

# Cuda Lattice Gauge Document

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# 1 Data

## 1.1 Index of lattice

### 1.1.1 UINT Index of lattice

Generally, in CLG, we have three kinds of indexes:

- site index
- link index
- fat index

Let the lattice have  $V = L_x \times L_y \times L_z \times L_t$  sites.

**Note: for  $D = 3$ , we assume  $L_x = 1, L_{y,z,t} > 1$ ; for  $D = 2$ , we assume  $L_x = L_y = 1, L_{z,t} > 1$ .**

For a site at  $(x, y, z, t)$

$$siteIndex = x \times L_y \times L_z \times L_t + y \times L_z \times L_t + z \times L_t + t \quad (1)$$

For a link at direction  $dir$ , link with site at  $(x, y, z, t)$ , and on a lattice with number of directions of links is  $dirCount$ ,

$$linkIndex = siteIndex \times dirCount + dir \quad (2)$$

**Note: we do NOT assume dimension equal number of links. For example for  $D = 2$  triangle lattice, number of directions of links is 6, for  $D = 2$  hexagon number of directions of links is 3. Only for square lattice, number of links equal dimension.**

For a link at direction  $dir$ , link with site at  $(x, y, z, t)$ , and on a lattice with number of directions of links is  $dirCount$ ,

$$fatIndex = \begin{cases} siteIndex \times (dirCount + 1); & \text{for site.} \\ siteIndex \times (dirCount + 1) + (dir + 1); & \text{for link} \end{cases} \quad (3)$$

### 1.1.2 SIndex of lattice

### 1.1.3 Index and boundary condition, a int2 or a uint2 structure

In CLGLib, sometimes, the index function return a uint2 structure.

**1.1.4 Index walking**

**1.2 CParemers**

## 2 Update scheme

### 2.1 HMC

HMC is abbreviation for hybrid Monte Carlo.

#### 2.1.1 The Fermion action

Cooperating with HMC, the fermion is usually the 'Pseudofermions'.

We begin with Eq. (1.85) and Eq. (1.86) of Ref. [1].

$$Z = \int \mathcal{D}[U] \prod_{f=1}^{N_f} \mathcal{D}[\bar{\psi}_f] \mathcal{D}[\psi_f] \exp \left( -S_G[U] - \sum_{f=1}^{N_f} \bar{\psi}_f \left( \hat{D}_f \right) \psi_f \right) \quad (4)$$

where  $\hat{D}_f = D + m_f$ . (Note that, there seems a typo in Eq. (1.85) of Ref. [1] and Eq. (8.31) of Ref. [2], we have  $S_F = +\bar{\psi}D\psi$ , see also Eqs. (2.5) and (8.39) of Ref. [2] and Eq. (7.6) of Ref. [3], Eq. (3.75) of Ref. [1], etc.)

It can be evaluated as Eq. (1.86) of Ref. [1] (or Eq. (4.19) of Ref. [4]) (Note, there is another minus sign in Eq. (5.28) of Ref. [2])

$$\begin{aligned} \int \mathcal{D}\bar{\psi}\psi \exp(-\bar{\psi}A\psi) &= \det(A), \\ Z &= \prod_{f=1}^{N_f} \det(\hat{D}_f) \int \mathcal{D}[U] \exp(-S_G[U]). \end{aligned} \quad (5)$$

On the other hand, with the help of Gaussian integral of complex vectors Eq. (3.17) of Ref. [4]

$$\int d\mathbf{v}^\dagger d\mathbf{v} \exp(-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}) = \pi^N (\det \mathbf{A})^{-1} \quad (6)$$

which is (3.31) of Ref. [1]

$$\frac{1}{\det(\mathbf{A})} = \int \mathcal{D}[\eta] \exp(-\eta^\dagger \mathbf{A} \eta) \quad (7)$$

where  $\eta$  now is a complex Bosonic field, and the normalization

$$\mathcal{D}[\eta] = \prod \frac{d\text{Re}(\eta_i) d\text{Im}(\eta_i)}{\pi}, \quad 1 = \int \mathcal{D}[\eta] \exp(-\eta^\dagger \eta) \quad (8)$$

is assumed. With the condition such that

$$\lambda(\mathbf{A} + \mathbf{A}^\dagger) > 0. \quad (9)$$

where  $\lambda(\mathbf{M})$  denoted as eigen-values of  $\mathbf{M}$ .

We now, concentrate on two degenerate fermion flavours. i.e. considering

$$S_F = \bar{\psi}_u \hat{D} \psi_u + \bar{\psi}_d \hat{D} \psi_d. \quad (10)$$

Using  $\det(DD^\dagger) = \det(D) \det(D^\dagger)$  and  $\det(M^{-1}) = (\det(M))^{-1}$  and  $\det(D) = \det(D^\dagger)$  (Only for Wilson Fermions or  $\gamma_5$ -hermiticity fermions,  $\hat{D}^\dagger = \gamma_5 D \gamma_5 + m = \gamma_5 (D + m) \gamma_5 = \gamma_5 \hat{D} \gamma_5$ , and  $\det(\hat{D}^\dagger) = \det(\gamma_5) \det(\hat{D}) \det(\gamma_5) = \det(\hat{D})$ . See also Ref. [5].), one can show Eq. (8.9) of Ref. [2] (Eq. (2.77) of Ref. [6])

$$\int \mathcal{D}[\bar{\psi}] \mathcal{D}[\psi] \exp \left( -\bar{\psi}_u \hat{D} \psi_u - \bar{\psi}_d \hat{D} \psi_d \right) = \det(\hat{D} \hat{D}^\dagger) = \int \mathcal{D}[\phi] \exp \left( -\phi^\dagger \left( \hat{D} \hat{D}^\dagger \right)^{-1} \phi \right) \quad (11)$$

where  $\phi$  now is a complex Bosonic field. (Note that, there is a sign typo in Eq. (8.31) of Ref. [2], see also Eqs. (8.38) and (8.39) of Ref. [2] )

So, generally, we are using HMC to evaluate the action with 'Pseudofermions', or in other words, we are working with an action including only gauge and bosons.

$$S = S_G + S_{pf} = S_G + \phi^\dagger \left( \hat{D} \hat{D}^\dagger \right)^{-1} \phi \quad (12)$$

where  $pf$  is short for pseudofermion.

### 2.1.2 Basic idea, force from gauge field

The basic idea is to use a molecular dynamics simulation, i.e, it is a integration of Langevin equation.

Treating  $SU(N)$  matrix  $U$  on links as coordinate, HMC will generate a pair of configurations,  $(P, U)$ , where  $P$  is momentum and  $P \in \mathfrak{su}(N)$ .

One can:

1. Create a random  $P = i \sum_a \omega_a T_a$ , where  $\omega_a \in \mathbb{R}$ .
  2. Obtain  $\dot{P}, \dot{U}$ . Note that, dot is  $d/d\tau$ , where  $\tau$  is 'Markov time'.
  3. Numerically evaluate the differential equation, and use a Metropolis accept / reject to update.
- About the randomized  $P$



The randomized  $P$  is chosen according to normal distribution  $\exp(-P^2/2)$

Note that, here  $P$  corresponds to  $Q$ , not  $U$ , for  $U = \exp(i \sum q_a T^a)$ , there are 8 **real** variables denoting as  $\omega_i$ .

Using  $P = \sum \omega_a T^a$ ,  $\text{tr}((T^a) \cdot (T^b)) = \frac{1}{2} \delta_{ab}$ . So one have  $\frac{1}{2} \sum_a \omega_a^2 = \text{tr}[P^2]$ .

It is usually written as distribution  $\exp(-\text{tr}(P^2))$  (where  $P$  is a matrix, and  $\text{tr}[P^2] = \frac{1}{2} p^2$  where  $p = (\omega_1, \omega_2, \dots, \omega_8)$ ).

Using the property of normal distribution

$$\begin{aligned} \text{if } \{X\} &\sim N(\mu_X, \sigma_X^2), \quad \{Y\} \sim N(\mu_Y, \sigma_Y^2), \\ \{X + Y\} &\sim N(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2). \end{aligned} \quad (13)$$

One can randomize  $\omega_a$  using  $\exp(-\omega_a \omega_a)$ . Then using  $P = \frac{1}{\sqrt{8N}} \sum \omega_a T^i$ , where  $N$  is the number of links.

**Note: Here is a difference between Refs. [2] and [1] and Bridge++ [7]**

Note, by Eq. (8.16) of Ref. [2],  $P^2 = \sum_{n \in \Lambda} P^2(n)$ , so when the lattice is large,  $P$  become very small. See also the definition of  $\langle P, P \rangle$  below Eq. (2.42) of Ref. [1].

However, in Bridge++, it uses distribution  $\exp(-\text{tr}(P^2)/DOF)$ , where ‘DOF’ is the degrees of freedom, i.e., number of links.

We use the distribution same as in Bridge++. Imagining that for a very small (hot)  $\beta \rightarrow 0$ , the force is also almost 0 so momentum is unchanged when evolution. Considering a very large lattice such that the momentum is very small when using distribution  $\exp(-\text{tr}(P^2))$ , the gauge field will stay near the initial value rather than becoming hot (randomized). So we think it should be  $\exp(-\text{tr}(P^2)/DOF)$ .

- Force

Defined by Newton,  $dp/dt$  is a force, so  $\dot{P}$  is called ‘force’. See Eqs. (2.53), (2.56) and (2.57) of Ref. [1], for  $SU(N)$ ,

$$\begin{aligned} S_G[U_\mu(n)] &= -\frac{\beta}{N} \text{Retr}[U_\mu(n) \Sigma_\mu^\dagger(n)] \\ \Sigma_\mu(n) &= \sum_{\mu \neq \nu} (U_\nu(n) U_\mu(n + a\nu) U_\nu^{-1}(n + a\mu) + U_\nu^{-1}(n - a\nu) U_\mu(n - a\nu) U_\nu(n - a\nu + a\mu)) \end{aligned} \quad (14)$$

**Note that**  $S_G \neq \sum_{\mu, n} S_G[U_\mu(n)]$ .  $S_G[U_\mu(n)]$  is convenient for derivate which collecting all terms related to the specified bond. For plaquettes with 4 edges,  $S_G = \frac{1}{4} \sum_{\mu, n} S_G[U_\mu(n)]$ .

$S_G$  the action for a particular  $U_\mu(n)$ .  $\Sigma$  is the ‘staple’(see Eq. (??)). The staple for  $U_\mu(n)$  is independent of  $U_\mu(n)$ , denoting

$$U_\mu(n) = \exp \left( i \sum_a \omega_a(\mu, n) T_a \right) U_\mu^0(n) \quad (15)$$

so

$$\begin{aligned} \frac{\partial}{\partial \omega_a(\mu, n)} S_G &= -\frac{\beta}{N} \text{Retr} \left[ \frac{\partial}{\partial \omega_a} U_\mu(n) \Sigma_\mu^\dagger(n) \right] = -\frac{\beta}{2N} \text{tr} \left[ \frac{\partial}{\partial \omega_a} (U_\mu(n) \Sigma_\mu^\dagger(n) + \Sigma_\mu(n) U_\mu^\dagger(n)) \right] \\ &= -i \frac{\beta}{2N} \text{tr} [T_a U_\mu(n) \Sigma_\mu^\dagger(n) - \Sigma_\mu(n) T_a^\dagger U_\mu^\dagger(n)] = -i \frac{\beta}{2N} \text{tr} [T_a (U_\mu(n) \Sigma_\mu^\dagger(n) - \Sigma_\mu(n) U_\mu^\dagger(n))] \\ &= \frac{\beta}{N} \text{Im tr} [T_a U_\mu(n) \Sigma_\mu^\dagger(n)] \end{aligned} \quad (16)$$

This is the Eq. (8.41) of Ref. [2].

Using (Checked by Mathematica that Eq. (8.42) of Ref. [2] is incompatible with our notation, but replacing the  $UA - A^\dagger U^\dagger$  of Eq. (8.42) with  $\{UA\}_{TA}$  is correct. Also, Eq. (2.58) of Ref. [1] is different from ours, in our formulism, it is correct by replacing  $2T_a \text{Re}[tr[T_a \cdot W]]$  of Eq. (2.58) with  $2iT_a \text{Im}[tr[T_a \cdot W]]$ )

$$\begin{aligned} \sum_a \text{tr} [T_a (U_\mu(n) \Sigma_\mu^\dagger(n) - \Sigma_\mu(n) U_\mu^\dagger(n))] T_a &= 2i \sum_a \text{Im} [T_a U_\mu(n) \Sigma_\mu^\dagger(n)] T_a = \{U_\mu(n) \Sigma_\mu^\dagger(n)\}_{TA} \\ \{W\}_{TA} &= \frac{W - W^\dagger}{2} - \text{tr} \left( \frac{W - W^\dagger}{2N} \right) \mathbb{I} \end{aligned} \quad (17)$$

where  $\mathbb{I}$  is identity matrix. Therefor

$$\begin{aligned} \dot{\omega}_a &= -\frac{\partial}{\partial \omega_a(\mu, n)} S_G \\ F_\mu(x) = \dot{P}_\mu(x) &= i \sum \dot{\omega}_a T_a = -i \frac{\partial}{\partial \omega_a(\mu, n)} S_G T_a = -\frac{\beta}{2N} \{U_\mu(n) \Sigma_\mu^\dagger(n)\}_{TA} \end{aligned} \quad (18)$$

Note that,  $\dot{\omega}_a = \frac{\beta}{N} \text{Im}[tr[T_a \cdot W]]$  is still a **real** number.

Eq. (18) is same as Eqs. (2.53), (2.56) and (2.57) of Ref. [1].

- Integrator

Knowing  $\dot{P}$ , and  $\dot{U}$ , to obtain  $U$  and  $P$  is simply

$$U(\tau + d\tau) \approx \dot{U} d\tau + U(\tau), \quad P(\tau + d\tau) \approx \dot{P} d\tau + P(\tau) \quad (19)$$

A more accurate calculation is done by integrator, for example, the leap frog integrator, the  $M$  step leap frog integral is described in Ref. [2],

$$\epsilon = \frac{\tau}{M} \quad (20a)$$

$$U_\mu(x, (n+1)\epsilon) = U_\mu(x, n\epsilon) + \epsilon P_\mu(x, n\epsilon) + \frac{1}{2} F_\mu(x, n\epsilon) \epsilon^2 \quad (20b)$$

$$P_\mu(x, (n+1)\epsilon) = P_\mu(x, n\epsilon) + \frac{1}{2} (F_\mu(x, (n+1)\epsilon) + F_\mu(x, n\epsilon)) \epsilon \quad (20c)$$

So, knowing  $U(n\epsilon)$  we can calculate  $F(n\epsilon)$  using Eq. (18). Knowing  $U(n\epsilon), P(n\epsilon), F(n\epsilon)$ , we can calculate  $U((n+1)\epsilon)$  using Eq. (20).b. Then we are able to calculate  $F((n+1)\epsilon)$  again using Eq. (18). Then we can calculate  $P((n+1)\epsilon)$  using Eq. (20).c.

### 2.1.3 Force of pseudofermions

For important sampling, one can generate both  $U$  and  $\phi$  by  $e^{-S}$ . In molecular dynamics simulation, it can be simplified as:

1. Evaluate  $U$  use force of  $U$  and  $\phi$  on  $U$ .
2. Evaluate  $\phi$  use force of  $U$  and  $\phi$  on  $\phi$ .

The second step can be simplified as, generating random complex numbers  $\phi$  according to  $\exp(-\phi^\dagger (\hat{D}\hat{D}^\dagger)^{-1} \phi) = \exp(-\phi^\dagger (\hat{D}^\dagger)^{-1} \hat{D}^{-1} \phi)$ .  $D[U]$  is a function of  $U$ .

**How to get randomized  $\phi$ ?** Let  $\chi$  be random **complex** numbers according to  $\exp(-\chi^\dagger \chi)$ . Let  $\hat{D}^{-1} \phi = \chi$ ,  $\phi$  is the random **complex** number satisfying distribution we want ( $\exp(-\phi^\dagger (\hat{D}^\dagger)^{-1} \hat{D}^{-1} \phi)$ ). So, first get  $\chi$  and then let  $\phi = D\chi$ .

Using the Wilson Fermion action

$$\begin{aligned} \hat{D} &= C(D+1) \\ D &= -\kappa \sum_\mu ((1-\gamma_\mu)U_\mu(x_L)\delta_{x_L, (x+\mu)_R} + (1+\gamma_\mu)U_\mu^{-1}(x_L-\mu)\delta_{x_L, (x-\mu)_R}) \end{aligned} \quad (21)$$

with  $C = m_f + (4/a) = 1/2a\kappa$  and  $\kappa = 1/(2am_f + 8)$ . One can rescale the field and set  $C = 1$ .

