

Comparison of different source calculations in two-nucleon channel at large quark mass

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Abstract. We investigate a systematic error coming from higher excited state contributions in the energy shift of light nucleus in the two-nucleon channel by comparing two different source calculations with the exponential and wall sources. Since it is hard to obtain a clear signal of the wall source correlation function in a plateau region, we employ a large quark mass as the pion mass is 0.8 GeV in quenched QCD. We discuss the systematic error in the spin-triplet channel of the two-nucleon system, and the volume dependence of the energy shift.

1 Introduction

We carried out an exploratory study of the direct calculation of the binding energy of the light nuclei with the atomic mass number less than or equal to four in quenched lattice QCD [1, 2]. These studies were followed by several calculations [3–9]. All the recent calculations at $m_\pi > 0.3$ GeV, which were obtained from the calculations with the exponential or gaussian source, suggest the existence of a bound state in the two-nucleon channels.

HALQCD [10] suggested that there is a sizable systematic error in the energy shift in the two-nucleon channels obtained from the ratio of the correlation functions. They compared the two results with the exponential and wall sources, and found discrepancies in the effective energy shifts. However, it is well known that the wall source needs the longest temporal extent to obtain a plateau even in the single nucleon mass. In this comparison a high precision calculation is necessary.

The purpose of this work is to investigate the systematic error coming from excited states by comparing the exponential and wall source calculations in the spin-triplet two-nucleon channel in a high precision calculation using a large quark mass of $m_\pi = 0.8$ GeV in the quenched approximation. To determine a plateau of the ratio of the correlation functions, we focus on an important condition in the direct calculation, which will be explained below, though it is trivial in lattice QCD calculation. The results in this report are the updated ones from the last conference [11]. All the results in this report are preliminary.

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2 Important condition of direct calculation

In the direct calculation [1–9] of the two-nucleon channel, the energy shift $\Delta E_{NN} = 2m_N - E_{NN}$ with the nucleon mass m_N and two-nucleon ground state energy E_{NN} is determined from a plateau region of the ratio of the correlation functions $R(t) = C_{NN}(t)/C_N^2(t)$ with the two-nucleon correlation function $C_{NN}(t)$ in the spin-triplet channel and the single nucleon correlation function $C_N(t)$. An important condition of this determination is that ΔE_{NN} should be determined in a region where both $C_{NN}(t)$ and $C_N^2(t)$ have each plateau. It means that it is not enough to determine a plateau region from only $R(t)$, but we need to investigate plateaus for $C_{NN}(t)$ and $C_N^2(t)$.

If one chooses a plateau from only $R(t)$, it might cause an incorrect determination of ΔE_{NN} , as discussed in the later sections. For example, when statistics is not enough, $R(t)$ using the wall source has a plateau like behavior in early t region, where $C_{NN}(t)$ and $C_N^2(t)$ do not have plateaus.

In the following sections, we shall call the minimum t of the plateau region for $C_{NN}(t)$, $C_N(t)$, and $R(t)$ as t_N^S , t_{NN}^S , and t_R^S , respectively, using the source $S = E$ (exponential) or W (wall).

3 Simulation parameters

We calculate the two-nucleon correlation function $C_{NN}(t)$ in the spin-triplet channel as well as the single nucleon correlation function $C_N(t)$ in the quenched approximation. In this calculation, we employ Iwasaki gauge action at $\beta = 2.416$, corresponding to $a = 0.128$ fm [12]. The quark propagators are calculated with a tad-pole improved Wilson action with $c_{SW} = 1.378$ at $\kappa_{ud} = 0.13482$ corresponding to $m_\pi = 0.8$ GeV and $m_N = 1.62$ GeV. The actions and parameters are the same as in our previous works [1, 2]. The temporal lattice size is fixed to 64, while the spatial size L is chosen to be 16, 20, and 32.

