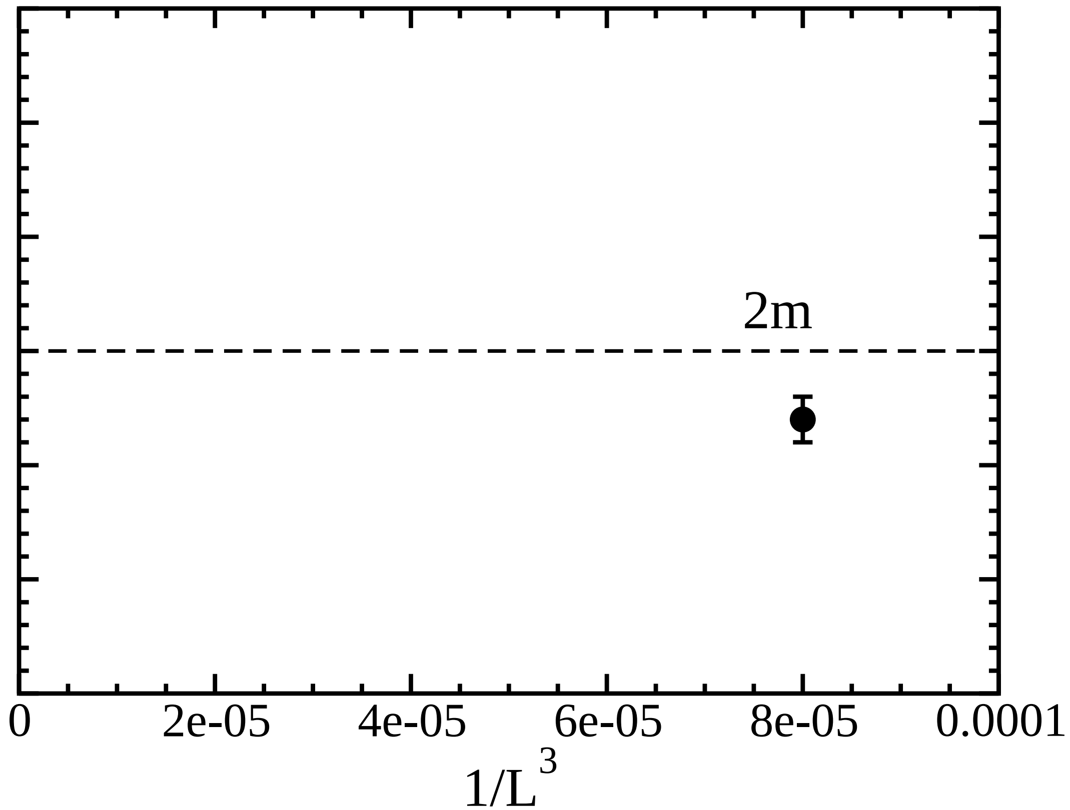
Identification of bound state in finite volume

$$\langle 0|\mathrm{He}(t)\overline{\mathrm{He}}(0)|0\rangle \xrightarrow[t\gg 1]{} Ce^{-Et} \quad (\mathrm{He:}\ J^P = 0^+, I = 0)$$

Measured state is whether bound state or not?

Example) Two-particle system

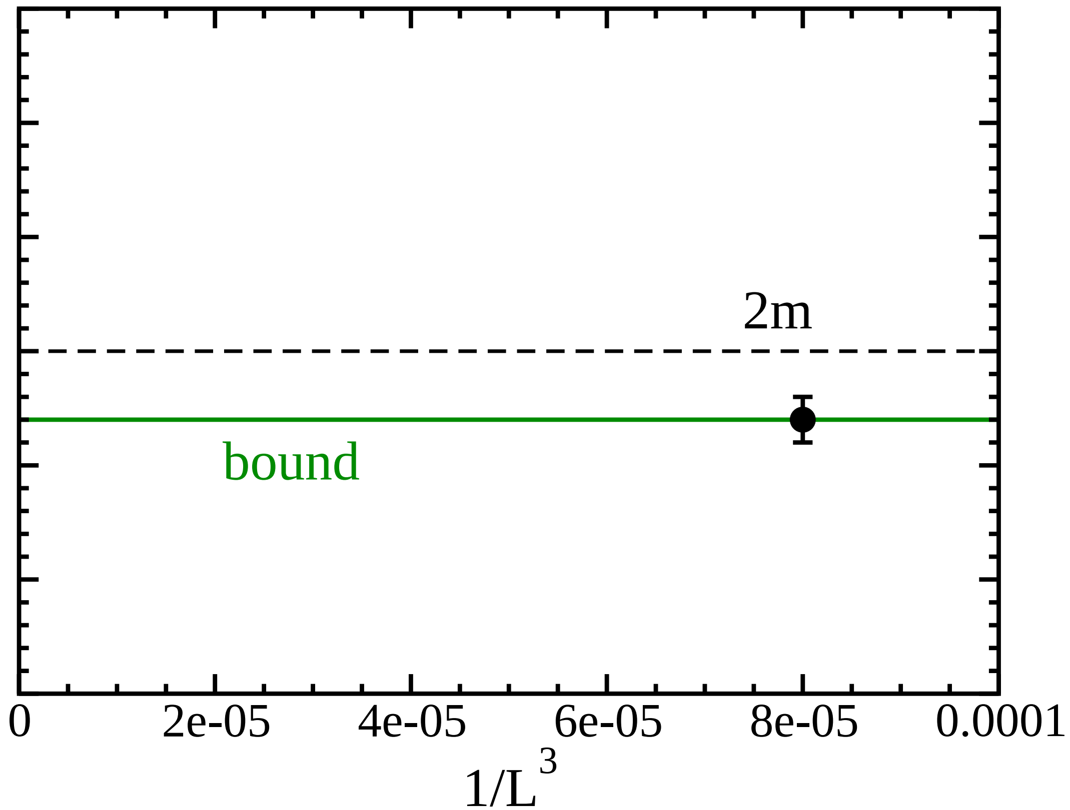
observe small $\Delta E = E - 2m < 0$ at single L



