Direct calculation of two-nucleon energy

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Frontiers in Lattice QCD and related topics

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Outline

- Introduction
  - Two-nucleon bound state calculation
  - Direct calculation of two-nucleon energy
- Simulation parameters in $N_f = 0$ at $m_\pi = 0.8$ GeV
- Preliminary result of comparison of two sources
- Very preliminary anaysis
- Summary

Introduction

Final goal: Qunantitave understanding of nucleus property from QCD

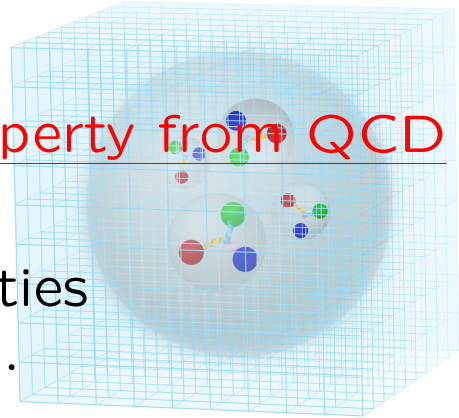


figure from Irie-san

Lattice QCD reproduced several single hadron properties

mass, decay constant, form factor, $\cdots$

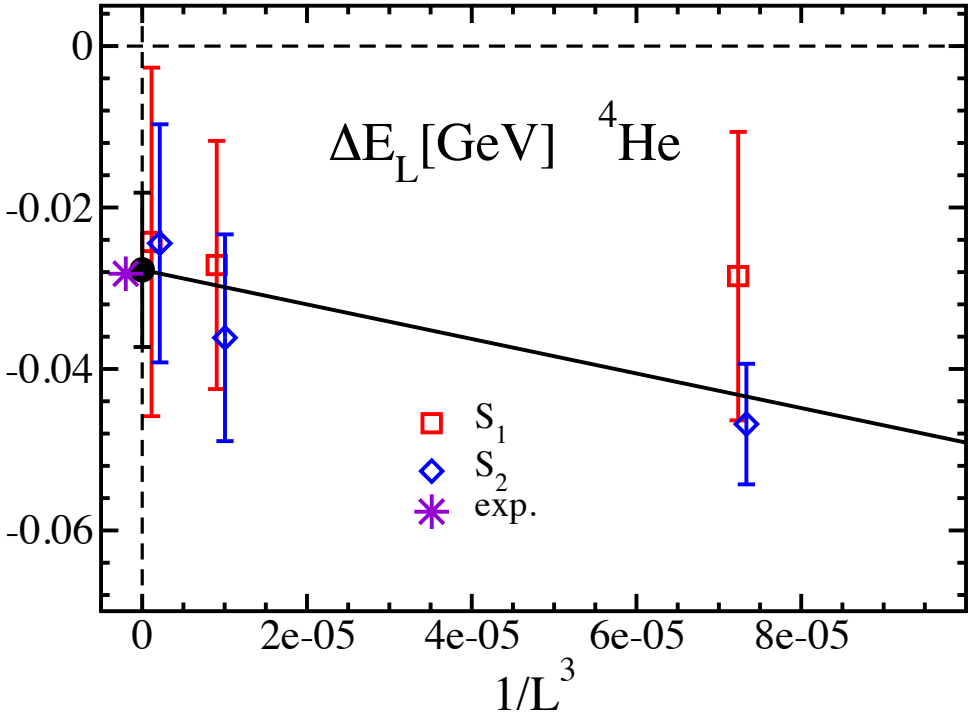
Lattice calculation of light nuclei started at 2009

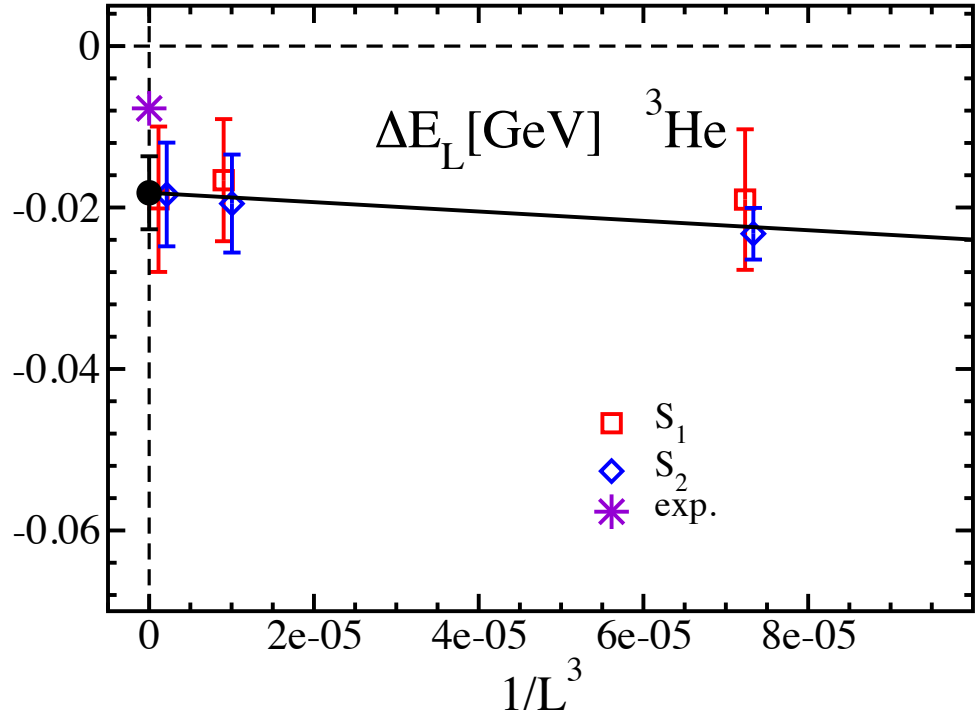
[PACS-CS PRD81:111504(R)(2010)]

Exploratory study of three- and four-nucleon systems

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

Identification of bound state from volume dependence of ΔE





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

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

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

Encouraging result as a first step

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[PACS-CS PRD81:111504(R)(2010)]

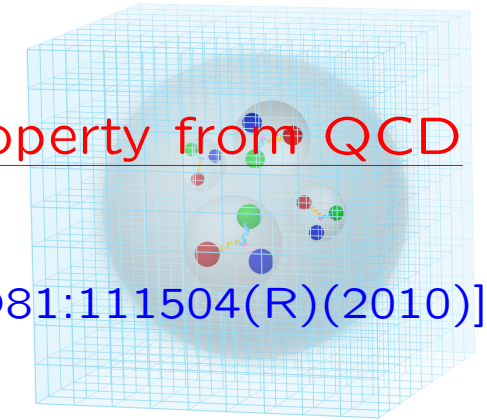


figure from Irie-san

Direct calculation of NN binding energy

Exponential source

PACS-CS, $N_f = 0$ $m_\pi = 0.8$ GeV [PRD84:054506(2011)]

TY *et al.*, $N_f = 2+1$ $m_\pi = 0.5$ GeV [PRD86:074514(2012)]

TY *et al.*, $N_f = 2+1$ $m_\pi = 0.3$ GeV [PRD92:014501(2015)]

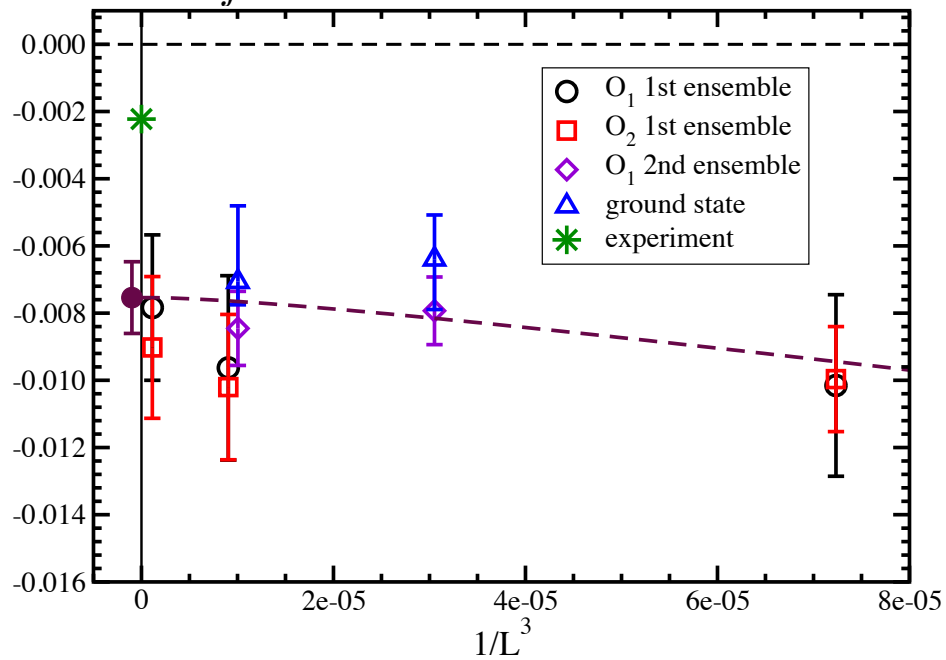
Gaussian source

'12 NPLQCD, '15 CalLat $N_f = 3$ $m_\pi = 0.81$ GeV; '15 NPLQCD $N_f = 2+1$ $m_\pi = 0.45$ GeV

Introduction

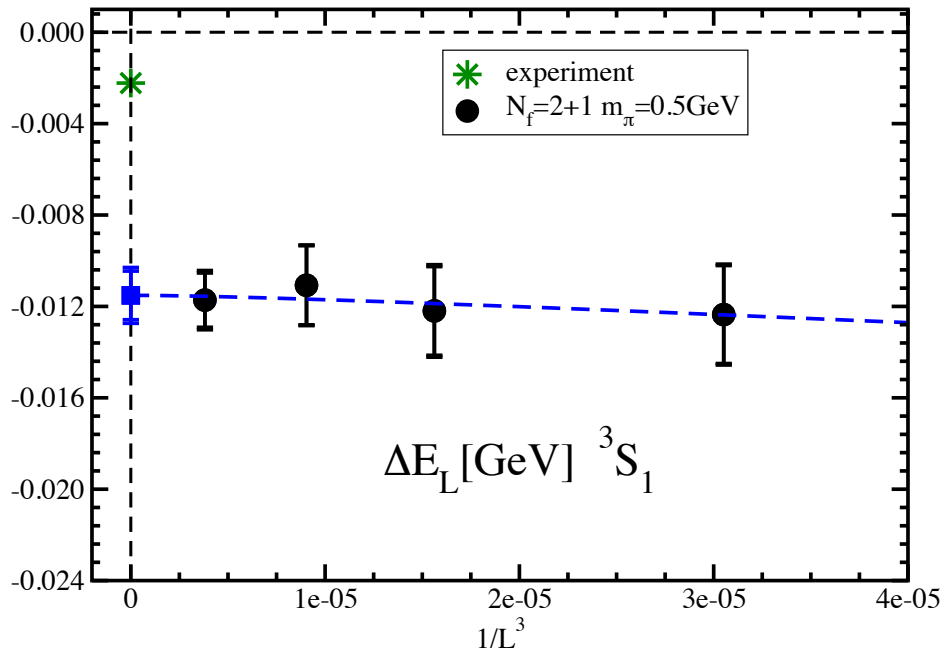
Energy shift ΔE_{NN} in $^3S_1$ channel

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



PRD84:054506(2011)

$N_f = 2+1$ $m_\pi = 0.5$ GeV



PRD86:074514(2012)

Bound state observed in $^3S_1$ channel and also $^1S_0$ channel

Similar results are obtained in other works

'15 TY *et al.* $N_f = 2+1$ $m_\pi = 0.3$ GeV [PRD92:014501(2015)]

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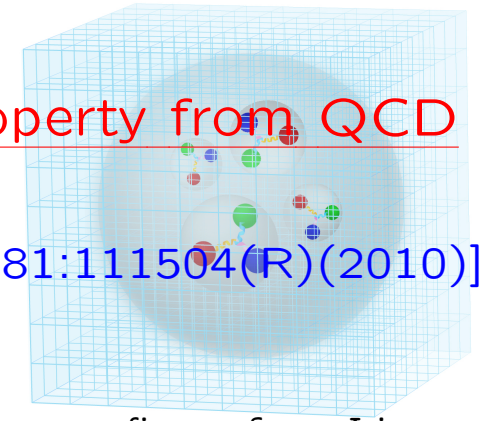

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Gaussian source

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Nucleus found in $^3S_1$ and $^1S_0$ at $m_\pi > m_\pi^{\rm phys}$

Effective potential from HALQCD method

'07 HALQCD and various works

No nucleus found in $^3S_1$ and $^1S_0$ at $m_\pi > m_\pi^{\rm phys}$

Urgent task: Reproduce nature at $m_\pi^{\rm phys}$

$\rightarrow$ deuteron only in $^3S_1$ and its binding energy

Important for reliability check of calculation method

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Lattice calculation of light nuclei started at 2009

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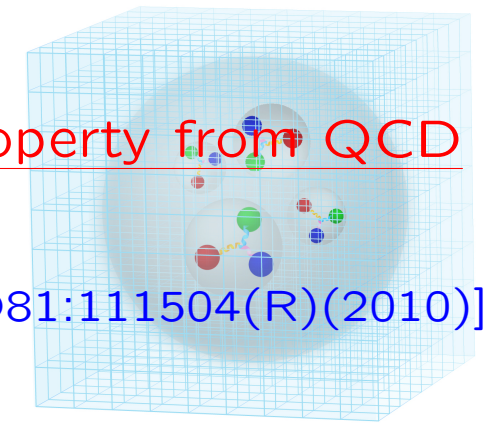

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'12 NPLQCD, '15 CalLat $N_f = 3$ $m_\pi = 0.81$ GeV; '15 NPLQCD $N_f = 2+1$ $m_\pi = 0.45$ GeV

Direct calculations have been carried out exponential or Gaussian source

HALQCD : Large source operator dependence of binding energy

[HALQCD, JHEP1610(2016)101;JHEP1903(2019)007]

Introduction

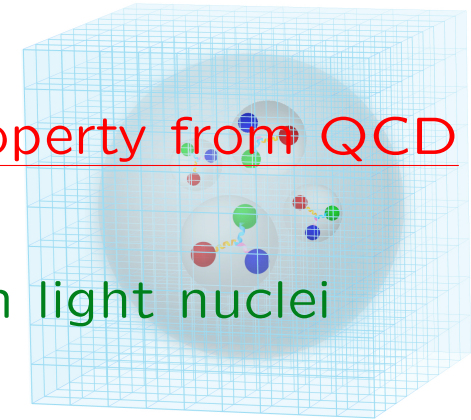


figure from Irie-san

Final goal: Qunantitave understanding of nucleus property from QCD

Lattice calculation of light nuclei started at 2009

Current purpose: Reproduce binding energy of known light nuclei

Direct calculation of NN binding energy

Direct calculations have been carried out exponential or Gaussian source

HALQCD : Large source operator dependence of binding energy

[HALQCD, JHEP1610(2016)101;JHEP1903(2019)007]

Comparing exponential and wall sources

Wall source is known to need longest time for plateau.

