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Abstract

The computation of the determinant for Wilson-Dirac operator contains two steps: 1) analytical reduction from the determinant of the original sparse matrix to that of lower order dense matrix, and 2) numerical evaluation of the latter determinant. The first part was already done by Ref. [1] and we use their reduction. In this report, we present a efficient technique for the computation of the determinant of the lower order dense matrix. Furthermore we address a reduction of Dirac-spinor space and its implementation. The algorithm shown here was used in Ref. [2].

Contents

1 Definition of problem

Our purpose here is to compute the determinant of the Wilson-Dirac operator in 4-dimensional Euclidean system with finite chemical potential μ for one-flavor,

$$D_{x,y}(\mu) = \delta_{x,y} - \kappa \sum_{\nu=1}^{4} [e^{\mu a \delta_{\nu,4}}(1-\gamma_\nu)U_\nu(x)\delta_{x+\hat{\nu},y} + e^{-\mu a \delta_{\nu,4}}(1+\gamma_\nu)U_\nu^\dagger(y)\delta_{x-\hat{\nu},y}], \tag{1}$$

where γ_ν ($\nu = 1,2,3,4$) are the gamma-matrix in the system, κ is the hopping parameter and $U_\nu(x)$ are link variables. The determinant of the operator[1] in a time-blocked form with temporal lattice size $N_\mathrm{T} = 8$ is given by,

$$\det D(\mu) = \det \left(\begin{array}{ccc|c|c|ccc|c} d_{(1)} & d_{(12)} & 0 & 0 & 0 & 0 & 0 & e^{-\mu/T} d_{(18)} \\ d_{(21)} & d_{(2)} & d_{(23)} & 0 & 0 & 0 & 0 & 0 \\ 0 & d_{(32)} & d_{(3)} & d_{(34)} & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & d_{(43)} & d_{(4)} & d_{(45)} & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & d_{(54)} & d_{(5)} & d_{(56)} & 0 & 0 \\ 0 & 0 & 0 & 0 & d_{(65)} & d_{(6)} & d_{(67)} & 0 \\ 0 & 0 & 0 & 0 & 0 & d_{(76)} & d_{(7)} & d_{(78)} \\ \hline e^{\mu/T} d_{(81)} & 0 & 0 & 0 & 0 & 0 & d_{(87)} & d_{(8)} \end{array} \right), \tag{2}$$

where we have defined the matrices of order $12N_\mathrm{L}^3$ (where N_L is the spatial lattice linear size). For example, the block diagonal elements $d_{(t)}$ for $t = 1,2,3,...,N_\mathrm{T}(=8)$ are three-dimensional Wilson-Dirac operator. The block off-diagonal elements for $t = 1,2,...,N_\mathrm{T}-1(=7)$ are hopping term for the time-direction,

$$\begin{aligned} d_{(t+1,t)} &= -2\kappa P_+ U_4^\dagger(t)\delta_{\mathbf{x},\mathbf{y}}, & (3)\\ d_{(t,t+1)} &= -2\kappa P_- U_4(t)\delta_{\mathbf{x},\mathbf{y}}, & (4)\end{aligned}$$

and for $t = N_\mathrm{T}(= 8)$ due to the anti-periodic boundary condition for fermion field, the corner elements are given by (additional minus sign cancels the original sign)

$$\begin{aligned} d_{(1,N_\mathrm{T})} &= 2\kappa P_+ U_4^\dagger(N_\mathrm{T})\delta_{\mathbf{x},\mathbf{y}}, & (5)\\ d_{(N_\mathrm{T},1)} &= 2\kappa P_- U_4(N_\mathrm{T})\delta_{\mathbf{x},\mathbf{y}}, & (6)\end{aligned}$$

where we denote $U_4(t) = U_{\nu=4}(x_0 = t, \mathbf{x})$ is the link-variable for time-direction and $P_\pm = (1\pm\gamma_4)/2$. The details of the Dirac-gamma matrices are given in appendix Appendix A.

By making use of the domain decomposition representation[2],

$$\det D(\mu) = \det \left(\begin{array}{c|c|c|c} D_{(1)} & D_{(12)} & 0 & e^{-\mu/T} D_{(14)} \\ \hline D_{(21)} & D_{(2)} & D_{(23)} & 0 \\ \hline 0 & D_{(32)} & D_{(3)} & D_{(34)} \\ \hline e^{\mu/T} D_{(41)} & 0 & D_{(43)} & D_{(4)} \end{array} \right), \tag{12}$$

[1]Inclusion of the clover term is straightforward.

[2]Decomposed into four domains:

$$\begin{aligned} &\text{domain (1) :} && \text{for} && t = 1,2,3, & (7)\\ &\text{domain (2) :} && \text{for} && t = 4, & (8)\\ &\text{domain (3) :} && \text{for} && t = 5,6,7, & (9)\\ &\text{domain (4) :} && \text{for} && t = 8, & (10)\\ &&&&&& (11)\end{aligned}$$

and the reduction for the time direction [1], the determinant may be written as

$$\det D(\mu) = A_0 \det[1 - H_0 - e^{\mu/T} H_+ - e^{-\mu/T} H_-], \tag{13}$$

where

$$\begin{aligned}
A_0 &= \det D_{(1)} \det D_{(3)} \det D_{(2*2)} \det D_{(4*4)}, & (14)\\
H_0 &= D^{-1}_{(4*4)} D_{(412)} D^{-1}_{(2*2)} D_{(214)} + D^{-1}_{(4*4)} D_{(432)} D^{-1}_{(2*2)} D_{(234)}, & (15)\\
H_+ &= D^{-1}_{(4*4)} D_{(412)} D^{-1}_{(2*2)} D_{(234)}, & (16)\\
H_- &= D^{-1}_{(4*4)} D_{(432)} D^{-1}_{(2*2)} D_{(214)}, & (17)
\end{aligned}$$

with

$$\begin{aligned}
D_{(2*2)} &= D_{(2)} - D_{(21)} D^{-1}_{(1)} D_{(12)} - D_{(23)} D^{-1}_{(3)} D_{(32)}, & (18)\\
D_{(4*4)} &= D_{(4)} - D_{(41)} D^{-1}_{(1)} D_{(14)} - D_{(43)} D^{-1}_{(3)} D_{(34)}, & (19)\\
D_{(412)} &= D_{(41)} D^{-1}_{(1)} D_{(12)}, & (20)\\
D_{(432)} &= D_{(43)} D^{-1}_{(3)} D_{(32)}, & (21)\\
D_{(214)} &= D_{(21)} D^{-1}_{(1)} D_{(14)}, & (22)\\
D_{(234)} &= D_{(23)} D^{-1}_{(3)} D_{(34)}. & (23)
\end{aligned}$$

In this note, we do not derive this form, but we address how to numerically compute the expression eq.(13) in an efficient way. Now, our task is to compute the following matrix products

$$D_{(21)} D^{-1}_{(1)} D_{(12)}, \tag{24}$$
$$D_{(21)} D^{-1}_{(1)} D_{(14)}, \tag{25}$$
$$D_{(41)} D^{-1}_{(1)} D_{(14)}, \tag{26}$$
$$D_{(41)} D^{-1}_{(1)} D_{(12)}, \tag{27}$$

and

$$D_{(43)} D^{-1}_{(3)} D_{(34)}, \tag{28}$$
$$D_{(43)} D^{-1}_{(3)} D_{(32)}, \tag{29}$$
$$D_{(23)} D^{-1}_{(3)} D_{(32)}, \tag{30}$$
$$D_{(23)} D^{-1}_{(3)} D_{(34)}. \tag{31}$$

An algorithm to compute them will be given in section 2.1. On the other hand, the computation of A_0 in eq.(14) will be addressed in section 2.2.

In the rest of this section, we explain a key idea in the computation of eq.(24-27). For $N_{\mathrm{T}} = 8$ case, $D_{(12)}$, $D_{(14)}$, $D_{(21)}$ and $D_{(41)}$ are given in a block form

$$\begin{aligned}
D_{(12)} &= \begin{pmatrix} 0 \\ 0 \\ * \end{pmatrix}, & (32)\\
D_{(14)} &= \begin{pmatrix} * \\ 0 \\ 0 \end{pmatrix}, & (33)\\
D_{(21)} &= \begin{pmatrix} 0 & 0 & * \end{pmatrix}, & (34)\\
D_{(41)} &= \begin{pmatrix} * & 0 & 0 \end{pmatrix}, & (35)
\end{aligned}$$

where each block element is a matrix with the size $12N_{\mathrm{L}}^3$ and there are many zeros. Thus, we need only four corner elements ($*$ element) of $D_{(1)}^{-1}$,

$$D_{(1)}^{-1} = \left(\begin{array}{ccc} * & - & * \\ - & - & - \\ * & - & * \end{array} \right). \tag{36}$$

Usually, LU decomposition algorithm automatically computes all elements of $D_{(1)}^{-1}$, but we need only small fraction of them. The same goes for eq.(28-31) where $D_{(3)}^{-1}$ appears instead of $D_{(1)}^{-1}$. Question now is how to compute only the corners without computing others. This report provides an answer to this demand and the details will be given in section 2.1.