Identification of bound state in finite volume (cont'd)

Example) Two-particle system

observe small $\Delta E = E - 2m < 0$ at single L



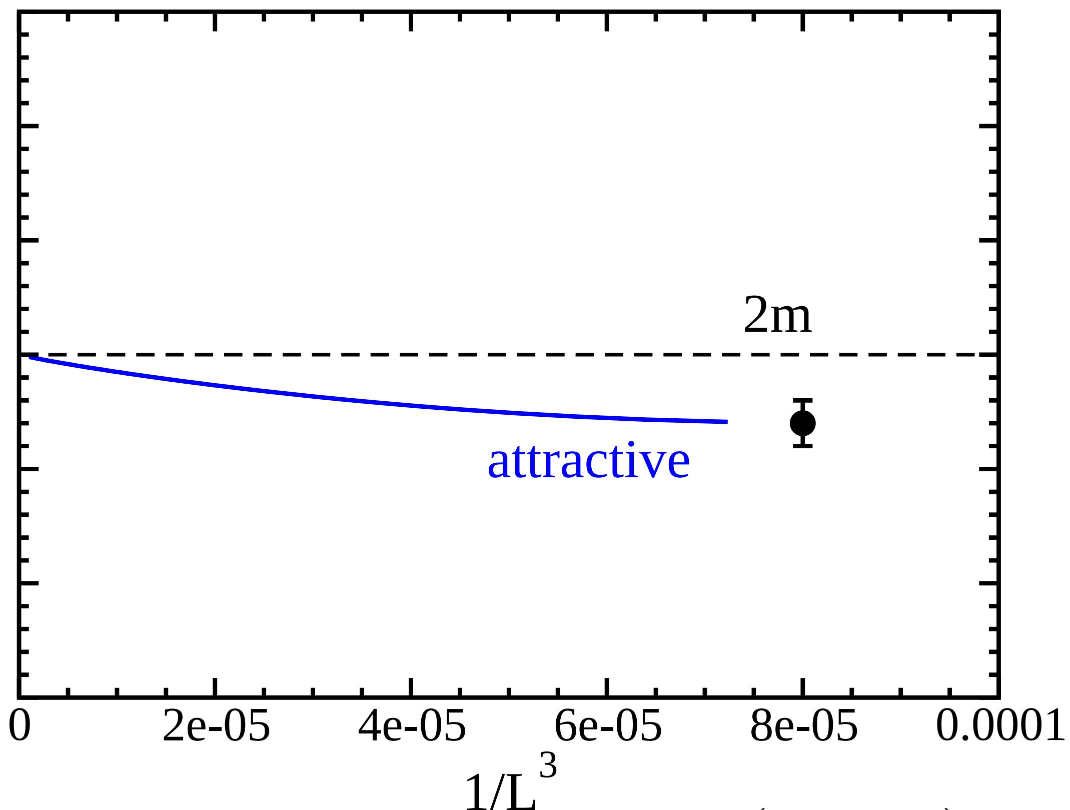
Bound state : $\Delta E = -\Delta E_{\text{bind}} + O(\mathrm{e}^{-\gamma L}) < 0$

Beane *et al.*, PLB585:106(2004), Sasaki & TY, PRD74:114507(2006)

Identification of bound state in finite volume (cont'd)

Example) Two-particle system

observe small $\Delta E = E - 2m < 0$ at single L



Attractive scattering state : $\Delta E = O\left(-\frac{a_0}{ML^3}\right) < 0 \quad (a_0 > 0)$

Lüscher, CMP105:153(1986), NPB354:531(1991)

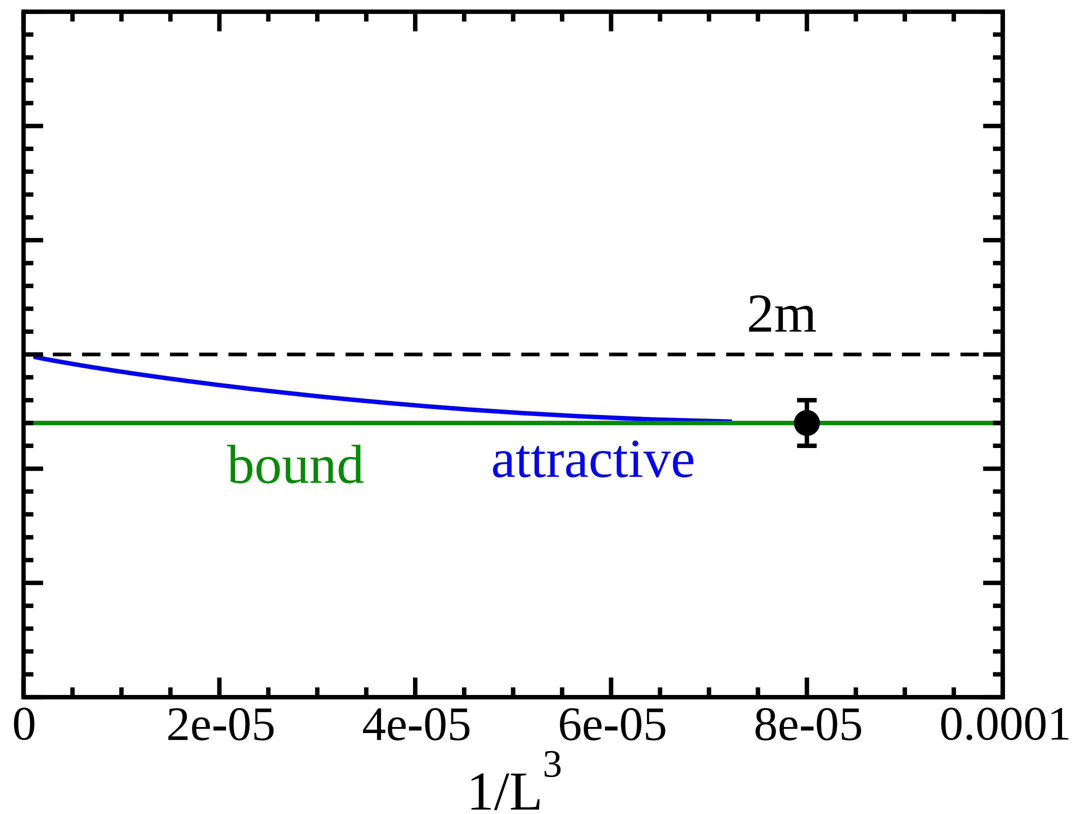
c.f.) N-particle scattering state : $\Delta E = E_{\text{scat}} - Nm = O\left(-\frac{{}_N C_2\, a_0}{ML^3}\right)$