In order to compare results with different source operators, we employ the exponential and wall sources. The exponential source at the time slice t is defined by

$$q'(\mathbf{x}, t) = q(\mathbf{x}, t) + A \sum_{\mathbf{y} \neq \mathbf{x}} \exp(-B|\mathbf{y} - \mathbf{x}|)q(\mathbf{y}, t), \quad (1)$$

where $q(\mathbf{x}, t)$ is the local quark field. The parameters A and B are chosen to obtain an early plateau of the effective nucleon mass on each volume. At the sink time slice, each nucleon operator is projected to zero momentum using the local quark field as in our previous calculations [2, 5, 7]. The number of the measurement of the correlation functions is tabulated in Table 1.

L	16	20	32
Exp	6,272,000	5,504,000	4,736,000
Wall	8,307,200	8,960,000	4,473,600

Table 1. Numbers of the measurement on each L with the exponential (Exp) and wall sources.

4 Results

In this section we present the results for twice the effective nucleon mass $2m_N^{\text{eff}}$, the effective two-nucleon energy E_{NN}^{eff} , and the effective energy shift $\Delta E_{NN}^{\text{eff}}$ evaluated from $C_N(t)$, $C_{NN}(t)$, and $R(t)$, respectively, on each volume. The volume dependence of ΔE_{NN} is also presented.

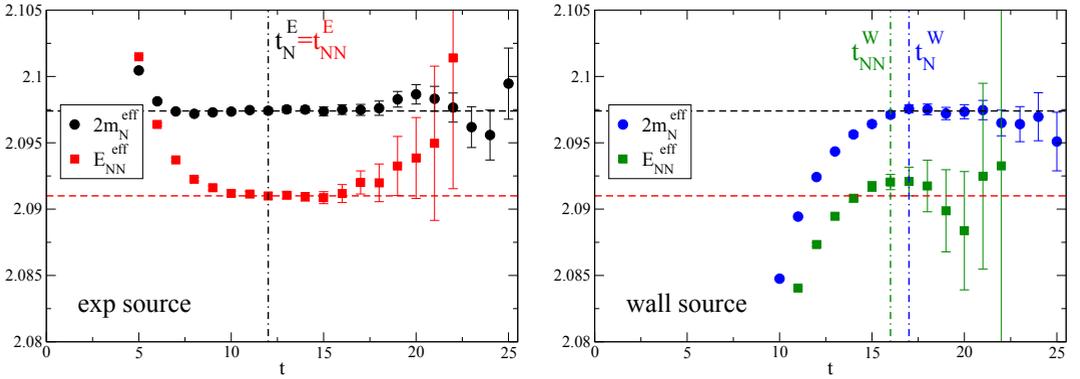


Figure 1. Effective twice nucleon mass $2m_N^{\text{eff}}$ (circle) and effective two-nucleon energy E_{NN}^{eff} (square) in the spin-triplet channel using the exponential (left panel) and wall (right panel) sources on $L = 20$. The vertical dot-dashed lines denote t_N^S and t_{NN}^S for $S = E, W$ explained in the text. The horizontal dashed lines express the values of each plateau in the exponential source in both the panels.

4.1 $L = 20$

First we present the results of $2m_N^{\text{eff}}$, E_{NN}^{eff} , and $\Delta E_{NN}^{\text{eff}}$ in both the exponential and wall sources on $L = 20$ as a typical result.

Figure 1 shows the results for $2m_N^{\text{eff}}$ and E_{NN}^{eff} using the exponential (left panel) and wall (right panel) sources. The results of the exponential source have plateaus, which start from $t = 12$ as denoted by vertical dot-dashed line in the left panel. It means that $t_N^E = t_{NN}^E = 12$ in this case. The horizontal dashed lines in black and red represent the values of the plateaus for $2m_N^{\text{eff}}$ and E_{NN}^{eff} , respectively.

The wall source results need longer t than the exponential source to have plateaus as shown in the right panel of Fig. 1. We determine $t_N^W = 17$ and $t_{NN}^W = 16$ from each plateau region, which are expressed by vertical dot-dashed lines. The same horizontal lines as in the left panel are shown in the right panel. Those lines are in good agreement with each plateau.

As discussed in Sec. 2, t_R^S , the minimum t of the plateau region of $\Delta E_{NN}^{\text{eff}}$, should be larger or equal to t_N^S and t_{NN}^S . Thus, $t_R^E = t_N^E = t_{NN}^E$, and $t_R^W = t_N^W$, in this case. Figure 2 presents that $\Delta E_{NN}^{\text{eff}}$ of the exponential source has a reasonable plateau after t_R^E . On the other hand, the result of the wall source has a non-monotonic t dependence in $t < 15$.