The force of  $\phi$  on  $U$  is obtained as  $\partial_{\omega_a} S_{pf}$ . The result for Wilson Fermion action is shown

in Eqs. (8.39), (8.44) and (8.45) of Ref. [2] as

$$\begin{aligned}
F &= i \sum_a \dot{\omega}_a T_a = i \sum_a (-\partial_{\omega_a} (S_G[U_\mu(n)] + S_{pf}[U_\mu(n)])) T_a = F_G + F_{pf}. \\
F_{pf} &= i \sum_a (-\partial_{\omega_a} S_{pf}[U_\mu(n)]) T_a = -i \sum_a T^a \frac{\partial}{\partial \omega_a} \left( \phi^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi \right). \\
\frac{\partial}{\partial \omega_a} \left( \phi^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) &= - \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right)^\dagger \left( \frac{\partial \hat{D}}{\partial \omega_\mu^a} \hat{D}^\dagger + \hat{D} \frac{\partial \hat{D}^\dagger}{\partial \omega_\mu^a} \right) \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right). \\
\frac{\partial \hat{D}}{\partial \omega_\mu^a} &= \left( \frac{\partial D}{\partial \omega_\mu^a} \right)_{x_L, x_R} = -i\kappa \{ (1 - \gamma_\mu) T^a U_\mu(x) \delta_{x, x_L} \delta_{x, (x+\mu)_R} - (1 + \gamma_\mu) U_\mu^{-1}(x) T^a \delta_{x, (x+\mu)_L} \delta_{x, x_R} \} \\
\hat{D}^\dagger &= \gamma_5 \hat{D} \gamma_5, \quad \frac{\partial \hat{D}^\dagger}{\partial \omega_\mu^a} = \gamma_5 \frac{\partial D}{\partial \omega_\mu^a} \gamma_5
\end{aligned} \tag{22}$$

where  $F_G$  is force from  $U$  introduced in Sec. 2.1.2,  $T^a$  are  $SU(3)$  generators.  $x_L, x_R$  are coordinate index of the left and right pseudofermion field. And

$$\begin{aligned}
U_\mu &= \exp(i \sum_a \omega_\mu^a T^a) U_0, \quad \frac{\partial U_\mu}{\partial \omega_\mu^a} = iT^a U_\mu, \quad \frac{\partial U_\mu^\dagger}{\partial \omega_\mu^a} = -iU_\mu^\dagger T^a, \\
(T^a)^\dagger &= T^a, \quad \frac{\partial M^{-1}}{\partial \omega_\mu^a} = -M^{-1} \frac{\partial M}{\partial \omega_\mu^a} M^{-1}
\end{aligned} \tag{23}$$

are used. (Note that, Eq. (8.45) of Ref. [2] has a sign typo, see also Eq. (2.82) of Ref. [6])

We can simplify it further by  $(\hat{D}^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi)^\dagger = ((\hat{D} \hat{D}^\dagger)^{-1} \phi)^\dagger \hat{D}$ , so

$$\begin{aligned}
\phi_1 &= \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right), \quad \phi_2 = \hat{D}^\dagger \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) = D^{-1} \phi, \quad \phi_1^\dagger D = \phi_2^\dagger, \\
\frac{\partial}{\partial \omega_a} \left( \phi^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) &= - \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right)^\dagger \left( \frac{\partial \hat{D}}{\partial \omega_\mu^a} \hat{D}^\dagger + \hat{D} \frac{\partial \hat{D}^\dagger}{\partial \omega_\mu^a} \right) \left( (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) \\
&= - \left( \phi_1^\dagger \frac{\partial D}{\partial \omega_\mu^a} \phi_2 + \phi_2^\dagger \frac{\partial D^\dagger}{\partial \omega_\mu^a} \phi_1 \right) = -2\text{Re} \left[ \left( \phi_1^\dagger \frac{\partial D}{\partial \omega_\mu^a} \phi_2 \right) \right]
\end{aligned} \tag{24}$$

and

$$\begin{aligned}
\frac{\partial D}{\partial \omega_\mu^a} &= -i\kappa M_a, \\
(M_a)_{x_L, x_R} &= \{ (1 - \gamma_\mu) T^a U_\mu \delta_{x_L, (x+\mu)_R} - (1 + \gamma_\mu) U_\mu^{-1} T^a \delta_{(x+\mu)_L, x_R} \} \\
\frac{\partial}{\partial \omega_a} \left( \phi^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) &= -2\kappa \text{Im} \left[ \left( \phi_1^\dagger M \phi_2 \right) \right]
\end{aligned} \tag{25}$$

Again,  $\dot{\omega}$  is a **real** number, and

$$F_{pf} = -i \sum_a T^a \frac{\partial}{\partial \omega_a} \left( \phi^\dagger (\hat{D} \hat{D}^\dagger)^{-1} \phi \right) = 2i\kappa \sum_a \text{Im} \left[ \left( \phi_1^\dagger M_a \phi_2 \right) \right] T_a \quad (26)$$

So we can calculate  $\phi_1$  first, then  $\phi_2 = \hat{D}^\dagger \phi_1$ . Then contract the spinor and color space with  $\partial D / \partial \omega$ .

Note that,  $D$  is changing when integrating the Langevin equation.

The last part is how to calculate  $(\hat{D} \hat{D}^\dagger)^{-1}$ .

- Anti-Hermitian traceless of the force

See from Eq. (18), the force from the gauge field is an anti-Hermitian traceless matrix.

The result above can be further simplified. Note that

$$\begin{aligned} \phi_{L1}(n) &= \phi_1(n), \quad \phi_{R1}(n) = (1 - \gamma_\mu) \phi_2(n + \mu), \\ \phi_{L2}(n) &= \phi_1(n + \mu), \quad \phi_{R1}(n) = (1 + \gamma_\mu) \phi_2(n), \end{aligned} \quad (27)$$

One have

$$\begin{aligned} \text{Im} \left[ \phi_1^\dagger M \phi_2 \right]_\mu^a(n) &= \text{Im} \left[ \phi_{L1}^\dagger T^a U_\mu(n) \phi_{R1} \right] - \text{Im} \left[ \phi_{L2}^\dagger U_\mu^\dagger(n) T^a \phi_{R2} \right] \\ &= \text{Im} \left[ \phi_{L1}^\dagger T^a U_\mu(n) \phi_{R1} \right] + \text{Im} \left[ \phi_{R2}^\dagger T^a U_\mu(n) \phi_{L2} \right] \end{aligned} \quad (28)$$

For any vector

$$\text{Im} [L^\dagger T U R] = \text{Im} \left[ \sum_{\alpha, \beta, \rho} L_\alpha^* T_{\alpha\beta} U_{\beta\rho} R_\rho \right] = \text{Im} \left[ \sum_{\alpha, \beta, \rho} T_{\alpha\beta} U_{\beta\rho} R_\rho L_\alpha^* \right] = \text{Im} [\text{tr} [T U (R L^\dagger)]] \quad (29)$$

So

$$\begin{aligned} F_\mu^{pf}(n) &= 2i\kappa \text{Im} \left[ \phi_1^\dagger M \phi_2 \right]_\mu(n) = \kappa \left( 2i \sum_a \text{Imtr} \left[ T^a U_\mu(n) \left( \phi_{R1} \phi_{L1}^\dagger + \phi_{R2} \phi_{L2}^\dagger \right) \right] T^a \right) \\ &= \kappa \left\{ U_\mu(n) \left( \phi_{R1} \phi_{L1}^\dagger + \phi_{R2} \phi_{L2}^\dagger \right) \right\} \Big|_{TA} \end{aligned} \quad (30)$$

which is also an anti-Hermitian traceless matrix.

**So, the momentum is always anti-Hermitian traceless..**

For anti-Hermitian traceless matrix  $M$ , the  $\exp(M)$  can be simplified as Appendix. A of Ref. [8].

### 2.1.4 Solver in HMC

To calculate  $(\hat{D}\hat{D}^\dagger)^{-1}$ , we need a solver. The detail of solvers will be introduced in Sec. 3. Here we establish a simple introduction.

Let  $M$  be a matrix operating on a vector, for example,  $M = (\hat{D}\hat{D}^\dagger)$ , the goal of the solver is to find  $x$  such  $b = M \cdot x$ , and therefor  $x = (\hat{D}\hat{D}^\dagger)^{-1}b$ .

We first introduce the CG algorithm for real vector and real matrix, define

$$Q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T \cdot A \cdot \mathbf{x} - \mathbf{x}^T \mathbf{b}. \quad (31)$$

so that one can try to find the minimum of  $Q$ , and at the minimum

$$\frac{\partial}{\partial \mathbf{x}} Q(\mathbf{x}) = 0 = A \cdot \mathbf{x} - \mathbf{b}. \quad (32)$$

To find the minimum, one can use gradient. Starting from a random point on a curve, calculate the falling speed and move it until it is stable.

For complex vector, one can use BiCGStab in Table. 6.2 in Ref. [2]. It can be described as

---

**Algorithm 1** BiCGStab, note that, the numbers are **complex** number.

---

```

x = b ▷ Use b as trail solution and start.
for  $i = 0$  to  $r$  do
    r = b -  $A\mathbf{x}$  ▷ Restart  $r$  times
     $\mathbf{r}_h = \mathbf{r}$ 
    for  $j = 0$  to  $itera$  do
         $\rho = \mathbf{r}_h^* \cdot \mathbf{r}_j$ 
        if  $j = 0$  then
             $\mathbf{p} = \mathbf{r}$ 
        else
             $\beta = \alpha \times \rho / (\omega \times \rho_p)$ 
             $\mathbf{p} = \mathbf{r} + \beta(\mathbf{p} - \omega \mathbf{v})$ 
        end if
         $\mathbf{v} = A\mathbf{p}$ 
         $\alpha = \rho / (\mathbf{r}_h^* \cdot \mathbf{v})$ 
         $\mathbf{s} = \mathbf{r} - \alpha \mathbf{v}$ 
        if  $0 \neq j$  and  $0 = \text{mod}(j, 5)$  then
             $er = \|\mathbf{s}\|$  ▷ Check deviation every 5 steps
            if  $er < \epsilon$  then
                return x
            end if
        end if
         $\mathbf{t} = A\mathbf{s}$ 
         $\omega = \mathbf{s}^* \cdot \mathbf{t} / \|\mathbf{t}\|$ 
         $\mathbf{r} = \mathbf{s} - \omega \mathbf{t}$ 
         $\mathbf{x} = \mathbf{x} + \alpha \mathbf{p} + \omega \mathbf{s}$ 
         $\rho_p = \rho$  ▷ Preserve the last calculated  $\rho$  because we still need it
    end for
end for

```

---

### 2.1.5 Leap frog integrator

In Sec. 2.1.2, the basic idea is introduced. However, the implementation is slightly different.

$$U_\mu(0, x) = gauge(x), \quad P_\mu(0, x) = \sum_a r_a(\mu, x) T_a \quad (33a)$$

$$F_\mu(n\epsilon, x) = -\frac{\beta}{2N} \{U_\mu(n\epsilon, x) \Sigma_\mu(n\epsilon, x)\}_{TA} \quad (33b)$$

$$P_\mu(\frac{1}{2}\epsilon, x) = P_\mu(0, x) + \frac{\epsilon}{2} F_\mu(0, x) \quad (33c)$$

$$U_\mu((n+1)\epsilon, x) = \exp(i\epsilon P_\mu((n+\frac{1}{2})\epsilon, x)) U_\mu(n\epsilon, x) \quad (33d)$$

$$P_\mu((n+\frac{1}{2})\epsilon, x) = P_\mu((n-\frac{1}{2})\epsilon, x) + \epsilon F_\mu(n\epsilon, x) \quad (33e)$$

Note that, the sign of  $F$  is '+' here which is different from Ref. [2], because in Ref. [2],  $F = \partial_{\mu,n} S = -\dot{P}$ . Here we define  $F = \dot{P} = -\partial_{\mu,n} S$ .

Or simply written as

$$P_\epsilon \circ U_\epsilon \circ P_{\frac{1}{2}\epsilon}(P_0, U_0) \quad (34)$$

The pseudo code can be written as

---

**Algorithm 2** leap-frog integration

---

$\mathbf{f} = CalculateForce(actions, \mathbf{U})$

$\mathbf{p} = \mathbf{p} + 0.5 \times \epsilon \mathbf{f}$

**for**  $i = 1$  to  $n$  **do**

$\mathbf{U} = \exp(\epsilon \mathbf{p}) \mathbf{U}$

$\mathbf{f} = CalculateForce(actions, \mathbf{U})$

**if**  $i = n$  **then**

$\mathbf{p} = \mathbf{p} + 0.5 \times \epsilon \mathbf{f}$

        ▷ We still need to update  $\mathbf{p}$  for the Metropolis step.

**else**

$\mathbf{p} = \mathbf{p} + \epsilon \mathbf{f}$

**end if**

**end for**

---

### 2.1.6 A summary of HMC with pseudofermions

Now, every part is ready. We summary the HMC following the Sec.8.2.3 in Ref. [2]. The HMC with fermions can be divided into 6 steps.



1. Generate a complex Bosonic field with  $\chi \sim \exp(-\chi^\dagger \chi)$ , and  $\phi = \hat{D}\chi$ .
  2. Generate a momentum field  $P$  by  $\exp(-tr(P^2))$ .
  3. Calculate  $E = tr(P^2) + S_G(U) + S_{pf}(U, \phi)$ .
  4. Use  $U_0$  to calculate  $F$ , evaluate  $P$  and  $U$  using integrator. Here,  $\phi$  is treated as a constant field.
  5. Finally, use  $P', U'$  to calculate  $E' = tr(P'^2) + S_G(U') + S_{pf}(U', \phi)$ . Use a Metropolis to accept or reject the result (configurations) **Note, by Refs. [2] and [6] ‘reject’ means add a duplicated old configuration..**
  6. Iterate from 1 to 5, until the number of configurations generated is sufficient.
- More on Metropolis step:

If the hybrid Monte Carlo can be implemented exactly, then, when equilibrium is reached,  $H$  should be unchanged, so, in some implementation, the Metropolis step can be ignored to archive a better accept rate. The parameter `Metropolis` of parameter `Updater` can be set to 1 if Metropolis step is enabled and 0 otherwise.

## 2.2 Optimization of HMC

### 2.2.1 Omelyan integrator

The Omelyan integrator can be simply written as (c.f. Eq. (2.80) of Ref. [1])

$$P_{\lambda\epsilon} \circ U_{\frac{1}{2}\epsilon} \circ P_{(1-2\lambda)\epsilon} \circ U_{\frac{1}{2}\epsilon} \circ P_{\lambda\epsilon}(P_0, U_0) \quad (35)$$

with

$$\lambda = \frac{1}{2} - \frac{(2\sqrt{326} + 36)^{\frac{1}{3}}}{12} + \frac{1}{6(2\sqrt{326} + 36)^{\frac{1}{3}}} \approx 0.19318332750378364 \quad (36)$$

In practical, the  $\lambda$  is a tunable parameter, and usually,  $2\lambda = 0.3 \sim 0.5$  [6]. The `Omelyan2Lambda` parameter of `Updater` is a input parameter to set  $2\lambda$ , which if left blank is set to be 0.38636665500756728 by default.

Usually, for each sub-step, it is 2 times slower then leap-frog, and for one trajectory, it is 1.5 time faster [6], implying the number of sub-step needed is about 1/3 of leap-frog.

### 2.2.2 Omelyan force-gradient integrator

Start from the approximation

$$\log \left( \exp\left(\frac{\epsilon S}{6}\right) \exp\left(\frac{\epsilon T}{2}\right) \exp\left(\frac{2}{3}\epsilon S + \frac{\epsilon^3}{72}[S, [S, T]]\right) \exp\left(\frac{\epsilon T}{2}\right) \exp\left(\frac{\epsilon S}{6}\right) \right) = S + T + \mathcal{O}(\epsilon^4) + \mathcal{O}(\epsilon^6) \quad (37)$$

with [9]

$$\mathcal{O}(\epsilon^4) \sim 10^{-4} \epsilon^4 \quad (38)$$

The other 4 steps are the usual ones, except for  $\exp\left(\frac{2}{3}\epsilon S + \frac{\epsilon^3}{72}[S, [S, T]]\right)$  which correspond to

$$\begin{aligned} \omega_i &\rightarrow \omega_i - \frac{2}{3}\tau \frac{\partial}{\partial \omega_i} S + \frac{1}{36}\tau^3 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j} \frac{\partial}{\partial \omega_i} S \\ p_i &= \sum_a \omega_i^a T^a \end{aligned} \quad (39)$$

Use the approximation [10]

$$\begin{aligned} &\frac{2}{3}\tau \frac{\partial}{\partial \omega_i} S - \frac{1}{36}\tau^3 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j} \frac{\partial}{\partial \omega_i} S \\ &= \frac{2}{3}\tau \exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) \frac{\partial}{\partial \omega_i} S + \mathcal{O}(\tau^5) \end{aligned} \quad (40)$$

Let  $U'$  be a function of  $U$ , solving

$$\begin{aligned} &\frac{2}{3}\tau \exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) \frac{\partial}{\partial \omega_i} S(U) = \frac{2}{3}\tau \frac{\partial}{\partial \omega_i} S(U') \\ &\exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) \frac{\partial}{\partial \omega_i} U \frac{\partial S(U)}{\partial U} = \frac{\partial}{\partial \omega_i} U' \frac{\partial S(U')}{\partial U'} \\ &\frac{\partial}{\partial \omega_i} \left( \exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) U \right) = \frac{\partial}{\partial \omega_i} U' \\ &\exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) U = U', \\ &U' = \exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) \frac{\partial}{\partial \omega_j}\right) U = \exp\left(-\frac{1}{24}\tau^2 \sum_j \left( \frac{\partial}{\partial \omega_j} S \right) T_i\right) U \end{aligned} \quad (41)$$

This approximation can be divided into 3 steps:

1. Calculate  $U' = \exp\left(-\frac{1}{24}\tau^2 \sum_j \left(\frac{\partial}{\partial \omega_j} S\right) T_i\right) U$ .
2. Use  $S[U']$  and  $\frac{2}{3}\tau$  to update  $P$ .
3. Restore  $U$ .

It is easy to implement, we do not need to calculate second derivative, and  $\sum_j \left(\frac{\partial}{\partial \omega_j} S\right) T_i$  is already implemented, it is nothing but the **force**.

It is almost as accurate as force-gradient, see the compare in Ref. [11]

### 2.2.3 Multi-rate integrator (nested integrator)

Following Ref. [11]

Assuming the action is  $S = S_F + S_G$  with  $S_G \gg S_F$ , one can evaluate  $S_G$  more often than  $S_F$ . In the case of lattice QCD, often, the  $S_G$  is the cheap gauge force, and  $S_F$  is the expensive fermion force.

The nested scheme is different for leap-frog Omelyan and force-gradient integrator, but they are similar

- Nested leap-frog

$$\begin{aligned} \Delta(h) &= \exp\left(\frac{h}{2} S_F\right) \Delta_m(h) \exp\left(\frac{h}{2} S_F\right), \\ \Delta_m(h) &= \left( \exp\left(\frac{h}{2m} S_G\right) \exp\left(\frac{h}{m} T\right) \exp\left(\frac{h}{2m} S_G\right) \right)^m. \end{aligned} \quad (42)$$

- Nested Omelyan

$$\begin{aligned} \Delta(h) &= \exp(\lambda h S_F) \Delta_m\left(\frac{h}{2}\right) \exp((1 - 2\lambda)h S_F) \Delta_m\left(\frac{h}{2}\right) \exp(\epsilon h S_F), \\ \Delta_m(h) &= \left( \exp\left(\frac{\lambda h}{m} S_G\right) \exp\left(\frac{h}{2m} T\right) \exp\left(\frac{1 - 2\lambda}{m} h S_G\right) \exp\left(\frac{h}{2m} T\right) \exp\left(\frac{\lambda h}{m} S_G\right) \right)^m. \end{aligned} \quad (43)$$

**Note, it is  $\Delta_m(\frac{h}{2})$  in the first line.**

- Nested force-gradient

$$\Delta(h) = \exp(\frac{h}{6}S_F)\Delta_m(\frac{h}{2})\exp(\frac{2}{3}hS_F + \frac{1}{72}h^3C_F)\Delta_m(\frac{h}{2})\exp(\frac{h}{6}S_F),$$

$$\Delta_m(\textcolor{red}{h}) = \left( \exp(\frac{h}{6m}S_G)\exp(\frac{h}{2m}T)\exp\left(\frac{2}{3}\frac{h}{m}S_G + \frac{1}{72}\left(\frac{h}{m}\right)^3C_G\right)\exp(\frac{h}{2m}T)\exp(\frac{h}{6m}S_G) \right)^m. \quad (44)$$

**Note about the integrator:** when analyzing the error of the integrators, it is assumed  $e^T$ ,  $e^{S_G}$  and  $e^{S_F}$  can be calculated accurately. It is almost true for  $e^{S_G}$ , and almost true for  $e^T$  as long as  $\epsilon$  is not too large, but it is not true for  $e^{S_F}$ . Typically, using an optimized integrator, it needs more accurate criterion for solvers.