Beane *et al.*, PRD76:074507(2007)

Identification of bound state in finite volume (cont'd)

Example) Two-particle system

observe small $\Delta E = E - 2m < 0$ at single L



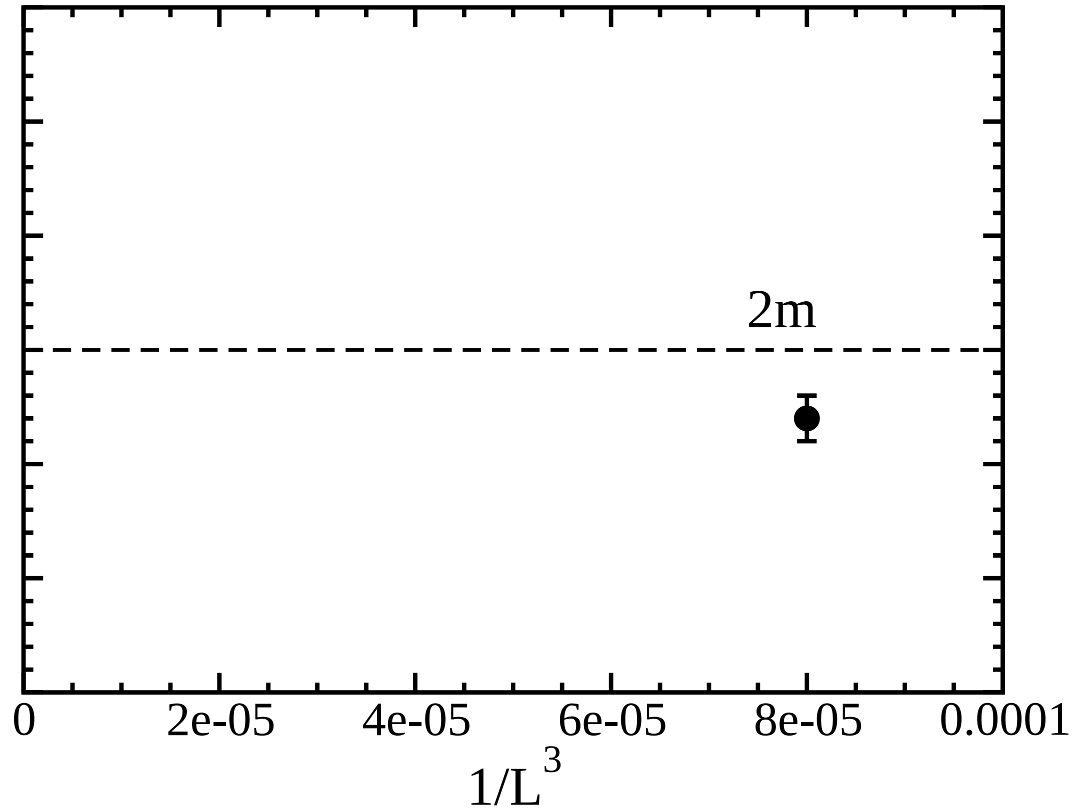
Hard to distinguish at single L

Bound state and Attractive scattering state

Identification of bound state in finite volume (cont'd)

Example) Two-particle system

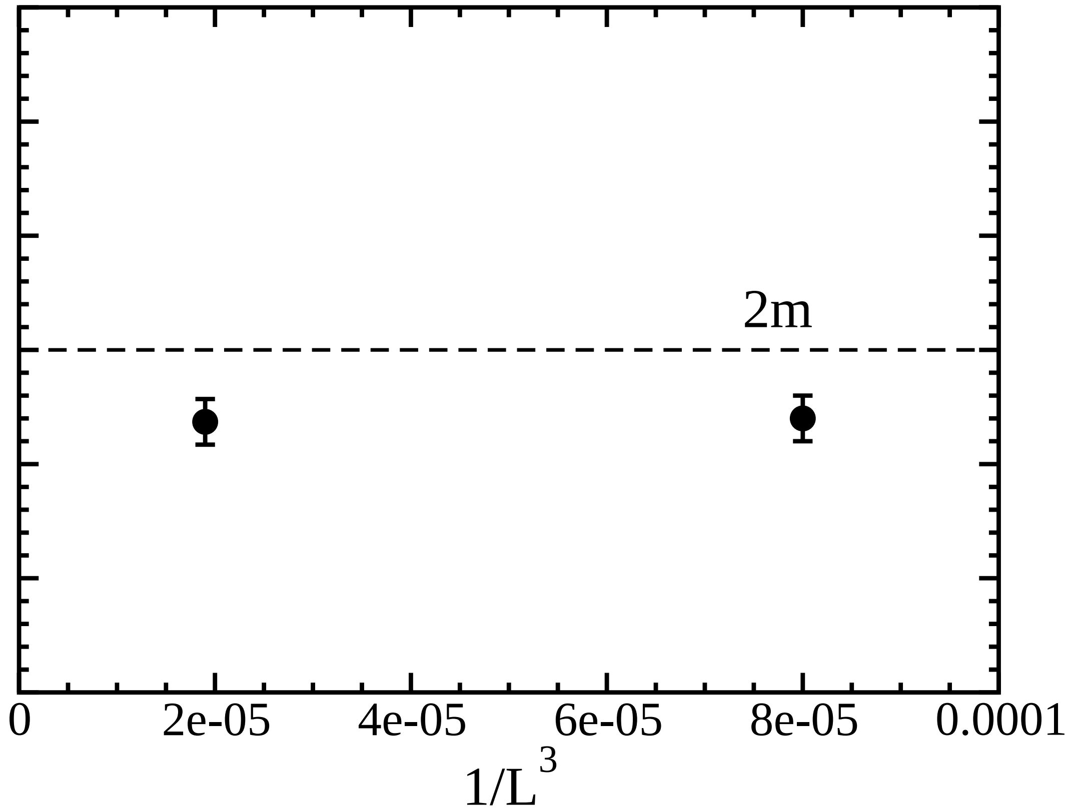
observe small $\Delta E = E - 2m < 0$ at several L