2 Time reduced case

2.1 How to compute corner blocks of an inverse matrix

2.1.1 For lower corners

2-block for lower corners

First of all, consider 2-block size matrix,

$$\alpha_2 = \left(\begin{array}{cc} d_{(1)} & d_{(12)} \\ d_{(21)} & d_{(2)} \end{array} \right). \tag{37}$$

By using the formula in eq.(178) in appendix Appendix B, the inverse matrix of α_2 (in a block form) is given by

$$\alpha_2^{-1} = \left(\begin{array}{cc} d_{(1)}^{-1} + d_{(1)}^{-1} d_{(12)} B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1} & -d_{(1)}^{-1} d_{(12)} B_{2(2)}^{-1} \\ -B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1} & B_{2(2)}^{-1} \end{array} \right), \tag{38}$$

where the "B"ackward (hopping domains (2) $\rightarrow$ (1) $\rightarrow$ (2)) matrix is given by

$$B_{2(2)} = d_{(2)} - d_{(21)} d_{(1)}^{-1} d_{(12)}. \tag{39}$$

While the second index of $B_{2(2)}$ refers to the lattice domain (it is (2)), the first index refers the block size (it is 2) of α_2, although $B_{2(2)}$ itself is 1-block size. We call the first index "level".

In the end, we obtain lower corner block elements

$$(2,2) \text{ element of } \alpha_2^{-1} = B_{2(2)}^{-1}, \tag{40}$$

$$(2,1) \text{ element of } \alpha_2^{-1} = -B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1}, \tag{41}$$

for 2-block size case.

In principle, one can compute other (upper) corner elements, but it requires additional calculation. As we will see later in section 2.1.2, other decomposition is useful for the computation of the upper corner elements.

3-block for lower corners

For 3-block size case,

$$\alpha_3 = \left(\begin{array}{ccc} d_{(1)} & d_{(12)} & 0 \\ d_{(21)} & d_{(2)} & d_{(23)} \\ 0 & d_{(32)} & d_{(3)} \end{array} \right). \tag{42}$$

By using eq.(178), the inverse matrix of α_3 (in a block form) is given by

$$
\begin{aligned}
&\alpha_3^{-1} \\
&= \left(\begin{array}{cc|c} \multicolumn{2}{c|}{\alpha_2} & \begin{array}{c} 0 \\ d_{(23)} \end{array} \\ \hline 0 & d_{(32)} & d_{(3)} \end{array}\right)^{-1} \qquad (43) \\
&= \left(\begin{array}{c|c} \alpha_2^{-1} + \alpha_2^{-1} \begin{bmatrix} 0 \\ d_{(23)} \end{bmatrix} B_{3(3)}^{-1} \begin{bmatrix} 0 & d_{(32)} \end{bmatrix} \alpha_2^{-1} & -\alpha_2^{-1} \begin{bmatrix} 0 \\ d_{(23)} \end{bmatrix} B_{3(3)}^{-1} \\ \hline -B_{3(3)}^{-1} \begin{bmatrix} 0 & d_{(32)} \end{bmatrix} \alpha_2^{-1} & B_{3(3)}^{-1} \end{array}\right) \qquad (44) \\
&= \left(\begin{array}{cc|c} * & * & d_{(1)}^{-1} d_{(12)} B_{2(2)}^{-1} d_{(23)} B_{3(3)}^{-1} \\ * & * & -B_{2(2)}^{-1} d_{(23)} B_{3(3)}^{-1} \\ \hline B_{3(3)}^{-1} d_{(32)} B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1} & -B_{3(3)}^{-1} d_{(32)} B_{2(2)}^{-1} & B_{3(3)}^{-1} \end{array}\right), \qquad (45)
\end{aligned}
$$

where the backward (hopping domains (3) $\to$ (2) $\to$ (3)) at level 3 matrix is given by

$$
\begin{aligned}
B_{3(3)} &= d_{(3)} - (0, d_{(32)}) \alpha_2^{-1} \begin{pmatrix} 0 \\ d_{(23)} \end{pmatrix}, \\
&= d_{(3)} - d_{(32)} B_{2(2)}^{-1} d_{(23)}, \qquad (46)
\end{aligned}
$$

which can be obtained from $B_{2(2)}$ that is the backward matrix at level 2 in eq.(39).

Thus we can see that

$$
\begin{aligned}
(3,3) \text{ element of } \alpha_3^{-1} &= B_{3(3)}^{-1}, \qquad (47) \\
(3,1) \text{ element of } \alpha_3^{-1} &= B_{3(3)}^{-1} d_{(32)} B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1}, \qquad (48)
\end{aligned}
$$

for 3-block size case.

4-block for lower corners

For

$$
\alpha_4 = \begin{pmatrix} d_{(1)} & d_{(12)} & 0 & 0 \\ d_{(21)} & d_{(2)} & d_{(23)} & 0 \\ 0 & d_{(32)} & d_{(3)} & d_{(34)} \\ 0 & 0 & d_{(43)} & d_{(4)} \end{pmatrix}. \qquad (49)
$$

Then

$$
\begin{aligned}
(4,4) \text{ element of } \alpha_4^{-1} &= B_{4(4)}^{-1} = (d_{(4)} - d_{(43)} B_{3(3)}^{-1} d_{(34)})^{-1}, \qquad (50) \\
(4,1) \text{ element of } \alpha_4^{-1} &= -B_{4(4)}^{-1} d_{(43)} B_{3(3)}^{-1} d_{(32)} B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1}, \qquad (51)
\end{aligned}
$$

for 4-block size case.

t-block for lower corners

Here we show only the results for t-block size case.

$$
\begin{aligned}
(t,t) \text{ element of } \alpha_t^{-1} &= B_{t(t)}^{-1} = (d_{(t)} - d_{(t,t-1)} B_{t-1(t-1)}^{-1} d_{(t-1,t)})^{-1}, \qquad (52) \\
(t,1) \text{ element of } \alpha_t^{-1} &= (-)^{t+1} B_{t(t)}^{-1} d_{(t,t-1)} B_{t-1(t-1)}^{-1} d_{(t-1,t-2)} \dots B_{2(2)}^{-1} d_{(21)} d_{(1)}^{-1}. \qquad (53)
\end{aligned}
$$

If one wants to obtain those of $D_{(3)}^{-1}$, one has to shift the domain in eq.(52) and (53)

$$
(t) \longrightarrow (t + N_{\mathrm{T}}/2), \qquad (54)
$$

but the level is intact.

2.1.2 For upper corners

2-block for upper corners

First of all, consider 2-block size matrix with $n = N_{\mathrm{T}}/2 - 1$

$$\beta_2 = \begin{pmatrix} d_{(n-1)} & d_{(n-1,n)} \\ d_{(n,n-1)} & d_{(n)} \end{pmatrix}. \tag{55}$$

By using the above formula, the inverse matrix of β_2 (in a block form) is given by

$$\beta_2^{-1} = \begin{pmatrix} F_{2(n-1)}^{-1} & -F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1} \\ -d_{(n)}^{-1} d_{(n,n-1)} F_{2(n-1)}^{-1} & d_{(n)}^{-1} + d_{(n)}^{-1} d_{(n,n-1)} F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1} \end{pmatrix}, \tag{56}$$

where the "F"orward (hopping domains $(n-1) \to (n) \to (n-1)$) matrix is given by

$$F_{2(n-1)} = d_{(n-1)} - d_{(n-1,n)} d_{(n)}^{-1} d_{(n,n-1)}. \tag{57}$$

In the end, we obtain the upper corner block elements

$$(1,1) \text{ element of } \beta_2^{-1} = F_{2(n-1)}^{-1}, \tag{58}$$

$$(1,2) \text{ element of } \beta_2^{-1} = -F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1}, \tag{59}$$

for 2-block size case.

3-block for upper corners

For 3-block size case,

$$\beta_3 = \begin{pmatrix} d_{(n-2)} & d_{(n-2,n-1)} & 0 \\ d_{(n-1,n-2)} & d_{(n-1)} & d_{(n-1,n)} \\ 0 & d_{(n,n-1)} & d_{(n)} \end{pmatrix}. \tag{60}$$

By using eq.(180), the inverse matrix of β_3 (in a block form) is given by

$$\beta_3^{-1}$$

$$= \left(\begin{array}{c|cc} d_{(n-2)} & d_{(n-2,n-1)} & 0 \\ \hline d_{(n-1,n-2)} & \multicolumn{2}{c}{\multirow{2}{*}{β_2}} \\ 0 & & \end{array}\right)^{-1} \tag{61}$$

$$= \left(\begin{array}{c|cc} F_{3(n-2)}^{-1} & \multicolumn{2}{c}{-F_{3(n-2)}^{-1} \left[\begin{array}{cc} d_{(n-2,n-1)} & 0 \end{array}\right] \beta_2^{-1}} \\ \hline * & * & * \\ * & * & * \end{array}\right) \tag{62}$$

$$= \left(\begin{array}{c|cc} F_{3(n-2)}^{-1} & * & F_{3(n-2)}^{-1} d_{(n-2,n-1)} F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1} \\ \hline * & * & * \\ * & * & * \end{array}\right), \tag{63}$$

where the forward (hopping domains $(n-2) \to (n-1) \to (n-2)$) at level 3 matrix is given by

$$F_{3(n-2)} = d_{(n-2)} - d_{(n-2,n-1)} F_{2(n-1)}^{-1} d_{(n-1,n-2)}, \tag{64}$$

which can be obtained from $F_{2(n-1)}$ that is the forward matrix at level 2 in eq.(57).

Thus we can see that

$$(1,1) \text{ element of } \beta_3^{-1} = F_{3(n-2)}^{-1}, \tag{65}$$

$$(1,3) \text{ element of } \beta_3^{-1} = F_{3(n-2)}^{-1} d_{(n-2,n-1)} F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1}, \tag{66}$$

for 3-block size case.