#### 2.2.4 Cached solution

The pseudo fermion field is generate only once for a trajectory and is not changed. Also, the gauge field is changing slowly in one trajectory, this make the solutions for  $\mathbf{x}_1 = D^{-1}\mathbf{b}$  or  $\mathbf{x}_2 = (DD^\dagger)^{-1}\mathbf{b}$ , where  $D$  depends on  $U$  and  $\mathbf{b}$  is the pseudo fermion field, only change slowly.

So, once  $\mathbf{x}_{1,2}$  is obtained, in the same trajectory,  $\mathbf{x}_{1,2}$  can be set as the initial trail solution for the solver.

### 3 Sparse linear algebra solver

Given a matrix  $A$  and a vector  $\mathbf{b}$ . The solver works out the solution

$$\mathbf{b} = A\mathbf{x}, \quad \mathbf{x} = A^{-1}\mathbf{b}. \quad (45)$$

#### 3.1 Krylov subspace

In short, the Krylov subspace methods assumes

$$\mathbf{x} \approx \sum_{l=0}^{k-1} C_l A^l \mathbf{b} \in K_k = \text{span} \{ \mathbf{b}, A\mathbf{b}, \dots, A^{k-1}\mathbf{b} \}. \quad (46)$$

with finite  $k$ , where  $C_k$  are coefficients. The equation  $0 = \mathbf{b} - A\mathbf{x}$  becomes

$$\|\mathbf{b} - \sum_{l=0}^{k-1} C_l A^{l+1} \mathbf{b}\| = 0 \quad (47)$$

This is a problem in  $k + 1$  dimension, where  $k$  is independent of the dimension of  $\mathbf{b}$ , and usually significantly smaller than the dimension of  $\mathbf{b}$ . The Eq. (47) can be understand that, if  $\mathbf{x}_k \approx A^{-1}\mathbf{b}$  is approximation of the solution in  $k$  dimension, in the  $k + 1$  dimension

$$(\mathbf{b} - A\mathbf{x})_{k+1} \perp K_k \quad (48)$$

That is, if we have a multi-dimension vector  $v_n$ , and its projection in 3-dimension ( $D = k + 1$ ) is a vector  $\mathbf{v}_3$ , if we want to find a plane ( $D = k$ ) such that the projection of  $v_n$  in the plane is minimized, the plane is chosen to be the one orthogonal to  $\mathbf{v}_3$ .

#### 3.2 GMRES

This section we follow Refs. [12] and [13].

Assume a set of basis has been found. For example, if the subspace is found by using modified Gram-Schmidt as

**Algorithm 3** Arnoldi with modified Gram-Schmidt

---

```

 $\mathbf{v}^{(0)} = \mathbf{x}_0 / \|\mathbf{x}_0\|$ 
for  $i = 0$  to  $k - 1$  do
   $\mathbf{w} = A\mathbf{v}^{(i)}$ 
  for  $j = 0$  to  $i$  do
     $c = \mathbf{v}^{(j)*} \cdot \mathbf{w}$ 
     $\mathbf{w} - = c\mathbf{v}^{(j)}$ 
     $h[j, i] = c$ 
  end for
   $h[i + 1, i] = \|\mathbf{w}\|$ 
   $\mathbf{v}^{(i+1)} = \mathbf{w} / \|\mathbf{w}\|$ 
end for

```

---

Note that  $(\mathbf{w} - (\mathbf{v}_i^* \cdot \mathbf{w}) \mathbf{v}_i)^* \cdot \mathbf{v}_i = 0$ , and  $\mathbf{x}_0$  is a trail solution, which can be set to be  $\mathbf{b}$  at first. Now we obtain  $k + 1$  unitary orthogonal vectors, such that

$$\mathbf{v}_i^* \cdot \mathbf{v}_j = \delta_{ij}, \quad A\mathbf{v}_{i-1} = \sum_{j=0}^i h[j, i-1] \mathbf{v}_j, \quad (49)$$

That is

$$\begin{pmatrix} Av_0 \\ Av_1 \\ Av_2 \\ \dots \\ Av_{k-1} \end{pmatrix} = (v_0, v_1, \dots, v_{k-1}, v_k) \begin{pmatrix} h[0,0] & h[0,1] & \dots & h[0,k-2] & h[0,k-1] \\ h[1,0] & h[1,1] & \dots & h[1,k-2] & h[1,k-1] \\ 0 & h[2,1] & \dots & h[2,k-2] & h[2,k-1] \\ 0 & 0 & \dots & \dots & \dots \\ \dots & \dots & \dots & h[k-1,k-2] & h[k-1,k-1] \\ 0 & 0 & \dots & 0 & h[k,k-1] \end{pmatrix} \quad (50)$$

which can be written as

$$(Av)_k = v_{k+1} H \quad (51)$$

The solution can be written as

$$\mathbf{x} = \mathbf{x}_0 + \sum_{i=0}^{k-1} y_i \mathbf{v}_i = \mathbf{x}_0 + \mathbf{y} = \mathbf{x}_0 + v_k y, \quad (52)$$

Using  $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$ , to minimize  $\|\mathbf{b} - A\mathbf{x}\|$  is to minimize  $\|\mathbf{r}_0 - A\mathbf{y}\|$ . We always choose  $\mathbf{v}_0 = \mathbf{r}_0 / \|\mathbf{r}_0\|$ , denote  $\beta = \|\mathbf{r}_0\|$ , it is to minimize

$$\operatorname{argmin} \|\beta \mathbf{e}_0 - H\mathbf{y}\|. \quad (53)$$

Or, to solve an equation in  $k$  dimension

$$\beta \mathbf{e}_0 - Hy = 0, \quad y = H^{-1} \beta \mathbf{e}_0 = H^{-1} g \quad (54)$$

Now, we need to solve  $H^{-1}$ , we can do this by applying rotation matrix, defining (This is also called **Givens rotation**)

$$J_0 = \begin{pmatrix} R & 0 \\ 0 & \mathbb{I}_{k-2} \end{pmatrix}_{D=k} = \begin{pmatrix} c_0^* & s_0^* & 0 & \dots & 0 \\ -s_0 & c_0 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}_{D=k} \quad (55)$$

**Note that  $c_0^*$  and  $s_0^*$  is necessary to keep unitary. ( $s_0^*$  seems not necessary? we only need to keep the length of  $g$  unchanged)** So that

$$0 = g - Hy \rightarrow 0 = J_0 g - J_0 Hy \quad (56)$$

with (Note that the first 2 lines are changed entirely)

$$H' = \begin{pmatrix} h'_{0,0} & h'_{0,1} & h'_{0,2} & \dots & h'_{0,k-1} \\ 0 & h'_{1,1} & h'_{1,2} & \dots & h'_{1,k-1} \\ 0 & h_{2,1} & h_{2,2} & \dots & h_{2,k-1} \\ 0 & 0 & \dots & \dots & 0 \\ 0 & 0 & 0 & 0 & h_{k,k-1} \end{pmatrix} \quad (57)$$

$$g' = (c_0^* \beta, -s_0 \beta, 0, \dots)$$

$$c_0 = \frac{h_{00}}{\sqrt{h_{00}^2 + h_{10}^2}}, \quad s_0 = \frac{h_{10}}{\sqrt{h_{00}^2 + h_{10}^2}}$$

where  $\mathbb{I}_l$  is dimension  $l$  identity matrix. Similarly, after this, one can rotation matrices

$$J_1 = \begin{pmatrix} \mathbb{I}_1 & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & \mathbb{I}_{k-3} \end{pmatrix}_{D=k}, J_2 = \begin{pmatrix} \mathbb{I}_2 & 0 & 0 \\ 0 & R & 0 \\ 0 & 0 & \mathbb{I}_{k-4} \end{pmatrix}_{D=k}, \dots \quad (58)$$

To make  $H$  triangular.

The algorithm is

---

**Algorithm 4** Rotate H

---

```

 $g[0] = \beta$ 
for  $i = 0$  to  $k - 1$  do
   $d = 1/\sqrt{|h[i, i]|^2 + |h[i + 1, i]|^2}$ 
   $cs = h[i, i] \times d, sn = h[i + 1, i] \times d$ 
  for  $j = i$  to  $k - 1$  do
     $h_{ij} = h[i, j]$ 
     $h[i, j] = cs^* \times h_{ij} + sn^* \times h[i + 1, j]$ 
     $h[i + 1, j] = cs \times h[i + 1, j] - sn \times h_{ij}$ 
  end for
   $minus_g = -g[i]$ 
   $g[i] = cs^* \times g[i]$ 
   $g[i + 1] = sn \times minus_g$ 
end for

```

---

After the rotation,  $g[k]$  is the residue. If it is small enough, the last step is to solve  $y = H^{-1}g$ , where  $H$  is a upper triangular matrix. It can be iterated as

$$y[k - 1] = \frac{g[k - 1]}{h[k - 1, k - 1]} \cdot y[k - 2] = \frac{1}{h[k - 2, k - 2]} (g[k - 2] - h[k - 2, k - 1]y[k - 1]), \dots \quad (59)$$

The algorithm is backward substitution

---

**Algorithm 5** Solve Y

---

```

for  $i = k - 1$  to  $0$  do
  for  $j = i + 1$  to  $k - 1$  do
     $g[i] - = h[i, j] \times y[j]$ 
  end for
   $y[i] = g[i]/h[i, i]$ 
end for
return  $\mathbf{x}_0 + \sum_{i=0}^{k-1} y[i] \mathbf{v}^{(i)}$ 

```

---

Note that, the first step, the modified Gram-Schmidt step will produce more and more unitary normalized vectors, so the GMRES usually has a restart step. Let  $r$  denote the restart times, for example, the full algorithm with  $k$  is (GMRES(m) means GMRES with modified Gram-Schmidt, there is also GMRES with Household, etc)



**Algorithm 6** GMRES(m)

---

```

x0 = b ▷ Use b as trail and start
for i = 1 to r do
  r0 = b − Ax0
  β = ||r0||
  v(0) = r0/β
  for i = 0 to k − 1 do
    w = Av(i)
    for j = 0 to i do
      c = v(j)* · w
      w− = cv(j)
      h[j, i] = c
    end for
    h[i + 1, i] = ||w||
    v(i+1) = w/||w||
  end for
  RotateH(k)
  x = SolveY(k)
  if |g[k] < ε then
    return x ▷ Succeed, with the solution
  end if
  x0 = x ▷ Use the last solution as trail and restart
end for
return x ▷ Failed, with the last best solution

```

---

where *RotateH*(*k*) and **x** = *SolveY*(*k*) is described in Algorithms. 4 and 5.

### 3.3 GCR

This section we follow Ref. [13].

The GCR solver is similar to GMRES in Sec. 3.2, but the orthogonal basis are obtained in a different way. If one have a set of orthogonal basis such that

$$A\mathbf{p}_i^* \cdot A\mathbf{p}_j = \delta_{ij}, \quad (60)$$

The solution  $\mathbf{x}$  is the residue projected into this basis (Note, here we do NOT assume the basis are normalized)

$$\begin{aligned} \mathbf{r}_0 &= \mathbf{b} - A\mathbf{x}_0 \\ \mathbf{x} &= \mathbf{x}_0 + \sum_{i=0}^{\infty} \frac{\mathbf{r}_0^* \cdot A\mathbf{p}_i}{\|A\mathbf{p}_i\|} \mathbf{p}_i \end{aligned} \quad (61)$$

So, the iteration is

$$\mathbf{x} \approx \mathbf{x}_k = \mathbf{x}_0 + \sum_{i=0}^k \frac{\mathbf{r}_0^* \cdot A\mathbf{p}_i}{\|A\mathbf{p}_i\|} \mathbf{p}_i \quad (62)$$

which can be obtained order by order as

$$\mathbf{x}_k = \mathbf{x}_{k-1} + \frac{(\mathbf{b} - A\mathbf{x}_{k-1})^* \cdot A\mathbf{p}_{k-1}}{\|A\mathbf{p}_{k-1}\|} \mathbf{p}_{k-1} \quad (63)$$

There are GCR, ORTHOMIN, ORTHODIR. Both GCR and ORTHOMIN have oscillation (tested with random Gaussian pseudo fermion field and random gauge field), when iterating, sometimes,  $\|\mathbf{p}^i\| \gg \|\mathbf{p}^{i-1}\|$ , and  $\|\mathbf{p}^{i+1}\| \ll \|\mathbf{p}^i\|$  and  $\|\mathbf{p}^{i+2}\| \gg \|\mathbf{p}^{i+1}\|$ , so we use ORTHODIR. The algorithm is

---

**Algorithm 7** incomplete GCR with restart

---

```

x = b ▷ Use b as trail and start
for  $i = 0$  to  $r$  do ▷ restart r times
  r = b - Ax, p0 = r
  for  $j = 0$  to  $k - 1$  do
     $\alpha = (A\mathbf{p}_j)^* \cdot \mathbf{r} / \|A\mathbf{p}_j\|^2$ 
    x = x +  $\alpha \mathbf{p}_j$ 
    r = r -  $\alpha A\mathbf{p}_j$ 
    if  $\|\mathbf{r}\| < \epsilon$  then return x ▷ Success
    end if
    p $j+1$  =  $A\mathbf{p}_j$ 
    for  $k = j - l + 1$  to  $j$  do
       $\beta = (A\mathbf{p}_k)^* \cdot A^2\mathbf{p}_j / \|A\mathbf{p}_k\|^2$ 
      p $j+1$  = p $j+1$  +  $\beta \mathbf{p}_k$ 
    end for
  end for
end for
return x ▷ Failed with the closest result

```

---

Note that, GCR is much slower than GMRES and BiCGStab. A strategy to improve the speed is to restart quickly.

### 3.4 GCRO-DR and GMRES-MDR

‘A comparison with the methods seen in the previous chapter indicates that in many cases, GMRES will be faster if the problem is well conditioned, resulting in a moderate number of steps required to converge. If many steps (say, in the hundreds) are required, then BICGSTAB and TFQMR may perform better. If memory is not an issue, GMRES or DQGMRES, with a large number of directions, is often the most reliable choice. The issue then is one of trading robustness for memory usage. In general, a sound strategy is to focus on finding a good preconditioner rather than the best accelerator’. [13].

That might be because the Krylov space will converge to the domain eigen-vector.

From Fig. 1. 9 of Ref. [14], the low mode is the most critical problem, so CLGLib first implement low mode deflation preconditioner.

In the following, we follow Ref. [15].

#### 3.4.1 Brief introduction to deflation preconditioner

In short, the preconditioner means, one solve

$$M^{-1}Ax = M^{-1}b, \quad (64)$$

or

$$\begin{cases} AM^{-1}u = b \\ x = M^{-1}u \end{cases} \quad (65)$$

instead of  $Ax = b$ . If  $M$  is chosen carefully, it is usually faster.

Now, considering  $A \in \mathbb{C}^{n \times n}$  and a matrix  $Z \in \mathbb{C}^{n \times k}$  such that  $Z = (v_1, v_2, \dots, v_k)$  and each row is a vector  $v_i \in \mathbb{C}^n$  such that  $v_i^\dagger v_j = \delta_{ij}$ . So  $Z$  acts like a Unitary matrix  $Z^\dagger Z = \mathbb{I}^{k \times k}$ . Then we can use  $Z$  to project  $A$  on a subspace, as

$$T = Z^\dagger A Z, \quad Z^\dagger A = T Z^\dagger \quad (66)$$

so

$$\begin{aligned} Ax = b &\Rightarrow (\mathbb{I} + Z (T^{-1} - \mathbb{I}) Z^\dagger) Ax = (\mathbb{I} + Z (T^{-1} - \mathbb{I}) Z^\dagger) b \\ &\Rightarrow (A - Z Z^\dagger A) x + Z T^{-1} Z^\dagger A x = b - Z Z^\dagger b + Z T^{-1} Z^\dagger b \end{aligned} \quad (67)$$

Note that  $ZZ^\dagger \in \mathbb{C}^{n \times n}$  is not identity matrix (**also not a unitary matrix, but is an Hermitian matrix**).  $T \in \mathbb{C}^{k \times k}$  is a small matrix. And then, one can solve

$$\begin{aligned} ZT^{-1}Z^\dagger Ax &= ZT^{-1}Z^\dagger b, \quad Z^\dagger A = TZ^\dagger \\ ZT^{-1}TZ^\dagger x &= ZT^{-1}Z^\dagger b \\ x &= ZT^{-1}Z^\dagger b \end{aligned} \tag{68}$$

exactly, while solving  $(A - ZZ^\dagger A)x = b - ZZ^\dagger b$  by iteration methods such as GMRES.

This is the so-called **subspace deflation**.

### 3.4.2 Brief intro to GCRO-DR

Start from Eq. (51). Assume after the first-step GMRES, we have the orthogonal-normal basis  $v_i$  which can be written as a matrix  $V_m \in \mathbb{C}^{n \times m}$ ,  $V_{m+1} \in \mathbb{C}^{n \times (m+1)}$ ,  $H \in \mathbb{C}^{(m+1) \times m}$ . On the other hand, will be introduced later, we have a set of deflation vectors, or a matrix  $P_k \in \mathbb{C}^{m \times k}$ , such that

$$\begin{aligned} AV_m P_k &= V_{m+1} H P_k \\ \tilde{Y}_k &\equiv V_m P_k \in \mathbb{C}^{n \times k} \end{aligned} \tag{69}$$

Then  $\tilde{Y}_k$  is the deflation matrix.

Consider the matrix  $HP_k = QR$ , where  $QR$  is the QR factorization, with  $Q \in \mathbb{C}^{(m+1) \times k}$  and  $R \in \mathbb{C}^{k \times k}$ . And define

$$C_k \equiv V_{m+1} Q \in \mathbb{C}^{n \times k}. \tag{70}$$

So, if  $R$  which is a small upper triangular matrix such that  $R^{-1}$  can be easily calculated, it is

$$\begin{aligned} AV_m P_k &= A\tilde{Y}_k = V_{m+1} H P_k = V_{m+1} Q R = C_k R \\ C_k &= A\tilde{Y}_k R^{-1} = AU, \quad U \equiv \tilde{Y}_k R^{-1} \in \mathbb{C}^{n \times k} \end{aligned} \tag{71}$$

Finally, the problem in GMRES Eq. (51) is changed as

$$\begin{aligned}
\tilde{U}_k &= U_k D_k = U_k \begin{pmatrix} \frac{1}{\|\mathbf{u}_1\|} & 0 & 0 & 0 \\ 0 & \frac{1}{\|\mathbf{u}_2\|} & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \frac{1}{\|\mathbf{u}_k\|} \end{pmatrix} \in \mathbb{C}^{n \times k} \\
V_m^{(1)} &= (U_k, V_{m-k}) \in \mathbb{C}^{n \times m} \\
V_{m+1}^{(2)} &= (C_k, V_{m-k+1}) \in \mathbb{C}^{n \times (m+1)} \\
H' &= \begin{pmatrix} D_k & B_{m-k} \\ 0 & H_{m-k} \end{pmatrix} \in \mathbb{C}^{(m+1) \times m} \\
AV_m^{(1)} &= V_{m+1}^{(2)} H'
\end{aligned} \tag{72}$$

where  $V$  are orthogonal-normal basis obtained in GMRES, and  $B_{m-k} = AV_{m-k}$ . Note that  $B_{m-k} \in \mathbb{C}^{(m-k) \times k}$  but  $H_{m-k} \in \mathbb{C}^{(m-k+1) \times (m-k)}$ .