Identification of bound state in finite volume (cont'd)

Example) Two-particle system

observe small $\Delta E = E - 2m < 0$ at several L



Identification of bound state in finite volume (cont'd)

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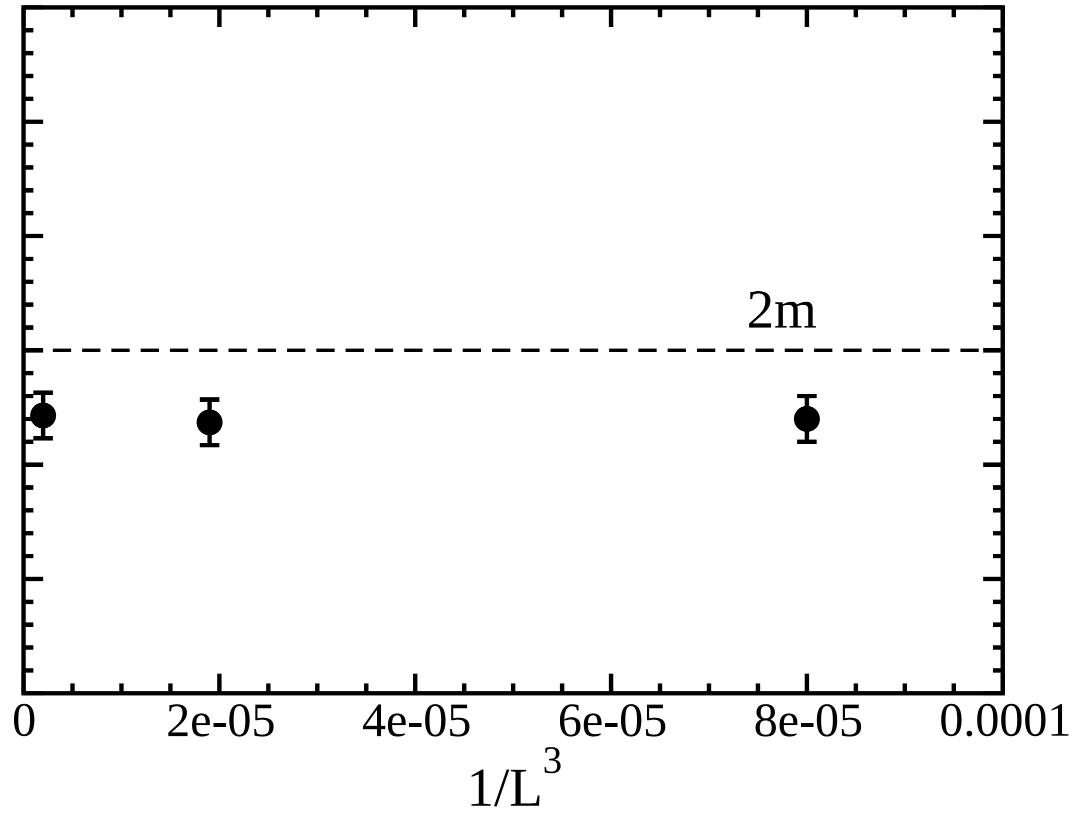

Identification of bound state in finite volume (cont'd)

Example) Two-particle system

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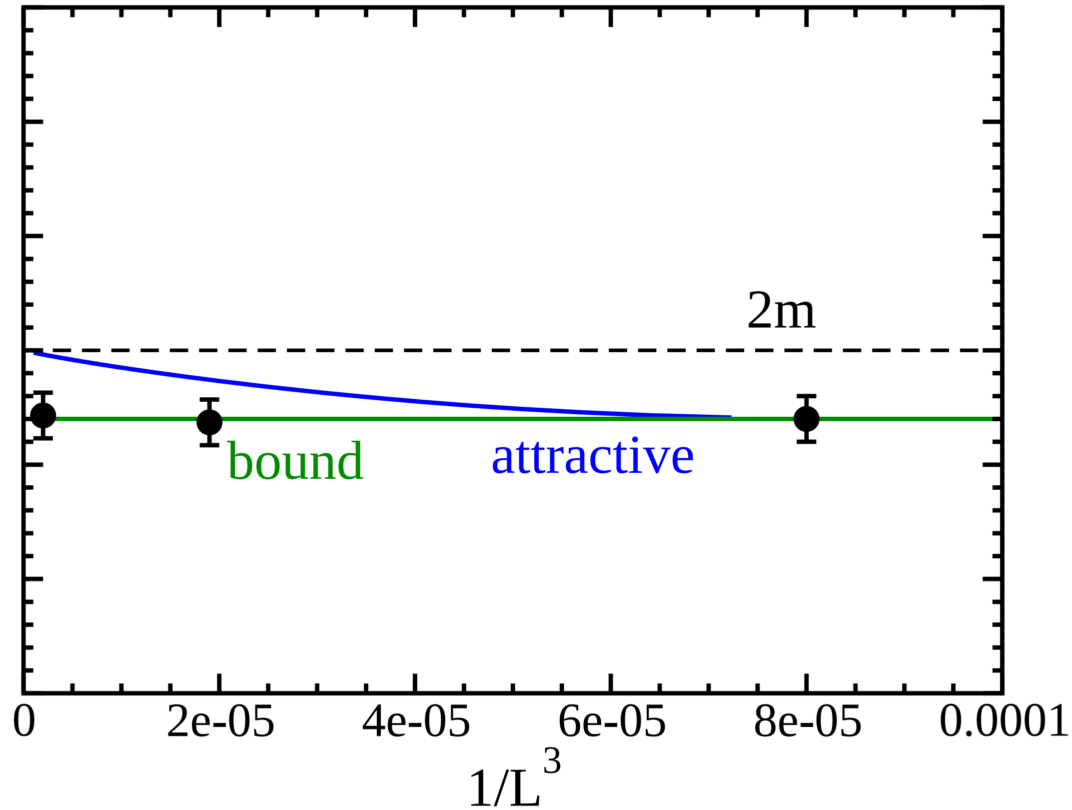