4-block for upper corners

For

$$\beta_4 = \begin{pmatrix} d_{(n-3)} & d_{(n-3,n-2)} & 0 & 0 \\ d_{(n-2,n-3)} & d_{(n-2)} & d_{(n-2,n-1)} & 0 \\ 0 & d_{(n-1,n-2)} & d_{(n-1)} & d_{(n-1,n)} \\ 0 & 0 & d_{(n,n-1)} & d_{(n)} \end{pmatrix}. \tag{67}$$

Then

$$\begin{aligned} (1,1) \text{ element of } \beta_4^{-1} &= F_{4(n-3)}^{-1} = (d_{(n-3)} - d_{(n-3,n-2)} F_{3(n-2)}^{-1} d_{(n-2,n-3)})^{-1}, && (68) \\ (1,4) \text{ element of } \beta_4^{-1} &= -F_{4(n-3)}^{-1} d_{(n-3,n-2)} F_{3(n-2)}^{-1} d_{(n-2,n-1)} F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1}, && (69) \end{aligned}$$

for 4-block size case.

t-block for upper corners

Here we show only the results for t-block ($n = N_{\mathrm{T}}/2 - 1$) size case.

$$\begin{aligned} (1,1) \text{ element of } \beta_t^{-1} &= F_{t(n-t+1)}^{-1} \\ &= (d_{(n-t+1)} - d_{(n-t+1,n-t+2)} F_{t-1(n-t+2)}^{-1} d_{(n-t+2,n-t+1)})^{-1}, && (70) \\ (1,t) \text{ element of } \beta_t^{-1} &= (-)^{t+1} F_{t(n-t+1)}^{-1} d_{(n-t+1,n-t+2)} F_{t-1(n-t+2)}^{-1} d_{(n-t+2,n-t+3)} \cdots \\ &\quad \times F_{2(n-1)}^{-1} d_{(n-1,n)} d_{(n)}^{-1}. && (71) \end{aligned}$$

If one wants to obtain those of $D_{(3)}^{-1}$, one has to shift the domain in eq.(70) and (71) as that of eq.(54).

2.1.3 Flow

We can obtain the corners of $D_{(1)}^{-1}$ by the following recursion method.

```
B_0 ⇐ d_(1)^-1          ···★
L_0 ⇐ d_(1)^-1
F_0 ⇐ d_(N_T/2-1)^-1
U_0 ⇐ d_(N_T/2-1)^-1
do t = 2 ~ N_T/2 - 1
    get d_(t), d_(t,t-1) and d_(t-1,t)
    B_1 ⇐ d_(t) - d_(t,t-1) B_0 d_(t-1,t)
    B_1 ⇐ inverse of B_1          ···★
    L_1 ⇐ -B_1 d_(t,t-1) L_0
    B_0 ⇐ B_1 copy
    L_0 ⇐ L_1 copy
    get d_(N_T/2-t), d_(N_T/2-t,N_T/2-t+1) and d_(N_T/2-t+1,N_T/2-t)
    F_1 ⇐ d_(N_T/2-t) - d_(N_T/2-t,N_T/2-t+1) F_0 d_(N_T/2-t+1,N_T/2-t)
    F_1 ⇐ inverse of F_1
    U_1 ⇐ -F_1 d_(N_T/2-t,N_T/2-t+1) U_0
    F_0 ⇐ F_1 copy
    U_0 ⇐ U_1 copy
enddo
```

Although B-L loop and F-U loop are independent each other, we show them in a combined form just for a convenience of writing in note. This loop can be parallelized in an actual implementation.

The symbol $\star$ means that in the process with it the sub determinant can be computed as will be discussed in section 2.2 for the evaluation of A_0. In the end, all corner elements are obtained by

$$
\begin{aligned}
(N_{\rm T}/2-1, N_{\rm T}/2-1) \text{ element of } D_{(1)}^{-1} &= B_1, & (72)\\
(N_{\rm T}/2-1, 1) \text{ element of } D_{(1)}^{-1} &= L_1, & (73)\\
(1, 1) \text{ element of } D_{(1)}^{-1} &= F_1, & (74)\\
(1, N_{\rm T}/2-1) \text{ element of } D_{(1)}^{-1} &= U_1. & (75)
\end{aligned}
$$

For $D_{(3)}^{-1}$ case, the domain of $d_{(*)}$ has to be shifted as in eq.(54) compared with the previous one,

$B_0 \Leftarrow d_{(N_{\rm T}/2+1)}^{-1}$ $\quad\cdots\star$
$L_0 \Leftarrow d_{(N_{\rm T}/2+1)}^{-1}$
$F_0 \Leftarrow d_{(N_{\rm T}-1)}^{-1}$
$U_0 \Leftarrow d_{(N_{\rm T}-1)}^{-1}$
do $t = 2 \sim N_{\rm T}/2-1$
  get $d_{(N_{\rm T}/2+t)}$, $d_{(N_{\rm T}/2+t, N_{\rm T}/2+t-1)}$ and $d_{(N_{\rm T}/2+t-1, N_{\rm T}/2+t)}$
  $B_1 \Leftarrow d_{(N_{\rm T}/2+t)} - d_{(N_{\rm T}/2+t, N_{\rm T}/2+t-1)} B_0 d_{(N_{\rm T}/2+t-1, N_{\rm T}/2+t)}$
  $B_1 \Leftarrow$ inverse of B_1 $\quad\cdots\star$
  $L_1 \Leftarrow -B_1 d_{(N_{\rm T}/2+t, N_{\rm T}/2+t-1)} L_0$
  $B_0 \Leftarrow B_1$ copy
  $L_0 \Leftarrow L_1$ copy
  get $d_{(N_{\rm T}-t)}$, $d_{(N_{\rm T}-t, N_{\rm T}-t+1)}$ and $d_{(N_{\rm T}-t+1, N_{\rm T}-t)}$
  $F_1 \Leftarrow d_{(N_{\rm T}-t)} - d_{(N_{\rm T}-t, N_{\rm N}-t+1)} F_0 d_{(N_{\rm T}-t+1, N_{\rm T}-t)}$
  $F_1 \Leftarrow$ inverse of F_1
  $U_1 \Leftarrow -F_1 d_{(N_{\rm T}-t, N_{\rm T}-t+1)} U_0$
  $F_0 \Leftarrow F_1$ copy
  $U_0 \Leftarrow U_1$ copy
enddo

In the end, all corner elements are obtained by

$$
\begin{aligned}
(N_{\rm T}/2-1, N_{\rm T}/2-1) \text{ element of } D_{(3)}^{-1} &= B_1, & (76)\\
(N_{\rm T}/2-1, 1) \text{ element of } D_{(3)}^{-1} &= L_1, & (77)\\
(1, 1) \text{ element of } D_{(3)}^{-1} &= F_1, & (78)\\
(1, N_{\rm T}/2-1) \text{ element of } D_{(3)}^{-1} &= U_1. & (79)
\end{aligned}
$$

2.2 How to compute A_0

For the computation of A_0 in eq.(14), we need

$$
\begin{aligned}
&\det D_{(1)}, & (80)\\
&\det D_{(3)}. & (81)
\end{aligned}
$$

To evaluate the first one, for the expression in eq.(42) where the time slice is $n = N_\mathrm{T}/2 - 1 = 3$, we use eq.(183)

$$
\begin{aligned}
\det D_{(1)} &= \det \alpha_3 \\
&= \det \begin{pmatrix} d_{(1)} & d_{(12)} & 0 \\ d_{(21)} & d_{(2)} & d_{(23)} \\ 0 & d_{(32)} & d_{(3)} \end{pmatrix} \\
&= \det \left(\begin{array}{cc|c} \multicolumn{2}{c|}{\multirow{2}{*}{α_2}} & 0 \\ & & d_{(23)} \\ \hline 0 & d_{(32)} & d_{(3)} \end{array}\right) \\
&= \det \alpha_2 \cdot \det \left[d_{(3)} - (0, d_{(32)}) \alpha_2^{-1} \begin{pmatrix} 0 \\ d_{(23)} \end{pmatrix} \right].
\end{aligned} \tag{82}
$$

The first factor in eq.(82) is given by

$$
\begin{aligned}
\det \alpha_2 &= \det \begin{pmatrix} d_{(1)} & d_{(12)} \\ d_{(21)} & d_{(2)} \end{pmatrix} \\
&= \det d_{(1)} \cdot \det \left[d_{(2)} - d_{(21)} d_{(1)}^{-1} d_{(12)} \right] \\
&= \det B_{1(1)} \cdot \det B_{2(2)}, \because \text{eq.}(39),
\end{aligned} \tag{83}
$$

where we have defined $B_{1(1)} = d_{(1)}$. The second factor in eq.(82) is given by

$$
\begin{aligned}
\det \left[d_{(3)} - (0, d_{(32)}) \alpha_2^{-1} \begin{pmatrix} 0 \\ d_{(23)} \end{pmatrix} \right] &= \det \left[d_{(3)} - d_{(32)} B_{2(2)}^{-1} d_{(23)} \right] \because \text{eq.}(38) \\
&= \det B_{3(3)} \because \text{eq.}(46).
\end{aligned} \tag{84}
$$

So in the end, eq.(82) is given by

$$
\det D_{(1)} = \det B_{1(1)} \det B_{2(2)} \det B_{3(3)}. \tag{85}
$$

In general, for any n it is given by

$$
\det D_{(1)} = \prod_{t=1}^{n} \det B_{t(t)}. \tag{86}
$$

The $\det B_{t(t)}$ can be computed in the process of the $B_{t(t)}^{-1}$ by the LU decomposition. This computation of $\det B_{t(t)}$ is not so crucial. The computation of $\det D_{(3)}$ can be done in the exactly same way. Furthermore, $\det D_{(2*2)}$ and $\det D_{(4*4)}$ can be also computed in the process of the their inverse calculation by the LU decomposition.