From Eq. (72), we find

- The subspace is  $k$  dimension subspace of  $m$  dimension Krylov space.
- With  $H$ ,  $V$  and  $P$  known, we are able to calculate  $QR = HP$ ,  $U = V_m PR^{-1}$ ,  $C = V_{m+1} Q$ .

### 3.4.3 The choice of deflation subspace

In the above, we have assumed  $P_k \in \mathbb{C}^{m \times k}$  is already known. Now we concentrate on this part.

Let  $A \in \mathbb{C}^{n \times n}$ ,  $V \in \mathbb{C}^{n \times k}$ , If  $V$  is formed as orthogonal normal basis of subspace  $S$ , then, if  $(\lambda, w \in \mathbb{C}^m)$  is eigen-pair of  $V^\dagger AV$ ,  $(\lambda, u = V^\dagger w \in \mathbb{C}^n)$  is eigen-pair of  $A$ .

$$\begin{aligned}
H_m p_i &= \lambda_i p_i, \quad H_m = V_m^\dagger A V_m \\
A(V_m p_i) &= V_m H_m p_i = \lambda_i (V_m p_i)
\end{aligned} \tag{73}$$

Therefor,  $P_k$  is a matrix with  $k$  rows, and each row is a eigen-vector of  $H_m$  ( $H_m$  denoting the first  $m$  row of  $H_{m+1}$ ), then,  $V P_k$  is a matrix with  $k$  rows such that each row is a eigen-vector of  $A$  (approximately since  $AV \approx VH \Rightarrow H \approx V^\dagger AV$ ).

The first GMRES cycle will generate  $H_m$  (denoting the first  $m$  row of  $H_{m+1}$ ), and  $H_m \omega = \theta \omega$  is solved. However, starting from the second cycle of GCRO-DR, it is not  $AV_m = V_{m+1} H_{m+1}$  but  $AV_m^{(1)} = V_{m+1}^{(2)} H'_{m+1}$ , such that  $V_{m+1}^{(2)}$  are orthogonal basis but

$V_m^{(1)}$  are not orthogonal basis! (Therefor  $V^\dagger AV$  does not hold!). In this case, it is another eigen-problem which should be solved. This will be listed below without explain.

By Ref. [15], there are three strategies, Ritz eigen-vector (REV), harmonic Ritz eigen vector (HEV) and singular value decomposition (SVD). Either it is  $REV > HEV > SVD$  or  $SVD > HEV > REV$ , so we only list REV and SVD here.

Note that  $\tilde{U}_k$  is the normalized  $U_k$ ,  $H_{m+1}$  means the  $H_{m+1}$  of GMRES procedure, and  $H'_{m+1}$  means  $H'_{m+1}$  obtained in GCRO-DR procedure,  $H_m$  and  $H'_m$  means the upper  $m$  rows of  $H_{m+1}$  and  $H'_{m+1}$ .

- REV

The  $k$  small eigen value of  $m$ , such that  $m$  is

$$\begin{cases} H_m \omega = \theta \omega, \\ \begin{pmatrix} \tilde{U}_k^\dagger C_k & \tilde{U}_k^\dagger V_{m-k+1} \\ 0 & (I_{m-k}, 0) \end{pmatrix} H'_{m+1} \omega = \theta \begin{pmatrix} \tilde{U}_k^\dagger \tilde{U}_k & \tilde{U}_k^\dagger V_{m-k} \\ V_{m-k}^\dagger \tilde{U}_k & I_{m-k} \end{pmatrix} \omega, \end{cases} \quad (74)$$

- HEV

The  $k$  larger eigen value of  $m$ , such that  $m$  is

$$\begin{cases} H_m^\dagger \omega = \theta H_{m+1}^\dagger H_{m+1} \omega, \\ H'_{m+1}^\dagger \begin{pmatrix} C_k^\dagger \tilde{U}_k & 0 \\ V_{m-k+1}^\dagger \tilde{U}_k & \begin{pmatrix} I_{m-k} \\ 0 \end{pmatrix} \end{pmatrix} \omega = \theta H'_{m+1}^\dagger H'_{m+1} \omega, \end{cases} \quad (75)$$

- SVD

The  $k$  small eigen value of  $m$ , such that  $m$  is

$$\begin{cases} H_m^\dagger H_m \omega = \theta \omega, \\ H'_{m+1}^\dagger H'_{m+1} \omega = \theta \begin{pmatrix} \tilde{U}_k^\dagger \tilde{U}_k & 0 \\ 0 & I_{m-k} \end{pmatrix} \omega, \end{cases} \quad (76)$$

Although  $H_m$  is usually a small matrix, we still need to know how to calculate the eigen-value and eigen-vectors.

Note that the second line of REV and SVD, and both line of HEV, that is a **generalized eigen-value problem (GEV)**.

### 3.4.4 Eigen solver

The eigen solver is implemented following Ref. [16].

There are many strategies. The most common algorithm is to transform a matrix to a **Hessenberg matrix**.

- Householder reflection

Tested that householder reduction is faster than symmetric or unsymmetric Lanczos method when the matrix is large. On the other hand, for a Hermitian matrix, Householder can also produce Hermitian tri-diagonal matrix.

**Note that this might be not true when the matrix is huge, and Hessenberg reduction is not a full reduction. In our case, we concentrate on matrix with  $5 < m < 50$ . Tested when about  $7 < m < 30$  ( $30 \times 30 \approx 1024$  is the maximum thread count on test machine), Householder is faster.**

Also, as tested, the quality of QR factorization affects the QR iteration very much. At the same time, compared with QR iteration, the QR factorization is relatively cheap, so we also use Householder to do the QR factorization.

The householder reduction is to insert zeros into a vector, which can be briefly written as

$$\mathbf{v} = \begin{pmatrix} x_1 + e^{i \arg x_1} |\mathbf{x}| \\ x_2 \\ \dots \\ x_n \end{pmatrix}, \quad U = \mathbb{I} - \frac{2\mathbf{v}\mathbf{v}^\dagger}{\mathbf{v}^\dagger\mathbf{v}}, \quad U \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix} = \begin{pmatrix} \frac{|x_1|}{x_1^*} |\mathbf{x}| \\ 0 \\ \dots \\ 0 \end{pmatrix}, \quad (77)$$

Note that  $U$  is at the same time unitary and Hermitian. Since it is unitary, it can be used as QR factorization,  $A = QR$  where  $Q$  is unitary and  $R$  is upper triangular, and to transform a matrix to Henssenberg matrix  $A = U^\dagger H U$ , where  $U$  is unitary and  $H$  is upper Henssenberg matrix.

The algorithm is not listed, the procedure can be written as

$$\begin{aligned}
A_0 &= U_0^\dagger U_0 A_0 = U_0^\dagger A_1, \quad U_0 A_0 = \left( \mathbb{I} - \frac{2\mathbf{v}\mathbf{v}^\dagger}{\mathbf{v}^\dagger \mathbf{v}} \right) A_0 = A_1 = \begin{pmatrix} + & + & + & + \\ 0 & + & + & + \\ 0 & + & + & + \\ 0 & + & + & + \end{pmatrix} \\
A_0 &= U_0^\dagger U_1^\dagger U_1 A_1, \quad U_1 A_1 = \begin{pmatrix} \mathbb{I}_1 & 0 \\ 0 & \mathbb{I} - \frac{2\mathbf{v}\mathbf{v}^\dagger}{\mathbf{v}^\dagger \mathbf{v}} \end{pmatrix} A_1 = A_2 = \begin{pmatrix} + & + & + & + \\ 0 & + & + & + \\ 0 & 0 & + & + \\ 0 & 0 & + & + \end{pmatrix} \\
A_0 &= U_0^\dagger U_1^\dagger U_2^\dagger R, \quad R = U_2 A_2 = \begin{pmatrix} \mathbb{I}_2 & 0 \\ 0 & \mathbb{I} - \frac{2\mathbf{v}\mathbf{v}^\dagger}{\mathbf{v}^\dagger \mathbf{v}} \end{pmatrix} A_2 = R = \begin{pmatrix} + & + & + & + \\ 0 & + & + & + \\ 0 & 0 & + & + \\ 0 & 0 & 0 & + \end{pmatrix}
\end{aligned} \tag{78}$$

Similarly, note that if only insert zeroes from the second row

$$UA = \begin{pmatrix} \mathbb{I}_1 & 0 \\ 0 & \mathbb{I} - \frac{2\mathbf{v}\mathbf{v}^\dagger}{\mathbf{v}^\dagger \mathbf{v}} \end{pmatrix} A = \begin{pmatrix} + & + & + & + \\ + & + & + & + \\ 0 & + & + & + \\ 0 & + & + & + \end{pmatrix} \tag{79}$$

then

$$UAU^\dagger = UA \begin{pmatrix} \mathbb{I}_1 & 0 \\ 0 & @ \end{pmatrix} = \begin{pmatrix} + & + & + & + \\ + & + & + & + \\ 0 & + & + & + \\ 0 & + & + & + \end{pmatrix} \begin{pmatrix} \mathbb{I}_1 & 0 \\ 0 & @ \end{pmatrix} = \begin{pmatrix} + & +@ & +@ & +@ \\ + & +@ & +@ & +@ \\ 0 & +@ & +@ & +@ \\ 0 & +@ & +@ & +@ \end{pmatrix} \tag{80}$$

So that it is kept Henssenberg.

- Shifted QR iteration

Let  $A = U_0^\dagger H_0 U_0$  where  $H$  is a Henssenberg matrix, then, let  $H_0 = U_1 R$ , it can be shown that  $H_1 = RU_1 = U_1^\dagger (U_1 R) U_1$  is still a Henssenberg.

Also,  $H = U_1 H_1 U_1^\dagger$ , so  $A = (U_0^\dagger U_1) H_1 (U_1^\dagger U_0)$ .

So,  $H_1$  has same eigen-value as  $A$ .



Apart from that,  $H_i$  can approach a upper triangular matrix. It is noted that, if the QR factorization is performed to a shifted matrix  $H - \sigma I$ , where  $\sigma$  is an approximate eigen-value of  $H$ , it will converge much fast.

In CLGLib, we use Wilkinson shift, which is the eigen-value of the right-bottom  $2 \times 2$  irreducible matrix, and is the one closer to the right-bottom corner element. It can be written as

---

**Algorithm 8** Shifted QR Iteration

---

**for**  $H$  is not a triangular **do**

$\sigma$  be the eigen-value of the  $2 \times 2$  matrix of right-bottom matrix which is closer to the right bottom element.

$$QR = H - \sigma I$$

$$H' = RQ + \sigma I$$

**if**  $H_{n-1,n} \approx 0$  **then**

        Reduce to a  $n - 1$  Henssenberg matrix problem.

**end if**

**end for**

---

Once the upper triangular matrix is obtained, the eigen-values are just the diagonal elements.

- Implicit shifted QR iteration

The **Implicit shifted QR iteration** sometimes also called **Double shifted QR iteration** or **Double shifted QR iteration**.

The details are not listed here, it uses Householder to chase the zero to the bottom and right, it is a little bit better convergent, and is said to be more stable. It can be written as

**Algorithm 9** Implicit shifted QR iteration

---

**for**  $T$  a Hessenberg matrix with  $n \geq 3$ . (In the case of  $n = 2$ , the eigen-value can be directly obtained.) **do**

$$H \text{ a irreducible Hessenberg matrix with } n \geq 3. \quad T = \begin{pmatrix} + & + & + \\ 0 & H & + \\ 0 & 0 & + \end{pmatrix} \quad \triangleright \text{ In the case of}$$

$n = 2$ , the eigen-value can be directly obtained.

$H_{2 \times 2}$  be the  $2 \times 2$  matrix of right-bottom matrix.  $s = \text{tr}(H_{2 \times 2})$  and  $t = \det(H_{2 \times 2})$

$$x = H_{1,1}(H_{1,1} - s) + H_{1,2}H_{2,1} + t$$

$$y = H_{2,1}(H_{1,1} + H_{2,2} - s)$$

$$z = H_{2,1}H_{3,2}$$

$$H' = RQ + \sigma I$$

**for**  $k = 0$  to  $n - 3$  **do**

$h$  be Householder matrix to zero  $\mathbf{v} = (x, y, z)^T \rightarrow (|\mathbf{v}|, 0, 0)^T$ .

$$q = \max(1, k), \quad H(k+1 : k+3, q : n) = hH(k+1 : k+3, q : n).$$

$$r = \min(k+4, n), \quad H(1 : 4, k+1 : k+3) = H(1 : 4, k+1 : k+3)h^\dagger. \quad \triangleright \text{ Note that}$$

$$h^\dagger = h$$

$$x = H(k+2, k+1), y = H(k+3, k+1)$$

**if**  $k < n - 3$  **then**

$$z = H(k+4, k+1)$$

**end if**

**end for**

$h$  be Householder matrix to zero  $\mathbf{v} = (x, y)^T \rightarrow (|\mathbf{v}|, 0)^T$ .

$$H(n-1 : n, n-2 : n) = hH(n-1 : n, n-2 : n), \quad H(1 : n, n-1 : n) = H(1 : n, n-1 : n)h^\dagger.$$

**end for**

---

- Inverse power iteration

Once the eigen-values are obtained, one can calculate the approximate eigen-vector correspond the the eigen-value using inverse power iteration. The inverse power iteration performs well with the original matrix  $A$ .

---

**Algorithm 10** Inverse power Iteration

---

$\mathbf{v}$  is a normalized vector.

**for**  $\|(A - \sigma I)\mathbf{v}\| > \epsilon$  **do**

$QR = (A - \sigma I)$

$\mathbf{v} = R^{-1}Q^\dagger \mathbf{v}$

$\mathbf{v} = \mathbf{v}/\|\mathbf{v}\|$

**end for**

---

The  $R$  is upper triangular, so  $R^{-1}$  is just a modification of Algorithm. 5.

---

**Algorithm 11** Backward substitution

---

**for**  $i = k - 1$  to  $0$  **do**

**for**  $j = i + 1$  to  $k - 1$  **do**

$\mathbf{y}[i] -= r[i, j]\mathbf{y}[j]$

**end for**

$\mathbf{y}[i] = \mathbf{y}[i]/r[i, i]$

**end for**

**return**  $\mathbf{u}[k] = \mathbf{y}[k]$ .

---

- Eigen vector of upper triangular matrix

The inverse power iteration is incompatible with upper triangular matrix, because  $R - \lambda I$  is singular, for the inverse power iteration,  $R - \lambda I$  is only nearly singular, however, for a upper triangular, it is almost exactly a singular. Although one can shift the eigen value a little bit, but one can also obtain eigen vector exactly. by the procedure below.

Suppose

$$\begin{pmatrix} r_{1,1} - \lambda_k & \dots & r_{1,k-1} \\ 0 & \dots & \dots \\ 0 & 0 & r_{k-1,k-1} - \lambda_k \end{pmatrix} \begin{pmatrix} x_1 \\ \dots \\ x_{k-1} \end{pmatrix} = \begin{pmatrix} y_1 \\ \dots \\ y_{k-1} \end{pmatrix} \quad (81)$$

$(R - \lambda_k \mathbb{I})\mathbf{x} = 0$  can be written as

$$\begin{pmatrix} r_{1,1} - \lambda_k & \dots & r_{1,k-1} & r_{1,k} & \dots \\ 0 & \dots & \dots & \dots & \dots \\ 0 & 0 & r_{k-1,k-1} - \lambda_k & r_{k-1,k} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & \dots \end{pmatrix} \begin{pmatrix} x_1 \\ \dots \\ x_{k-1} \\ 1 \\ 0 \\ \dots \end{pmatrix} = \begin{pmatrix} y_1 + r_{1,k} \\ \dots \\ y_{k-1} + r_{k-1,k} \\ 0 \\ \dots \end{pmatrix} = 0 \quad (82)$$

leads to the equation

$$\begin{pmatrix} r_{1,1} - \lambda_k & \dots & r_{1,k-1} \\ 0 & \dots & \dots \\ 0 & 0 & r_{k-1,k-1} - \lambda_k \end{pmatrix} \begin{pmatrix} x_1 \\ \dots \\ x_{k-1} \end{pmatrix} = \begin{pmatrix} -r_{1,k} \\ \dots \\ -r_{k-1,k} \end{pmatrix} \quad (83)$$

which can be solved using backward shift, i.e. Algorithm. 11.

- Generalized eigen-value problem

The generalized eigen-value problem can be transformed to a eigen-value problem

$$A\mathbf{v} = \lambda B\mathbf{v} \Rightarrow B = QR \Rightarrow R^{-1}Q^\dagger A\mathbf{v} = \lambda \mathbf{v} \quad (84)$$

### 3.4.5 Implementation of GCRO-DR

Now, we concentrate on the implementation of GCRO-DR. First of all, we need to know how to apply  $\mathbf{x} - AB^\dagger \mathbf{v}$ , where  $A, B \in \mathbb{C}^{n \times k}$  and  $\mathbf{v} \in \mathbb{C}^n$ .

---

**Algorithm 12**  $\mathbf{x} = \mathbf{x} - AB^\dagger \mathbf{v}$

---

**for**  $i = 0$  to  $k - 1$  **do**

$\mathbf{x} = \mathbf{x} - (\mathbf{b}_k^\dagger \mathbf{x}) \mathbf{a}_k$

**end for**

**return**  $\mathbf{x}$

---

The second thing is QR decompose of  $\mathbb{C}^{n \times k}$  and  $\mathbb{C}^{(m+1) \times k}$  matrix. For the  $\mathbb{C}^{n \times k}$  matrix, the usually Arnoldi with modified Gram-Schmidt, i.e. Algorithm. 3 can be used.

---

**Algorithm 13** modified Gram-Schmidt for QR factorization decompose of  $A\tilde{Y}_k$ 


---

```

for  $i = 0$  to  $k - 1$  do
     $y_i = Ay_i$ 
end for
 $\mathbf{v}^{(0)} = y_0 / \|\mathbf{y}_0\|$ 
for  $i = 0$  to  $k - 1$  do
     $\mathbf{w} = \mathbf{y}_{i+1}$ 
    for  $j = i + 1$  to  $k - 1$  do
         $c = \mathbf{v}^{(j)*} \cdot \mathbf{w}$ 
         $\mathbf{w} = \mathbf{w} - c\mathbf{v}^{(j)}$ 
         $r[j, i] = c$ 
    end for
     $\mathbf{v}^{(i+1)} = \mathbf{w} / r[i + 1, i + 1]$ 
end for
return  $Q = (\mathbf{v}_0, \dots, \mathbf{v}_{k-1}), R = r[i, j]$ .