One might choose $t_R^W \sim 14$, if it is determined from only the wall source data in Fig. 2. Moreover, if the statistics is much smaller than the current calculation, the data around $t = 5$ would be also regarded as a plateau. However, the data in the small t region contain excited state contributions as shown in the right panel of Fig. 1. It suggests that it is easy to mistake the plateau region, when it is determined from only $\Delta E_{NN}^{\text{eff}}$, especially in the case where $\Delta E_{NN}^{\text{eff}}$ has a non-monotonic t dependence, like the wall source data in the current study.

In the wall source, while the data in $t \geq t_R^W$ has the large error, it agrees with the plateau value of the exponential source within the error.

4.2 $L = 16$

The results for $2m_N^{\text{eff}}$ and E_{NN}^{eff} using the exponential and wall sources are plotted in the left and right panels of Fig. 3, respectively. The results are similar to the ones on $L = 20$ in the previous subsection.

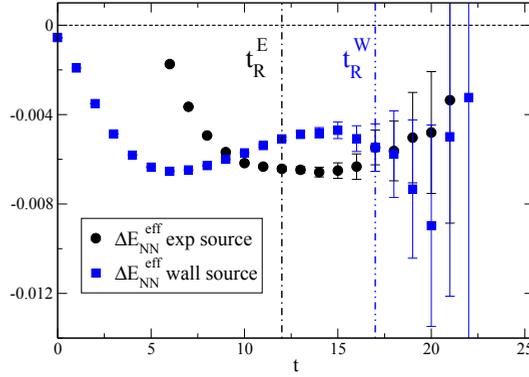


Figure 2. Effective energy shift $\Delta E_{NN}^{\text{eff}} = 2m_N^{\text{eff}} - E_{NN}^{\text{eff}}$ using the exponential (circle) and wall (square) sources on $L = 20$. The vertical dot-dashed and dot-dot-dashed lines express t_R^E and t_R^W , respectively, as explained in the text.

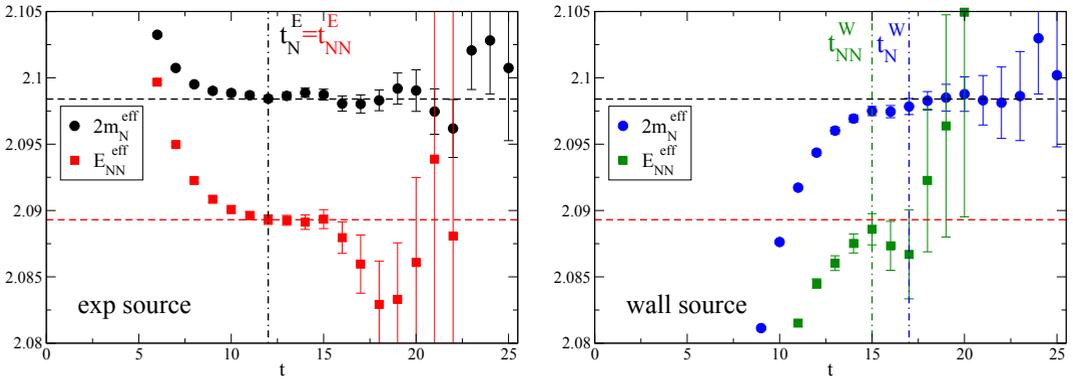


Figure 3. The same figures as Fig. 1, but in the $L = 16$ case.

The data of the exponential source have plateaus, which start from $t = 12$, and the ones of the wall source need longer t to have plateaus. It is noted that comparing with the results on $L = 20$ and 16 we observe 0.02% finite volume effect in m_N on this volume of the spatial extent 2.0 fm.

The results of $\Delta E_{NN}^{\text{eff}}$ are shown in Fig. 4. The exponential source has a reasonable plateau after $t_R^E = t_N^E = t_{NN}^E$ as in the $L = 20$ case. The t dependence of the wall source in the smaller t region becomes larger as the volume decreases comparing with the result in Fig. 2. While the error of the wall source is large after $t_R^W = t_N^W$, the data is consistent with the plateau value of the exponential source.