2.3 Comments

- Note that this method works for $N_\mathrm{T} \geq 6$.
- For Hermitian matrix $H_{(1)} = \gamma_5 D_{(1)}$, we do not need to compute U by the above recursion method, since it can be obtained by $U = L^\dagger$.
- Memory: The size of working matrix is $12N_\mathrm{L}^3$. This is a big reduction compared with the old method where the size $12N_\mathrm{L}^3(N_\mathrm{T}/2-1)$ was required. Thus, $O(N_\mathrm{T}^2/4)$ memory size reduction is achieved, and the memory size does not scale with N_T.
- Cost: The proposed method here needs $2 \times (N_\mathrm{T}/2 - 1)$ inverses for matrix whose size is $12N_\mathrm{L}^3$. Old method requires inverse of matrix whose size is $12N_\mathrm{L}^3(N_\mathrm{T}/2 - 1)$ and the cost is $(12N_\mathrm{L}^3(N_\mathrm{T}/2-1))^3$ for LU decomposition, while our case scales with $2(N_\mathrm{T}/2-1) \times (12N_\mathrm{L}^3)^3$. We obtain $N_\mathrm{T}^2/8$ reduction!!! Of course, we have to take into account the dense matrix-matrix multiplications $((12N_\mathrm{L}^3)^3 \times (N_\mathrm{T}/2-2) \times 2)$, but its cost is still proportional to linear of N_T.

- This method is useful for very large N_T case. The cost scales with N_T linearly and the required memory is independent of N_T.
- Note that loops for B and F are independent, thus this part can be paralleled.

N_L	4	6	8	10	12
memory (GB unit)	0.2	1.3	7.3	27.7	82.6

Table 1: We use 12 working matrices with size $12N_\mathrm{L}^3$ with the double precision complex number. Therefore the required memory size $12 \times 16 \times (12N_\mathrm{L}^3)^2$GB. $N_\mathrm{L} = 8$ is now feasible for any value of N_T.

3 Time reduced + Dirac-spinor reduced case

3.1 Reduction of spinor space

3.1.1 $D_{(1)}$ related case

For γ_5 multiplied Wilson-Dirac operator $H(\mu) = \gamma_5 D(\mu)$ case, by using eq.(3-6) with γ_5, the terms in eq.(24-27) are given by

$$\begin{aligned}
D_{(21)}D_{(1)}^{-1}D_{(12)} &= (0,..,0,d_{(N_\mathrm{T}/2,N_\mathrm{T}/2-1)})D_{(1)}^{-1}\begin{pmatrix} 0 \\ \vdots \\ 0 \\ d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2)} \end{pmatrix} \\
&= d_{(N_\mathrm{T}/2,N_\mathrm{T}/2-1)}B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)}d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2)} \\
&= (2\kappa)^2\gamma_5 P_+ U(N_\mathrm{T}/2-1)^\dagger B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)}U(N_\mathrm{T}/2-1)\gamma_5 P_-, \qquad (87)
\end{aligned}$$

$$\begin{aligned}
D_{(21)}D_{(1)}^{-1}D_{(14)} &= (0,..,0,d_{(N_\mathrm{T}/2,N_\mathrm{T}/2-1)})D_{(1)}^{-1}\begin{pmatrix} d_{(1,N_\mathrm{T})} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\
&= d_{(N_\mathrm{T}/2,N_\mathrm{T}/2-1)} \\
&\quad \left[(-)^{N_\mathrm{T}/2}B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)}d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2-2)}...d^{-1}_{(1)}\right]d_{(1,N_\mathrm{T})} \\
&= -(2\kappa)^2\gamma_5 P_+ U(N_\mathrm{T}/2-1)^\dagger\left[(-)^{N_\mathrm{T}/2}...\right]U(N_\mathrm{T})^\dagger\gamma_5 P_+, \qquad (88)
\end{aligned}$$

$$\begin{aligned}
D_{(41)}D_{(1)}^{-1}D_{(14)} &= (d_{(N_\mathrm{T},1)},0,...,0)D_{(1)}^{-1}\begin{pmatrix} d_{(1,N_\mathrm{T})} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\
&= d_{(N_\mathrm{T},1)}F^{-1}_{N_\mathrm{T}/2-1(1)}d_{(1,N_\mathrm{T})} \\
&= (-2\kappa)^2\gamma_5 P_- U(N_\mathrm{T})F^{-1}_{N_\mathrm{T}/2-1(1)}U(N_\mathrm{T})^\dagger\gamma_5 P_+, \qquad (89)
\end{aligned}$$

$$\begin{aligned}
D_{(41)}D_{(1)}^{-1}D_{(12)} &= (d_{(N_\mathrm{T},1)},0,...,0)D_{(1)}^{-1}\begin{pmatrix} 0 \\ \vdots \\ 0 \\ d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2)} \end{pmatrix} \\
&= d_{(N_\mathrm{T},1)}\left[(-)^{N_\mathrm{T}/2}F^{-1}_{N_\mathrm{T}/2-1(1)}d_{(12)}...d^{-1}_{(N_\mathrm{T}/2-1)}\right] \\
&\quad d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2)} \\
&= -(2\kappa)^2\gamma_5 P_- U(N_\mathrm{T})\left[(-)^{N_\mathrm{T}/2}...F^{-1}_{1(N_\mathrm{T}/2-1)}\right] \\
&\quad U(N_\mathrm{T}/2-1)\gamma_5 P_-. \qquad (90)
\end{aligned}$$

Note that the minus sign in eq.(88) and (90) whose origin is the anti-periodic boundary condition. From the above form, it is obvious that we need some fraction of spinor space since they are sandwiched by the spinor projections $P_\pm$. In the following, we treat them separately.

How to obtain $D_{(21)}D^{-1}_{(1)}D_{(12)}$

First by looking at

$$\begin{aligned} B_{t(t)} &= d_{(t)} - d_{(t,t-1)}B^{-1}_{t-1(t-1)}d_{(t-1,t)} \\ &= d_{(t)} - (2\kappa)^2\gamma_5 P_+ U(t-1)^\dagger B^{-1}_{t-1(t-1)}U(t-1)\gamma_5 P_- \\ &= d_{(t)} - (2\kappa)^2 U(t-1)^\dagger P_-\gamma_5 B^{-1}_{t-1(t-1)}\gamma_5 P_- U(t-1). \end{aligned} \tag{91}$$

The second term is sandwiched by the P_- together with γ_5 which interchange all element

$$\gamma_5 A\gamma_5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} A_{++} & A_{+-} \\ A_{-+} & A_{--} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} A_{--} & A_{-+} \\ A_{+-} & A_{++} \end{pmatrix}. \tag{92}$$

Therefore we need $++$ component of $B^{-1}_{t-1(t-1)}$ namely $(B^{-1}_{t-1(t-1)})_{++}$ in

$$B^{-1}_{t-1(t-1)} = \begin{pmatrix} (B^{-1}_{t-1(t-1)})_{++} & (B^{-1}_{t-1(t-1)})_{+-} \\ (B^{-1}_{t-1(t-1)})_{-+} & (B^{-1}_{t-1(t-1)})_{--} \end{pmatrix}. \tag{93}$$

Eq.(91) is given by

$$\begin{aligned} B_{t(t)} &= \left(\begin{array}{c|c} B_{t(t)++} & B_{t(t)+-} \\ \hline B_{t(t)-+} & B_{t(t)--} \end{array}\right) \\ &= \left(\begin{array}{c|c} d_{(t)++} & d_{(t)+-} \\ \hline d_{(t)-+} & d_{(t)--} - (2\kappa)^2 U(t-1)^\dagger (B^{-1}_{t-1(t-1)})_{++}U(t-1) \end{array}\right). \end{aligned} \tag{94}$$

In the next step $t+1$, one needs $++$ component of $B^{-1}_{t(t)}$ namely

$$\begin{aligned} (B^{-1}_{t(t)})_{++} &= (B_{t(t)++} - B_{t(t)+-}B^{-1}_{t(t)--}B_{t(t)-+})^{-1} \\ &= (d_{(t)++} - d_{(t)+-}B^{-1}_{t(t)--}d_{(t)-+})^{-1}, \end{aligned} \tag{95}$$

with

$$B_{t(t)--} = d_{(t)--} - (2\kappa)^2 U(t-1)^\dagger (B^{-1}_{t-1(t-1)})_{++}U(t-1). \tag{96}$$

In the end,

$$D_{(21)}D^{-1}_{(1)}D_{(12)} = \begin{pmatrix} 0 & 0 \\ 0 & (2\kappa)^2 U(N_\mathrm{T}/2-1)^\dagger (B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)})_{++}U(N_\mathrm{T}/2-1) \end{pmatrix}, \tag{97}$$

equivalently

$$(D_{(21)}D^{-1}_{(1)}D_{(12)})_{--} = (2\kappa)^2 U(N_\mathrm{T}/2-1)^\dagger (B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)})_{++}U(N_\mathrm{T}/2-1). \tag{98}$$

How to obtain $D_{(21)}D^{-1}_{(1)}D_{(14)}$

$$\begin{aligned} D_{(21)}D^{-1}_{(1)}D_{(14)} &= -(2\kappa)^2\gamma_5 P_+ U(N_\mathrm{T}/2-1)^\dagger \\ &\quad \left[(-)^{N_\mathrm{T}/2}B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)}d_{(N_\mathrm{T}/2-1,N_\mathrm{T}/2-1)}...d_{(21)}B^{-1}_{1(1)}\right] \\ &\quad U(N_\mathrm{T})^\dagger\gamma_5 P_+ \\ &= -(2\kappa)^2(-)^{N_\mathrm{T}/2}(-2\kappa)^{N_\mathrm{T}/2-2} \\ &\quad \gamma_5 P_+ U(N_\mathrm{T}/2-1)^\dagger B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2-1)} \\ &\quad \gamma_5 P_+ U(N_\mathrm{T}/2-2)^\dagger B^{-1}_{N_\mathrm{T}/2-2(N_\mathrm{T}/2-2)}\cdots \\ &\quad \gamma_5 P_+ U(2)^\dagger B^{-1}_{2(2)}\gamma_5 P_+ U(1)^\dagger B^{-1}_{1(1)}\gamma_5 P_+ U(N_\mathrm{T})^\dagger\gamma_5 P_+. \end{aligned} \tag{99}$$