```

---

Finally we have to calculate  $YR^{-1}$ . This is a forward substitution.

$$U = YR^{-1}, \quad UR = Y, \quad R^T U^T = Y^T \quad U^T = (R^T)^{-1} Y^T. \quad (85)$$

### 3.4.6 Implement of GCRO-DR

We present pseudo-code of GCRO-DR can be found in Ref. [15]. The only difference is that we always make sure  $C_k$  and  $V_{m-k+1}$  are orthogonal to each other. It can be written as

---

**Algorithm 14** GCRO-DR

---

**if**  $U_k$  is defined from solving a previous linear system **then**

Let  $[Q, R] = AU_k$  be QR decomposition or  $AU_k$ .

$C_k = Q$ .

$U_k = U_k R^{-1}$ .

$\mathbf{r}^{(0)} = A\mathbf{x}^{(0)} - \mathbf{b}$

**else**

Perform GMRES to get  $W_{m+1} = (C_k, V_{m-k+1})$

Update  $\mathbf{x}^{(0)}, \mathbf{r}^{(0)}$  as  $\mathbf{x}^{(0)} = \mathbf{x}^{(0)} + V_m y, \mathbf{r}^{(0)} = V_{m+1}(\beta \mathbf{e}_1 - H_{m+1} y)$ , which is in fact part of GMRES.

Compute eigen-vector problem and obtain  $P_k \in \mathbb{C}^{m \times k}$ .

$U_k = V_m P_k$

Let  $[Q, R] = H_{m+1} P_k$  be QR decomposition.

$C_k = V_{m+1} Q$

$U_k = U_k R^{-1}$

**end if**

**for**  $\hat{i} = 1$  to  $r$  **do** ▷ restart  $r$  times.

$\mathbf{x}^{(i-1)} = \mathbf{x}^{(i-1)} + U_k C_k^\dagger \mathbf{r}^{(i-1)}$

$\mathbf{r}^{(i-1)} = \mathbf{r}^{(i-1)} - C_k C_k^\dagger \mathbf{r}^{(i-1)}$

Reset  $H_{m+1} = 0$ .  $W_{m+1}(k) = V_{m-k+1}(0) = \mathbf{r}^{(i)} / \|\mathbf{r}^{(i)}\|$ .

$H_{m+1}(k, k) = 1 / \|U_k\|$ , normalize  $U_k$ .

Perform Arnoldi procedure on matrix  $(1 - CC^\dagger)A$ , to obtain  $V_{m-k+1}$ , and set  $H_{k:m+1, k:m}$ .

And  $H_{0:k, m} = C_k^\dagger A V_{m-k}$ .  $\hat{V} = (U_k, V_{m-k})$  and  $W_{m+1} = (C_k, V_{m-k+1})$ .

Solve  $\arg \min \|r\| \mathbf{e}_k - H_{m+1} y$ .

$\mathbf{x}^{(i)} = \mathbf{x}^{(i-1)} + \hat{V}_m y, \mathbf{r}^{(i)} = \mathbf{r}^{(i-1)} - W_{m+1} H_{m+1} y$ . ▷ Check the error here. If reach the criterion, return.

Compute eigen-vector problem and obtain  $P_k \in \mathbb{C}^{m \times k}$ .

$U_k = V_m P_k$

Let  $[Q, R] = H_{m+1} P_k$  be QR decomposition.

$C_k = V_{m+1} Q$

$U_k = U_k R^{-1}$

**end for**

---

### 3.4.7 Implement of GMRES-MDR

The GMRES-MDR is almost the same as GCRO-DR, except for 3 things.

1. It set a threshold on eigen-values to decrease  $k$  if a larger  $k$  is not necessary.
2. It check the speed of convergence to switch between REV and SVD.
3. At first iteration, if  $U_k$  is defined, it use another algorithm to obtain  $U_k$  and  $C_k$ .

---

**Algorithm 15** First iteration of GMRES-MDR if  $U_k$  is defined.

---

```

[Q, R] = U_k
if REV then
     $Q^\dagger A Q \omega = \theta \omega$ 
end if
if HEV then
     $Q^\dagger A^\dagger A Q \omega = \theta Q^\dagger A^\dagger Q \omega$ 
end if
if SVD then
     $Q^\dagger A^\dagger A Q \omega = \theta^2 \omega$ 
end if
 $U_k = Q \omega_k$ 

```

---

We only implement the third because the first two can be tunable by parameters.

### 3.4.8 Test of GCRO-DR and GMRES-MDR

It is tested that, for both GCRO-DR and GMRES-MDR are suitable for the low-mode case.

We run with unitary gauge and  $\kappa = 0.1249$ . ( $\kappa_c = 0.125$ ). GCRO-DR with  $m = 16$  and  $k = 4$  will run even faster than  $dim = 50$  GMRES.

**However, if it is not the low-mode case, GMRES is faster.**

## 4 Miscellaneous topics

### 4.1 Gauge Fixing

#### 4.1.1 Introduction of FFT before start

We may use 3D cuFFT to implement 4D FFT, however, before this can be done, we need to understand what FFT is.

FFT is to calculate Discrete Fourier Transform (DFT), in 1D, it is

$$\begin{aligned}\tilde{x}_m &= \sum_n x_n W_N^{mn} \\ W_N^j &\equiv \exp(-i \frac{2\pi j}{N})\end{aligned}\tag{86}$$

- Cooley-Tukey mapping

Let  $N = N_1 \times N_2$ , we first calculate DFT of subset  $I_{n_1} = \{n_2 N_1 + n_1\}$ , such that

$$\tilde{x}_m = \sum_{n_1} S_{n_1}, \quad S_{n_1} = \sum_{n_2} x_{n_2 N_1 + n_1} W_N^{m(n_2 N_1 + n_1)}\tag{87}$$

Note that,  $S_{n_1}$  can be further factorized as

$$\tilde{x}_m = \sum_{n_1} W_N^{mn_1} S'_{n_1}, \quad S'_{n_1} = \sum_{n_2} x_{n_2 N_1 + n_1} W_N^{mn_2 N_1}\tag{88}$$

then, note that,  $N$  can be divided by  $N_1$  (the result is  $N_2$ ), so  $W_N^{mn_2 N_1} = W_{N_2}^{mn_2}$ , so  $S'$  is just DFT of subset  $I_{n_1}$ . Then, we can also decompose

$$m = m_1 N_2 + m_2\tag{89}$$

to write

$$\tilde{x}_{m_1 N_2 + m_2} = \sum_{n_1} W_N^{n_1(m_1 N_2 + m_2)} S'_{n_1} = \sum_{n_1} W_{N_1}^{n_1 m_1} W_N^{n_1 m_2} S'_{n_1}\tag{90}$$

The  $W_N^{n_1 m_2}$  is twiddle factor, after 'twiddle',  $S''_{n_1} = W_N^{n_1 m_2} S'_{n_1}$ , the result is again a DFT with size  $N_1$

$$\tilde{x}_{m_1 N_2 + m_2} = \sum_{n_1} W_{N_1}^{n_1 m_1} S''_{n_1}\tag{91}$$



As an example, we show index mapping of a  $2 \times 3 \times 5 \times 7$  array

$$\begin{aligned}
 & x_1, \dots, x_{230} \\
 & (x_1, x_8, x_{15} \dots, x_{7 \times 29 + 1}), \dots, (x_{7i+j}, x_{7(i+1)+j}, \dots), \dots, (x_7, x_{7+7}, x_{14+7} \dots, x_{7 \times 29 + 7}) \\
 & ((x_1, x_{35+1}, x_{70+1}, x_{105+1}, x_{140+1}, x_{175+1}), (x_8, x_{35+8}, x_{70+8}, \dots) \dots, \dots) \\
 & (((x_1, x_{105+1}), (x_{35+1}, x_{140+1}), (x_{70+1}, x_{175+1}), \dots), \dots), \dots
 \end{aligned} \tag{92}$$

which can be index with 4D index

$$\begin{aligned}
 & (x_{1,1,1,1}, x_{1,1,1,2}, \dots) \\
 & (x_{1,1,1,1}, x_{1,1,2,1}, x_{1,1,3,1} \dots, x_{2,3,5,1}), \dots, (x_{1,1,1,j}, \dots), \dots, (x_{1,1,1,7}, \dots, x_{2,3,5,7}) \\
 & ((x_{1,1,1,1}, x_{1,2,1,1}, \dots, x_{2,3,1,1}), (x_{1,1,2,1} \dots, x_{2,3,2,1}), \dots) \\
 & (((x_{1,1,1,1}, x_{2,1,1,1}), (x_{1,2,1,1}, x_{2,2,1,1}), (x_{1,3,1,1}, x_{2,3,1,1})) \dots)
 \end{aligned} \tag{93}$$

- Good mapping

#### 4.1.2 Cornell Gauge Fixing

#### 4.1.3 FFT accelerated Cornell Gauge Fixing

#### 4.1.4 Landau Gauge

#### 4.1.5 Coulomb Gauge

## 5 Measurement

## 6 Programming

### 6.1 cuda

#### 6.1.1 blocks and threads

#### 6.1.2 device member function

According to <https://stackoverflow.com/questions/53781421/cuda-the-member-field-with-device-ptr-and-device-member-function-to-visit-it-i>

To call device member function, the content of the class should be on device.

- First, new a instance of the class.
- Then, create a device memory using cudaMalloc.
- Copy the content to the device memory

In other words, it will work as

```

1  __global__ void _kInitialArray(int* thearray)
2  {
3      int iX = threadIdx.x + blockDim.x * blockIdx.x;
4      int iY = threadIdx.y + blockDim.y * blockIdx.y;
5      int iZ = threadIdx.z + blockDim.z * blockIdx.z;
6      thearray[iX * 16 + iY * 4 + iZ] = iX * 16 + iY * 4 + iZ;
7  }
8
9  extern "C" {
10     void _cInitialArray(int* thearray)
11     {
12         dim3 block(1, 1, 1);
13         dim3 th(4, 4, 4);
14
15         _kInitialArray << <block, th >> > (thearray);
16         checkCudaErrors(cudaGetLastError());
17     }
18 }
19
20 class B
21 {
22 public:
```

```

23     B()
24     {
25         checkCudaErrors(cudaMalloc((void**)&m_pDevicePtr, sizeof(int) * 64));
26         _cInitialArray(m_pDevicePtr);
27     }
28     ~B()
29     {
30         cudaFree(m_pDevicePtr);
31     }
32     __device__ int GetNumber(int index)
33     {
34         m_pDevicePtr[index] = m_pDevicePtr[index] + 1;
35         return m_pDevicePtr[index];
36     }
37     int* m_pDevicePtr;
38 };
39
40 __global__ void _kAddArray(int* thearray1, B* pB)
41 {
42     int iX = threadIdx.x + blockDim.x * blockIdx.x;
43     int iY = threadIdx.y + blockDim.y * blockIdx.y;
44     int iZ = threadIdx.z + blockDim.z * blockIdx.z;
45     thearray1[iX * 16 + iY * 4 + iZ] = thearray1[iX * 16 + iY * 4 + iZ] + pB->GetNumber(iX * 16 +
        iY * 4 + iZ);
46 }
47
48 extern "C" {
49     void _cAddArray(int* thearray1, B* pB)
50     {
51         dim3 block(1, 1, 1);
52         dim3 th(4, 4, 4);
53         _kAddArray << <block, th >> > (thearray1, pB);
54         checkCudaErrors(cudaGetLastError());
55     }
56 }
57
58 class A
59 {
60 public:
61     A()
62     {
63         checkCudaErrors(cudaMalloc((void**)&m_pDevicePtr, sizeof(int) * 64));
64         _cInitialArray(m_pDevicePtr);
65     }
66     ~A()
67     {
68         checkCudaErrors(cudaFree(m_pDevicePtr));

```

```

69     }
70     void Add(B* toAdd/*this should be a device ptr(new on device function or created by cudaMalloc)
       */)
71     {
72         _cAddArray(m_pDevicePtr, toAdd);
73     }
74     int* m_pDevicePtr;
75 };
76
77
78
79 int main(int argc, char * argv[])
80 {
81     B* pB = new B();
82     A* pA = new A();
83     B* pDeviceB;
84     checkCudaErrors(cudaMalloc((void**)&pDeviceB, sizeof(B)));
85     checkCudaErrors(cudaMemcpy(pDeviceB, pB, sizeof(B), cudaMemcpyHostToDevice));
86     pA->Add(pDeviceB);
87     int* res = (int*)malloc(sizeof(int) * 64);
88     checkCudaErrors(cudaMemcpy(res, pA->m_pDevicePtr, sizeof(int) * 64, cudaMemcpyDeviceToHost));
89     printf("-----_A=");
90     for (int i = 0; i < 8; ++i)
91     {
92         printf("\n");
93         for (int j = 0; j < 8; ++j)
94             printf("res_%d=%d", i * 8 + j, res[i * 8 + j]);
95     }
96     printf("\n");
97     //NOTE: We are getting data from pB, not pDeviceB, this is OK, ONLY because m_pDevicePtr is a
           pointer
98     checkCudaErrors(cudaMemcpy(res, pB->m_pDevicePtr, sizeof(int) * 64, cudaMemcpyDeviceToHost));
99     printf("-----_B=");
100    for (int i = 0; i < 8; ++i)
101    {
102        printf("\n");
103        for (int j = 0; j < 8; ++j)
104            printf("res_%d=%d", i * 8 + j, res[i * 8 + j]);
105    }
106    printf("\n");
107    delete pA;
108    delete pB;
109    return 0;
110 }

```

Note: this is a copy of the original instance! It is ONLY OK to change the content of *pDevicePtr* → *m\_pOtherPtr*, NOT *pDevicePtr* → *somevalue*

### 6.1.3 device virtual member function

According to <https://stackoverflow.com/questions/26812913/how-to-implement-device-side-cuda-virtual-functions>

To call a device virtual member function, unlike Sec. 6.1.2, the pointer to the virtual function table should also be on device,

- First, cudaMalloc a sizeof(void\*), for the device pointer.
- Then, use a kernel function to new the instance on device, and assign it to the device pointer created by cudaMalloc.
- One can copy the pointer, by using cudaMemcpy(void\*\*, void\*\*, sizeof(void\*), device-todevice).
- When copy it to elsewhere, one need to copy it back to host, then copy it again to device. The example shows how to copy it to constant.

in other words, it will work as

```

1
2  class CA
3  {
4  public:
5      __device__ CA() { ; }
6      __device__ ~CA() { ; }
7      __device__ virtual void CallMe() { printf("This is A\n"); }
8  };
9
10 class CB : public CA
11 {
12 public:
13     __device__ CB() : CA() { ; }
14     __device__ ~CB() { ; }
15     __device__ virtual void CallMe() { printf("This is B\n"); }
16 };
17
18 __global__ void _kernelCreateInstance(CA** pptr)
19 {
20     (*pptr) = new CB();
21 }
22
23 __global__ void _kernelDeleteInstance(CA** pptr)
24 {

```

```

25     delete (*pptr);
26 }
27
28 extern "C" {
29     void _kCreateInstance(CA** pptr)
30     {
31         _kernelCreateInstance << <1, 1 >> >(pptr);
32     }
33
34     void _kDeleteInstance(CA** pptr)
35     {
36         _kernelDeleteInstance << <1, 1 >> >(pptr);
37     }
38 }
39
40 __constant__ CA* m_pA;
41
42 __global__ void _kernelCallConstantFunction()
43 {
44     m_pA->CallMe();
45 }
46
47
48 extern "C" {
49     void _cKernelCallConstantFunction()
50     {
51         _kernelCallConstantFunction << <1, 1 >> > ();
52     }
53 }
54
55 int main()
56 {
57     CA** pptr;
58     cudaMalloc((void**)&pptr, sizeof(CA*));
59     _kCreateInstance(pptr);
60
61     //I can NOT use a kernel to set m_pA = (*pptr), because it is constant.
62     //I can NOT use cudaMemcpyToSymbol(m_pA, (*pptr)), because * operator on host is incorrect when
        pptr is a device ptr.
63     //I can NOT use cudaMemcpyToSymbol(m_pA, (*pptr)) in kernel, because cudaMemcpyToSymbol is a
        __host__ function
64     //I have to at first copy it back to host, then copy it back back again to constant
65     CA* pptrHost[1];
66     cudaMemcpy(pptrHost, pptr, sizeof(CA**), cudaMemcpyDeviceToHost);
67     cudaMemcpyToSymbol(m_pA, pptrHost, sizeof(CA*));
68     _cKernelCallConstantFunction();
69

```

```
70     _kDeleteInstance(pptr);  
71     cudaFree(pptr);  
72     return 0;  
73 }
```

## 7 Testing

### 7.1 random number



## 8 Applications

### 8.1 Rotating Frame

We follow Ref. [17].