$\rightarrow$ Hard to satisfy important condition of direct calculation

Purpose: Examine source dependence in high precision calculation

Important condition of binding energy calculation

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

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

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

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

Choice of two-nucleon operator in direct method

Two-nucleon scattering state with $p \sim 0$
well overlap to $\sum_{x,y} N(x)N(y)(= O_{NN})$

Two-nucleon bound state
better overlap to $\sum_{x} N(x)N(x)(= O_L)$ than O_{NN}

But $\langle 0|O_L(t)\overline{O}_L(0)|0\rangle$ is not good for bound state energy calculation
all $N(p)N(-p)$ states also equally contribute $\rightarrow$ much late plateau

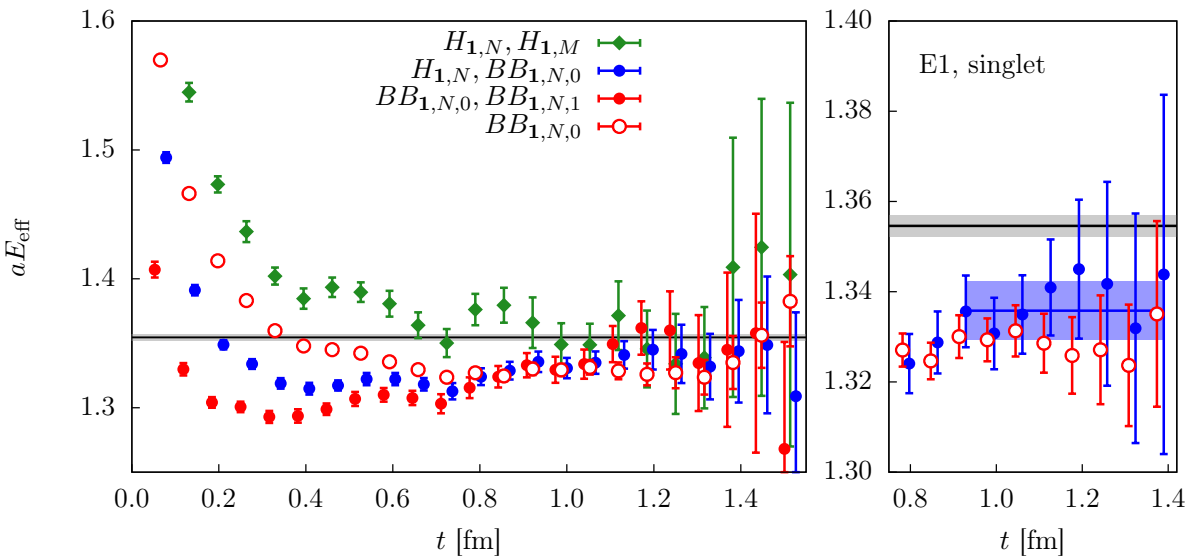
$\Rightarrow$ $\langle 0|O_{NN}(t)\overline{O}_L(0)|0\rangle$ is used for bound state energy calculations
[PACS, NPLQCD, CalLat, (Mains)]

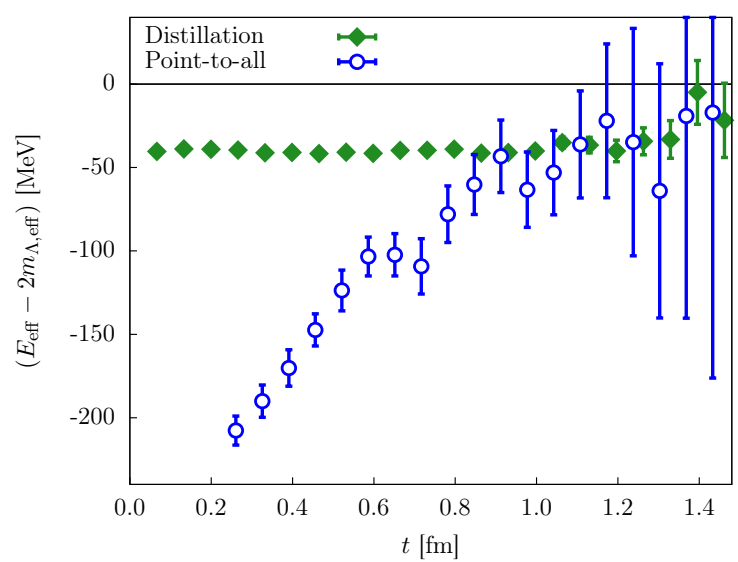
Variational analysis is desirable, but calculation cost is large.

Variational analysis by Mains group

Fransis *et al.*, arXiv:1805.03966

H-dibaryon channel $N_f = 3$ $m_\pi = 0.96$ GeV





Compare $\langle 0|O_{BB}(t)\overline{O}_L(0)|0\rangle$ and variational analysis
$\rightarrow$ good agreement

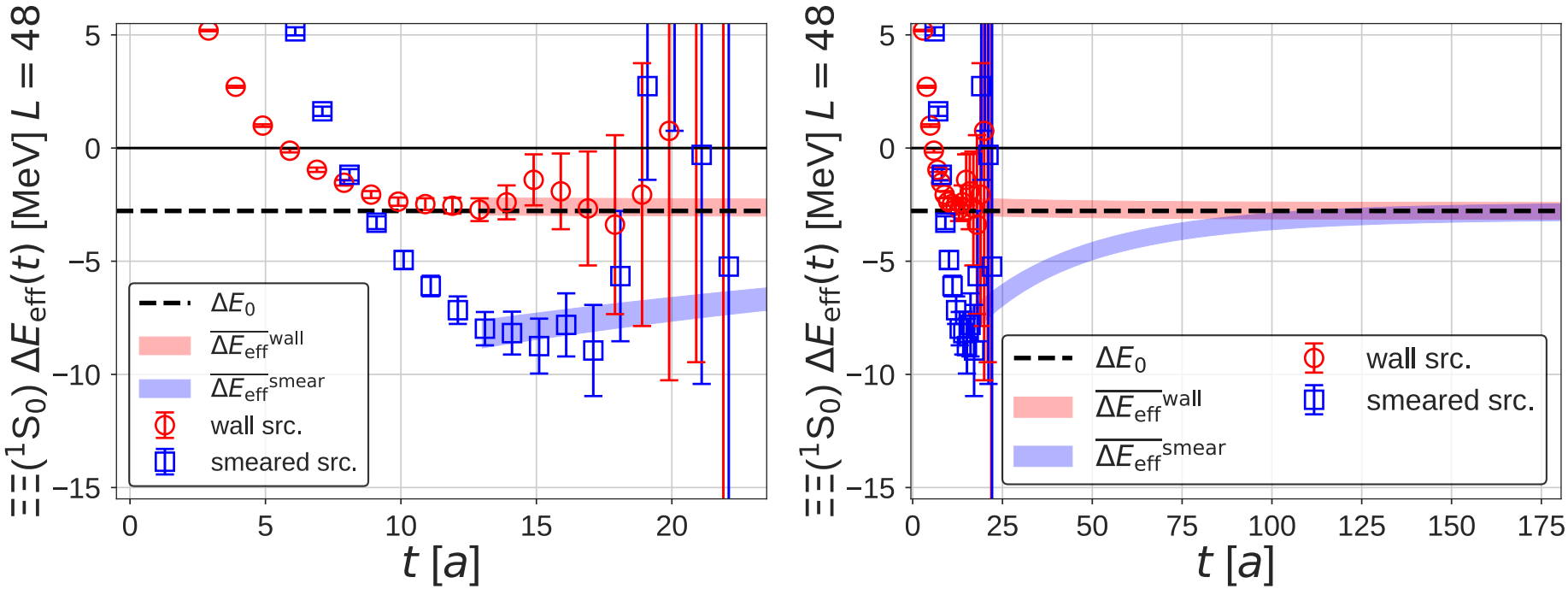
Compare high precision $\langle 0|O_{BB}(t)\overline{O}_{BB}(0)|0\rangle$ and variational analysis
$\rightarrow$ statistically consistent

$\Rightarrow$ $\langle 0|O_{BB}(t)\overline{O}_L(0)|0\rangle$ could give a correct ΔE.

Different ΔE^{eff} from two sources

[HALQCD, JHEP1610(2016)101;JHEP1903(2019)007]

Wall and Exp sources give different ΔE



Based on HALQCD potential

$\Delta E_{NN}^{\text{exp}}$ has large contamination from excited states

$\Delta E_{NN}^{\text{wall}}$ is almost flat

Important: check using variational analysis $\rightarrow$ large computational cost

This work: check with high precision calculation

Comments on HALQCD method

1. Derivative expansion [TY and Kuramashi, PRD96(2017)11:114511]

- Not systematic expansion and need convergence ckeck
- Truncation causes input k dependence of coefficients.

$$(\Delta + k^2)\phi_k(r) = \sum_{n=0}^{\infty} V_n(r)\Delta^n\phi_k(r) = \sum_{n=0}^{N} \overline{V}_n(r)\Delta^n\phi_k(r)$$

$V_n(r) \neq \overline{V}_n(r)$ and $\overline{V}_n(r)$ depends on input k

2. Time-dependent HALQCD method

[TY and Kuramashi, PRD98(2018)3:038502]

- $\overline{V}_n(r)$ has operator dependence if t is not large enough.

Number of operator = Number of states in 4-point functions

$\Rightarrow$ Same condition to variational analysis

- Even if the condition is satisfied, $\overline{V}_n(r)$ give correct amplitude at k determined from state energy in 4-point functions
- Time-dependent HALQCD method cannot dtermine the energy.

Simulation parameters

High precison calculation in $N_f = 0$ $m_\pi = 0.8$ GeV

Iwasaki gauge ($\beta = 2.416$, $a^{-1} = 1.541$ GeV) + tadpole imporved Wilson fermion actions
same action as '02 CP-PACS, PRD81:111504(R)(2010); PRD84:054506(2011)

Compare exponential and wall sources in NN $^3S_1$ channel
roughly correspond to $\langle 0|O_{NN}(t)\overline{O}_L(0)|0\rangle$ and $\langle 0|O_{NN}(t)\overline{O}_{NN}(0)|0\rangle$

L	T	source	N_{meas}
16	64	Exp	15,544,000
		Wall	8,307,200
20	64	Exp	5,504,000
		Wall	4,480,000
32	64	Exp	10,496,000
		Wall	8,307,200

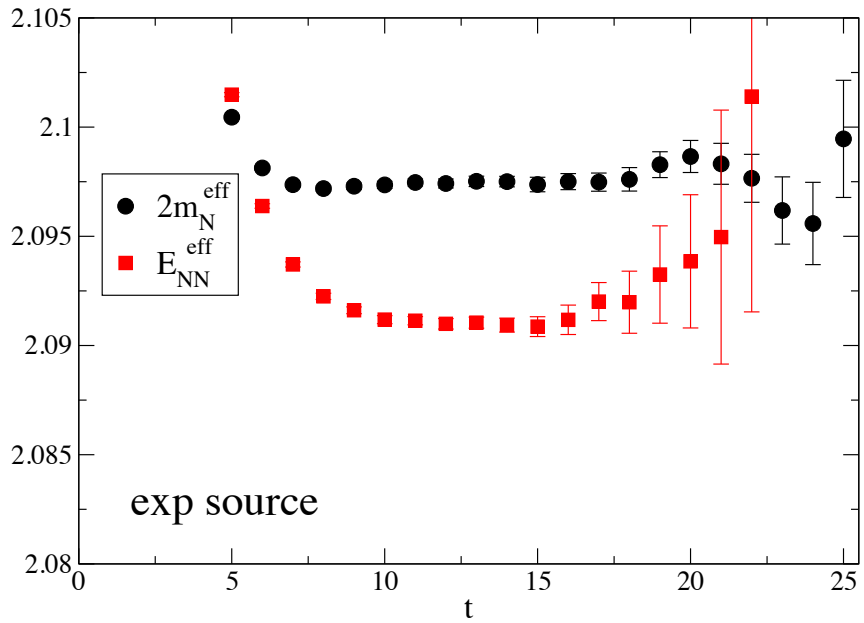
All results are preliminary.

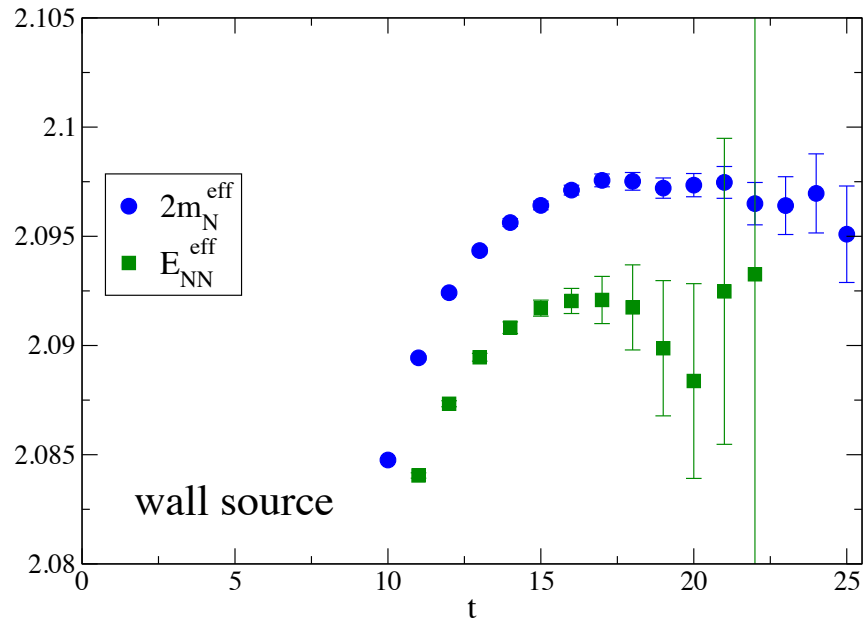
Computational resources (HPCI System Research Project: hp160124)
COMA and HA-PACS(U. of Tsukuba), FX10 and Reedbush (U. of Tokyo), Tatara (Kyushu U.),
FX100 and CX400(Nagoya U.), OFP(JCAHPC)

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $L = 20$

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

Effective $2m_N$ and E_{NN}





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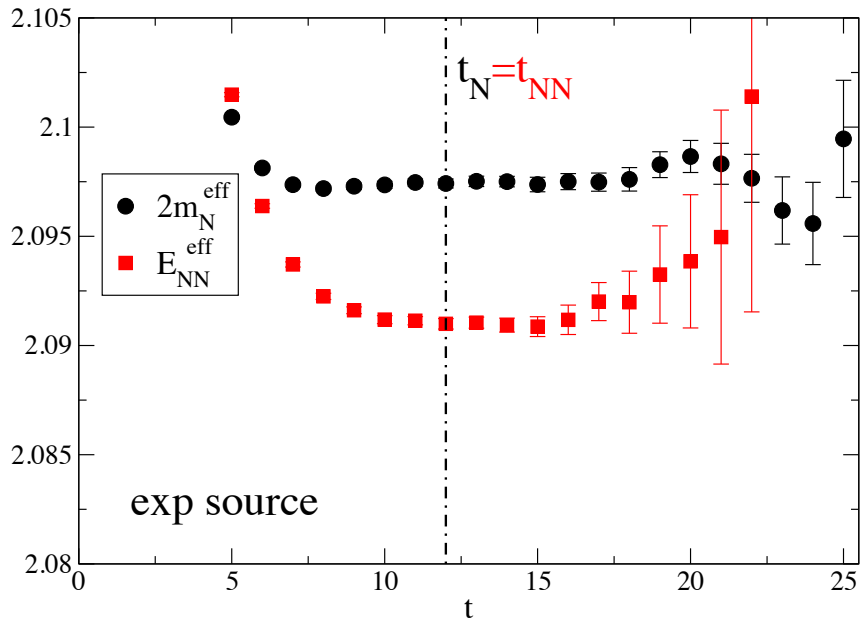
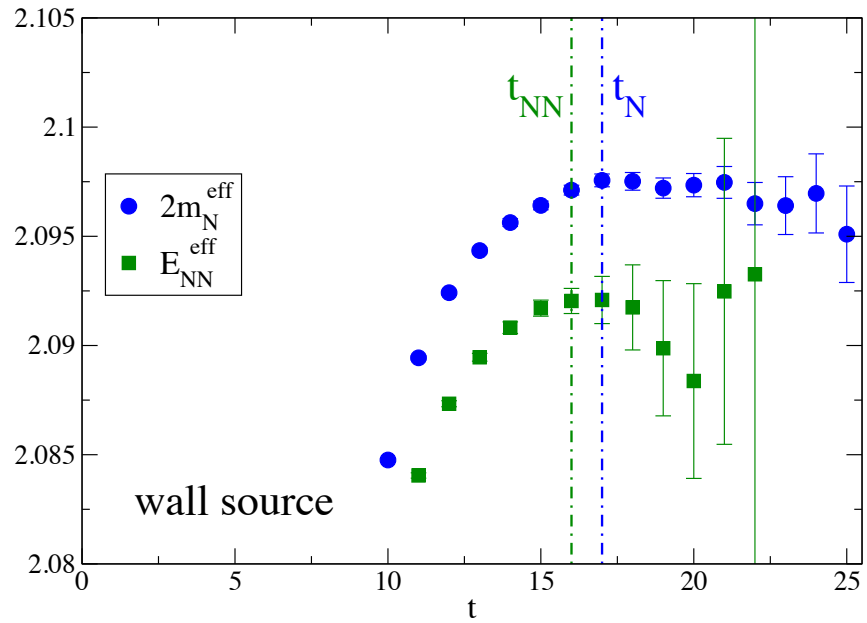