By using a property

$$\gamma_5 P_+ A \gamma_5 P_+ = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} A_{++} & A_{+-} \\ A_{-+} & A_{--} \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ A_{+-} & 0 \end{pmatrix}, \tag{100}$$

we obtain

$$\begin{aligned} (D_{(21)} D^{-1}_{(1)} D_{(14)})_{-+} &= -(-)^{N_{\rm T}} (2\kappa)^{N_{\rm T}/2} U(N_{\rm T}/2-1)^\dagger (B^{-1}_{N_{\rm T}/2-1(N_{\rm T}/2-1)})_{+-} \\ & \quad U(N_{\rm T}/2-2)^\dagger (B^{-1}_{N_{\rm T}/2-2(N_{\rm T}/2-2)})_{+-} \cdots \\ & \quad U(2)^\dagger (B^{-1}_{2(2)})_{+-} U(1)^\dagger (B^{-1}_{1(1)})_{+-} U(N_{\rm T})^\dagger, \end{aligned} \tag{101}$$

with

$$\begin{aligned} (B^{-1}_{t(t)})_{+-} &= -(B^{-1}_{t(t)})_{++} B_{t(t)+-} B^{-1}_{t(t)--} \\ &= -(B^{-1}_{t(t)})_{++} d_{(t)+-} B^{-1}_{t(t)--}, \end{aligned} \tag{102}$$

where $(B^{-1}_{t(t)})_{++}$ and $B_{t(t)--}$ are defined in eq.(95) and eq.(96) respectively. Note that there is the minus sign in eq.(101) due to the anti-periodic boundary condition.

How to obtain $D_{(41)} D^{-1}_{(1)} D_{(14)}$

First looking at

$$\begin{aligned} F_{t(n-t+1)} &= d_{(n-t+1)} - d_{(n-t+1,n-t+2)} F^{-1}_{t-1(n-t+2)} d_{(n-t+2,n-t+1)} \\ &= d_{(n-t+1)} - (2\kappa)^2 \gamma_5 P_- U(n-t+1) F^{-1}_{t-1(n-t+2)} U(n-t+1)^\dagger \gamma_5 P_+ \\ &= d_{(n-t+1)} - (2\kappa)^2 U(n-t+1) P_+ \gamma_5 F^{-1}_{t-1(n-t+2)} \gamma_5 P_+ U(n-t+1)^\dagger. \end{aligned} \tag{103}$$

The second term is sandwiched by the P_+ together with γ_5. Therefore we need $--$ component of $F^{-1}_{t-1(n-t+2)}$ namely $(F^{-1}_{t-1(n-t+2)})_{--}$ in

$$F^{-1}_{t-1(n-t+2)} = \begin{pmatrix} (F^{-1}_{t-1(n-t+2)})_{++} & (F^{-1}_{t-1(n-t+2)})_{+-} \\ (F^{-1}_{t-1(n-t+2)})_{-+} & (F^{-1}_{t-1(n-t+2)})_{--} \end{pmatrix}. \tag{104}$$

Eq.(103) is given by

$$\begin{aligned} & F_{t(n-t+1)} \\ &= \left(\begin{array}{c|c} F_{t(n-t+1)++} & F_{t(n-t+1)+-} \\ \hline F_{t(n-t+1)-+} & F_{t(n-t+1)--} \end{array} \right) \\ &= \left(\begin{array}{c|c} d_{(n-t+1)++} - (2\kappa)^2 U(n-t+1) (F^{-1}_{t-1(n-t+2)})_{--} U(n-t+1)^\dagger & d_{(n-t+1)+-} \\ \hline d_{(n-t+1)-+} & d_{(n-t+1)--} \end{array} \right). \end{aligned} \tag{105}$$

In the next step $t+1$, one needs $--$ component of $F^{-1}_{t(n-t+1)}$ namely

$$\begin{aligned} (F^{-1}_{t(n-t+1)})_{--} &= (F_{t(n-t+1)--} - F_{t(n-t+1)-+} F^{-1}_{t(n-t+1)++} F_{t(n-t+1)+-})^{-1} \\ &= (d_{(n-t+1)--} - d_{(n-t+1)-+} F^{-1}_{t(n-t+1)++} d_{(n-t+1)+-})^{-1}, \end{aligned} \tag{106}$$

with

$$F_{t(n-t+1)++} = d_{(n-t+1)++} - (2\kappa)^2 U(n-t+1) (F^{-1}_{t-1(n-t+2)})_{--} U(n-t+1)^\dagger. \tag{107}$$

In the end,

$$D_{(41)} D^{-1}_{(1)} D_{(14)} = \begin{pmatrix} (2\kappa)^2 U(N_{\rm T}) (F^{-1}_{N_{\rm T}/2-1(1)})_{--} U(N_{\rm T})^\dagger & 0 \\ 0 & 0 \end{pmatrix}, \tag{108}$$

equivalently

$$(D_{(41)} D^{-1}_{(1)} D_{(14)})_{++} = (2\kappa)^2 U(N_{\rm T}) (F^{-1}_{N_{\rm T}/2-1(1)})_{--} U(N_{\rm T})^\dagger. \tag{109}$$

How to obtain $D_{(41)}D_{(1)}^{-1}D_{(12)}$

This can be obtained by Hermite conjugate of $D_{(21)}D_{(1)}^{-1}D_{(14)}$, therefore we do not discuss it here.

3.1.2 $D_{(3)}$ related case

For γ_5 multiplied Wilson-Dirac operator $H(\mu) = \gamma_5 D(\mu)$ case, by using eq.(3-6) with γ_5, the terms in eq.(28-31) are given by

$$
\begin{aligned}
D_{(43)}D_{(3)}^{-1}D_{(34)} &= (0, .., 0, d_{(N_{\mathrm{T}},N_{\mathrm{T}}-1)})D_{(3)}^{-1}\begin{pmatrix} 0 \\ \vdots \\ 0 \\ d_{(N_{\mathrm{T}}-1,N_{\mathrm{T}})} \end{pmatrix} \\
&= d_{(N_{\mathrm{T}},N_{\mathrm{T}}-1)}B^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}-1)}d_{(N_{\mathrm{T}}-1,N_{\mathrm{T}})} \\
&= (2\kappa)^2\gamma_5 P_+ U(N_{\mathrm{T}}-1)^\dagger B^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}-1)}U(N_{\mathrm{T}}-1)\gamma_5 P_-, \qquad (110)\\
D_{(43)}D_{(3)}^{-1}D_{(32)} &= (0, .., 0, d_{(N_{\mathrm{T}},N_{\mathrm{T}}-1)})D_{(3)}^{-1}\begin{pmatrix} d_{(N_{\mathrm{T}}/2+1,N_{\mathrm{T}}/2)} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\
&= d_{(N_{\mathrm{T}},N_{\mathrm{T}}-1)} \\
&\quad \left[(-)^{N_{\mathrm{T}}/2}B^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}-1)}d_{(N_{\mathrm{T}}-1,N_{\mathrm{T}}-2)}...d^{-1}_{(N_{\mathrm{T}}/2+1)}\right]d_{(N_{\mathrm{T}}/2+1,N_{\mathrm{T}}/2)} \\
&= (2\kappa)^2\gamma_5 P_+ U(N_{\mathrm{T}}-1)^\dagger\left[(-)^{N_{\mathrm{T}}/2}...\right]U(N_{\mathrm{T}}/2)^\dagger\gamma_5 P_+, \qquad (111)\\
D_{(23)}D_{(3)}^{-1}D_{(32)} &= (d_{(N_{\mathrm{T}}/2,N_{\mathrm{T}}/2+1)}, 0, ..., 0)D_{(3)}^{-1}\begin{pmatrix} d_{(N_{\mathrm{T}}/2+1,N_{\mathrm{T}}/2)} \\ 0 \\ \vdots \\ 0 \end{pmatrix} \\
&= d_{(N_{\mathrm{T}}/2,N_{\mathrm{T}}/2+1)}F^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}/2+1)}d_{(N_{\mathrm{T}}/2+1,N_{\mathrm{T}}/2)} \\
&= (2\kappa)^2\gamma_5 P_- U(N_{\mathrm{T}}/2)F^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}/2+1)}U(N_{\mathrm{T}}/2)^\dagger\gamma_5 P_+, \qquad (112)\\
D_{(23)}D_{(3)}^{-1}D_{(34)} &= (d_{(N_{\mathrm{T}}/2,N_{\mathrm{T}}/2+1)}, 0, ..., 0)D_{(3)}^{-1}\begin{pmatrix} 0 \\ \vdots \\ 0 \\ d_{(N_{\mathrm{T}}-1,N_{\mathrm{T}})} \end{pmatrix} \\
&= d_{(N_{\mathrm{T}}/2,N_{\mathrm{T}}/2+1)}\left[(-)^{N_{\mathrm{T}}/2}F^{-1}_{N_{\mathrm{T}}/2-1(N_{\mathrm{T}}/2+1)}d_{(N_{\mathrm{T}}/2+1,N_{\mathrm{T}}/2+2)}...d^{-1}_{(N_{\mathrm{T}}-1)}\right] \\
&\quad d_{(N_{\mathrm{T}}-1,N_{\mathrm{T}})} \\
&= (2\kappa)^2\gamma_5 P_- U(N_{\mathrm{T}}/2)\left[(-)^{N_{\mathrm{T}}/2}...F^{-1}_{1(N_{\mathrm{T}}-1)}\right] \\
&\quad U(N_{\mathrm{T}}-1)\gamma_5 P_-. \qquad (113)
\end{aligned}
$$

Note that there is no minus sign in eq.(111) and (113) compared with eq.(88) and (90). The above equations are obtained by just shifting the domains as in eq.(54). In the following, we treat them separately.