The matrix element can be written as

$$\mathcal{M} = \int \mathcal{D}(A_\mu \psi) \exp \left( i \int d^4x \mathcal{L} \right) \quad (94)$$

with

$$\mathcal{L} = \bar{\psi} (i \not{D} - m) \psi - \frac{1}{4} (F_{\mu\nu}^a)^2, \quad D_\mu \equiv \partial_\mu + i g_{YM} \sum_a T_a A_\mu^a \quad (95)$$

The first few steps are as usual, defining

$$A_\mu = g_{YM} \sum_a T_a A_\mu^a, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu + i[A_\mu, A_\nu] \quad (96)$$

using  $\text{tr}[T_i T_j] = \frac{1}{2} \delta_{ij}$

$$\begin{aligned} F_{\mu\nu} &= g_{YM} \sum_a T_a F_{\mu\nu}^a \\ \frac{1}{4} (F_{\mu\nu}^a)^2 &= \frac{1}{2g_{YM}^2} \text{tr} [F_{\mu\nu}^2] \end{aligned} \quad (97)$$

and

$$\begin{aligned} \mathcal{L} &= \bar{\psi} (i \not{D} - m) \psi - \frac{1}{2g_{YM}^2} \text{tr} [F_{\mu\nu}^2] \\ D_\mu &= \partial_\mu + i A_\mu \end{aligned} \quad (98)$$

For rotational frame, the metric and frame can be defined as

$$\begin{aligned}
 h_{\mu\nu} &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \\
 g_{\mu\nu} &= \begin{pmatrix} 1 - r^2\Omega^2 & +y\Omega & -x\Omega & 0 \\ y\Omega & -1 & 0 & 0 \\ -x\Omega & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \sqrt{-g_{\mu\nu}} = 1 \\
 e_0 &= (1, y\Omega, -x\Omega, 0) \\
 e_1 &= (0, 1, 0, 0) \\
 e_2 &= (0, 0, 1, 0) \\
 e_3 &= (0, 0, 0, 1)
 \end{aligned} \tag{99}$$

### 8.1.1 The rotating gauge action

Considering the case of pure gauge, the action can be written as

$$\begin{aligned}
 \mathcal{L}_G &= -\sqrt{\det(-g_{\alpha\beta})} \frac{1}{2g_{YM}^2} g^{\mu\nu} g^{\rho\sigma} \text{tr}[F_{\mu\rho} F_{\nu\sigma}] \\
 &= -\frac{1}{2g_{YM}^2} \left( \sum_{ijkl=0}^3 h_{ij} h_{kl} \text{tr}[F_{ik} F_{jl}] + 2\Omega^2 \text{tr}[(xF_{01} + yF_{02})^2 + r^2 F_{03}^2] \right. \\
 &\quad \left. - 4\Omega(x\text{tr}[F_{01}F_{12}] + y\text{tr}[F_{02}F_{12}] + y\text{tr}[F_{03}F_{13}] - x\text{tr}[F_{03}F_{23}]) \right)
 \end{aligned} \tag{100}$$

- Wick rotation of gauge action

The Wick rotation

$$t \rightarrow -i\tau, \quad \Omega \rightarrow i\Omega, \quad A_\mu \rightarrow (iA_0, A_1, A_2, A_3), \quad F_{0i} \rightarrow iF_{0i} \tag{101}$$

and substitute  $x = (t, x, y, z) \rightarrow x_E = (x, y, z, \tau)$ . After Wick rotation, we are expecting

$$\exp(-S_G) = \exp(i \int d^4x \mathcal{L}_G) \tag{102}$$

the result is

$$\begin{aligned}
-S_G &= i \int d^4x \mathcal{L}_G \\
S_G &= \int d^4x_E \frac{1}{2g_{YM}^2} \left( \sum_{ij=1}^4 \text{tr}[F_{ij}F_{ij}] + 2\Omega^2 \text{tr}[(xF_{14} + yF_{24})^2 + r^2 F_{34}^2] \right. \\
&\quad \left. + 4\Omega(x\text{tr}[F_{14}F_{12}] + y\text{tr}[F_{24}F_{12}] + y\text{tr}[F_{34}F_{13}] - x\text{tr}[F_{34}F_{23}]) \right)
\end{aligned} \tag{103}$$

Therefor  $S_G$  is real. The  $\sum_{ij=1}^4 \text{tr}[F_{ij}F_{ij}]$  is the gauge action in rest frame.

- Discretization of gauge action

The discretized version can be derived using compact gauge group

$$U_\mu(x) = \exp(iaA_\mu(x)), \quad U_{-\mu}(x) = U_\mu^{-1}(x - \mu). \tag{104}$$

As usual,

$$\begin{aligned}
U_{\mu,\nu}(n) &\equiv U_\mu(n)U_\nu(n + a\mu)U_\mu^{-1}(n + a\nu)U_\nu^{-1}(n) = \exp(ia^2F_{\mu\nu} + \mathcal{O}(a^3)). \\
\text{Re}[U_{\mu\nu}(n)] &= \mathbb{I}_{N_c \times N_c} - \frac{a^4}{2}F_{\mu\nu}^2 + \mathcal{O}(a^6) \\
\frac{1}{2g_{YM}^2} \sum_{\mu \neq \nu} \text{tr}[F_{\mu\nu}^2] &= \frac{1}{a^4g_{YM}^2} \sum_{\mu \neq \nu} \text{Retr}[1 - U_{\mu\nu}(n)] = \frac{2}{a^4g_{YM}^2} \sum_{\mu > \nu} \text{Retr}[1 - U_{\mu\nu}(n)]
\end{aligned} \tag{105}$$

For those plaquette with coordinate as coefficients, we use the average of plaquette

$$\begin{aligned}
\bar{U}_{\mu,\nu}(n) &\equiv \frac{1}{4} (U_{\mu,\nu}(n) + U_{-\mu,\nu}(n) + U_{\mu,-\nu}(n) + U_{-\mu,-\nu}(n)) \\
\text{Retr}[\bar{U}_{\mu,\nu}(n)] &= N_c - \frac{a^4}{2} \text{tr}[F_{\mu\nu}^2] + \mathcal{O}(a^6), \quad \frac{1}{2g_{YM}^2} \text{tr}[F_{\mu\nu}^2] = \frac{2}{a^4g_{YM}^2} \frac{1}{2} \text{Retr}[1 - \bar{U}_{\mu,\nu}(n)]
\end{aligned} \tag{106}$$

The remaining are those has the form  $\text{tr}[F_{ab}F_{bc}]$ , using

$$\begin{aligned}
U_{\mu\nu}^{-1}(n) &= U_\nu(n)U_\mu(n + a\nu)U_\nu^{-1}(n + a\mu)U_\mu^{-1}(n) = U_{\nu\mu}(n) = \exp(-ia^2F_{\mu\nu}) + \mathcal{O}(a^6) \\
U_{a,b}(n)(U_{b,c}(n) - U_{c,b}(n)) &= \exp(-ia^2(F_{ab} + F_{bc})) - \exp(-ia^2(F_{ab} - F_{bc})) \\
\frac{1}{2} \text{Re}[U_{a,b}(n)(U_{c,b}(n) - U_{b,c}(n))] &= a^4 F_{ab}F_{bc} + \mathcal{O}(a^6)
\end{aligned} \tag{107}$$

Note that  $b$  is not summed.

We can have a more symmetric form to use

$$U_{c,b}(n) = U_{b,-c}(n) + \mathcal{O}(a^4) \tag{108}$$

then it is a chair-type.

$$\frac{1}{2}\text{Re}[U_{a,b}(n)(U_{b,-c}(n) - U_{b,c}(n))] = a^4 F_{ab} F_{bc} + \mathcal{O}(a^6) \quad (109)$$

Similarly, we can use the average of chairs, and define

$$\begin{aligned} V_{\mu\nu\sigma} &= \frac{1}{8} ((U_{\mu,\nu} - U_{-\mu,\nu})(U_{\nu,\sigma} - U_{\nu,-\sigma}) + (U_{\mu,-\nu} - U_{-\mu,-\nu})(U_{-\nu,\sigma} - U_{-\nu,-\sigma})) \\ \text{Retr}[V_{\mu\nu\rho}] &= -a^4 \text{tr}[F_{\mu\nu} F_{\nu\rho}] + \mathcal{O}(a^6), \quad \frac{1}{2g_{YM}^2} \text{tr}[F_{\mu\nu} F_{\nu\rho}] = -\frac{2}{a^4 g_{YM}^2} \frac{1}{4} \text{Retr}[V_{\mu\nu\rho}] \end{aligned} \quad (110)$$

- Final result of gauge action

The discretized and Wick rotated gauge action is

$$\begin{aligned} S_G &= \frac{2}{a^4 g_{YM}^2} \sum_n \left( \sum_{\mu > \nu} \text{Retr}[1 - U_{\mu\nu}(n)] + \Omega (x \text{Retr}[V_{412} + V_{432}] - y \text{Retr}[V_{421} + V_{431}]) \right. \\ &\quad \left. + \Omega^2 (x^2 \text{Retr}[1 - \bar{U}_{14}(n)] + y^2 \text{Retr}[1 - \bar{U}_{24}(n)] + r^2 \text{Retr}[1 - \bar{U}_{34}(n)] + xy \text{Retr}[V_{142}]) \right) \\ &= \frac{\beta}{N_c} \sum_n \left( \sum_{\mu > \nu} \text{Retr}[1 - U_{\mu\nu}(n)] + \Omega (x \text{Retr}[V_{412} + V_{432}] - y \text{Retr}[V_{421} + V_{431}]) \right. \\ &\quad \left. + \Omega^2 (x^2 \text{Retr}[1 - \bar{U}_{14}(n)] + y^2 \text{Retr}[1 - \bar{U}_{24}(n)] + r^2 \text{Retr}[1 - \bar{U}_{34}(n)] + xy \text{Retr}[V_{142}]) \right) \end{aligned} \quad (111)$$

with  $\frac{\beta}{N_c} \equiv \frac{2}{a^4 g_{YM}^2}$ .

### 8.1.2 Rotating Fermion action

$$D_R = \left[ i\gamma^\mu \left( (\partial_\mu + ieA_\mu) - \frac{i}{4} \sigma^{ij} w_{\mu ij} \right) - m \right] \quad (112)$$

with

$$\begin{aligned} w_{\mu ij} &= g_{\alpha\beta} e_i^\alpha (\partial_\mu e_j^\beta + \Gamma_{\mu\nu}^\beta e_j^\nu) \\ \Gamma_{\mu\nu}^\beta &= \frac{1}{2} g^{\beta\alpha} \left( \frac{\partial g_{\alpha\mu}}{\partial x^\nu} + \frac{\partial g_{\alpha\nu}}{\partial x^\mu} - \frac{\partial g_{\mu\nu}}{\partial x^\alpha} \right) \\ \sigma^{ij} &= \frac{i}{2} [\gamma^i, \gamma^j] \end{aligned} \quad (113)$$

so

$$\frac{i}{4} \sigma^{ij} w_{\mu ij} = \left( \frac{i}{2} \Omega \sigma^{12}, 0, 0, 0 \right) \quad (114)$$

and

$$D_R = \left[ i\gamma^x(\partial_x + ieA_x) + i\gamma^y(\partial_y + ieA_y) + i\gamma^z(\partial_z + ieA_z) + i\gamma^t(\partial_t + ieA_t - \frac{i}{2}\Omega\sigma^{12}) - m \right] \quad (115)$$

using  $\gamma^\mu = \gamma^i e_i^\mu$ , it is

$$D_R = \left[ i(\gamma^1 + y\Omega\gamma^0)(\partial_x + ieA_x) + i(\gamma^2 - x\Omega\gamma^0)(\partial_y + ieA_y) + i\gamma^3(\partial_z + ieA_z) + i\gamma^0(\partial_t + ieA_t - \frac{i}{2}\Omega\sigma^{12}) - m \right] \quad (116)$$

- The Wick rotation of Fermion action

The Wick rotation

$$t \rightarrow -i\tau, \quad \gamma_i^M \rightarrow i\gamma_i^E, \quad \gamma_4 = \gamma_0, \quad \gamma_5 = \gamma_1\gamma_2\gamma_3\gamma_4, \quad A_t \rightarrow iA_\tau, \quad \partial_t \rightarrow i\partial_\tau, \quad \Omega \rightarrow i\Omega \quad (117)$$

where the superscript of gamma matrix stands for Minkowski or Euclidian. So

$$\begin{aligned} D_R &= -[(\gamma_1 + y\Omega\gamma_4)(\partial_x + ieA_x) + (\gamma_2 - x\Omega\gamma_4)(\partial_y + ieA_y) + \gamma_3(\partial_z + ieA_z) \\ &\quad + \gamma_4(\partial_\tau + ieA_\tau - \frac{i}{2}\Omega\sigma^{12}) + m] \\ &= -[\gamma_1(\partial_x + ieA_x) + \gamma_2(\partial_y + ieA_y) + \gamma_3(\partial_z + ieA_z) + \gamma_4(\partial_\tau + ieA_\tau) + m \\ &\quad + \gamma_4(y\Omega(\partial_x + ieA_x) - x\Omega(\partial_y + ieA_y)) - \frac{i}{2}\gamma_4\Omega\sigma^{12}] \end{aligned} \quad (118)$$

And

$$\begin{aligned} -S_F &= i \int d^4x \sqrt{-g_{\alpha\beta}} \bar{\psi} D_R \psi \\ S_F &= \int d^4x_E \bar{\psi} [\gamma_1(\partial_x + ieA_x) + \gamma_2(\partial_y + ieA_y) + \gamma_3(\partial_z + ieA_z) + \gamma_4(\partial_\tau + ieA_\tau) + m \\ &\quad + \gamma_4(y\Omega(\partial_x + ieA_x) - x\Omega(\partial_y + ieA_y)) - \frac{i}{2}\gamma_4\Omega\sigma^{12}] \psi \end{aligned} \quad (119)$$

- The discretization of Fermion action

The naive discretization yields

$$\partial_\mu \psi(n) = \frac{\psi(n + a\mu) - \psi(n - a\mu)}{2a} \quad (120)$$

and

$$\begin{aligned}
U_\mu(n) &= \exp(iaA_\mu) \approx 1 + iaA_\mu(n), \quad U_\mu^{-1}(n) \approx 1 - iaA_\mu(n) \\
iA_\mu(n) &= \frac{2iaA_\mu(n)}{2a} \approx \frac{(U_\mu(n) - 1) - (U_\mu^{-1}(n) - 1)}{2a} \approx \frac{(U_\mu(n) - 1) - (U_{-\mu}(n) - 1)}{2a} \\
iA_\mu(n)\psi(n) &= \frac{(U_\mu(n) - 1)\psi(n + a\mu) - (U_{-\mu}(n) - 1)\psi(n - a\mu)}{2a} + \mathcal{O}(a)
\end{aligned} \tag{121}$$

Therefor

$$(\partial_\mu + iA_\mu)\psi(n) = \frac{U_\mu(n)\psi(n + a\mu) - U_{-\mu}(n)\psi(n - a\mu)}{2a} + \mathcal{O}(a) \tag{122}$$

The Wilson term is

$$W\psi(n) = - \sum_\mu \frac{U_\mu(n)\psi(n + a\mu) + U_{-\mu}(n)\psi(n - a\mu) - 2\psi(n)}{2a} \tag{123}$$

considering the rotation, we add a modified Wilson term as

$$\begin{aligned}
W_R\psi(n) &= - \sum_\mu \frac{U_\mu(n)\psi(n + a\mu) + U_{-\mu}(n)\psi(n - a\mu) - 2\psi(n)}{2a} \\
&\quad - y\Omega \frac{U_x(n)\psi(n + ax) + U_{-x}(n)\psi(n - ax) - 2\psi(n)}{2a} \\
&\quad + x\Omega \frac{U_y(n)\psi(n + ay) + U_{-y}(n)\psi(n - ay) - 2\psi(n)}{2a}
\end{aligned} \tag{124}$$

Similar as the Wilson term, the last two terms also decouples when approaching the continuum limit. And the Wilson-Dirac operator becomes

$$\begin{aligned}
S_F &= \sum_{n,m} \bar{\psi}(n) D_W(n|m) \psi(m) \\
D_W(n|m) &= \left( m + \frac{4}{a} + \frac{y\Omega}{a} - \frac{x\Omega}{a} \right) \delta_{n,m} - \sum_\mu \frac{(1 - \gamma_\mu)U_\mu(n)\delta_{n+a\mu,m} + (1 + \gamma_\mu)U_{-\mu}(n)\delta_{n-a\mu,m}}{2a} \\
&\quad - y\Omega \frac{(1 - \gamma_4)U_x(n)\delta_{n+ax,m} + (1 + \gamma_4)U_{-x}(n)\delta_{n-ax,m}}{2a} \\
&\quad + x\Omega \frac{(1 - \gamma_4)U_y(n)\delta_{n+ay,m} + (1 + \gamma_4)U_{-y}(n)\delta_{n-ay,m}}{2a} - \frac{i}{2}\gamma_4\Omega\sigma^{12}\delta_{n,m}
\end{aligned} \tag{125}$$

Note that,

$$\begin{aligned}
(U(1)\delta_{n+1,m,n=1,m=2})^\dagger &= U^\dagger(1)\delta_{n,m+1,n=2,m=1} = U^\dagger(m)\delta_{n,m+1} \text{ or } U^\dagger(n-1)\delta_{n-1,m} \\
(U_\mu(n)\delta_{n+a\mu,m})^\dagger &= U_\mu^{-1}(n - a\mu)\delta_{n,m+a\mu} = U_{-\mu}(n)\delta_{n-a\mu,m}
\end{aligned} \tag{126}$$

Let's check whether the periodic condition for gauge field or infinite lattice volume is necessary

$$\begin{aligned}
& \sum_{n=1,2,3,m=1,2,3} (U_\mu(n)\delta_{n+1,m} + U_{-\mu}(n)\delta_{n-1,m})^\dagger = (U_\mu(1))^\dagger + (U_\mu(2))^\dagger + (U_{-\mu}(2))^\dagger + (U_{-\mu}(3))^\dagger \\
& = U_\mu^{-1}(2-1) + U_\mu^{-1}(3-1) + (U_\mu^{-1}(1))^\dagger + (U_\mu^{-1}(2))^\dagger \\
& = U_{-\mu}(2) + U_{-\mu}(3) + U_\mu(1) + U_\mu(2) \\
& = \sum_{n=1,2,3,m=1,2,3} (U_\mu(n)\delta_{n+1,m} + U_{-\mu}(n)\delta_{n-1,m})
\end{aligned} \tag{127}$$

So we can conclude [The  \$\gamma\_5\$ -hermiticity is kept with open\(Dirichlet\) boundary condition and finite volume.](#)

[Both the naive discretization and the Wilson term satisfy the  \$\gamma\_5\$ -hermiticity \(separately\).](#)

$$\begin{aligned}
& \gamma_5 \gamma_\nu \gamma_5 = -\gamma_\nu, \quad \gamma_\mu^\dagger = \gamma_\mu, \quad \gamma_5^2 = 1 \\
& \sum_{n,m} (\gamma_\nu U_\mu(n)\delta_{n+a\mu,m} - \gamma_\nu U_{-\mu}(n)\delta_{n,m+a\mu})^\dagger = \sum_{n,m} (\gamma_5 \gamma_\nu \gamma_5 U_\mu(n)\delta_{n+a\mu,m} - \gamma_5 \gamma_\nu \gamma_5 U_{-\mu}(n)\delta_{n-a\mu,m}) \\
& \sum_{n,m} (U_\mu(n)\delta_{n+a\mu,m} + U_{-\mu}(n)\delta_{n,m+a\mu})^\dagger = \sum_{n,m} (\gamma_5^2 U_\mu(n)\delta_{n+a\mu,m} + \gamma_5^2 U_{-\mu}(n)\delta_{n-a\mu,m})
\end{aligned} \tag{128}$$

Apart from that

$$\left( \frac{i}{2} \gamma_4 \Omega \sigma^{12} \delta_{n,m} \right)^\dagger = \gamma_5 \frac{i}{2} \gamma_4 \Omega \sigma^{12} \delta_{n,m} \gamma_5 \tag{129}$$

Therefor, the new Wilson-Dirac operator is also  $\gamma_5$ -hermiticity.