Identify bound state from volume dependence of ΔE

observe constant in infinite volume limit with $L = 3.1, 6.1, 12.3$ fm

Other methods: spectral weight: Mathur *et al.*, PRD70:074508(2004)

anti-periodic boundary.: Ishii *et al.*, PRD71:034001(2005)

3. Simulation parameters

- Quenched Iwasaki gauge action at $\beta = 2.416$

  $$a^{-1} = 1.54 \text{ GeV with } r_0 = 0.49 \text{ fm}$$

- Tad-pole improved Wilson fermion action

  $$m_\pi = 0.8 \text{ GeV and } m_N = 1.62 \text{ GeV}$$

- Three volumes

L	L [fm]	$N_{\rm conf}$	$N_{\rm meas}$
24	3.1	2500	2
48	6.1	400	12
96	12.3	200	12

- Exponential smearing sources $q(\vec{x}) = A \exp(-B|\vec{x}|)$

  $$\begin{array}{ll} & \quad\quad\quad\quad S_1 \quad\quad\quad\quad\quad S_2 \\ (A,B) = & (0.5, 0.5),\ (0.5,\ 0.1) \text{ for } L = 24 \\ (A,B) = & (0.5, 0.5),\ (1.0,\ 0.4) \text{ for } L = 48, 96 \end{array}$$

- quark operator with non-relativistic projection in nucleon operator

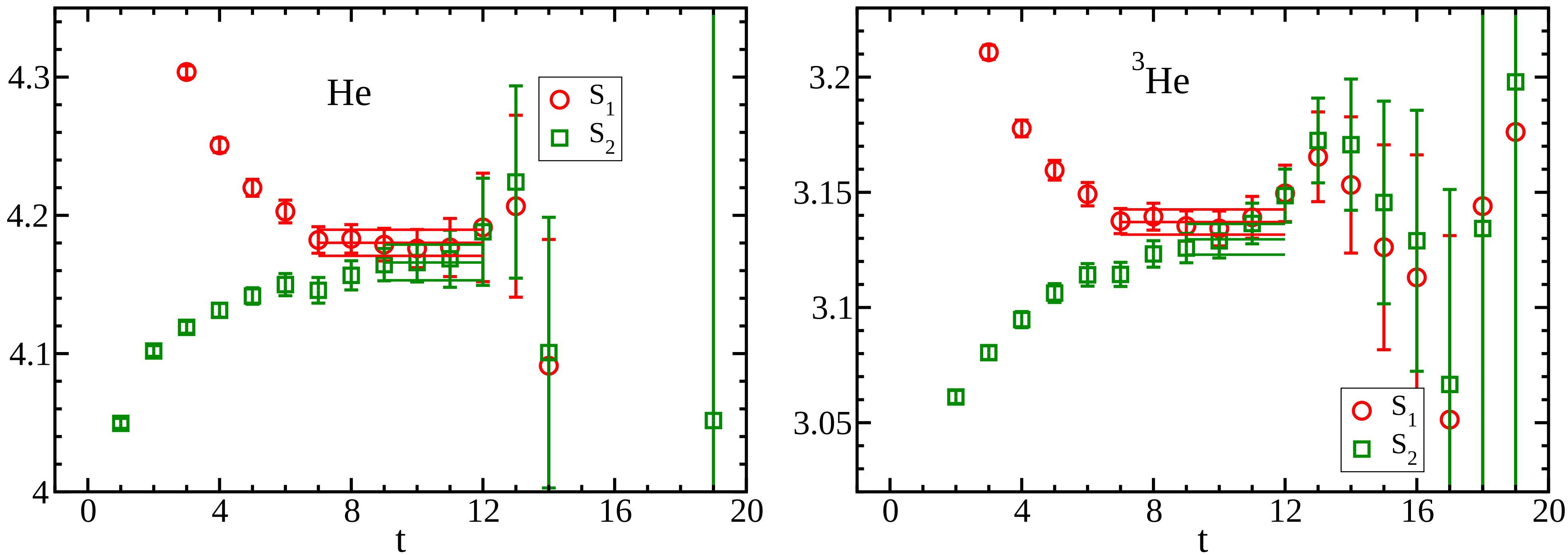
Simulations:

PACS-CS at Univ. of Tsukuba, and HA8000 at Univ. of Tokyo

4. Results

Effective mass of He and ^{3}He nuclei at $L = 48$

$$m_{\text{He}}(t) = \log\left(\frac{C_{\text{He}}(t)}{C_{\text{He}}(t+1)}\right)$$