It is noted that on $L = 16$ the consistent results with the exponential and wall sources are not obtained even in $2m_N^{\text{eff}}$, when the number of the measurement of the wall source is half of the current calculation. This suggests that a huge statistics is necessary to obtain statistically stable result from the wall source even in the single nucleon mass.

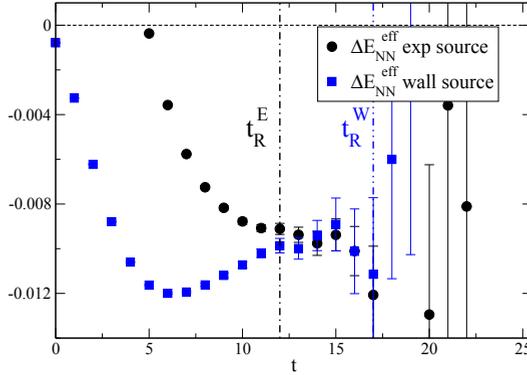


Figure 4. The same figures as Fig. 2, but in the $L = 16$ case.

4.3 $L = 32$

The left panel of Fig. 5 presents that the results for $2m_N^{\text{eff}}$ and E_{NN}^{eff} with the exponential source are similar to the ones in the $L = 16$ and 20 cases.

On the other hand, the wall source results look different from the ones on the other volumes. The result of E_{NN}^{eff} with the wall source in $t \leq 20$ is larger than the one with the exponential source represented by the red dashed line. One of the reasons is that the contribution of the two-nucleon scattering state with almost zero relative momentum, which corresponds to the first excited state in this system, becomes relatively larger than the one of the ground state in $C_{NN}(t)$ with the wall source as the volume increases. Another reason is that the energy of the first excited state is larger than $2m_N$ in this system, where one bound state exists [2]. Thus, it is harder to obtain the same plateau as the one of the exponential source, expressed by the red dashed line in the right panel of Fig. 5, from the wall source as the volume increases. From the data, we cannot determine t_{NN} of the wall source. In the following analysis, it is assumed that $t_N^W = t_{NN}^W$ in the wall source result.

From the above reasons, it is expected that on much larger volumes than the current calculation E_{NN}^{eff} of the wall source would become larger than $2m_N^{\text{eff}}$ in a large t region. Then, it would go down to agree with the plateau value of the exponential source in much larger t region.

Figure 6 shows the results of $\Delta E_{NN}^{\text{eff}}$ with both the sources. It is surprising that the wall source result has a mild t dependence in the small t region, although the data for $2m_N^{\text{eff}}$ and E_{NN}^{eff} largely depend on t in the same region as shown in the right panel of Fig. 5. If a plateau of $\Delta E_{NN}^{\text{eff}}$ is determined from only the wall source data in smaller statistics than the present calculation, one might choose much smaller t region as a plateau than t_R^W .

While it is not as good as the smaller volumes, we observe a plateau after t_R^E in the exponential source result on this volume. Although the wall source result has large error after t_R^W , it is not inconsistent with the plateau of the exponential source. We expect that the plateau of E_{NN}^{eff} with the wall source is obtained in a region of the much larger t than the smaller volumes. In order to confirm this expectation, it is an important future work to observe clear signal of the wall source after t_R^W .

From the comparisons including the ones in the smaller volumes, we conclude that the results using the exponential and wall source are consistent with each other in each plateau region. Thus, contaminations of excited states in $\Delta E_{NN}^{\text{eff}}$ obtained from the plateau region are negligible in our calculation.