$t_N \sim t_{NN} \sim 12$



$t_{NN} \sim 16, \; t_N \sim 17$

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $L = 20$

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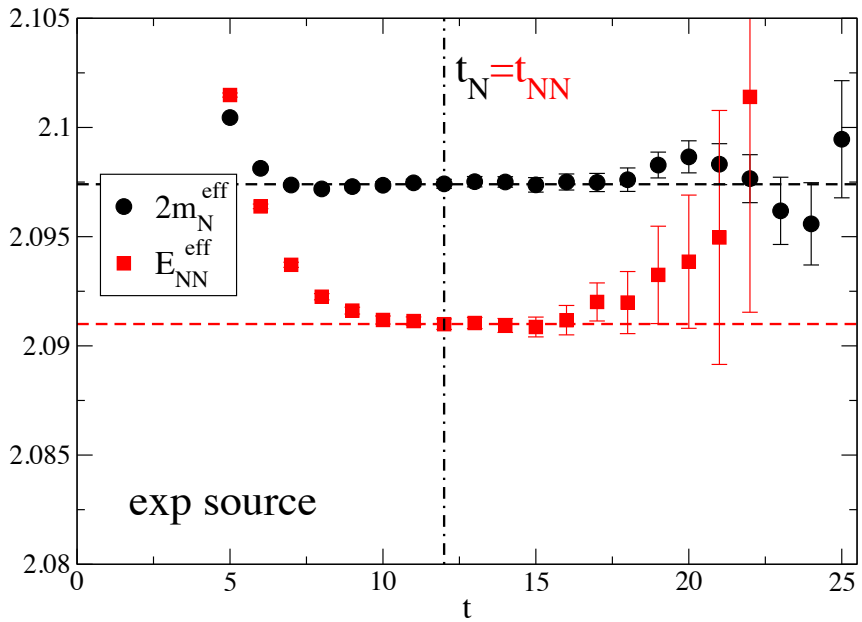
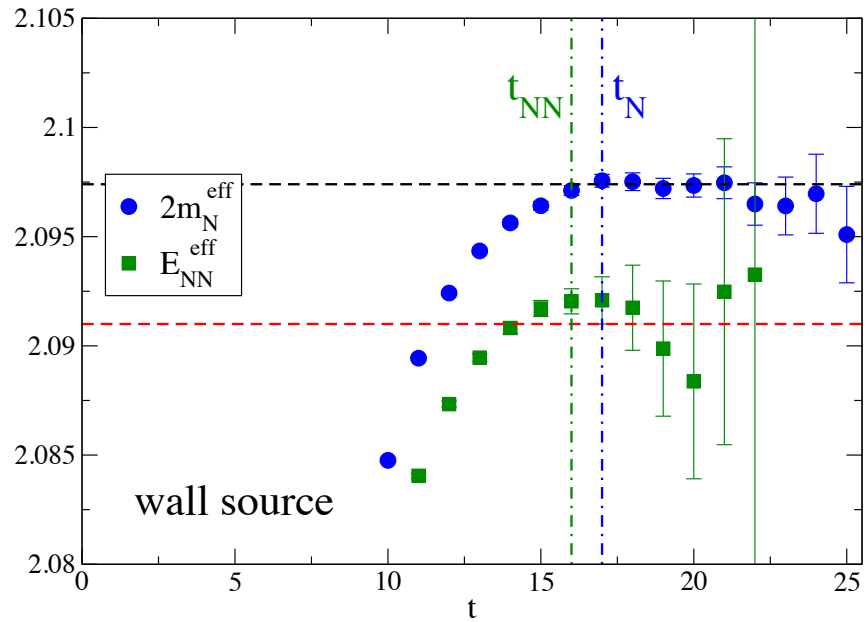
Effective $2m_N$ and E_{NN}





$t_N \sim t_{NN} \sim 12$

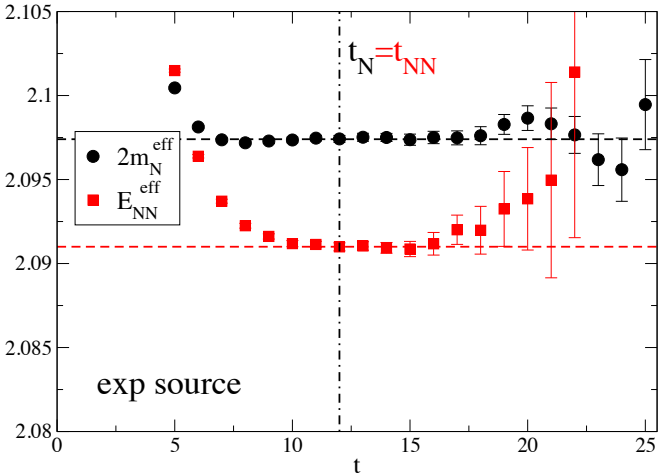
$t_{NN} \sim 16, \; t_N \sim 17$

dashed lines determined from exponential source

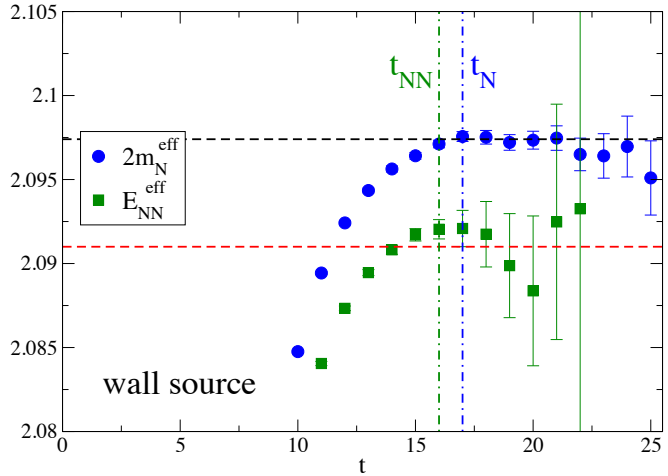
consistent with each other in plateau region

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $L = 20$

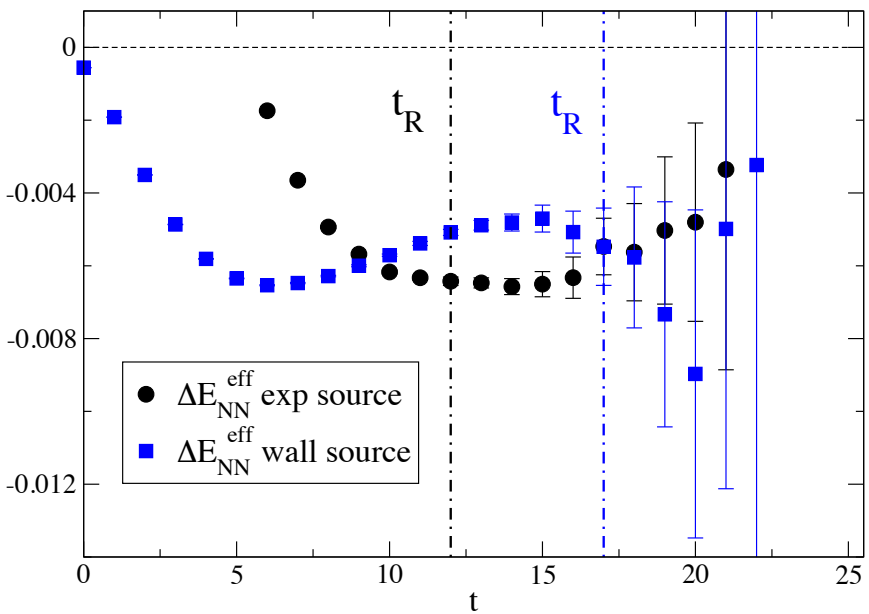
Effective $2m_N$ and E_{NN}



$t_N \sim t_{NN} \sim 12$



$t_{NN} \sim 16$, $t_N \sim 17$



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

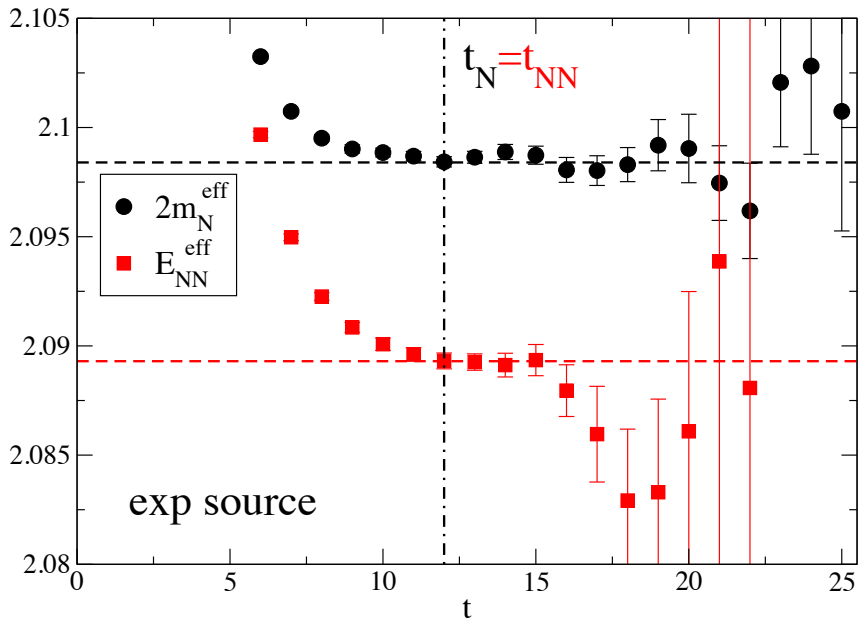
exp: reasonable plateau in $t \gtrsim t_{N,NN}$