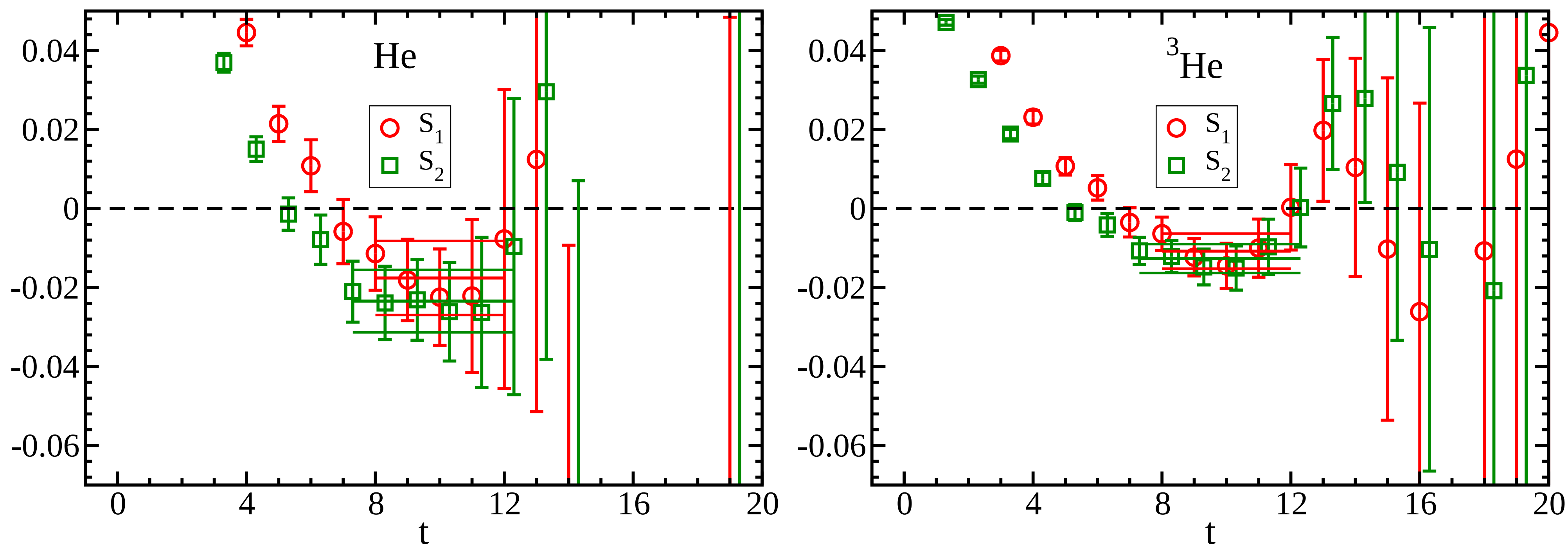


- Clear signal in $t < 12$, but larger error in $t \geq 12$
- consistent plateaus in $8 \lesssim t \leq 12$

4. Results (cont'd)

Effective energy shift $\Delta E_L = m_{\mathrm{He},{}^3\mathrm{He}} - N m_N$ of He nuclei at $L = 48$

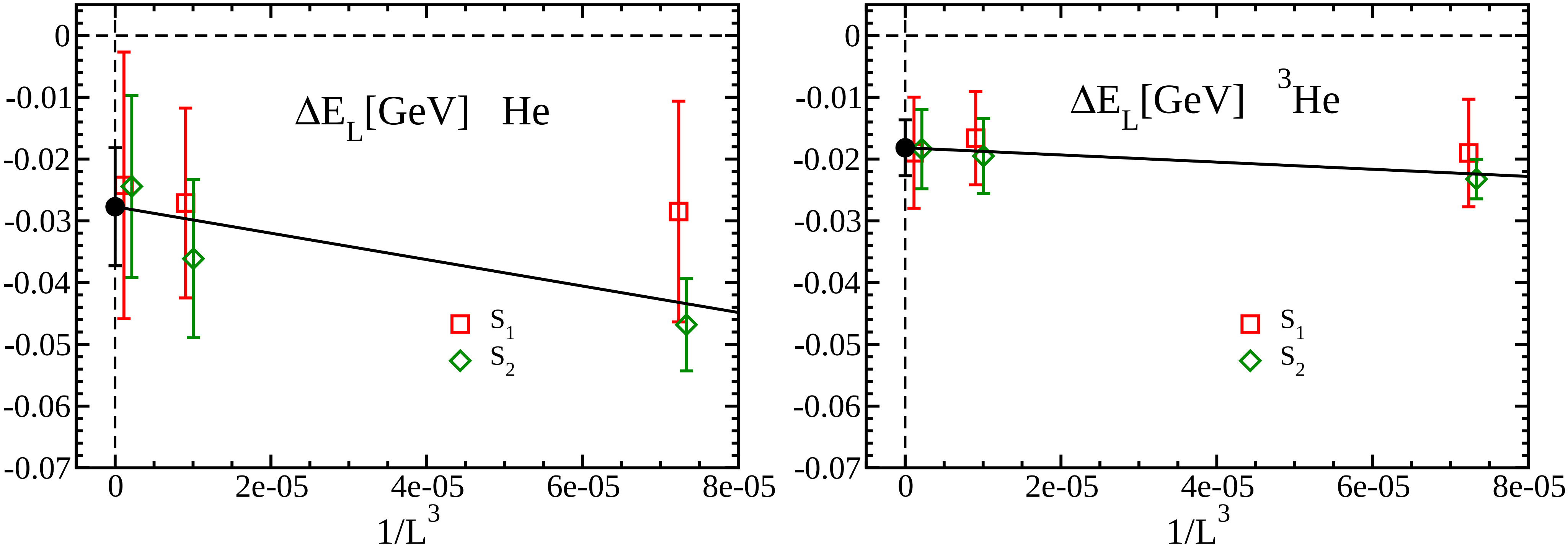
$$\Delta E_L(t) = \log\left(\frac{R(t)}{R(t+1)}\right), \quad R_{\mathrm{He}}(t) = \frac{C_{\mathrm{He}}(t)}{(C_N(t))^4}, \; R_{{}^3\mathrm{He}}(t) = \frac{C_{{}^3\mathrm{He}}(t)}{(C_N(t))^3}$$



- $\Delta E_L < 0$ in $8 \lesssim t \leq 12$
- consistent plateaus in $8 \lesssim t \leq 12$