How to obtain $D_{(43)}D^{-1}_{(3)}D_{(34)}$

$$D_{(43)}D^{-1}_{(3)}D_{(34)} = \begin{pmatrix} 0 & 0 \\ 0 & (2\kappa)^2 U(N_\mathrm{T}-1)^\dagger (B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}-1)})_{++} U(N_\mathrm{T}-1) \end{pmatrix}, \tag{114}$$

equivalently

$$(D_{(43)}D^{-1}_{(3)}D_{(34)})_{--} = (2\kappa)^2 U(N_\mathrm{T}-1)^\dagger (B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}-1)})_{++} U(N_\mathrm{T}-1). \tag{115}$$

How to obtain $D_{(43)}D^{-1}_{(3)}D_{(32)}$

$$\begin{aligned} (D_{(43)}D^{-1}_{(3)}D_{(32)})_{-+} &= (-)^{N_\mathrm{T}}(2\kappa)^{N_\mathrm{T}/2} U(N_\mathrm{T}-1)^\dagger (B^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}-1)})_{+-} \\ & U(N_\mathrm{T}-2)^\dagger (B^{-1}_{N_\mathrm{T}/2-2(N_\mathrm{T}-2)})_{+-} \cdots \\ & U(N_\mathrm{T}/2+2)^\dagger (B^{-1}_{2(N_\mathrm{T}/2+2)})_{+-} \\ & U(N_\mathrm{T}/2+1)^\dagger (B^{-1}_{1(N_\mathrm{T}/2+1)})_{+-} U(N_\mathrm{T}/2)^\dagger, \end{aligned} \tag{116}$$

with

$$\begin{aligned} (B^{-1}_{t(t')})_{+-} &= -(B^{-1}_{t(t')})_{++} B_{t(t')+-} B^{-1}_{t(t')--} \\ &= -(B^{-1}_{t(t')})_{++} d_{(t')+-} B^{-1}_{t(t')--}. \end{aligned} \tag{117}$$

Note that there is no minus sign in eq.(116).

How to obtain $D_{(23)}D^{-1}_{(3)}D_{(32)}$

$$D_{(23)}D^{-1}_{(3)}D_{(32)} = \begin{pmatrix} (2\kappa)^2 U(N_\mathrm{T}/2)(F^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2+1)})_{--} U(N_\mathrm{T}/2)^\dagger & 0 \\ 0 & 0 \end{pmatrix}, \tag{118}$$

equivalently

$$(D_{(23)}D^{-1}_{(3)}D_{(32)})_{++} = (2\kappa)^2 U(N_\mathrm{T}/2)(F^{-1}_{N_\mathrm{T}/2-1(N_\mathrm{T}/2+1)})_{--} U(N_\mathrm{T}/2)^\dagger. \tag{119}$$

How to obtain $D_{(23)}D^{-1}_{(3)}D_{(34)}$

This can be obtained by Hermite conjugate of $D_{(43)}D^{-1}_{(3)}D_{(32)}$, therefore we do not discuss it here.

3.1.3 Flow

We can obtain $D_{(2*2)--}$ and $(D_{(21)}D^{-1}_{(1)}D_{(14)})_{-+}$ which are $D^{-1}_{(1)}$ related quantities by the following recursion method.

get $d_{(1)--}$
$B_0 \Leftarrow$ inverse of $d_{(1)--}$ $\cdots\star$
$L_0 \Leftarrow B_0 U(N_{\mathrm{T}})^\dagger$
get $d_{(1)++}$, $d_{(1)+-}$ and $d_{(1)-+}$
$B_1 \Leftarrow d_{(1)++} - d_{(1)+-} B_0 d_{(1)-+}$
$B_1 \Leftarrow$ inverse of B_1 $\cdots\star$
$L_1 \Leftarrow d_{(1)+-} L_0$
$L_0 \Leftarrow B_1 \times L_1$
$L_1 \Leftarrow U(1)^\dagger L_0$
do $t = 2 \sim N_{\mathrm{T}}/2 - 1$
  get $d_{(t)--}$
  $B_0 \Leftarrow d_{(t)--} - (2\kappa)^2 U(t-1)^\dagger B_1 U(t-1)$
  $B_0 \Leftarrow$ inverse of B_0 $\cdots\star$
  $L_0 \Leftarrow B_0 \times L_1$
  get $d_{(t)++}$, $d_{(t)+-}$ and $d_{(t)-+}$
  $B_1 \Leftarrow d_{(t)++} - d_{(t)+-} B_0 d_{(t)-+}$
  $B_1 \Leftarrow$ inverse of B_1 $\cdots\star$
  $L_1 \Leftarrow d_{(t)+-} L_0$
  $L_0 \Leftarrow B_1 \times L_1$
  $L_1 \Leftarrow U(t)^\dagger L_0$
enddo
get $d_{(N_{\mathrm{T}}/2)--}$
$B_0 \Leftarrow d_{(N_{\mathrm{T}}/2)--} - (2\kappa)^2 U(N_{\mathrm{T}}/2-1)^\dagger B_1 U(N_{\mathrm{T}}/2-1)$
$L_0 \Leftarrow -(-)^{N_{\mathrm{T}}+N_{\mathrm{T}}/2-1}(2\kappa)^{N_{\mathrm{T}}/2} L_1$

Note the minus sign in the final step for L_0 due to the anti-periodic boundary condition. The number of required inversion is $2 + 2(N_{\mathrm{T}}/2 - 2)$. The symbol $\times$ shows the dense matrix multiplication, which is needed $1 + 2(N_{\mathrm{T}} - 2)$. The symbol $\star$ means that in the process with it the sub determinant can be computed as will be discussed in section 3.6 for the evaluation of A_0. In the end, B_0 and L_0 are

$$D_{(2*2)--} = B_0, \tag{120}$$
$$(D_{(21)} D_{(1)}^{-1} D_{(14)})_{-+} = L_0. \tag{121}$$

We can obtain $D_{(4*4)++}$ which is $D_{(1)}^{-1}$ related quantity by the following recursion method.

get $d_{(N_{\mathrm{T}}/2-1)++}$
$F_0 \Leftarrow$ inverse of $d_{(N_{\mathrm{T}}/2-1)++}$ $\cdots\star$
get $d_{(N_{\mathrm{T}}/2-1)--}$, $d_{(N_{\mathrm{T}}/2-1)+-}$ and $d_{(N_{\mathrm{T}}/2-1)-+}$
$F_1 \Leftarrow d_{(N_{\mathrm{T}}/2-1)--} - d_{(N_{\mathrm{T}}/2-1)+-} F_0 d_{(N_{\mathrm{T}}/2-1)-+}$
$F_1 \Leftarrow$ inverse of F_1 $\cdots\star$
do $t = 2 \sim N_{\mathrm{T}}/2 - 1$
  get $d_{(N_{\mathrm{T}}/2-t)++}$
  $F_0 \Leftarrow d_{(N_{\mathrm{T}}/2-t)++} - (2\kappa)^2 U(N_{\mathrm{T}}/2-t) F_1 U(N_{\mathrm{T}}/2-t)^\dagger$
  $F_0 \Leftarrow$ inverse of F_0 $\cdots\star$
  get $d_{(N_{\mathrm{T}}/2-t)--}$, $d_{(N_{\mathrm{T}}/2-t)-+}$ and $d_{(N_{\mathrm{T}}/2-t)+-}$
  $F_1 \Leftarrow d_{(N_{\mathrm{T}}/2-t)--} - d_{(N_{\mathrm{T}}/2-t)-+} F_0 d_{(N_{\mathrm{T}}/2-t)+-}$
  $F_1 \Leftarrow$ inverse of F_1 $\cdots\star$
enddo
get $d_{(N_{\mathrm{T}})++}$
$F_0 \Leftarrow d_{(N_{\mathrm{T}})++} - (2\kappa)^2 U(N_{\mathrm{T}}) F_1 U(N_{\mathrm{T}})^\dagger$

The number of required inversion is $2 + 2(N_{\mathrm{T}}/2 - 2)$. There is no dense matrix multiplication in this case. The symbol $\star$ means that in the process with it the sub determinant can be computed as will be discussed in section 3.6 for the evaluation of A_0. In the end, F_0 is

$$D_{(4*4)++} \quad = \quad F_0. \tag{122}$$

For $D_{(3)}^{-1}$ case, the domain of $d_{(*)}$ has to be shifted as in eq.(54) compared with the previous one and take into account the minus sign from the anti-periodic boundary condition. Actually, in this case there is no such a minus sign. We can obtain $D_{(4*4)--}$ and $(D_{(43)}D_{(3)}^{-1}D_{(32)})_{-+}$ which are $D_{(3)}^{-1}$ related quantities by the following recursion method.