- The doubler problem

Note that the naive action and Wilson term both satisfy the  $\gamma_5$ -hermiticity, the traditional Wilson term will also lead to a  $\gamma_5$ -hermiticity fermion action, with

$$\begin{aligned}
D_W(n|m) &= \left( m + \frac{4}{a} \right) \delta_{n,m} - \sum_\mu \frac{(1 - \gamma_\mu) U_\mu(n) \delta_{n+a\mu,m} + (1 + \gamma_\mu) U_{-\mu}(n) \delta_{n-a\mu,m}}{2a} \\
&+ y \Omega \frac{\gamma_4 U_x(n) \delta_{n+ax,m} - \gamma_4 U_{-x}(n) \delta_{n-ax,m}}{2a} - x \Omega \frac{\gamma_4 U_y(n) \delta_{n+ay,m} - \gamma_4 U_{-y}(n) \delta_{n-ay,m}}{2a} - \frac{i}{2} \gamma_4 \Omega \sigma^{12} \delta_{n,m}
\end{aligned} \tag{130}$$

This action also does not suffer from the doubler problem.

- The final action of fermions

As usual, we define the hopping parameter as  $\kappa = \frac{1}{2am+8}$ , then rescale the fermion field, the action is

$$\begin{aligned}
S_F &= \sum_{n,m} \bar{\psi}(n) D_W(n|m) \psi(m) \\
D_W(n|m) &= (1 + 2\kappa(y-x)\Omega) \delta_{n,m} - \kappa \sum_{\mu} ((1 - \gamma_{\mu}) U_{\mu}(n) \delta_{n+a\mu,m} + (1 + \gamma_{\mu}) U_{-\mu}(n) \delta_{n-a\mu,m}) \\
&\quad - \kappa y \Omega ((1 - \gamma_4) U_x(n) \delta_{n+ax,m} + (1 + \gamma_4) U_{-x}(n) \delta_{n-ax,m}) \\
&\quad + \kappa x \Omega ((1 - \gamma_4) U_y(n) \delta_{n+ay,m} + (1 + \gamma_4) U_{-y}(n) \delta_{n-ay,m}) - \kappa i \gamma_4 a \Omega \sigma^{12} \delta_{n,m}
\end{aligned} \tag{131}$$

### 8.1.3 The exponential chemical potential

On the other hand, the  $i\kappa\gamma_4\hat{\Omega}\sigma^{12}$  term can also be modified. The  $\sigma^{12}$  term can be considered as a chemical potential ( $\bar{\psi}\gamma_0\psi$  and then do the Wick rotation  $\gamma_0 \rightarrow \gamma_4$ . The sign is after Wick rotation and relative to the mass term)

$$\mu \bar{\psi} \gamma_4 \psi, \quad \mu = -\frac{i\Omega}{2} \sigma^{12} \tag{132}$$

and discretized as

$$\begin{aligned}
D_{\tau} + \mu \bar{\psi} \gamma_4 \psi &\rightarrow -\kappa (e^{\mu a} (1 - \gamma_4) U_{\tau}(n) \delta_{n,n+t} + e^{-\mu a} (1 + \gamma_4) U_{-\tau}(n) \delta_{n-t,n}) \\
&= -\kappa \left( e^{-\frac{ia\Omega\sigma^{12}}{2}} (1 - \gamma_4) U_{\tau}(n) \delta_{n,n+t} + e^{+\frac{ia\Omega\sigma^{12}}{2}} (1 + \gamma_4) U_{-\tau}(n) \delta_{n-t,n} \right)
\end{aligned} \tag{133}$$

**It looks not satisfy the  $\gamma_5$  -hermiticity.** However, using  $(\sigma^{12})^2 = 1$ , it is in fact

$$\begin{aligned}
D_{\tau} + \mu \bar{\psi} \gamma_4 \psi &\rightarrow -\kappa \left[ \left( \cos\left(\frac{a\Omega}{2}\right) - i \sin\left(\frac{a\Omega}{2}\right) \sigma^{12} \right) (1 - \gamma_4) U_{\tau}(n) \delta_{n,n+t} \right. \\
&\quad \left. + \left( \cos\left(\frac{a\Omega}{2}\right) + i \sin\left(\frac{a\Omega}{2}\right) \sigma^{12} \right) (1 + \gamma_4) U_{-\tau}(n) \delta_{n-t,n} \right]
\end{aligned} \tag{134}$$

The 1 in  $1 \pm \frac{ia\Omega\sigma^{12}}{2}$  is the usual  $D_{\tau}$ . So the additional term is in fact

$$\begin{aligned}
&-\kappa \left[ \left( \cos\left(\frac{a\Omega}{2}\right) - 1 - i \sin\left(\frac{a\Omega}{2}\right) \sigma^{12} \right) (1 - \gamma_4) U_{\tau}(n) \delta_{n,n+t} \right. \\
&\quad \left. + \left( \cos\left(\frac{a\Omega}{2}\right) - 1 + i \sin\left(\frac{a\Omega}{2}\right) \sigma^{12} \right) (1 + \gamma_4) U_{-\tau}(n) \delta_{n-t,n} \right]
\end{aligned} \tag{135}$$

In the case of  $a \ll 1$ , it is approximately

$$\begin{aligned}
&-\kappa \left[ \left( -i \frac{a\Omega}{2} \sigma^{12} \right) (1 - \gamma_4) U_{\tau}(n) \delta_{n,n+t} \right. \\
&\quad \left. + \left( i \frac{a\Omega}{2} \sigma^{12} \right) (1 + \gamma_4) U_{-\tau}(n) \delta_{n-t,n} \right]
\end{aligned} \tag{136}$$



The  $U_\tau$  is in fact added to keep gauge symmetry, originally it is

$$\begin{aligned}
& -\kappa \frac{ia\Omega\sigma^{12}}{2} ((\gamma_4 - 1)\delta_{n,n+t} + (\gamma_4 + 1)\delta_{n-t,n}) \\
& \approx -\kappa \frac{ia\Omega\sigma^{12}}{2} ((\gamma_4 - 1)\delta_{n,n} + (\gamma_4 + 1)\delta_{n,n}) \\
& = -\kappa\gamma_4 ia\Omega\sigma^{12}
\end{aligned} \tag{137}$$

which go back to the  $\sigma^{12}$  term.

We still check the  $\gamma_5$ -hermiticity, using

$$\begin{aligned}
& \sum_{n=1,2,3,m=1,2,3} (U_\mu(n)\delta_{n+1,m} + U_{-\mu}(n)\delta_{n-1,m})^\dagger = \sum_{n=1,2,3,m=1,2,3} (U_\mu(n)\delta_{n+1,m} + U_{-\mu}(n)\delta_{n-1,m}) \\
& \gamma_5\gamma_4\gamma_5 = -\gamma_4^\dagger \\
& \gamma_5 \frac{ia\Omega\sigma^{12}}{2} \gamma_5 = -\left(\frac{ia\Omega\sigma^{12}}{2}\right)^\dagger
\end{aligned} \tag{138}$$

It is  $\gamma_5$ -hermite.

#### 8.1.4 The final action of rotation

Defining  $\frac{\beta}{N_c} \equiv \frac{2}{a^4 g_{YM}^2}$ ,  $\kappa \equiv \frac{1}{2am+8}$ ,  $\hat{\mu} \equiv \frac{\mu}{a}$ ,  $\hat{\Omega} \equiv a\Omega$ , (here  $\mu = x, y, z, t$  is the coordinate) we have

$$Z = \exp(-S_G - S_F) \tag{139}$$

with

$$\begin{aligned}
S_G &= \frac{\beta}{N_c} \sum_n \left( \sum_{\mu > \nu} \text{Retr}[1 - U_{\mu\nu}(n)] + \hat{\Omega} (\hat{x} \text{Retr}[V_{412} + V_{432}] - \hat{y} \text{Retr}[V_{421} + V_{431}]) \right. \\
&\quad \left. + \hat{\Omega}^2 (\hat{x}^2 \text{Retr}[1 - \bar{U}_{14}(n)] + \hat{y}^2 \text{Retr}[1 - \bar{U}_{24}(n)] + (\hat{x}^2 + \hat{y}^2) \text{Retr}[1 - \bar{U}_{34}(n)] + \hat{x}\hat{y} \text{Retr}[V_{142}]) \right) \\
U_{\mu,\nu}(n) &\equiv U_\mu(n)U_\nu(n + a\hat{\mu})U_\mu^{-1}(n + a\hat{\nu})U_\nu^{-1}(n) \\
\bar{U}_{\mu,\nu}(n) &\equiv \frac{1}{4} (U_{\mu,\nu}(n) + U_{-\mu,\nu}(n) + U_{\mu,-\nu}(n) + U_{-\mu,-\nu}(n)) \\
V_{\mu\nu\sigma}(n) &= \frac{1}{8} ((U_{\mu,\nu}(n) - U_{-\mu,\nu}(n))(U_{\nu,\sigma}(n) - U_{\nu,-\sigma}(n)) \\
&\quad + (U_{\mu,-\nu}(n) - U_{-\mu,-\nu}(n))(U_{-\nu,\sigma}(n) - U_{-\nu,-\sigma}(n)))
\end{aligned} \tag{140}$$

and

$$\begin{aligned}
S_F &= \sum_{n,m} \bar{\psi}(n) D(n|m) \psi(m) \\
D(n|m) &= \left( 1 + 2\kappa(\hat{y} - \hat{x})\hat{\Omega} - i\kappa\gamma_4\hat{\Omega}\sigma^{12} \right) \delta_{n,m} \\
&\quad - \kappa \sum_{\mu} [(1 - \gamma_{\mu})U_{\mu}(n)\delta_{n+a\hat{\mu},m} + (1 + \gamma_{\mu})U_{-\mu}(n)\delta_{n-a\hat{\mu},m}] \\
&\quad - \kappa\hat{y}\hat{\Omega}((1 - \gamma_4)U_x(n)\delta_{n+a\hat{x},m} + (1 + \gamma_4)U_{-x}(n)\delta_{n-a\hat{x},m}) \\
&\quad + \kappa\hat{x}\hat{\Omega}((1 - \gamma_4)U_y(n)\delta_{n+a\hat{y},m} + (1 + \gamma_4)U_{-y}(n)\delta_{n-a\hat{y},m})
\end{aligned} \tag{141}$$

such that  $\gamma_5 D \gamma_5 = D^\dagger$ .

or (As in Ref. [17], the naive discretization is used.)

$$\begin{aligned}
S_F &= \sum_{n,m} \bar{\psi}(n) D(n|m) \psi(m) \\
D(n|m) &= \left( 1 - i\kappa\gamma_4\hat{\Omega}\sigma^{12} \right) \delta_{n,m} \\
&\quad - \kappa \sum_{\mu} ((1 - \gamma_{\mu})U_{\mu}(n)\delta_{n+a\hat{\mu},m} + (1 + \gamma_{\mu})U_{-\mu}(n)\delta_{n-a\hat{\mu},m}) \\
&\quad - \kappa\hat{y}\hat{\Omega}((- \gamma_4)U_x(n)\delta_{n+a\hat{x},m} + (+\gamma_4)U_{-x}(n)\delta_{n-a\hat{x},m}) \\
&\quad + \kappa\hat{x}\hat{\Omega}((- \gamma_4)U_y(n)\delta_{n+a\hat{y},m} + (+\gamma_4)U_{-y}(n)\delta_{n-a\hat{y},m})
\end{aligned} \tag{142}$$

If using the exponential spin coupling term it is

$$\begin{aligned}
S_F &= \sum_{n,m} \bar{\psi}(n) D(n|m) \psi(m) \\
D(n|m) &= \delta_{n,m} - \kappa \sum_{\mu} ((1 - \gamma_{\mu})U_{\mu}(n)\delta_{n+a\hat{\mu},m} + (1 + \gamma_{\mu})U_{-\mu}(n)\delta_{n-a\hat{\mu},m}) \\
&\quad - \kappa\hat{y}\hat{\Omega}((- \gamma_4)U_x(n)\delta_{n+a\hat{x},m} + (+\gamma_4)U_{-x}(n)\delta_{n-a\hat{x},m}) \\
&\quad + \kappa\hat{x}\hat{\Omega}((- \gamma_4)U_y(n)\delta_{n+a\hat{y},m} + (+\gamma_4)U_{-y}(n)\delta_{n-a\hat{y},m}) \\
&\quad - \kappa \frac{ia\Omega\sigma^{12}}{2} ((\gamma_4 - 1)U_{\tau}(n)\delta_{n,n+t} + (\gamma_4 + 1)U_{-\tau}(n)\delta_{n-t,n})
\end{aligned} \tag{143}$$

### 8.1.5 The force from gauge action

$$\begin{aligned}
U_{\mu,\nu}(n) &= U_\mu(n)U_\nu(n+a\mu)U_\mu^{-1}(n+a\nu)U_\nu^{-1}(n). \quad U_{\mu,\nu}^\dagger(n) = U_{\mu,\nu}^{-1}(n) \\
U_{\mu,\nu}^{-1}(n) &= U_\nu(n)U_\mu(n+a\nu)U_\nu^{-1}(n+a\mu)U_\mu^{-1}(n) = U_{\nu,\mu}(n). \\
\text{tr}[U_{\nu,\mu}(n)] &= \text{tr}[U_\nu(n)U_\mu(n+a\nu)U_\nu^{-1}(n+a\mu)U_\mu^{-1}(n)]. \\
\text{tr}[U_{-\mu,\nu}(n)] &= \text{tr}[U_\nu(n-a\mu)U_\mu^{-1}(n+a\nu+a\mu-a\mu)U_\nu^{-1}(n)U_{-\mu}(n)] \\
&= \text{tr}[U_\nu(n-a\mu)U_\mu(n+a\nu-a\mu)U_\nu^{-1}(n)U_\mu^{-1}(n-a\mu)] = \text{tr}[U_{\nu,\mu}(n-a\mu)] = \text{tr}[U_{\mu,\nu}^\dagger(n-a\mu)] \\
\text{tr}[U_{\mu,-\nu}(n)] &= \text{tr}[U_{-\nu,\mu}^\dagger(n)] = (\text{tr}[U_{-\nu,\mu}(n)])^* = (\text{tr}[U_{\mu,\nu}(n-a\nu)])^* = \text{tr}[U_{\mu,\nu}^\dagger(n-a\nu)] \\
\text{tr}[U_{-\mu,-\nu}(n)] &= \text{tr}[U_{\mu,\nu}(n-a\mu-a\nu)]
\end{aligned} \tag{144}$$

so

$$\text{Retr}[\bar{U}_{\mu,\nu}(n)] = \frac{1}{4}\text{Retr}[U_{\mu\nu}(n) + U_{\mu\nu}(n-a\mu) + U_{\mu\nu}(n-a\nu) + U_{\mu\nu}(n-a\mu-a\nu)] \tag{145}$$

and

$$\sum_n f(n)\text{Retr}[1 - \bar{U}_{\mu,\nu}(n)] = \sum_n \frac{f(n) + f(n+a\mu) + f(n+a\nu) + f(n+a\mu+a\nu)}{4}\text{Retr}[1 - U_{\mu\nu}(n)] \tag{146}$$

so (Note, this is for infinite lattice size, the boundary condition should be considered)

$$\begin{aligned}
\sum_n \hat{\Omega}^2 \hat{x}^2 \text{Retr}[1 - \bar{U}_{1,4}(n)] &= \sum_n \hat{\Omega}^2 \frac{2\hat{x}^2 + 2\hat{x} + 1}{2} \text{Retr}[1 - U_{1,4}(n)] \\
\sum_n \hat{\Omega}^2 \hat{y}^2 \text{Retr}[1 - \bar{U}_{2,4}(n)] &= \sum_n \hat{\Omega}^2 \frac{2\hat{y}^2 + 2\hat{y} + 1}{2} \text{Retr}[1 - U_{2,4}(n)] \\
\sum_n \hat{\Omega}^2 (\hat{x}^2 + \hat{y}^2) \text{Retr}[1 - \bar{U}_{3,4}(n)] &= \sum_n \hat{\Omega}^2 (\hat{x}^2 + \hat{y}^2) \text{Retr}[1 - U_{3,4}(n)]
\end{aligned} \tag{147}$$

Using

$$\begin{aligned}
\text{Retr}[U_{\mu,\nu}(n-a\nu)] &= \text{Retr}[U_\mu(n-a\nu)U_\nu(n+a\mu-a\nu)U_\mu^{-1}(n)U_\nu^{-1}(n-a\nu)] \\
&= \text{Retr}[U_\nu(n-a\nu)U_\mu(n)U_\nu^{-1}(n+a\mu-a\nu)U_\mu^{-1}(n-a\nu)] \\
&= \text{Retr}[U_\mu(n)U_\nu^{-1}(n+a\mu-a\nu)U_\mu^{-1}(n-a\nu)U_\nu(n-a\nu)]
\end{aligned} \tag{148}$$

$$\sum_n g(n) \text{Retr}[1 - U_{\mu,\nu}(n)] = N \times N_c - \sum_n \text{Retr}[U_\mu(n) \Sigma_\mu^\dagger(n)]$$

$$\Sigma_{\mu,i}(n, \nu) = g_i(n) U_\nu(n) U_\mu(n + a\nu) U_\nu^{-1}(n + a\mu) + g_i(n - a\nu) U_\nu^{-1}(n - a\nu) U_\mu(n - a\nu) U_\nu(n + a\mu - a\nu)$$
(149)

The product is just same as the definition of staples. However, there are two differences, (i) there is a coefficient function for each term of the sum. (ii) there is no sum over  $\nu$ .

The following is usual, with the new definition of the staple, one have

$$F_\mu(n) = -\frac{\beta}{2N_c} \left\{ U_\mu(n) \Sigma_{\mu,i}^\dagger(n, \nu) \right\}_{TA}$$
(150)

with  $i = 1, 2, 3$  and (**Note, this is for infinite lattice size, the boundary condition should be considered**)

$$g_1(n) = \frac{\Omega^2(2x^2 + 2x + 1)}{2}, \quad g_2(n) = \frac{\Omega^2(2y^2 + 2y + 1)}{2}, \quad g_3(n) = \Omega^2(x^2 + y^2),$$

$$F_{\mu=1,2,3}(n) = -\frac{\beta}{2N_c} \left\{ U_\mu(n) \Sigma_{\mu,\mu}^\dagger(n, 4) \right\}_{TA}$$
(151)

$$F_4(n) = -\frac{\beta}{2N_c} \left\{ U_4(n) \sum_{i=1,2,3} \Sigma_{4,i}^\dagger(n, i) \right\}_{TA}$$

Now we consider the force of  $V$

$$V_{\mu\nu\sigma} = \frac{1}{8} (U_{\mu,\nu} U_{\nu,\sigma} + U_{-\mu,\nu} U_{\nu,-\sigma} + U_{\mu,-\nu} U_{-\nu,\sigma} + U_{-\mu,-\nu} U_{-\nu,-\sigma}$$

$$- U_{\mu,\nu} U_{\nu,-\sigma} - U_{-\mu,\nu} U_{\nu,\sigma} - U_{\mu,-\nu} U_{-\nu,-\sigma} - U_{-\mu,-\nu} U_{-\nu,\sigma})$$
(152)

Using

$$\text{Retr}[U_{\mu,\nu} U_{\nu,\sigma}] = \text{Retr}[U_{\sigma,\nu} U_{\nu,\mu}], \quad \text{Retr}[U_{\mu,\nu} U_{\nu,-\sigma}] = \text{Retr}[U_{-\sigma,\nu} U_{\nu,\mu}]$$
(153)

one have

$$\text{Retr}[V_{\mu\nu\rho}] = \text{Retr}[V_{\rho\nu\mu}]$$
(154)

So we only need to calculate  $\frac{\partial}{\partial \omega_\mu} V_{\mu\nu\rho}$  and  $\frac{\partial}{\partial \omega_\nu} V_{\mu\nu\rho}$ .