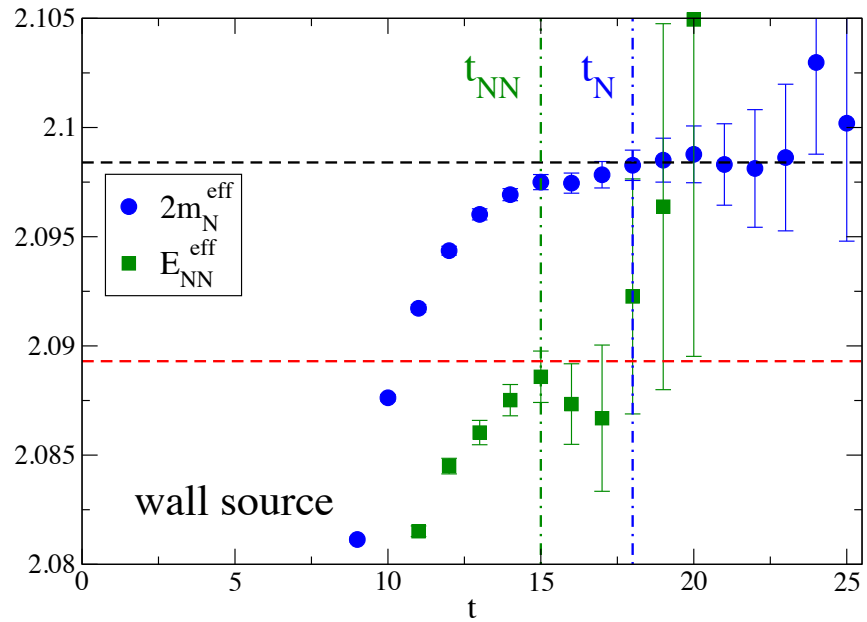
wall: non-monotonic behavior

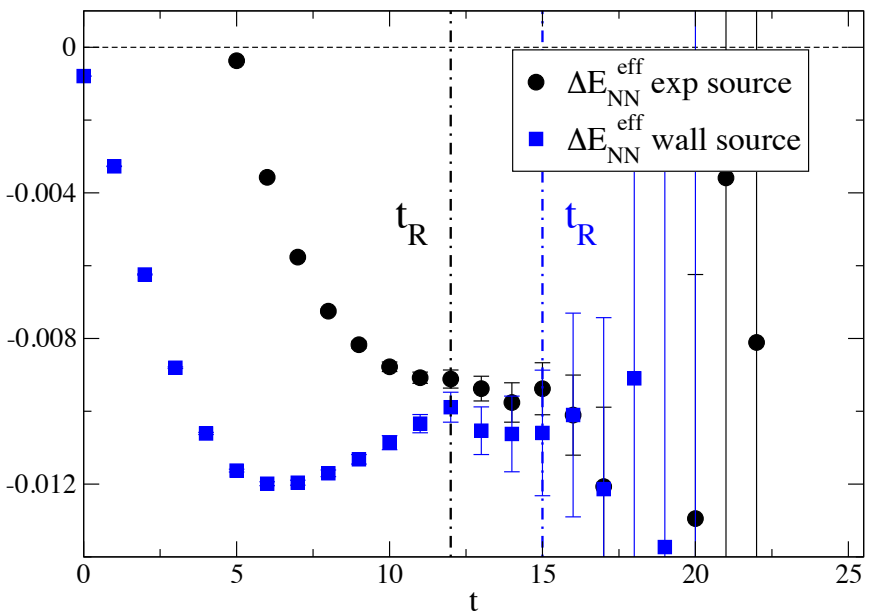
consistent with exp in $t \gtrsim t_N$

with large error

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $L = 16$







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

exp: reasonable plateau in $t \gtrsim t_{N,NN}$

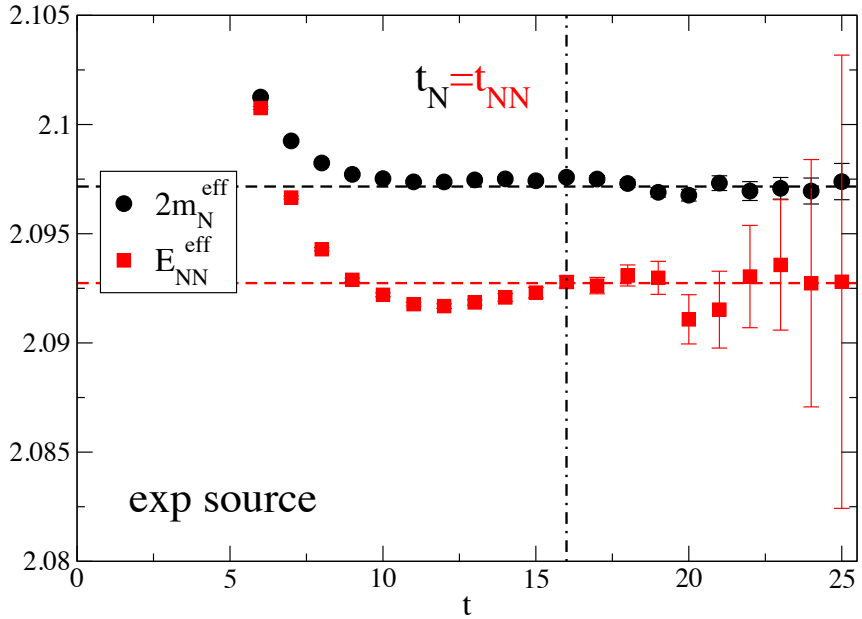
wall: non-monotonic behavior

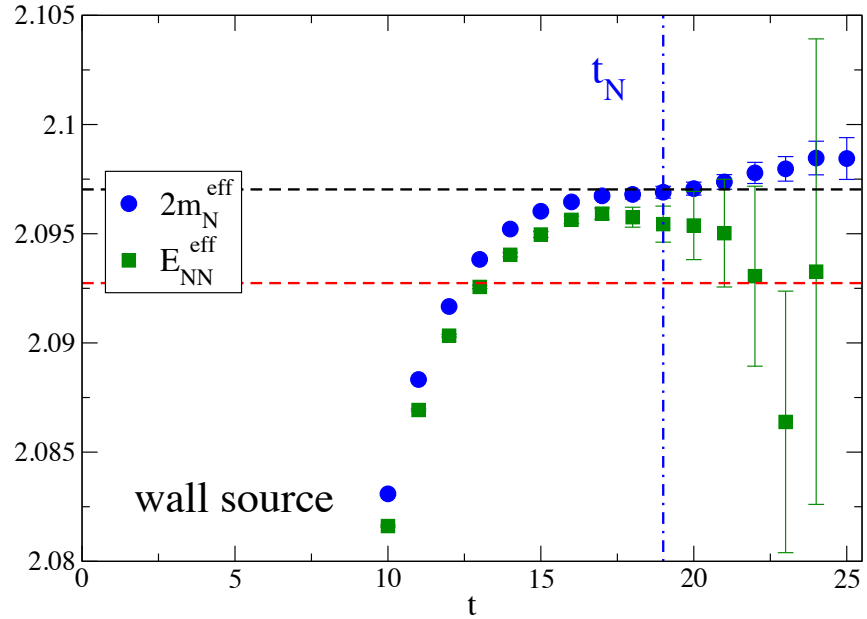
consistent with exp in $t \gtrsim t_N$

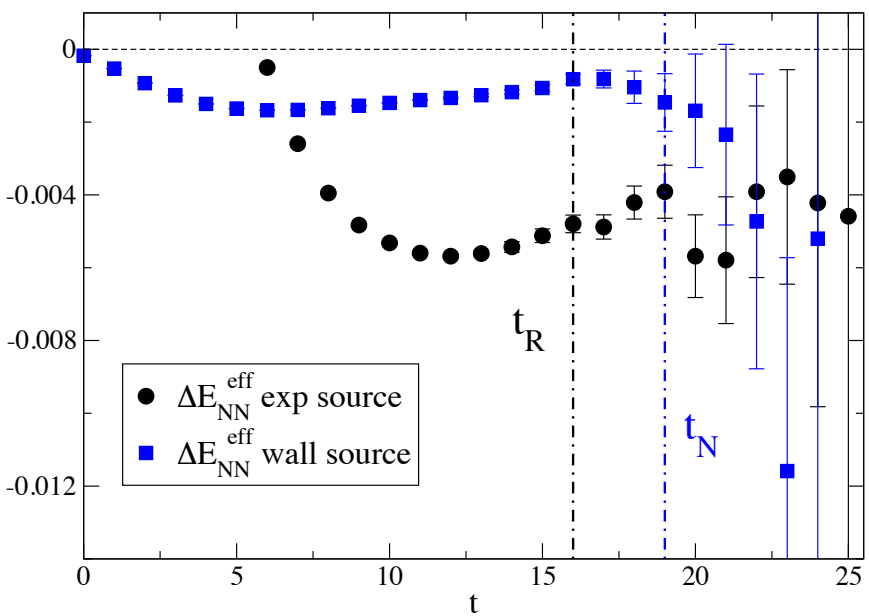
with large error

Similar result to $L = 20$

$R(t) = C_{NN}(t)/(C_N(t))^2$ in $L = 32$







exp: ΔE_{NN} in $t \gtrsim t_{N,NN}$

wall: non-monotonic behavior

downward trend in E_{NN}^{eff}

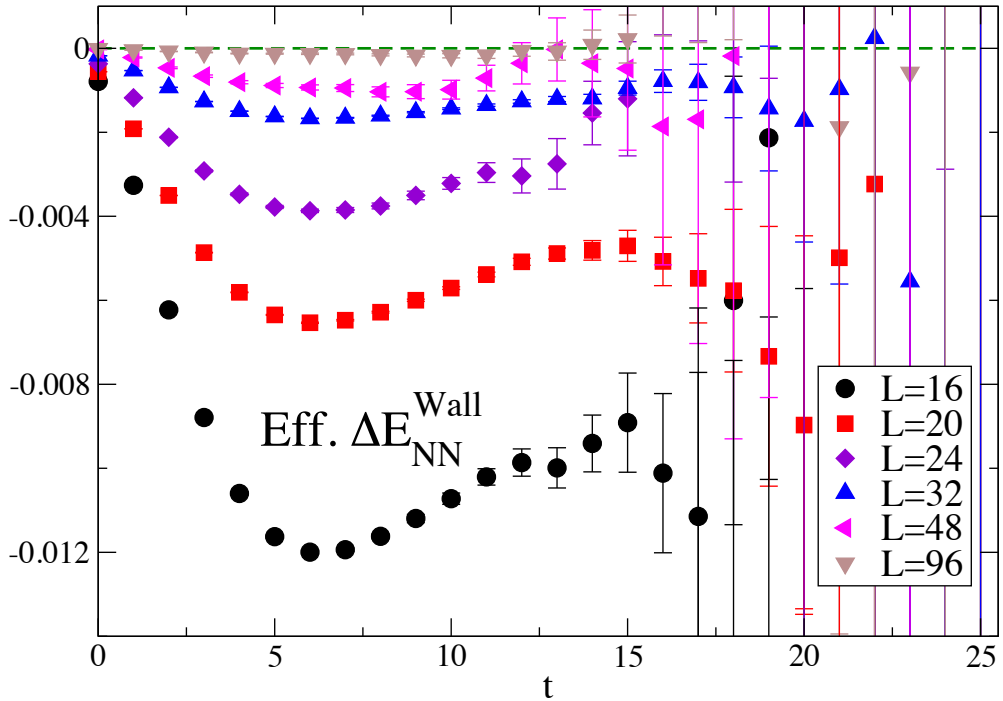
ΔE_{NN} plateau may appear $t > t_N$

Might become $\Delta E_{NN} = \Delta E_{NN}$

Why hard to observe consistency on larger volume?

Volume dependence of wall source

Preliminary result + pilot study of PRD84:054506(2011): $N_f = 0$ $m_\pi = 0.8$ GeV



Clear volume dependence + dip structure in small t

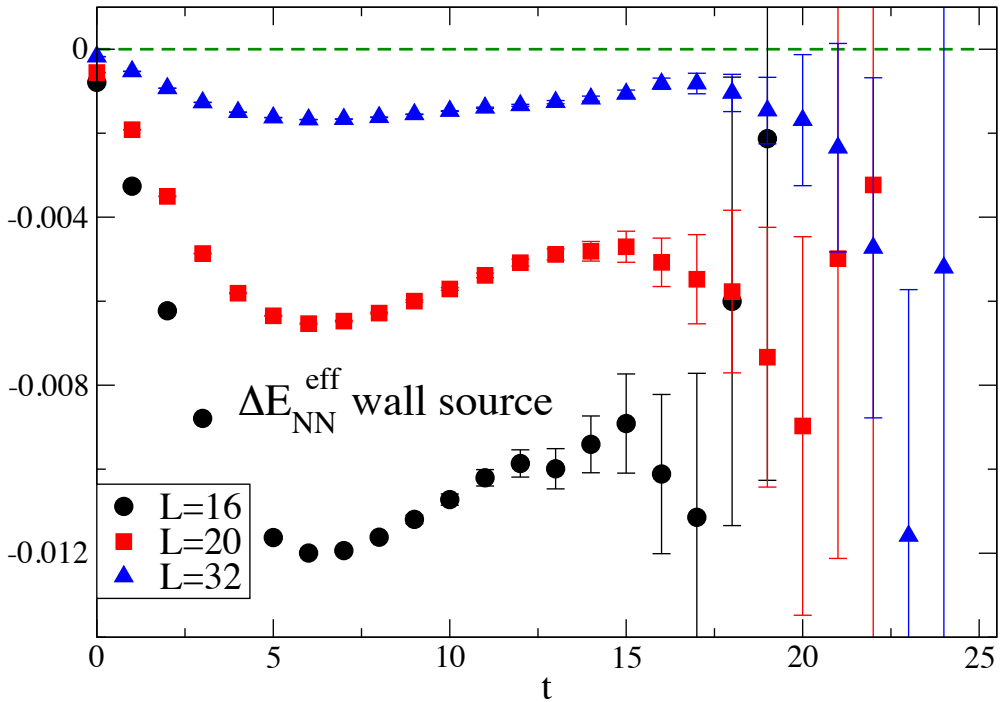
Dip becomes flat as volume increases

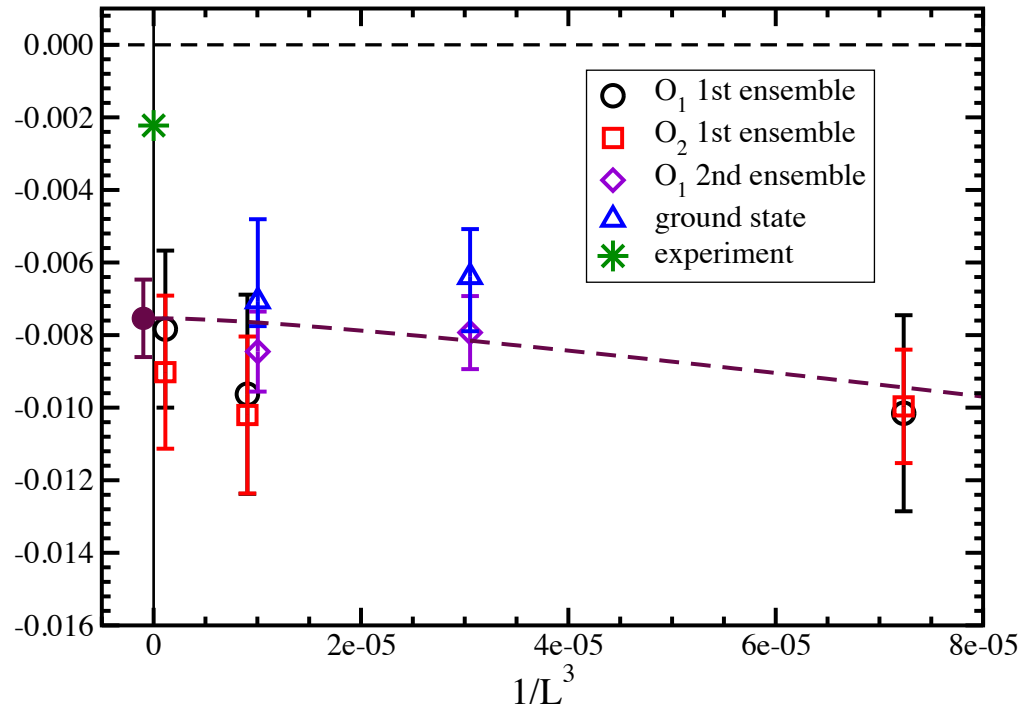
Bump appears in large t region in high precision data on $L = 20$ and 32

attempt to explain bump using ΔE_{NN} from exponential

Time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source (very preliminary)

Can understand time dependence with ΔE_{NN} from exponential?

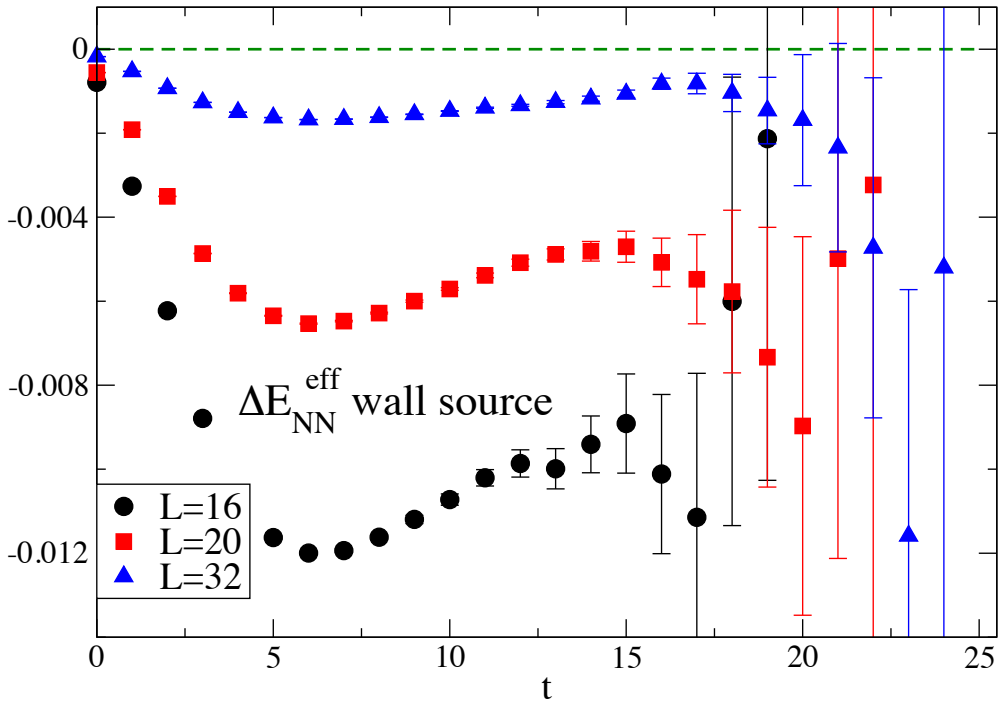


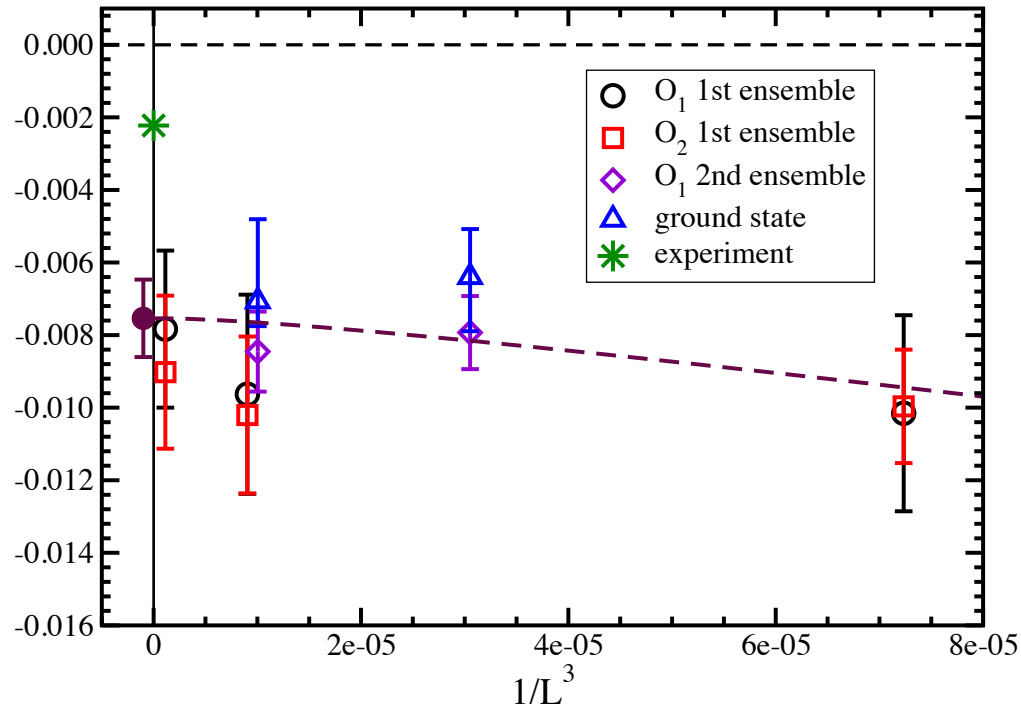


Bound state from $\Delta E_{NN}^{\text{exp}} = \Delta E_0$

Time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source (very preliminary)

Can understand time dependence with ΔE_{NN} from exponential?