get $d_{(N_\mathrm{T}/2+1)--}$
$B_0 \Leftarrow$ inverse of $d_{(N_\mathrm{T}/2+1)--}$ $\cdots\star$
$L_0 \Leftarrow B_0 U(N_\mathrm{T})^\dagger$
get $d_{(N_\mathrm{T}/2+1)++}$, $d_{(N_\mathrm{T}/2+1)+-}$ and $d_{(N_\mathrm{T}/2+1)-+}$
$B_1 \Leftarrow d_{(N_\mathrm{T}/2+1)++} - d_{(N_\mathrm{T}/2+1)+-} B_0 d_{(N_\mathrm{T}/2+1)-+}$
$B_1 \Leftarrow$ inverse of B_1 $\cdots\star$
$L_1 \Leftarrow d_{(N_\mathrm{T}/2+1)+-} L_0$
$L_0 \Leftarrow B_1 \times L_1$
$L_1 \Leftarrow U(N_\mathrm{T}/2+1)^\dagger L_0$
do $t = 2 \sim N_\mathrm{T}/2-1$
  get $d_{(N_\mathrm{T}/2+t)--}$
  $B_0 \Leftarrow d_{(N_\mathrm{T}/2+t)--} - (2\kappa)^2 U(N_\mathrm{T}/2+t-1)^\dagger B_1 U(N_\mathrm{T}/2+t-1)$
  $B_0 \Leftarrow$ inverse of B_0 $\cdots\star$
  $L_0 \Leftarrow B_0 \times L_1$
  get $d_{(N_\mathrm{T}/2+t)++}$, $d_{(N_\mathrm{T}/2+t)+-}$ and $d_{(N_\mathrm{T}/2+t)-+}$
  $B_1 \Leftarrow d_{(N_\mathrm{T}/2+t)++} - d_{(N_\mathrm{T}/2+t)+-} B_0 d_{(N_\mathrm{T}/2+t)-+}$
  $B_1 \Leftarrow$ inverse of B_1 $\cdots\star$
  $L_1 \Leftarrow d_{(N_\mathrm{T}/2+t)+-} L_0$
  $L_0 \Leftarrow B_1 \times L_1$
  $L_1 \Leftarrow U(N_\mathrm{T}/2+t)^\dagger L_0$
enddo
get $d_{(N_\mathrm{T})--}$
$B_0 \Leftarrow d_{(N_\mathrm{T})--} - (2\kappa)^2 U(N_\mathrm{T}-1)^\dagger B_1 U(N_\mathrm{T}-1)$
$L_0 \Leftarrow (-)^{N_\mathrm{T}+N_\mathrm{T}/2-1}(2\kappa)^{N_\mathrm{T}/2} L_1$

Note that there is no minus sign in the final step for L_0 compared with the $D_{(1)}^{-1}$ case. The number of required inversion is $2+2(N_\mathrm{T}/2-2)$. The symbol $\times$ shows the dense matrix multiplication, which is needed $1+2(N_\mathrm{T}-2)$. The symbol $\star$ means that in the process with it the sub determinant can be computed as will be discussed in section 3.6 for the evaluation of A_0. In the end, B_0 and L_0 are

$$D_{(4*4)--} \quad = \quad B_0, \tag{123}$$
$$(D_{(43)}D_{(3)}^{-1}D_{(32)})_{-+} \quad = \quad L_0. \tag{124}$$

We can obtain $D_{(2*2)++}$ which is $D_{(3)}^{-1}$ related quantity by the following recursion method.

get $d_{(N_{\rm T}-1)++}$
$F_0 \Leftarrow$ inverse of $d_{(N_{\rm T}-1)++}$ $\cdots\star$
get $d_{(N_{\rm T}-1)--}$, $d_{(N_{\rm T}-1)+-}$ and $d_{(N_{\rm T}-1)-+}$
$F_1 \Leftarrow d_{(N_{\rm T}-1)--} - d_{(N_{\rm T}-1)+-}F_0 d_{(N_{\rm T}-1)-+}$
$F_1 \Leftarrow$ inverse of F_1 $\cdots\star$
do $t = 2 \sim N_{\rm T}/2-1$
    get $d_{(N_{\rm T}-t)++}$
    $F_0 \Leftarrow d_{(N_{\rm T}-t)++} - (2\kappa)^2 U(N_{\rm T}-t)F_1 U(N_{\rm T}-t)^\dagger$
    $F_0 \Leftarrow$ inverse of F_0 $\cdots\star$
    get $d_{(N_{\rm T}-t)--}$, $d_{(N_{\rm T}-t)-+}$ and $d_{(N_{\rm T}-t)+-}$
    $F_1 \Leftarrow d_{(N_{\rm T}-t)--} - d_{(N_{\rm T}-t)-+}F_0 d_{(N_{\rm T}-t)+-}$
    $F_1 \Leftarrow$ inverse of F_1 $\cdots\star$
enddo
get $d_{(N_{\rm T}/1)++}$
$F_0 \Leftarrow d_{(N_{\rm T}/2)++} - (2\kappa)^2 U(N_{\rm T}/2)F_1 U(N_{\rm T}/2)^\dagger$

The number of required inversion is $2+2(N_{\rm T}/2-2)$. There is no dense matrix multiplication in this case. The symbol $\star$ means that in the process with it the sub determinant can be computed as will be discussed in section 3.6 for the evaluation of A_0. In the end, F_0 is

$$D_{(2*2)++} = F_0. \tag{125}$$

3.2 How to obtain $D^{-1}_{(2*2)}$ and $D^{-1}_{(4*4)}$

For

$$\begin{aligned} D_{(2*2)} &= \begin{pmatrix} D_{(2*2)++} & D_{(2*2)+-} \\ D_{(2*2)-+} & D_{(2*2)--} \end{pmatrix} \\ &= \begin{pmatrix} eq.(125) & d_{(N_{\rm T}/2)+-} \\ d_{(N_{\rm T}/2)-+} & eq.(120) \end{pmatrix}, \end{aligned} \tag{126}$$

by using eq.(180) the inverse matrix is

$$D^{-1}_{(2*2)} = \begin{pmatrix} (D^{-1}_{(2*2)})_{++} & (D^{-1}_{(2*2)})_{+-} \\ (D^{-1}_{(2*2)})_{-+} & (D^{-1}_{(2*2)})_{--} \end{pmatrix}, \tag{127}$$

with

$$(D^{-1}_{(2*2)})_{++} = (D_{(2*2)++} - d_{(N_{\rm T}/2)+-}D^{-1}_{(2*2)--}d_{(N_{\rm T}/2)-+})^{-1}, \tag{128}$$
$$(D^{-1}_{(2*2)})_{+-} = -(D^{-1}_{(2*2)})_{++}d_{(N_{\rm T}/2)+-}D^{-1}_{(2*2)--}, \tag{129}$$
$$(D^{-1}_{(2*2)})_{--} = D^{-1}_{(2*2)--}(1 - d_{(N_{\rm T}/2)-+}(D^{-1}_{(2*2)})_{+-}). \tag{130}$$

Note that for Hermite matrix A,

$$\begin{pmatrix} A_{++} & A_{+-} \\ A_{-+} & A_{--} \end{pmatrix}, \tag{131}$$

$$A_{++} = A^\dagger_{++}, \tag{132}$$
$$A_{--} = A^\dagger_{--}, \tag{133}$$
$$A_{-+} = A^\dagger_{+-}. \tag{134}$$

For

$$
\begin{aligned}
D_{(4*4)} &= \begin{pmatrix} D_{(4*4)++} & D_{(4*4)+-} \\ D_{(4*4)-+} & D_{(4*4)--} \end{pmatrix} \\
&= \begin{pmatrix} eq.(122) & d_{(N_\mathrm{T})+-} \\ d_{(N_\mathrm{T})-+} & eq.(123) \end{pmatrix}, \qquad (135)
\end{aligned}
$$

by using eq.(180) the inverse matrix is

$$
D^{-1}_{(4*4)} = \begin{pmatrix} (D^{-1}_{(4*4)})_{++} & (D^{-1}_{(4*4)})_{+-} \\ (D^{-1}_{(4*4)})_{-+} & (D^{-1}_{(4*4)})_{--} \end{pmatrix}, \qquad (136)
$$

with

$$
\begin{aligned}
(D^{-1}_{(4*4)})_{++} &= (D_{(4*4)++} - d_{(N_\mathrm{T})+-} D^{-1}_{(4*4)--} d_{(N_\mathrm{T})-+})^{-1}, && (137) \\
(D^{-1}_{(4*4)})_{+-} &= -(D^{-1}_{(4*4)})_{++} d_{(N_\mathrm{T})+-} D^{-1}_{(4*4)--}, && (138) \\
(D^{-1}_{(4*4)})_{--} &= D^{-1}_{(4*4)--}(1 - d_{(N_\mathrm{T})-+}(D^{-1}_{(4*4)})_{+-}). && (139)
\end{aligned}
$$

3.3 How to obtain H_0 and $H_\pm$

For

$$
\begin{aligned}
H_0 &= \begin{pmatrix} H_{0++} & H_{0+-} \\ H_{0-+} & H_{0--} \end{pmatrix}, && (140) \\
H_+ &= \begin{pmatrix} 0 & H_{+,+-} \\ 0 & H_{+,--} \end{pmatrix}, && (141) \\
H_- &= \begin{pmatrix} H_{-,++} & 0 \\ H_{-,-+} & 0 \end{pmatrix}, && (142)
\end{aligned}
$$

the elements are given by

$$
\begin{aligned}
H_{0++} &= (D^{-1}_{4*4})_{++} D_{(412)+-} (D^{-1}_{2*2})_{--} D_{(214)-+}, && (143) \\
H_{0-+} &= (D^{-1}_{4*4})_{-+} D_{(412)+-} (D^{-1}_{2*2})_{--} D_{(214)-+}, && (144) \\
H_{0+-} &= (D^{-1}_{4*4})_{+-} D_{(432)-+} (D^{-1}_{2*2})_{++} D_{(234)+-}, && (145) \\
H_{0--} &= (D^{-1}_{4*4})_{--} D_{(432)-+} (D^{-1}_{2*2})_{++} D_{(234)+-}, && (146) \\
H_{+,+-} &= (D^{-1}_{4*4})_{++} D_{(412)+-} (D^{-1}_{2*2})_{-+} D_{(234)+-}, && (147) \\
H_{+,--} &= (D^{-1}_{4*4})_{-+} D_{(412)+-} (D^{-1}_{2*2})_{-+} D_{(234)+-}, && (148) \\
H_{-,++} &= (D^{-1}_{4*4})_{+-} D_{(432)-+} (D^{-1}_{2*2})_{+-} D_{(214)-+}, && (149) \\
H_{-,-+} &= (D^{-1}_{4*4})_{--} D_{(432)-+} (D^{-1}_{2*2})_{+-} D_{(214)-+}. && (150)
\end{aligned}
$$