4. Results (cont'd)

Volume dependence of ΔE_L of He nuclei

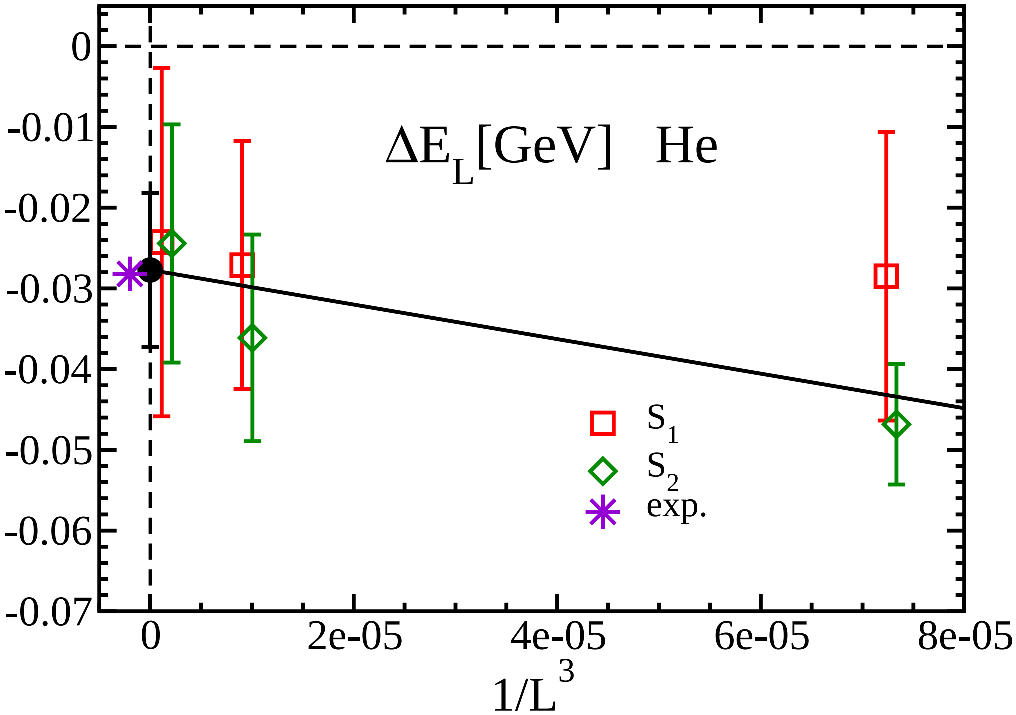


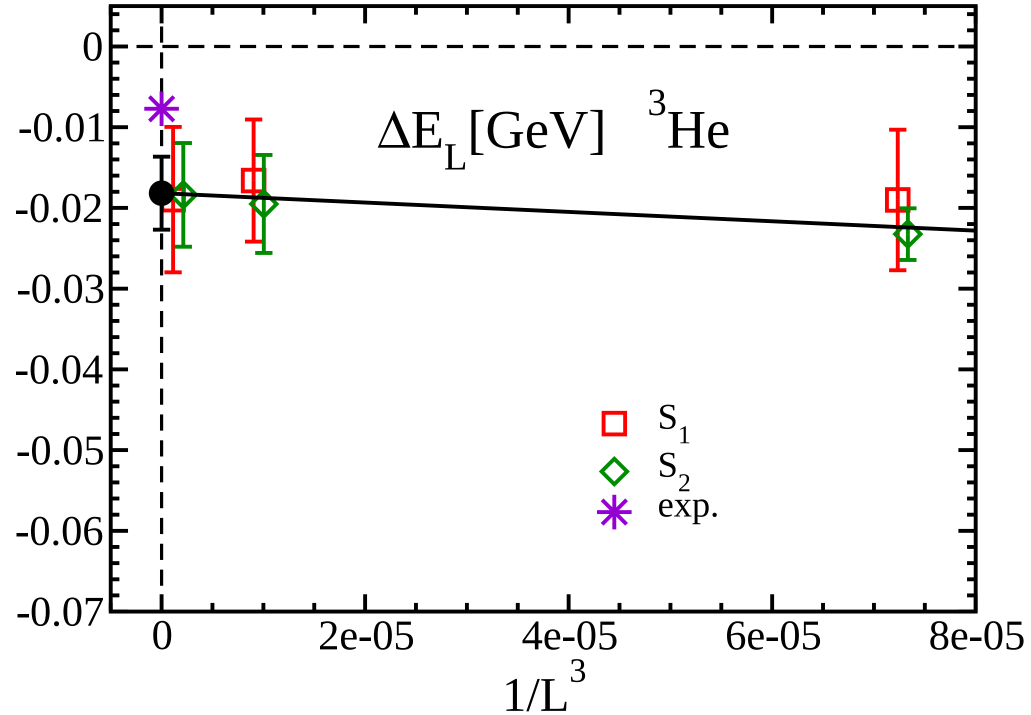
$\Delta E_{\text{He}} = 27.7(7.8)(5.5)$ MeV $\qquad$ $\Delta E_{^3\text{He}} = 18.2(3.5)(2.9)$ MeV

- $\Delta E_L < 0$ in three volumes $\Leftarrow$ statistically independent ensembles
- Small volume dependence
- Infinite volume limit with $\Delta E_L = -\Delta E_{\text{bind}} + C/L^3$
- Non-zero binding energy in infinite volume limit

4. Results (cont'd)

Volume dependence of ΔE_L of He nuclei





$\Delta E_{\mathrm{He}} = 27.7(7.8)(5.5)$ MeV $\quad$ $\Delta E_{^3\mathrm{He}} = 18.2(3.5)(2.9)$ MeV

- Same order to experimental values
- Binding increases as mass number in experiment, but inconsistent

  $\Delta E_{\mathrm{He}}/4 = 6.9(2.0)(1.4)$ MeV and $\Delta E_{^3\mathrm{He}}/3 = 6.1(1.2)(1.0)$ MeV

  mainly caused by heavy quark mass in calculation, probably

5. Summary

- Exploratory study of helium nuclei in quenched lattice QCD
- Unphysically heavy quark mass
- Reduction of calculation cost with some techniques
- Volume dependence of energy shift from free multi-nucleon state