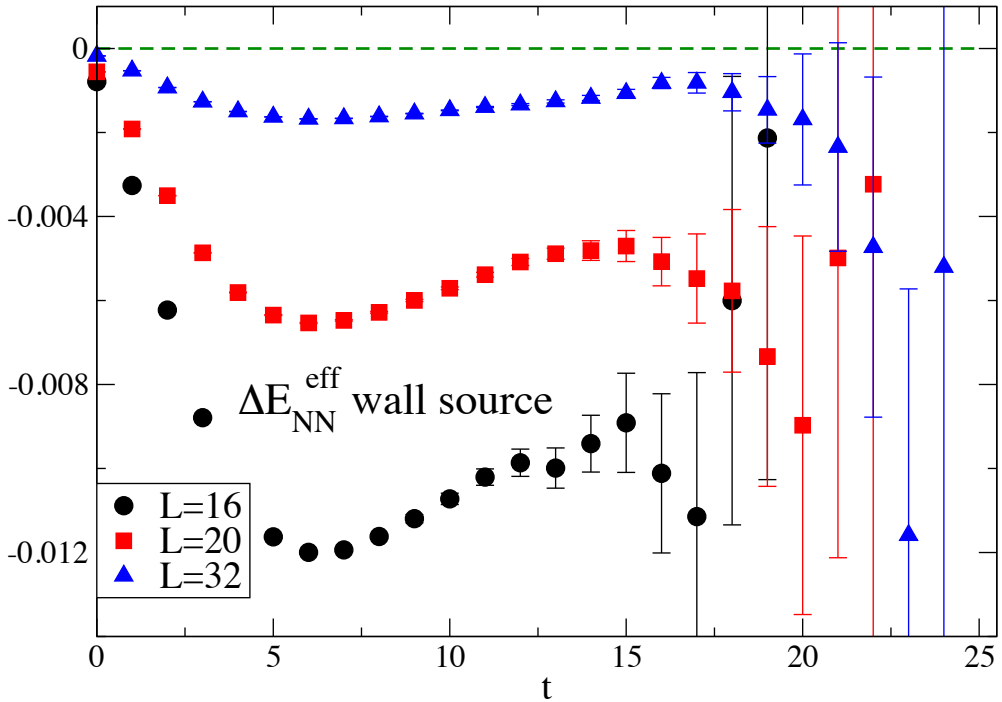


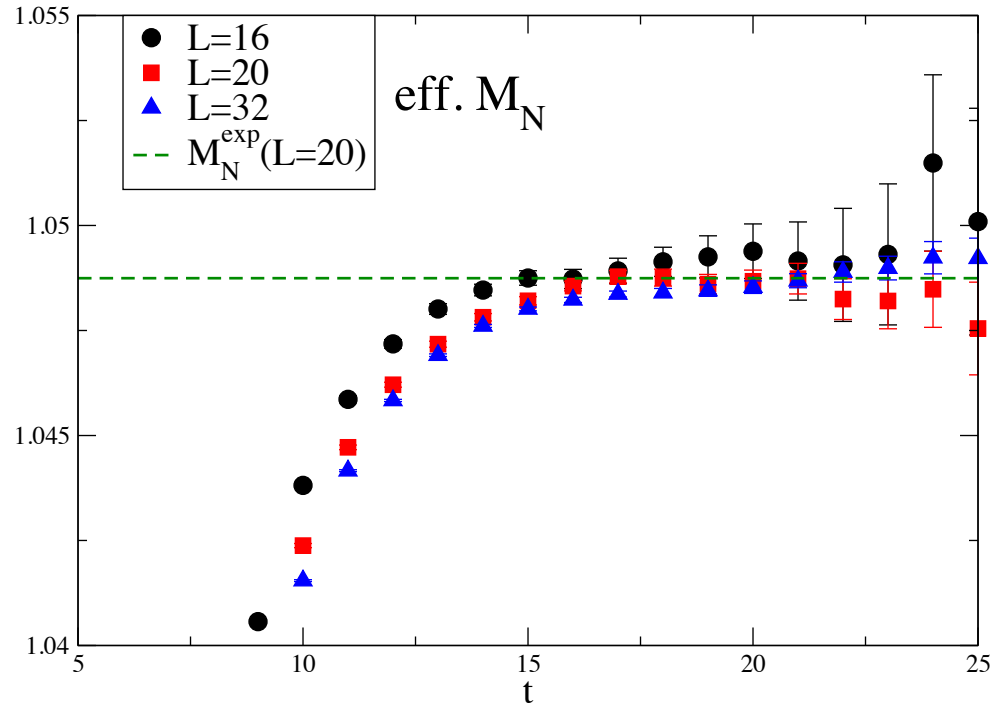
Bound state from $\Delta E_{NN}^{\text{exp}} = \Delta E_0 \to a_0 < 0$

lowest NN scattering state $\Delta E_1 = AL^{-3} > 0$

Time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source (very preliminary)

Can understand time dependence with ΔE_{NN} from exponential?





Bound state from $\Delta E_{NN}^{\text{exp}} = \Delta E_0 \to a_0 < 0$

lowest NN scattering state $\Delta E_1 = AL^{-3} > 0$

Wall source: next leading excited state contribution in $R(t) \Rightarrow NN'$

$$\Delta E_2 = \Delta E_{NN'} = m_{N'} - m_N$$

$\because$ suppress $p \neq 0$ baryon and large N' contribution in $C_N^W(t)$

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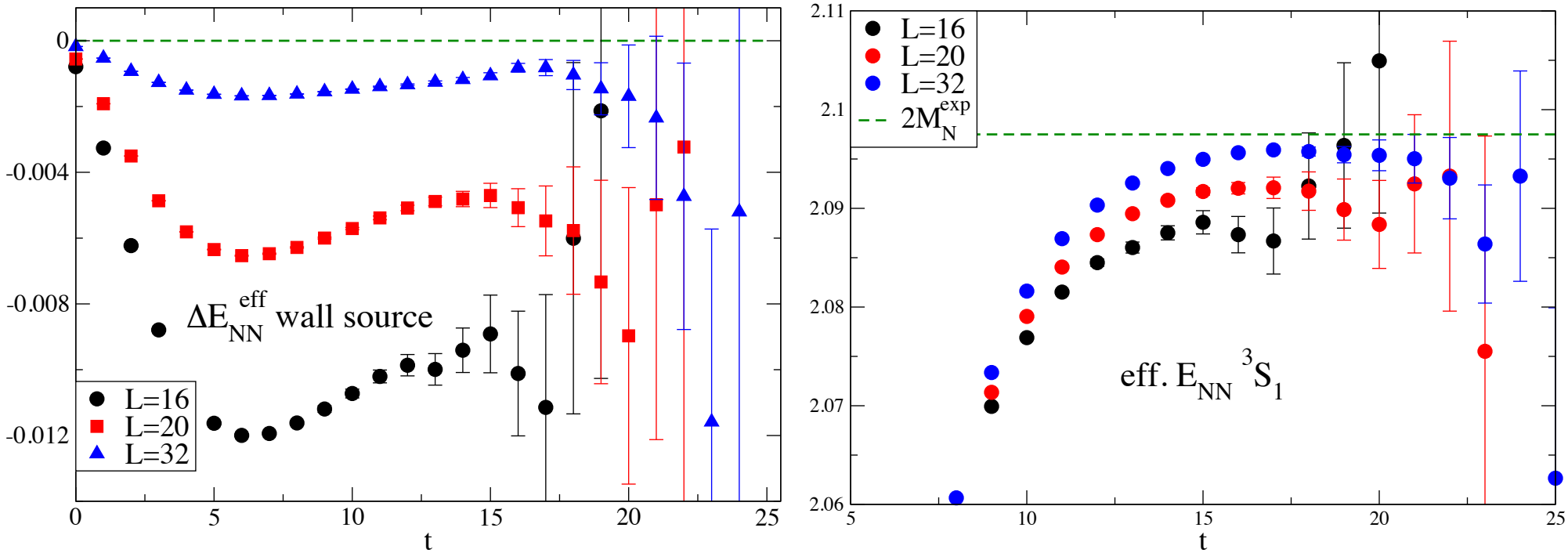

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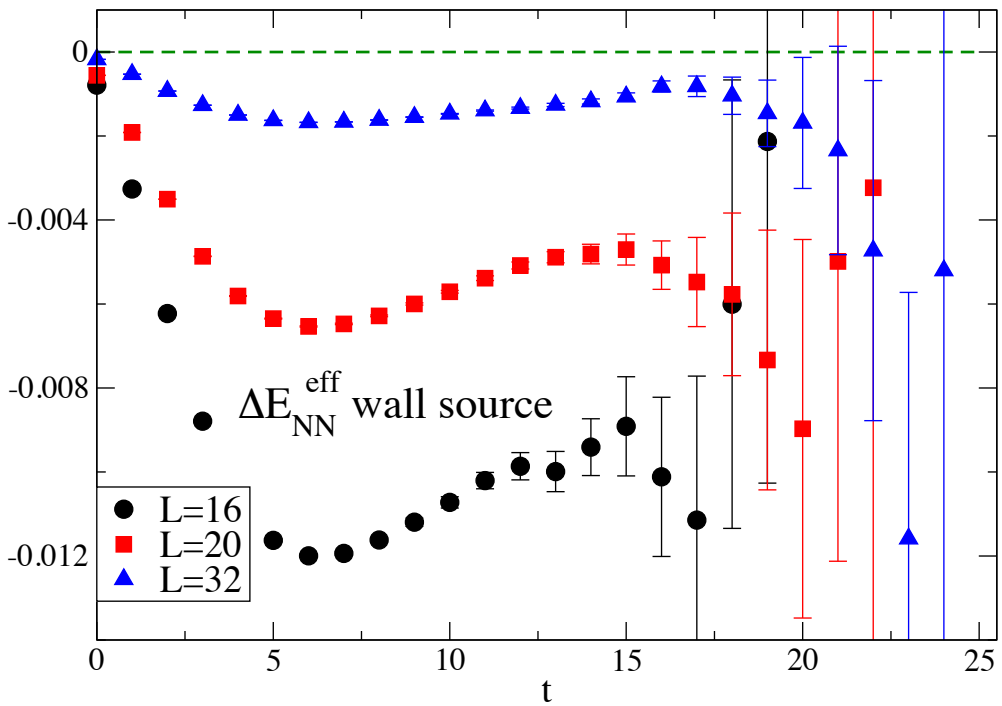

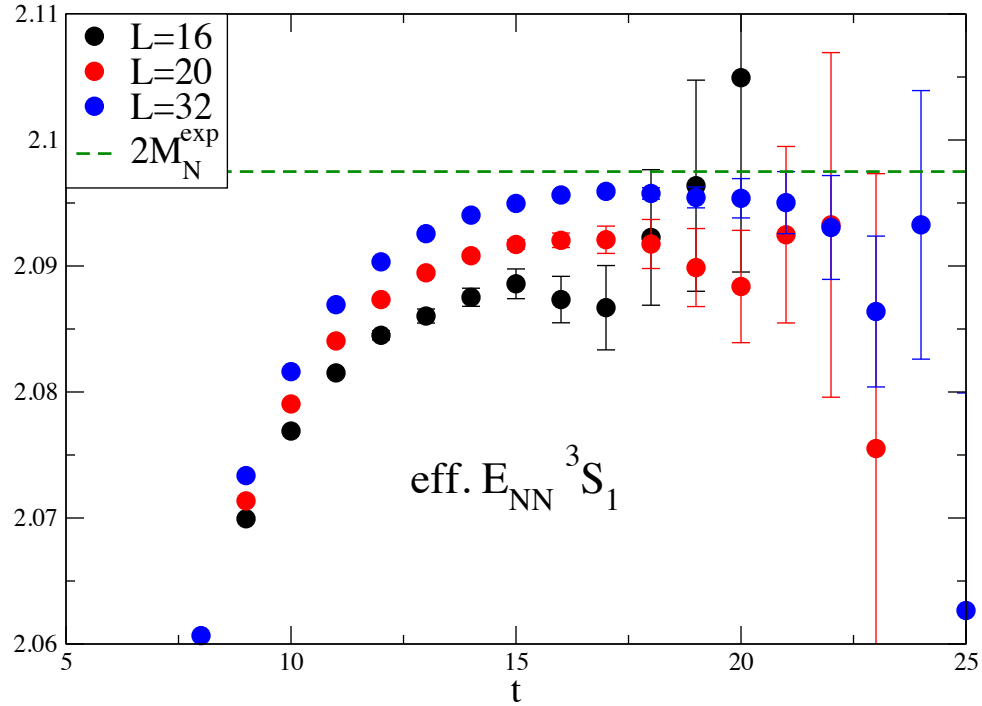

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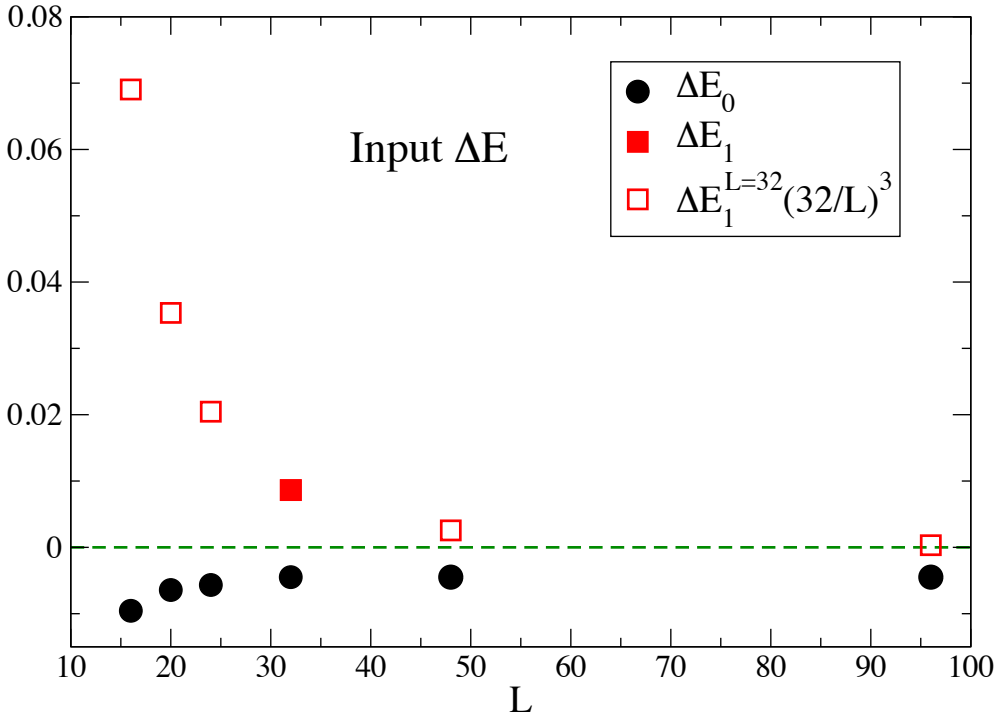
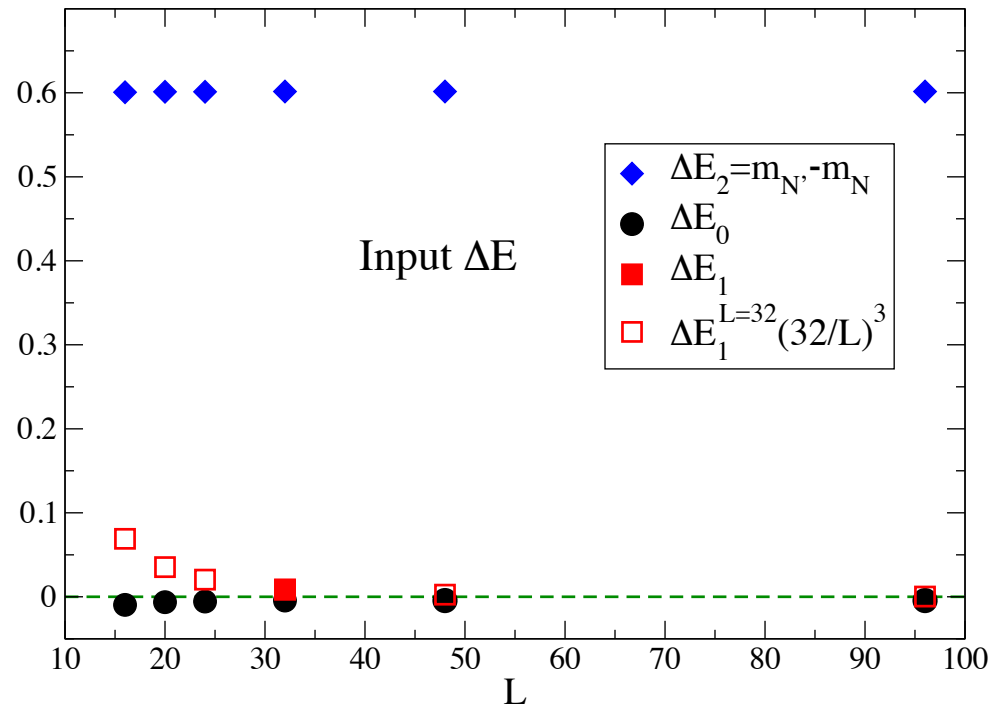
Explain $R(t)$ in $12 \lesssim t \leq 20$ by $\Delta E_0, \Delta E_1, \Delta E_2$