This can be written in a systematic way

$$
\begin{aligned}
H_{0++} &= APZP^\dagger, && (151) \\
H_{0-+} &= BPZP^\dagger, && (152) \\
H_{0+-} &= B^\dagger QXQ^\dagger, && (153) \\
H_{0--} &= CQXQ^\dagger, && (154) \\
H_{+,+-} &= APYQ^\dagger, && (155) \\
H_{+,--} &= BPYQ^\dagger, && (156) \\
H_{-,++} &= B^\dagger QY^\dagger P^\dagger, && (157) \\
H_{-,-+} &= CQY^\dagger P^\dagger. && (158)
\end{aligned}
$$

One needs $4(H_0)+2(H_+)+2(H_-)+3(ABC)+3(XYZ)+2(PQ) = 16$ matrices and $4+8+4 = 16$ matrix multiplications.

3.4 How to obtain $\hat{V}_{(q)}$

To compute the truncated $V_{(q)}$

$$\begin{aligned}
\hat{V}_{(0)} &= \mathrm{tr}[H_0] + \frac{1}{2}\mathrm{tr}[(H_0)^2] + \mathrm{tr}[H_+H_-], &(159)\\
\hat{V}_{(q)} &= \frac{1}{q}\mathrm{tr}[(H_+)^q] + \mathrm{tr}[(H_+)^q H_0], &(160)
\end{aligned}$$

we need

$$\begin{aligned}
\mathrm{tr}[H_0] &= \mathrm{tr}[H_{0++}] + \mathrm{tr}[H_{0--}], &(161)\\
\mathrm{tr}[(H_0)^2] &= \mathrm{tr}[(H_{0++})^2 + H_{0+-}H_{0-+}] + \mathrm{tr}[(H_{0--})^2 + H_{0-+}H_{0+-}], &(162)\\
\mathrm{tr}[H_+H_-] &= \mathrm{tr}[H_{+,+-}H_{-,-+}], &(163)\\
(H_+)^q &= \begin{pmatrix} 0 & H_{+,+-}H_{+,--}^{q-1} \\ 0 & H_{+,--}^q \end{pmatrix}, &(164)\\
\mathrm{tr}[(H_+)^q] &= \mathrm{tr}[(H_{+,--})^q], &(165)\\
\mathrm{tr}[(H_+)^q H_0] &= \mathrm{tr}[H_{+,+-}(H_{+,--})^{q-1}H_{0-+}] + \mathrm{tr}[(H_{+,--})^q H_{0--}]. &(166)
\end{aligned}$$

3.5 Comment

- A gain for each LU decomposition and matrix-matrix multiplication is $(1/2)^3 = 1/8$ but we need twice, so total cost is proportional to $1/8 \times 2 = 1/4$.
- Since in the time reduced case, lapack is clever enough to skip zero element part, this spin reduction is not so impressive compared with the time reduction case.

3.6 Computation of A_0

When one computes eq.(86)

$$\det D_{(1)} = \prod_{t=1}^{N_{\mathrm{T}}/2-1} \det B_{t(t)}, \qquad (167)$$

the computation of

$$\det B_{t(t)}, \qquad (168)$$

is needed. This can be obtained by the spin decomposition form together with eq.(184)

$$\begin{aligned}
\det B_{t(t)} &= \det \begin{pmatrix} B_{t(t)++} & B_{t(t)+-} \\ B_{t(t)-+} & B_{t(t)--} \end{pmatrix} \\
&= \det B_{t(t)--} \det \left[B_{t(t)++} - B_{t(t)+-} B_{t(t)--}^{-1} B_{t(t)-+} \right]. &(169)
\end{aligned}$$

The first term can be obtained when one computes $B_{t(t)--}^{-1}$ in eq.(96). The second term can be obtained when one computes $(B_{t(t)}^{-1})_{++}$ in eq.(95).

4 Benchmark

The actual benchmark was done on K computer and the computational cost is plotted as a function of the lattice size in Fig.1. We find reduction method is several tens times faster than naive method. Using reduction method algorithm changes from one matrix inversion for a matrix of order $12N_{\rm L}^3N_{\rm T}$ to $5\times4\times(N_{\rm T}/2-1)+2$ matrix-matrix multiplications and $2\times4\times(N_{\rm T}/2-1)+2$ matrix inversions for matrices of order $6N_{\rm L}^3$. So numerical cost is reduced from

$$6\times(12N_{\rm L}^3N_{\rm T})^3 \tag{170}$$

to

$$6\times(6N_{\rm L}^3)^3\times\left[28\times(N_{\rm T}/2-1)+4\right]. \tag{171}$$

In reduction method we use pzgemm, pzgetrf and pzgetri of ScaLAPACK optimized for the K computer to compute matrix-matrix multiplication and matrix inversion which operates at $\sim$50% and $\sim$5% efficiency against the theoretical peak performance, respectively. Since most of computation is done by higher performance pzgemm, one might get more speed-up, e.g. by a factor of O(100) at $N_{\rm T}=6$. Our speed-up factor, however, is not such high because there are number of matrix copying and making inside of determinant calculation to save memory in our implementation.

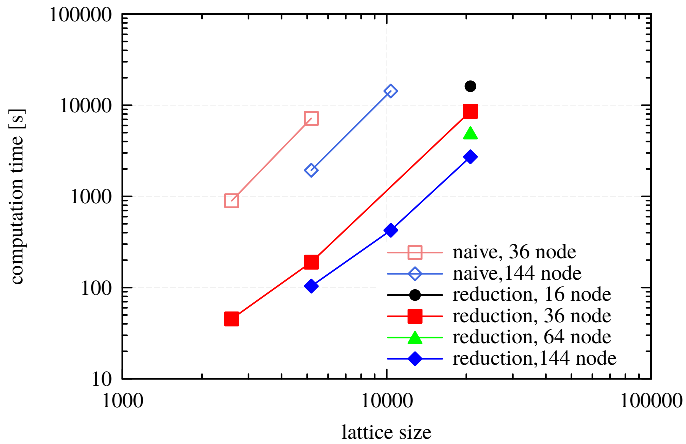

Figure 1: Computational cost [s] as function of lattice size $N_{\rm L}^3N_{\rm T}$. The lattice size is changed from the left to right in the following ordering, $12\times6\times6\times6$, $12\times12\times6\times6$, $12\times12\times12\times6$, $24\times12\times12\times6$. In the legend, "naive" means the determinant calculation without reduction, while "reduction" represents the calculation according to the reduction technique for time and spinor space shown in this report.

Acknowledgments

All the results are obtained by using the K computer at the RIKEN Advanced Institute for Computational Science.

References

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Appendix A
Dirac-gamma matrix notation

The Pauli matrices are

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{172}$$

The Dirac-gamma matrix in the non-relativistic representation are given by

$$\gamma_{1,2,3} = \begin{pmatrix} 0 & -i\sigma_{1,2,3} \\ i\sigma_{1,2,3} & 0 \end{pmatrix}, \quad \gamma_4 = \begin{pmatrix} 1_2 & 0 \\ 0 & -1_2 \end{pmatrix}, \tag{173}$$

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4 = \begin{pmatrix} 0 & 1_2 \\ 1_2 & 0 \end{pmatrix}, \tag{174}$$

$$\sigma_{\mu\nu} = \frac{i}{2}[\gamma_\mu, \gamma_\nu]. \tag{175}$$

$$\gamma_5 P_+ = \begin{pmatrix} 0 & 0 \\ 1_2 & 0 \end{pmatrix}, \quad \gamma_5 P_- = \begin{pmatrix} 0 & 1_2 \\ 0 & 0 \end{pmatrix}. \tag{176}$$

Appendix B
Formula for block matrix

In this note, the following formula is useful. For inverse matrix,

$$\begin{aligned}
&\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} \\
&= \begin{pmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix} && (177) \\
&= \begin{pmatrix} A^{-1} + A^{-1}BX^{-1}CA^{-1} & -A^{-1}BX^{-1} \\ -X^{-1}CA^{-1} & X^{-1} \end{pmatrix} && (178) \\
&= \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -D^{-1}C(A - BD^{-1}C)^{-1} & D^{-1} + D^{-1}C(A - BD^{-1}C)^{-1}BD^{-1} \end{pmatrix} && (179) \\
&= \begin{pmatrix} Y^{-1} & -Y^{-1}BD^{-1} \\ -D^{-1}CY^{-1} & D^{-1} + D^{-1}CY^{-1}BD^{-1} \end{pmatrix}, && (180)
\end{aligned}$$

with

$$X = D - CA^{-1}B, \tag{181}$$

$$Y = A - BD^{-1}C. \tag{182}$$

For determinant

$$\det \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \det A \det[D - CA^{-1}B] \tag{183}$$

$$= \det D \det[A - BD^{-1}C]. \tag{184}$$