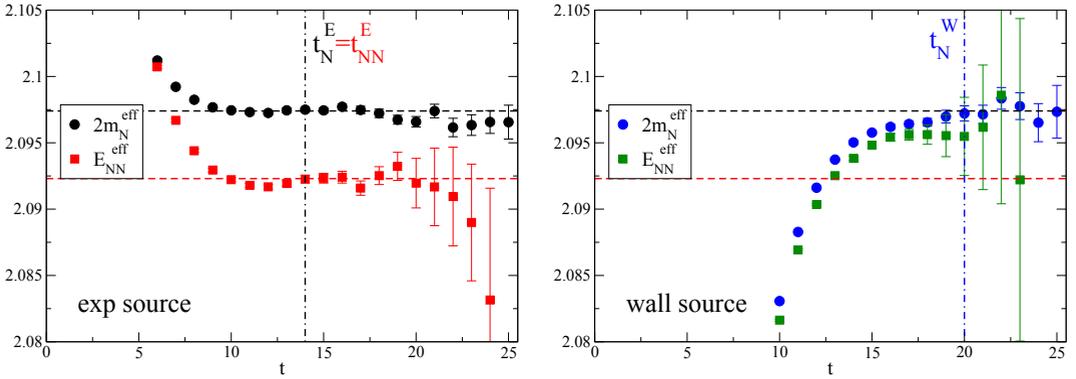


Figure 5. The same figures as Fig. 1, but in the $L = 32$ case.

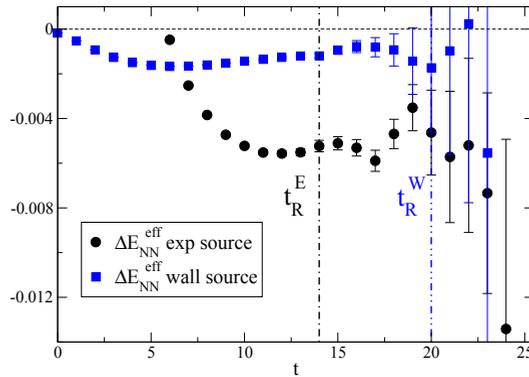


Figure 6. The same figures as Fig. 2, but in the $L = 32$ case.

4.4 Volume dependence

The result of ΔE_{NN} on the three volumes with the exponential source are plotted in Fig. 7 together with our previous result [2]. We neglect the wall source data in the following due to the much larger error. The result of the current calculation denoted by the filled circle has much smaller statistical error, and is reasonably consistent with the fit curve using the previous data, so that the result indicates that the existence of a bound state in this system.

Recently HALQCD Collaboration suggested that the volume dependence of ΔE_{NN} obtained from the direct calculation is too small comparing to the one expected from the effective range expansion [13]. However, this argument is assumed that the effective range expansion is valid in $p^2 < 0$ region in the continuum theory, and there is no finite volume effect in the two-nucleon interaction. In the comparison between the expectation in the ideal case and the lattice data, there could be several sources of systematic errors, such as finite lattice spacing and finite volume effects, which may deform the two-nucleon interaction. In order to understand the current situation, it is an important future work to investigate such systematic errors in the ΔE_{NN} calculation.

It is noted that even if there is a finite volume effect in ΔE_{NN} , which cannot be treated by the finite volume method [14, 15], we consider that the signal of the existence of the bound state is meaningful

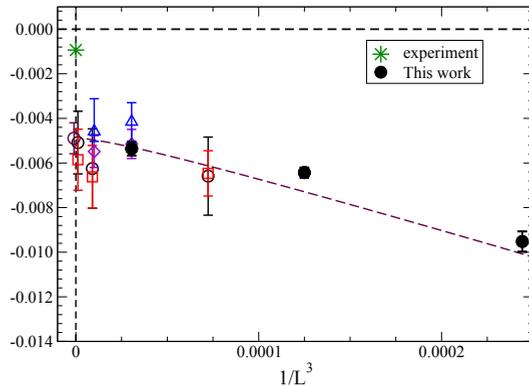


Figure 7. Volume dependence of the energy shift ΔE_{NN} using the exponential source. The horizontal axis is one over volume. The filled circles denote ΔE_{NN} on $L = 16, 20, 32$ in the current calculation. The open symbols and dashed curve are the results in our previous work [2]. The star symbol expresses the experimental value of the deuteron binding energy.

in our calculation, because we discuss the existence in the infinite volume limit, so that our result does not contain the finite volume effect.