Input for $\Delta E_0, \Delta E_1, \Delta E_2$





ΔE_0: exponetial source results

ΔE_1: a variational analysis result $\Delta E_1^{L=32} = 0.0086(^{+44}_{-14})$ PRD84(2011)054506

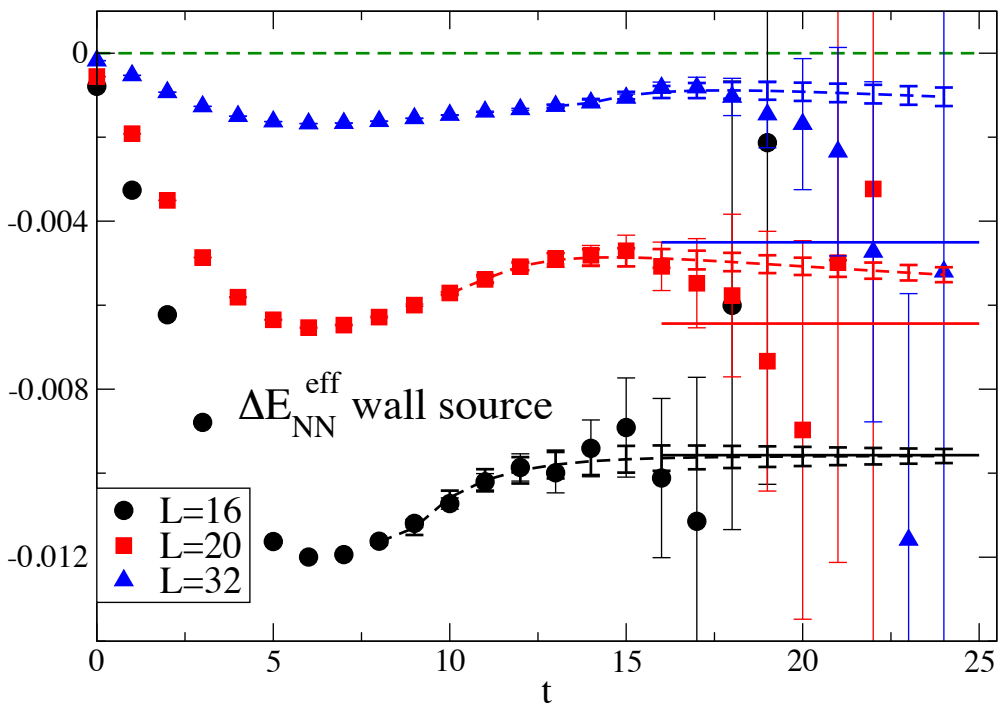
$$\Delta E_1^L = \Delta E_1^{L=32} \left(\frac{32}{L}\right)^3$$

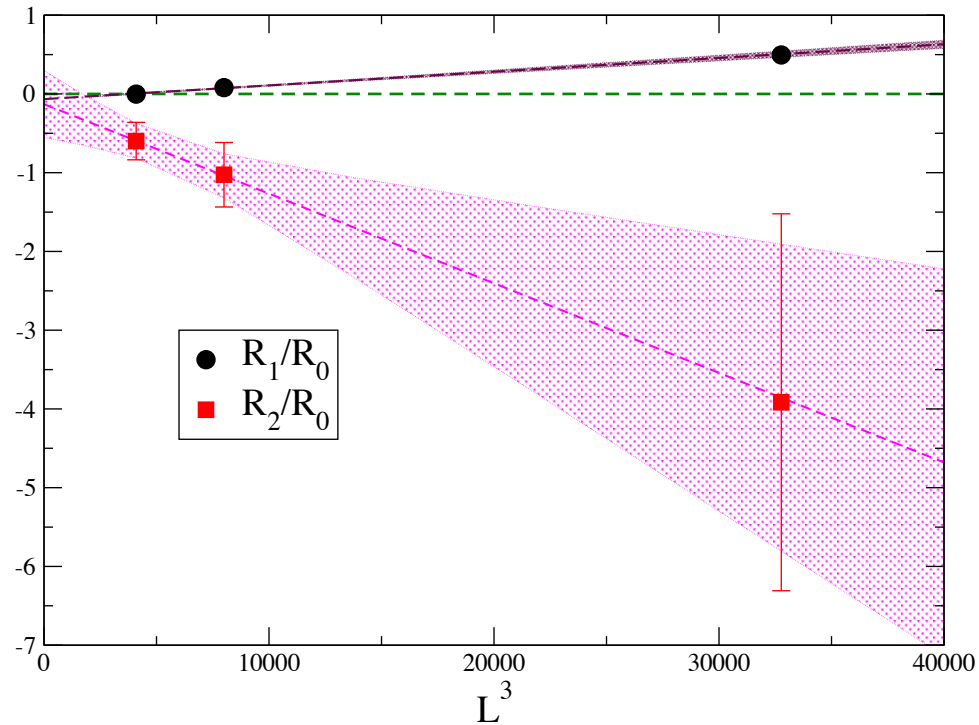
ΔE_2: $m_{N'} \sim 1.6$ estimated from $C_N^W(t)$

$\Delta E_2 = m_{N'} - m_N$ w/o finite volume effect

Fit results of $R(t)$ with wall source

Fit form: $R(t) = R_0 e^{-\Delta E_0 t} + R_1 e^{-\Delta E_1 t} + R_2 e^{-\Delta E_2 t}$





Bump in $t \sim 15$ can be explained by 3 states

Ratios for R_i/R_0 propotional to L^3

$\rightarrow$ consistent with [R_0 : bound state] and [$R_{1,2}$: scattering states]

c.f.) [Mathur *et al.*, PRD70(2004)074508]

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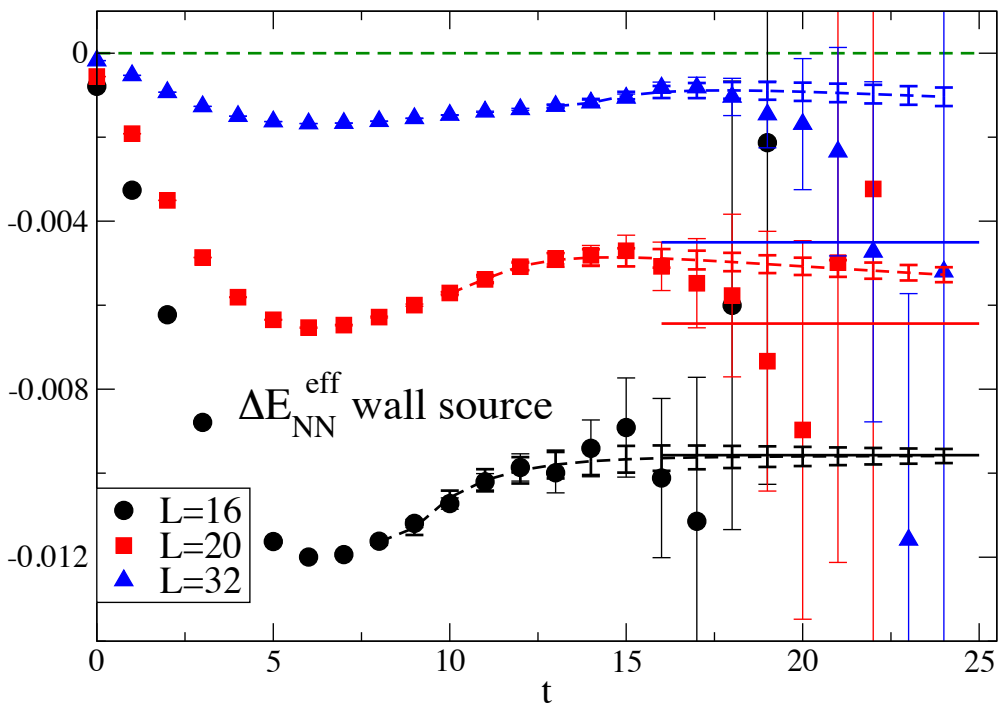

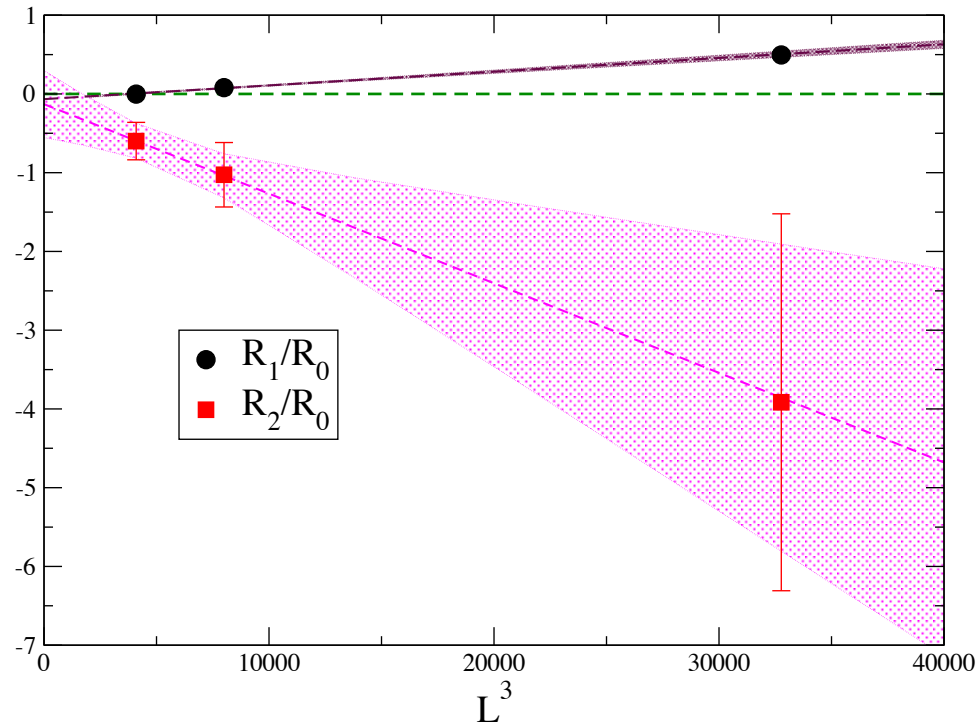

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t_{min} shifts to larger t as L

other scattering state contributions become non negligible

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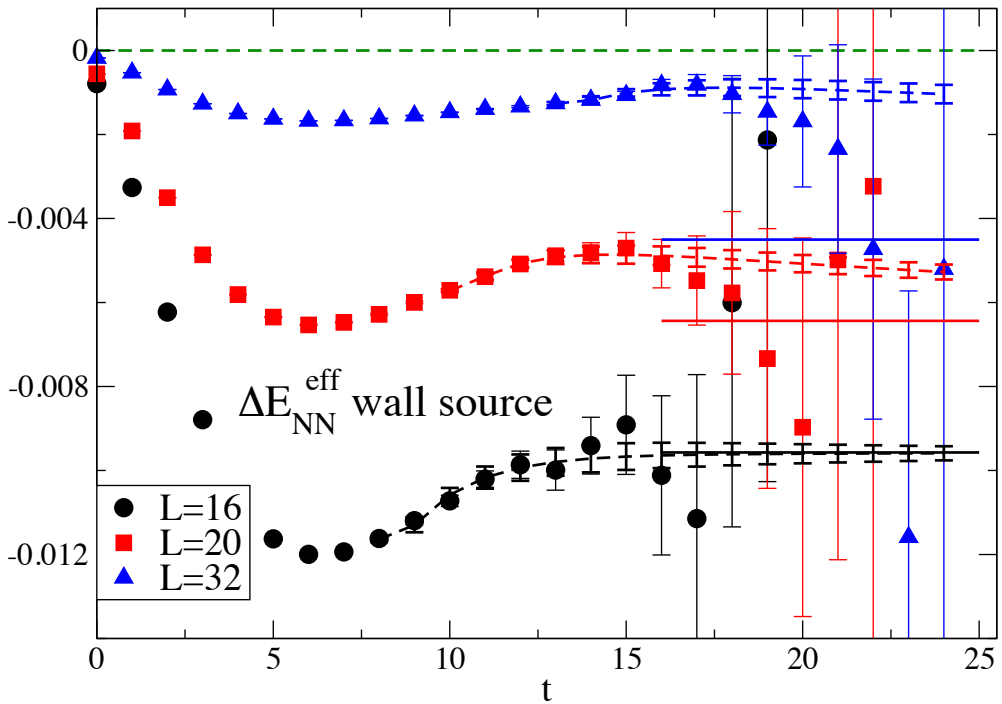
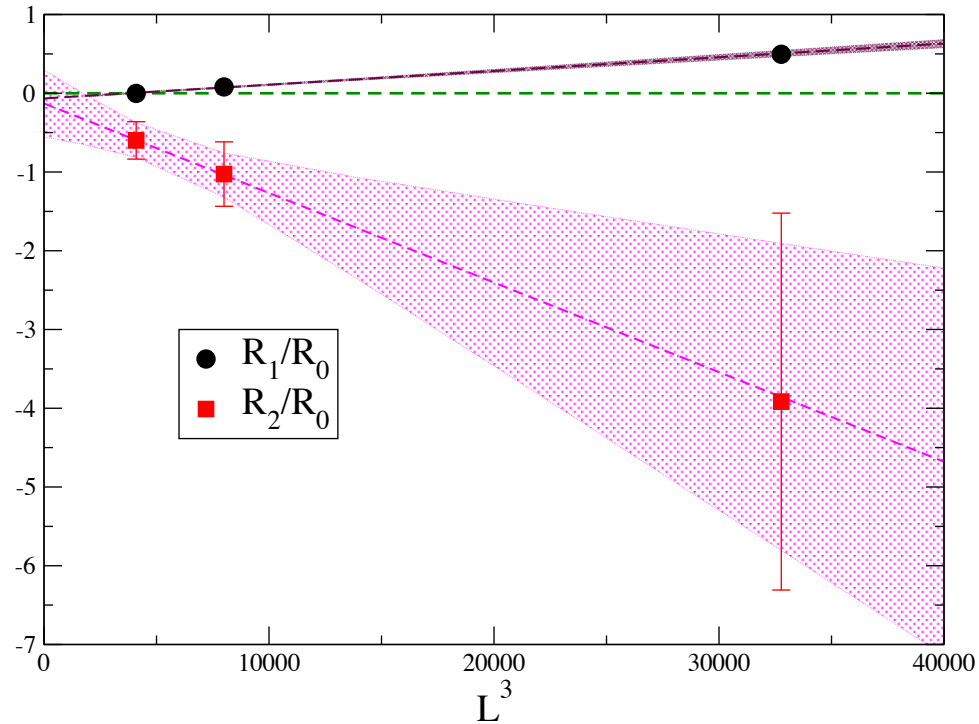