Non-zero energy shift in infinite volume limit
$\rightarrow$ He and ^{3}He are bound at $m_\pi = 0.8$ GeV

Future work

- Quark mass dependence of ΔE
- Reduction of statistical error
- Deuteron bound state
- Larger nuclei $\Leftarrow$ need other technique

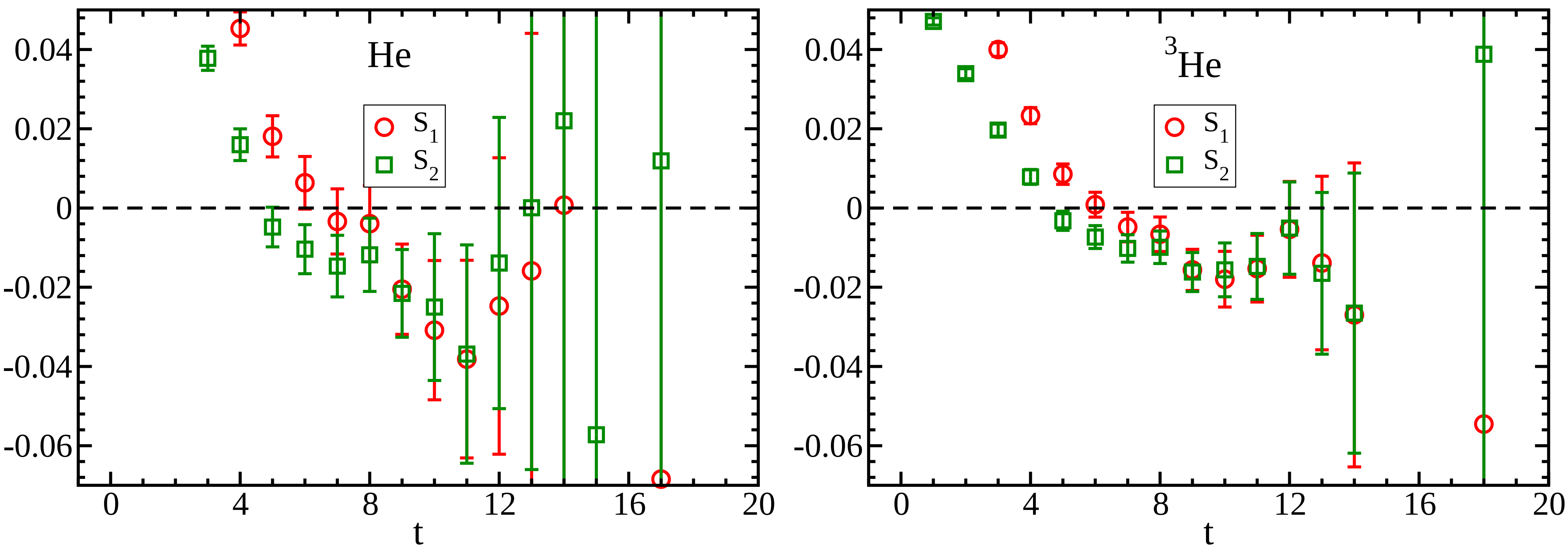
$$\mathrm{Li}^6 : (9!)^2 = 131681894400 \xrightarrow[\text{current method}]{} \sim 800000$$

- Dynamical quark effect

Back up

Effective energy shift $\Delta E_L = m_{\mathrm{He},{}^3\mathrm{He}} - N m_N$ of He nuclei at $L = 96$

$$\Delta E_L(t) = \log\left(\frac{R(t)}{R(t+1)}\right), \quad R_{\mathrm{He}}(t) = \frac{C_{\mathrm{He}}(t)}{(C_N(t))^4}, \ R_{{}^3\mathrm{He}}(t) = \frac{C_{{}^3\mathrm{He}}(t)}{(C_N(t))^3}$$



Lüscher's finite volume method

CMP105:153(1986), NPB354:531(1991)

$$p \cot \delta(p) = \frac{Z(1; q^2)}{L\pi}$$

$$Z(s; q^2) = \sum_{\mathbf{n}} \frac{1}{(\mathbf{n}^2 - q^2)^s}, \quad q = \frac{Lp}{2\pi}, \quad E = 2\sqrt{m^2 + p^2}$$

Expansion at $p^2 = 0$

$$\Delta E = \frac{p^2}{m} = -\frac{4\pi a_0}{mL^3} \left[1 + c_1 \frac{a_0}{L} + c_2 \left(\frac{a_0}{L} \right)^2 + \mathcal{O}(L^{-3}) \right]$$

$$c_1 = -2.837297, c_2 = 6.375183$$

Lücsher's method and bound state

Bound state: $p^2 = -\kappa^2 = -\gamma^2 \neq 0$ in $L \to \infty \iff q^2 = -q_*^2 \to -\infty$.

Behavior of zeta function at $q^2 \to -\infty$ Beane it et al., PLB585:106(2004)

$$Z(1;q^2) = -2\pi^2 q_* + \sum_{\vec{n}\in Z^3} \frac{\pi}{\sqrt{n^2}} \, \mathrm{e}^{-2\pi q_* \sqrt{n^2}}$$

at $q^2 < 0$ $(q_* > 0)$ Elizalde, CMP198:83(1998)

At large L

$$\begin{aligned} p \cot\delta(p) = \kappa \cot\sigma(\kappa) &= \frac{1}{L\pi}\left(-2\pi^2 q_* + \mathcal{O}\left(\mathrm{e}^{-q_*}\right)\right) \\ &= -\kappa - \mathcal{O}\left(\mathrm{e}^{-\kappa L}/L\right) \end{aligned}$$

$$\sigma(\gamma) = -\pi/4 \text{ only at } L \to \infty$$

Expansion at $p^2 = -\gamma^2$

$$\Delta E \approx -\frac{\kappa^2}{m} = -\frac{\gamma^2}{m} + \mathcal{O}\left(\mathrm{e}^{-\gamma L}/L\right)$$