5 Summary

We have carried out the high precision calculation of the spin-triplet two-nucleon channel at the large quark mass, corresponding to $m_\pi = 0.8$ GeV in the quenched approximation to investigate a systematic error of ΔE_{NN} coming from excited states by comparing the results with the two different source calculations using the exponential and wall sources on the three volumes. Though it might be a trivial, we discuss the important condition to calculate ΔE_{NN} . When the condition is satisfied, the two sources give the consistent results of $\Delta E_{NN}^{\text{eff}}$ in each plateau region, while the wall source data has the large error due to the late plateau. From this comparison, we have concluded that the systematic error from higher excited states is negligible in our calculation.

There are several important future works, such as comparing the current result with the one obtained from the generalized eigenvalue problem [16], and investigations of systematic errors in ΔE_{NN} . It is also an important future work to clarify the qualitative difference between the direct calculation and HALQCD method in the point of view of the definitions of the scattering amplitude in quantum field theory and quantum mechanics [17].

Acknowledgements

Numerical calculations for the present work have been carried out on the FX10 supercomputer system at Information Technology Center of the University of Tokyo, on the COMA cluster system under the “Interdisciplinary Computational Science Program” of Center for Computational Science at University of Tsukuba, on the Oakforest-PACS system of Joint Center for Advanced High Performance Computing, on the computer facilities of the Research Institute for Information Technology of Kyushu University, and on the FX100 and CX400 supercomputer systems at the Information Technology Center of Nagoya University. This research used computational resources of the HPCI system provided

by Information Technology Center of the University of Tokyo through the HPCI System Research Project (Project ID: hp160125). We thank the colleagues in the PACS Collaboration for providing us the code used in this work. This work is supported in part by Grants-in-Aid for Scientific Research from the Ministry of Education, Culture, Sports, Science and Technology (No. 16H06002).

References

- [1] T. Yamazaki, Y. Kuramashi, A. Ukawa (PACS-CS Collaboration), Phys. Rev. **D81**, 111504 (2010)
- [2] T. Yamazaki, Y. Kuramashi, A. Ukawa (PACS-CS Collaboration), Phys. Rev. **D84**, 054506 (2011)
- [3] S. Beane et al. (NPLQCD Collaboration), Phys. Rev. **D85**, 054511 (2012)
- [4] S. Beane, E. Chang, S. Cohen, W. Detmold, H. Lin et al. (NPLQCD Collaboration), Phys.Rev. **D87**, 034506 (2013)
- [5] T. Yamazaki, K.i. Ishikawa, Y. Kuramashi, A. Ukawa, Phys. Rev. **D86**, 074514 (2012)
- [6] E. Berkowitz, T. Kurth, A. Nicholson, B. Joo, E. Rinaldi, M. Strother, P.M. Vranas, A. Walker-Loud (CalLat Collaboration), Phys. Lett. **B765**, 285 (2017)
- [7] T. Yamazaki, K.i. Ishikawa, Y. Kuramashi, A. Ukawa, Phys. Rev. **D92**, 014501 (2015)
- [8] K. Orginos, A. Parreno, M.J. Savage, S.R. Beane, E. Chang, W. Detmold (NPLQCD Collaboration), Phys. Rev. **D92**, 114512 (2015)
- [9] M.L. Wagman, F. Winter, E. Chang, Z. Davoudi, W. Detmold, K. Orginos, M.J. Savage, P.E. Shanahan (2017), 1706.06550
- [10] T. Iritani et al. (HALQCD Collaboration), JHEP **10**, 101 (2016)
- [11] T. Yamazaki, K.I. Ishikawa, Y. Kuramashi, A. Ukawa (PACS), PoS **LATTICE2016**, 108 (2017)
- [12] A. Ali Khan et al. (CP-PACS Collaboration), Phys. Rev. **D65**, 054505 (2002)
- [13] T. Iritani, S. Aoki, T. Doi, T. Hatsuda, Y. Ikeda, T. Inoue, N. Ishii, H. Nemura, K. Sasaki, Phys. Rev. **D96**, 034521 (2017)
- [14] M. Lüscher, Commun. Math. Phys. **105**, 153 (1986)
- [15] M. Lüscher, Nucl. Phys. **B354**, 531 (1991)
- [16] M. Lüscher, U. Wolff, Nucl. Phys. **B339**, 222 (1990)
- [17] T. Yamazaki, Y. Kuramashi (2017), 1709.09779