Bump in $t \sim 15$ can be explained by 3 states

Ratios for R_i/R_0 propotional to L^3

t_{min} shifts to larger t as L

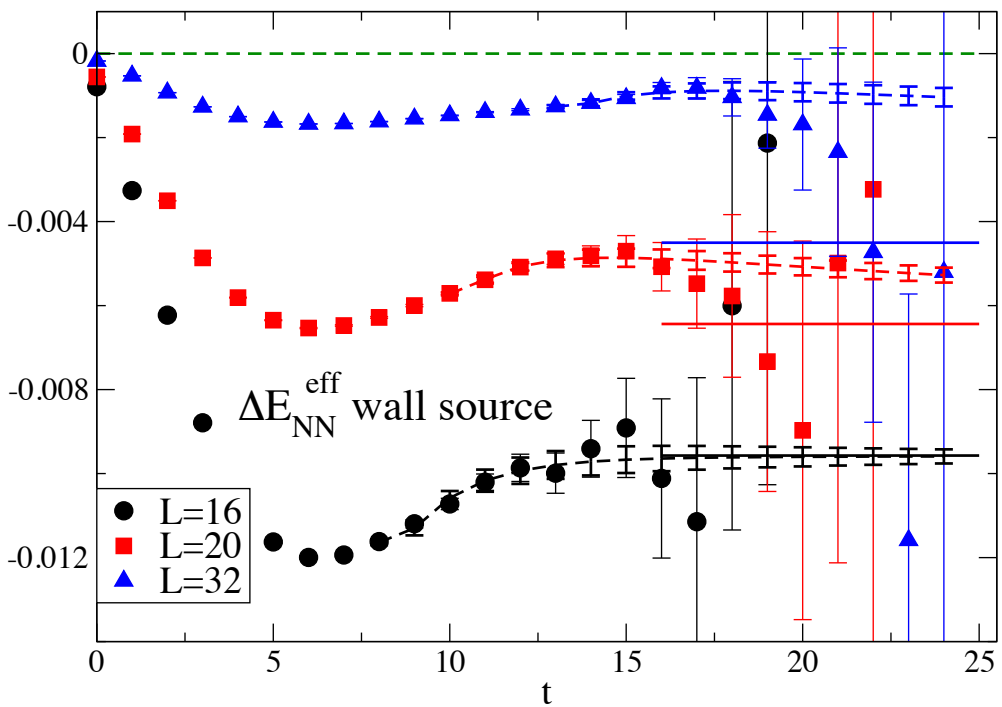
other scattering state contributions become non negligible

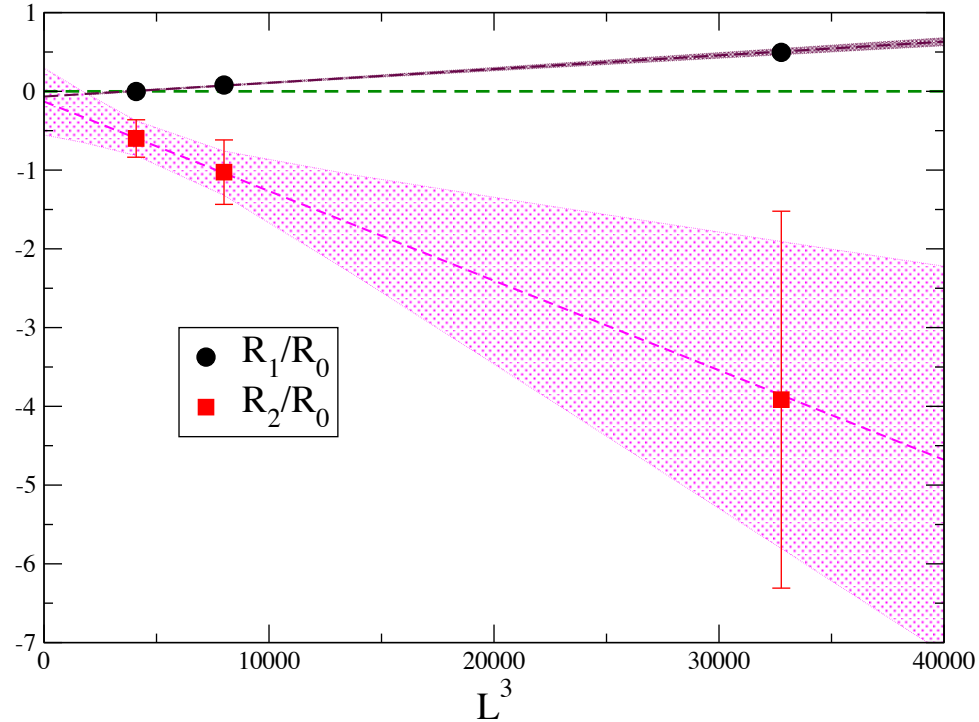
$L = 32$ needs much larger t to agree with ΔE_0^{exp}

$L = 20$ might need larger t to agree with ΔE_0^{exp}

Fit results of $R(t)$ with wall source

Fit form: $R(t) = R_0 e^{-\Delta E_0 t} + R_1 e^{-\Delta E_1 t} + R_2 e^{-\Delta E_2 t}$





Bump in $t \sim 15$ can be explained by 3 states

Smaller t: NN' contribution seen (upward)

Larger t: NN contribution seen (bump)

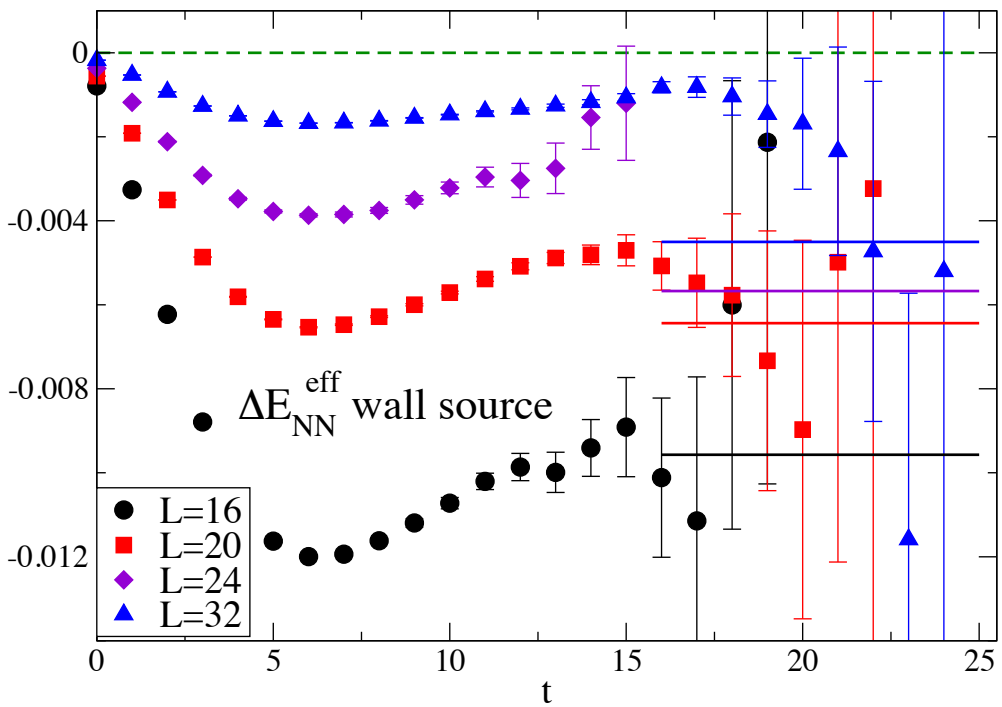
Volume dependence

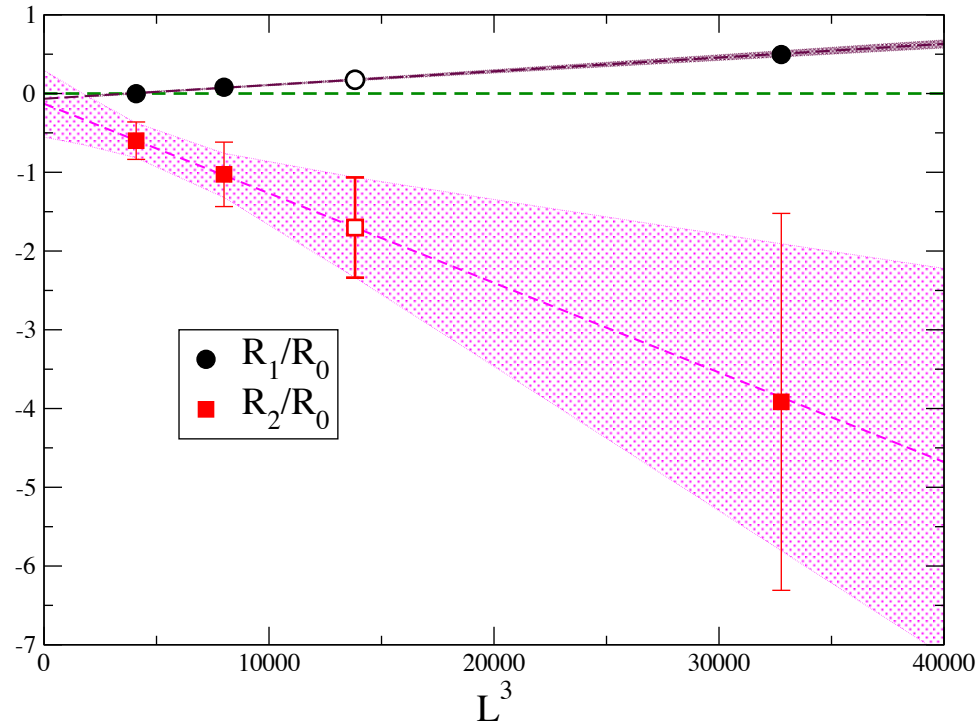
$\rightarrow$ Overlaps and ΔE_1 of NN state largely changed with L

Expected time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source

Estimate $\Delta E_{NN}^{\text{eff}}$ at $L = 24$

$$R(t)/R_0 = e^{-\Delta E_0 t} + R_1/R_0 e^{-\Delta E_1 t} + R_2/R_0 e^{-\Delta E_2 t}$$





R_i/R_0 estimated from linear interpolation

Expected time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source

Estimate $\Delta E_{NN}^{\text{eff}}$ at $L = 24$

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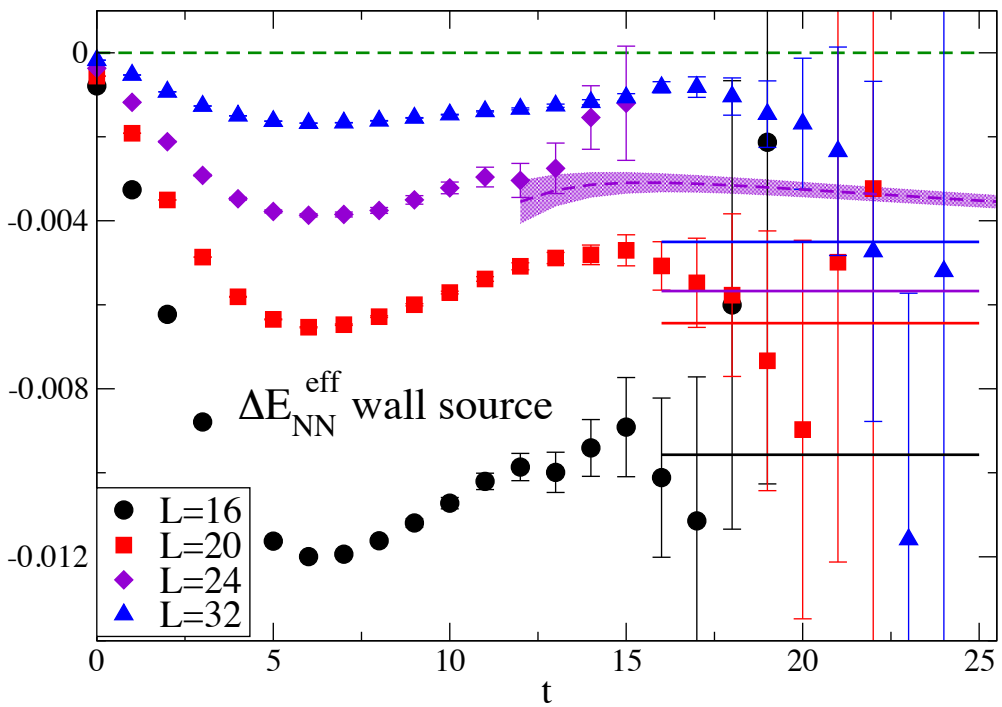
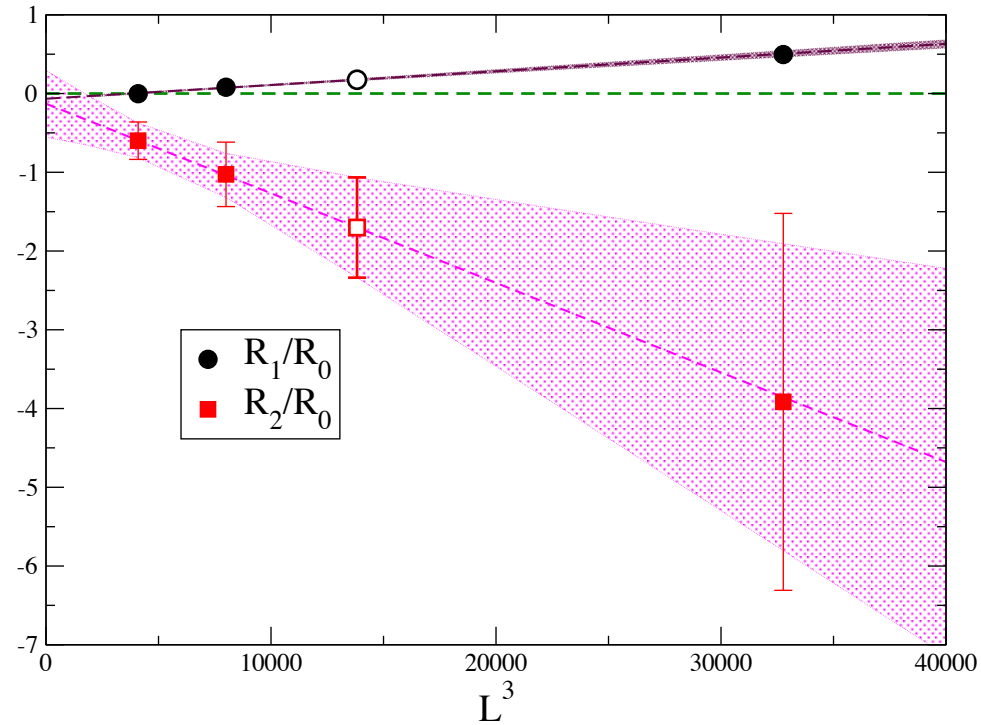




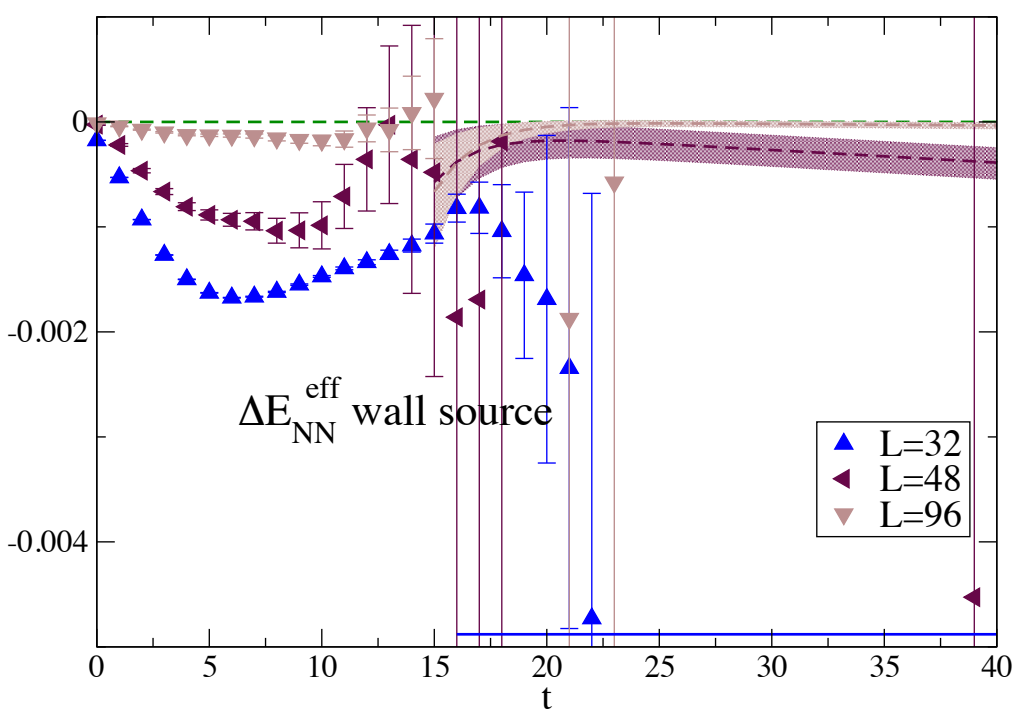
Could touch actual data

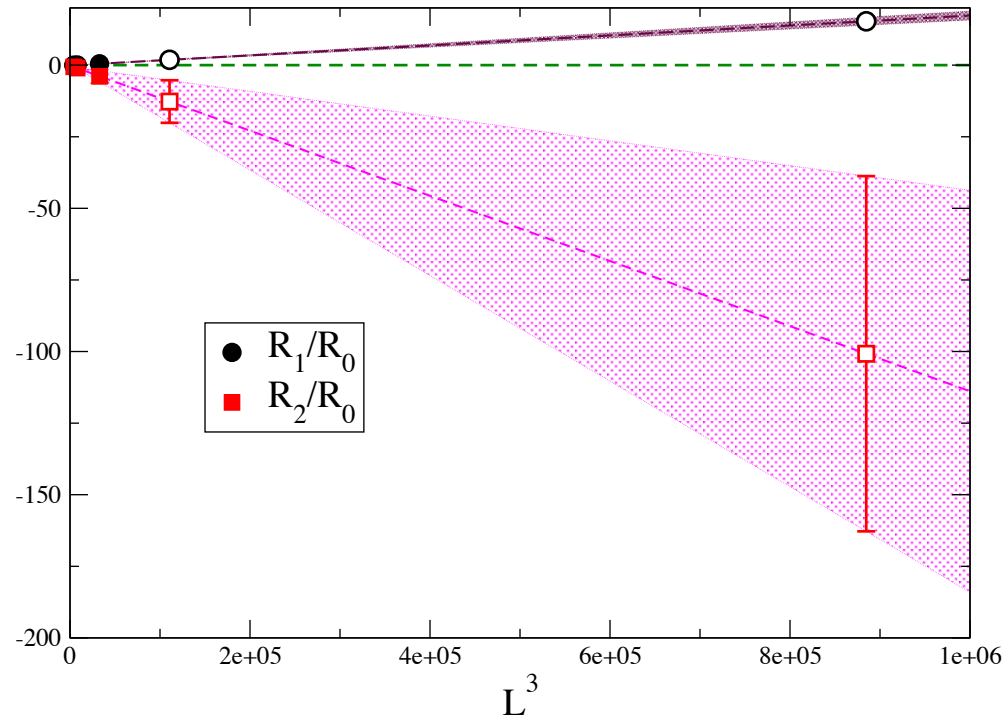
Large t needs to agree with ΔE_0^{exp}

Expected time dependence of $\Delta E_{NN}^{\text{eff}}$ with wall source

Estimate $\Delta E_{NN}^{\text{eff}}$ at $L = 48$ and 96

$$R(t)/R_0 = e^{-\Delta E_0 t} + R_1/R_0 e^{-\Delta E_1 t} + R_2/R_0 e^{-\Delta E_2 t}$$





R_i/R_0 estimated from linear extrapolation

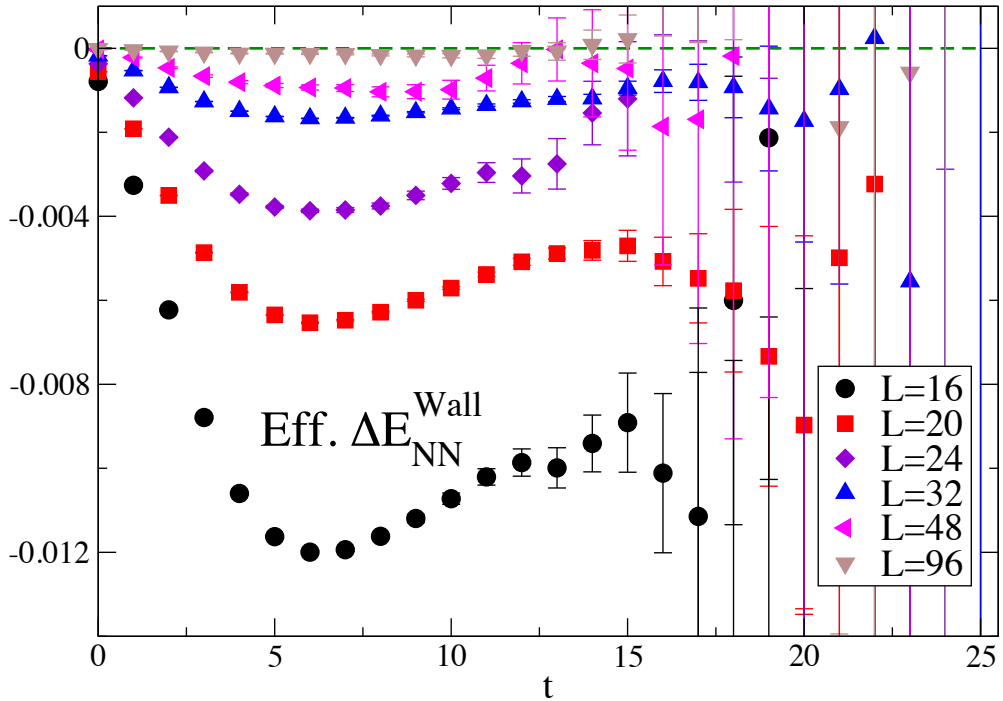
Could touch actual data

Much large t needs to agree with ΔE_0^{exp}

$\Delta E_{NN}^{\text{eff}} < 0$ on $L = 96$

Volume dependence of wall source

Preliminary result + pilot study of PRD84:054506(2011): $N_f = 0$ $m_\pi = 0.8$ GeV



Dip in small t + Bump in large t

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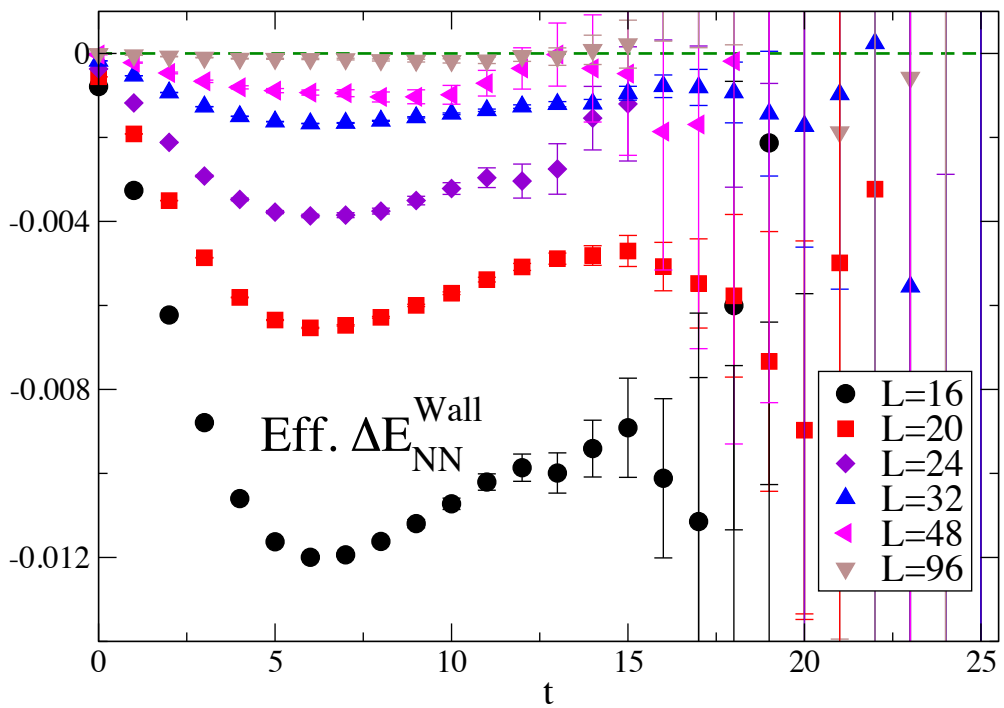
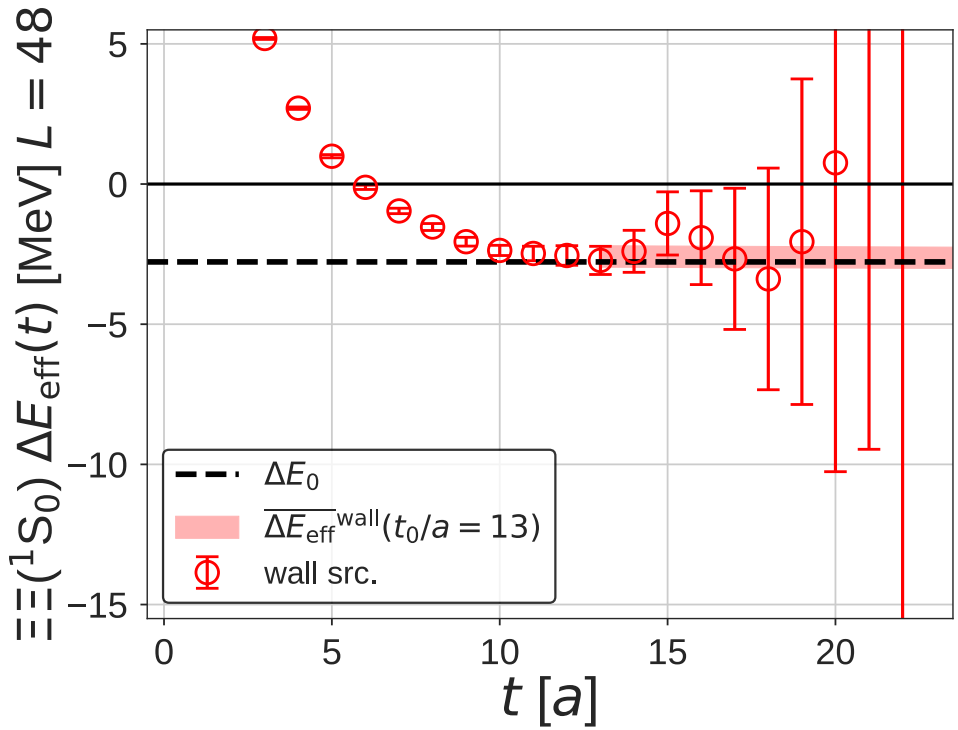




Dip in small t + Bump in large t

Different behavior from HALQCD expectation

[HALQCD, JHEP1903(2019)007]

Dip becomes flat as volume increases

$\Rightarrow$ looks plateau in large volume if statistics is not enough

Our expectation: In large statistics similar behavior will appear

Summary

Preliminary result

High precision NN calculation in $N_f = 0$ at $m_\pi = 0.8$ GeV

Souce dependence of $\Delta E_{NN}^{\text{eff}}$

exponential source: earlier plateau

walll source: non monotonic behavior

consistent with exponential source at large t

Volume dependence of $R(t)$ with wall source

Bump in large t can be explained by bound, NN, NN' states

Ratios of amplitudes propotional to L^3

$\rightarrow$ ground state is bound state, 1st and 2nd are scattering states

Expected $\Delta E_{NN}^{\text{eff}}$ on other L agrees with data

Dip becomes flat as volume increases

$\rightarrow$ looks plateau if statistics is not enough

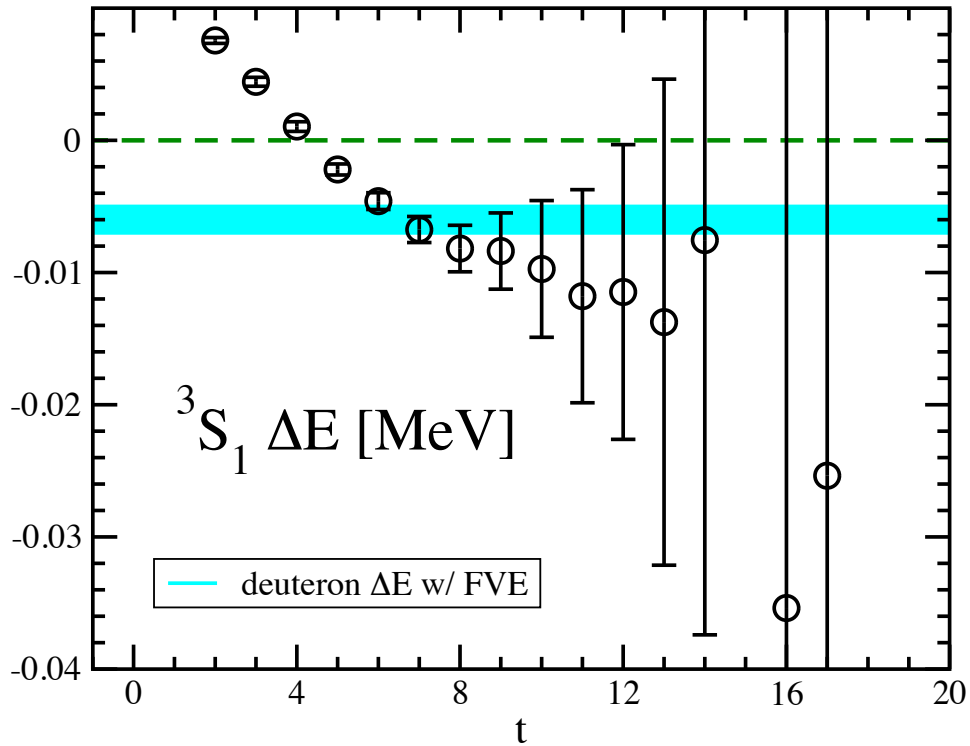
Wall source: hard to obtain bound state energy

large overlap to NN scattering state in large t

Need to check our expectation with variantional analysis

$N_f = 2 + 1$ $m_\pi = 0.146$ GeV on (8.1 fm)^3

$^3S_1$ effective ΔE with exponential source



118,080 measurements

roughly agree with deuteron ΔE with finite volume effect ~ 6 MeV

Might be hard to improve statistical error further

need better calculation method to imporve statistical error