One can find

$$\sum_n \text{Retr}[g(n) V_{\mu\nu\rho}(n)] \rightarrow S[U_\mu(n)] = \text{Retr}[U_\mu(n) M(n)]$$
(155)

with

$$\begin{aligned}
M(n) = & \frac{1}{8} ((g(n) + g(n + a\nu))U_\nu(n + a\mu)U_\mu^{-1}(n + a\nu)U_\rho(n + a\nu)U_\nu^{-1}(n + a\rho)U_\rho^{-1}(n) \\
& + (g(n) + g(n - a\nu))U_\nu^{-1}(n + a\mu - a\nu)U_\mu^{-1}(n - a\nu)U_\rho(n - a\nu)U_\nu(n - a\nu + a\rho)U_\rho^{-1}(n) \\
& + (g(n + a\mu - a\nu) + g(n + a\mu))U_\rho^{-1}(n + a\mu - a\rho)U_\nu^{-1}(n + a\mu - a\rho - a\nu) \\
& \times U_\rho(n + a\mu - a\rho - a\nu)U_\mu^{-1}(n - a\nu)U_\nu(n - a\nu) \\
& + (g(n + a\mu + a\nu) + g(n + a\mu))U_\rho^{-1}(n + a\mu - a\rho)U_\nu(n + a\mu - a\rho) \\
& \times U_\rho(n + a\mu - a\rho + a\nu)U_\mu^{-1}(n + a\nu)U_\nu^{-1}(n) \\
& - (g(n + a\mu) + g(n + a\mu + a\nu))U_\rho(n + a\mu)U_\nu(n + a\mu + a\rho)U_\rho^{-1}(n + a\mu + a\nu)U_\mu^{-1}(n + a\nu)U_\nu^{-1}(n) \\
& - (g(n + a\mu) + g(n + a\mu - a\nu))U_\rho(n + a\mu)U_\nu^{-1}(n + a\mu + a\rho - a\nu) \\
& \times U_\rho^{-1}(n + a\mu - a\nu)U_\mu^{-1}(n - a\nu)U_\nu(n - a\nu) \\
& - (g(n) + g(n + a\nu))U_\nu(n + a\mu)U_\mu^{-1}(n + a\nu)U_\rho^{-1}(n + a\nu - a\rho)U_\nu^{-1}(n - a\rho)U_\rho(n - a\rho) \\
& - (g(n) + g(n - a\nu))U_\nu^{-1}(n + a\mu - a\nu)U_\mu^{-1}(n - a\nu)U_\rho^{-1}(n - a\nu - a\rho)U_\nu(n - a\nu - a\rho)U_\rho(n - a\rho))
\end{aligned} \tag{156}$$

It can be simplified as

$$\begin{aligned}
M(n) = & \frac{1}{8} ((g(n) + g(n + a\nu))U_\nu(n + a\mu)U_\mu^{-1}(n + a\nu)S_1 \\
& + (g(n) + g(n - a\nu))U_\nu^{-1}(n + a\mu - a\nu)U_\mu^{-1}(n - a\nu)S_2 \\
& + (g(n + a\mu) + g(n + a\mu + a\nu))S_3U_\mu^{-1}(n + a\nu)U_\nu^{-1}(n) \\
& + (g(n + a\mu) + g(n + a\mu - a\nu))S_4U_\mu^{-1}(n - a\nu)U_\nu(n - a\nu)) \\
S_1 = & U_\rho(n + a\nu)U_\nu^{-1}(n + a\rho)U_\rho^{-1}(n) - U_\rho^{-1}(n + a\nu - a\rho)U_\nu^{-1}(n - a\rho)U_\rho(n - a\rho) \\
S_2 = & U_\rho(n - a\nu)U_\nu(n - a\nu + a\rho)U_\rho^{-1}(n) - U_\rho^{-1}(n - a\nu - a\rho)U_\nu(n - a\nu - a\rho)U_\rho(n - a\rho) \\
S_3 = & U_\rho^{-1}(n + a\mu - a\rho)U_\nu(n + a\mu - a\rho)U_\rho(n + a\mu - a\rho + a\nu) \\
& - U_\rho(n + a\mu)U_\nu(n + a\mu + a\rho)U_\rho^{-1}(n + a\mu + a\nu) \\
S_4 = & U_\rho^{-1}(n + a\mu - a\rho)U_\nu^{-1}(n + a\mu - a\rho - a\nu)U_\rho(n + a\mu - a\rho - a\nu) \\
& - U_\rho(n + a\mu)U_\nu^{-1}(n + a\mu + a\rho - a\nu)U_\rho^{-1}(n + a\mu - a\nu)
\end{aligned} \tag{157}$$

Similarly, one also have

$$\sum_n \text{Retr}[g(n)V_{\mu\nu\rho}(n)] \rightarrow S[U_\nu(n)] = \text{Retr}[U_\nu(n)N(n)] \tag{158}$$

where

$$\begin{aligned}
N(n) &= \frac{1}{8} \left\{ (g(n + a\mu) + g(n + a\nu + a\mu))U_\mu(n + a\nu)T_1U_\mu^{-1}(n) \right. \\
&\quad + (g(n - a\mu) + g(n + a\nu - a\mu))U_\mu^{-1}(n + a\nu - a\mu)T_2U_\mu(n - a\mu) \\
&\quad + (g(n + a\rho) + g(n + a\nu + a\rho))U_\rho(n + a\nu)T_3U_\rho^{-1}(n) \\
&\quad \left. + (g(n - a\rho) + g(n + a\nu - a\rho))U_\rho^{-1}(n + a\nu - a\rho)T_4U_\rho(n - a\rho) \right\}, \\
T_1 &= U_\rho^{-1}(n + a\nu + a\mu - a\rho)U_\nu^{-1}(n + a\mu - a\rho)U_\rho(n + a\mu - a\rho) \\
&\quad - U_\rho(n + a\nu + a\mu)U_\nu^{-1}(n + a\mu + a\rho)U_\rho^{-1}(n + a\mu), \\
T_2 &= U_\rho(n + a\nu - a\mu)U_\nu^{-1}(n - a\mu + a\rho)U_\rho^{-1}(n - a\mu) \\
&\quad - U_\rho^{-1}(n + a\nu - a\mu - a\rho)U_\nu^{-1}(n - a\mu - a\rho)U_\rho(n - a\mu - a\rho), \\
T_3 &= U_\mu^{-1}(n + a\nu + a\rho - a\mu)U_\nu^{-1}(n + a\rho - a\mu)U_\mu(n + a\rho - a\mu) \\
&\quad - U_\mu(n + a\nu + a\rho)U_\nu^{-1}(n + a\mu + a\rho)U_\mu^{-1}(n + a\rho), \\
T_4 &= U_\mu(n + a\nu - a\rho)U_\nu^{-1}(n - a\rho + a\mu)U_\mu^{-1}(n - a\rho) \\
&\quad - U_\mu^{-1}(n + a\nu - a\mu - a\rho)U_\nu^{-1}(n - a\mu - a\rho)U_\mu(n - a\mu - a\rho),
\end{aligned} \tag{159}$$

One can further reduce the dagger operation by defining

$$S[U_\mu(n)] = \text{Retr}[U_\mu(n)M^\dagger(n)], \quad S[U_\nu(n)] = \text{Retr}[U_\nu(n)N^\dagger(n)] \tag{160}$$

with

$$\begin{aligned}
M(n) &= \frac{1}{8} \left( (g(n) + g(n + a\nu))S_1U_\mu(n + a\nu)U_\nu^{-1}(n + a\mu) \right. \\
&\quad + (g(n) + g(n - a\nu))S_2U_\mu(n - a\nu)U_\nu(n + a\mu - a\nu) \\
&\quad + (g(n + a\mu) + g(n + a\mu + a\nu))U_\nu(n)U_\mu(n + a\nu)S_3 \\
&\quad \left. + (g(n + a\mu) + g(n + a\mu - a\nu))U_\nu^{-1}(n - a\nu)U_\mu(n - a\nu)S_4 \right) \\
S_1 &= U_\rho(n)U_\nu(n + a\rho)U_\rho^{-1}(n + a\nu) - U_\rho^{-1}(n - a\rho)U_\nu(n - a\rho)U_\rho(n + a\nu - a\rho) \\
S_2 &= U_\rho(n)U_\nu^{-1}(n - a\nu + a\rho)U_\rho^{-1}(n - a\nu) - U_\rho^{-1}(n - a\rho)U_\nu^{-1}(n - a\nu - a\rho)U_\rho(n - a\nu - a\rho) \\
S_3 &= U_\rho^{-1}(n + a\mu - a\rho + a\nu)U_\nu^{-1}(n + a\mu - a\rho)U_\rho(n + a\mu - a\rho) \\
&\quad - U_\rho(n + a\mu + a\nu)U_\nu^{-1}(n + a\mu + a\rho)U_\rho^{-1}(n + a\mu) \\
S_4 &= U_\rho^{-1}(n + a\mu - a\rho - a\nu)U_\nu(n + a\mu - a\rho - a\nu)U_\rho(n + a\mu - a\rho) \\
&\quad - U_\rho(n + a\mu - a\nu)U_\nu(n + a\mu + a\rho - a\nu)U_\rho^{-1}(n + a\mu)
\end{aligned} \tag{161}$$

and

$$\begin{aligned}
N(n) &= \frac{1}{8}(N(\mu, \rho)(n) + N(\rho, \mu)(n)) \\
N(\mu, \rho)(n) &= \{ (g(n + a\mu) + g(n + a\nu + a\mu))U_\mu(n)T_1U_\mu^{-1}(n + a\nu) \\
&\quad + (g(n - a\mu) + g(n + a\nu - a\mu))U_\mu^{-1}(n - a\mu)T_2U_\mu(n + a\nu - a\mu) \}, \\
T_1 &= U_\rho^{-1}(n + a\mu - a\rho)U_\nu(n + a\mu - a\rho)U_\rho(n + a\nu + a\mu - a\rho) \\
&\quad - U_\rho(n + a\mu)U_\nu(n + a\mu + a\rho)U_\rho^{-1}(n + a\nu + a\mu), \\
T_2 &= U_\rho(n - a\mu)U_\nu(n - a\mu + a\rho)U_\rho^{-1}(n + a\nu - a\mu) \\
&\quad - U_\rho^{-1}(n - a\mu - a\rho)U_\nu(n - a\mu - a\rho)U_\rho(n + a\nu - a\mu - a\rho),
\end{aligned} \tag{162}$$

**Note, instead of  $S_G[U_\mu] = -U_\mu \Sigma_\mu^\dagger$ , here it is  $S_G[U_\mu] = +U_\mu M_\mu^\dagger$  and  $S_G[U_\mu] = +U_\mu N_\mu^\dagger$ .**

### 8.1.6 The force from fermion action

The first step is to shift the second term to factorize  $U_\mu(n)$  out

$$\begin{aligned}
\sum_{m,n} g(n)(1 + \gamma_\mu)U_{-\mu}(n)\delta_{n-a\mu,m} &= \sum_{m,n} g(n)(1 + \gamma_\mu)U_\mu^{-1}(n - a\mu)\delta_{n-a\mu,m} \\
&= \sum_{m,n} g(n + a\mu)(1 + \gamma_\mu)U_\mu^{-1}(n)\delta_{n,m}
\end{aligned} \tag{163}$$

It is more convenient to split the  $D$  operator as (note that for  $yU_x$ ,  $g(n) = y$ , and  $g(n) = g(n + x)$ ,  $xU_y$  is similar. Also, note that, it is also true for open boundary)

$$\begin{aligned}
M^a &= \{ (1 - \gamma_\mu)T^a U_\mu \delta_{x_L, (x+\mu)_R} - (1 + \gamma_\mu)U_\mu^{-1}T^a \delta_{(x+\mu)_L, x_R} \} \\
&\quad - y\Omega\delta_{\mu,x} \{ (1 - \gamma_4)T^a U_\mu \delta_{x_L, (x+\mu)_R} - (1 + \gamma_4)U_\mu^{-1}T^a \delta_{(x+\mu)_L, x_R} \} \\
&\quad + x\Omega\delta_{\mu,y} \{ (1 - \gamma_4)T^a U_\mu \delta_{x_L, (x+\mu)_R} - (1 + \gamma_4)U_\mu^{-1}T^a \delta_{(x+\mu)_L, x_R} \} \\
F_{pf} &= 2i\kappa \sum_a \text{Im} \left[ \left( \phi_1^\dagger M_a \phi_2 \right) \right] T_a
\end{aligned} \tag{164}$$

with

$$\phi_1 = \left( \left( \hat{D} \hat{D}^\dagger \right)^{-1} \phi \right), \quad \phi_2 = \hat{D}^\dagger \phi_1, \tag{165}$$

similarly, with

$$\begin{aligned}
\phi_{L1}(n) &= \phi_1(n), \quad \phi_{R1}(n) = \{ (1 - \gamma_\mu) + (x\Omega\delta_{\mu,y} - y\Omega\delta_{\mu,x})(1 - \gamma_4) \} \phi_2(n + \mu), \\
\phi_{L2}(n) &= \phi_1(n + \mu), \quad \phi_{R1}(n) = \{ (1 + \gamma_\mu) + (x\Omega\delta_{\mu,y} - y\Omega\delta_{\mu,x})(1 + \gamma_4) \} \phi_2(n),
\end{aligned} \tag{166}$$

$$F_\mu^{pf}(n) = \kappa \left\{ U_\mu(n) \left( \phi_{R1} \phi_{L1}^\dagger + \phi_{R2} \phi_{L2}^\dagger \right) \right\} \Big|_{TA} \quad (167)$$

Note that **Both the force from gauge and fermion actions are kept anti-hermitian traceless.**

### 8.1.7 The angular momentum

The angular momentum operator is defined as

$$\begin{aligned} J &\equiv \left. \frac{\delta \mathcal{L}}{\delta \Omega} \right|_{\Omega=0} \\ &= J_G + J_{FL} + J_{FS} \\ J_G &= \frac{\beta}{N_c} \sum_n (\hat{x} \text{Retr}[V_{412}(n) + V_{432}(n)] - \hat{y} \text{Retr}[V_{421}(n) + V_{431}(n)]) \\ J_{FL} &= \bar{\psi} \{ -\kappa \hat{y} ((-\gamma_4) U_x(n) \delta_{n+a\hat{x},m} + (+\gamma_4) U_{-x}(n) \delta_{n-a\hat{x},m}) \\ &\quad + \hat{x} ((-\gamma_4) U_y(n) \delta_{n+a\hat{y},m} + (+\gamma_4) U_{-y}(n) \delta_{n-a\hat{y},m}) \} \\ &= -\kappa \bar{\psi} \gamma_4 (\hat{y} D_x - x D_y) \psi, \\ J_{FS} &= -i \kappa \bar{\psi} \gamma_4 \sigma^{12} \psi. \end{aligned} \quad (168)$$

The result is derived as  $\delta \mathcal{L} / \delta \hat{\Omega}$ , therefor, the result has unit as  $a^{-3}$ .

The measurement of  $\langle J_G \rangle$  is straightforward. The measurement of  $J_{FL}$  and  $J_{FS}$  are inertia mass densities of quark-antiquark pairs. So, for the  $u - \bar{u}$  pair. On the other hand,  $J$  is **NOT** a local operator.  $\langle J_F(n|m) \rangle$  can be written as (in the spinor space, where  $a, b$  are spinor indices)

$$\begin{aligned} \langle J_F(n|m) \rangle &= \langle \bar{u}(n) O(n|m) u(m) \rangle \\ &= \sum_{a,b} O_{a,b}(n|m) \langle \bar{u}_a(n) u_b(m) \rangle = - \sum_{a,b} O_{a,b}(n|m) \langle u_b(m) \bar{u}_a(n) \rangle \\ &= - \sum_{a,b} O_{a,b}(n|m) D^{-1}(m|n)_{b,a} = -\text{tr}_{c,s} [O(n|m) D^{-1}(m|n)] \end{aligned} \quad (169)$$

So the definition of local angular momentum density should be

$$\langle J_F(n) \rangle = - \sum_{a,b,m} O_{a,b}(n|m) D^{-1}(m|n)_{b,a} = -\text{tr}_{c,s,m} [O(n|m) D^{-1}(m|n)] \quad (170)$$

So, we need to calculate  $\sum_n O(m_0|n) D^{-1}(n|m_0)$  as a matrix in color and spinor space. It can be done by introduce the source

$$\phi_{m_0, c_2, s_2}^S(m)_{c,s} = \delta(m - m_0) \delta(c - c_2) \delta(s - s_2) \quad (171)$$



and  $D^{-1}(n|m_0)_{c,s}$  as a vector  $\vec{v}(n)$  can be written as

$$\begin{pmatrix} D_{1,cs}^{-1}(n) \\ D_{2,cs}^{-1}(n) \\ D_{3,cs}^{-1}(n) \\ \dots \\ D_{10,cs}^{-1}(n) \\ D_{11,cs}^{-1}(n) \\ D_{12,cs_2}^{-1}(n) \end{pmatrix} = \begin{pmatrix} D_{1,1}^{-1} & D_{1,2}^{-1} & \dots & D_{1,cs}^{-1}(n|m_0) & \dots & D_{1,11}^{-1} & D_{1,12}^{-1} \\ D_{2,1}^{-1} & D_{2,2}^{-1} & \dots & D_{2,cs}^{-1}(n|m_0) & \dots & D_{2,11}^{-1} & D_{2,12}^{-1} \\ D_{3,1}^{-1} & D_{3,2}^{-1} & \dots & D_{3,cs}^{-1}(n|m_0) & \dots & D_{3,11}^{-1} & D_{3,12}^{-1} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ D_{10,1}^{-1} & D_{10,2}^{-1} & \dots & D_{10,cs}^{-1}(n|m_0) & \dots & D_{10,11}^{-1} & D_{10,12}^{-1} \\ D_{11,1}^{-1} & D_{11,2}^{-1} & \dots & D_{11,cs}^{-1}(n|m_0) & \dots & D_{11,11}^{-1} & D_{11,12}^{-1} \\ D_{12,1}^{-1} & D_{12,2}^{-1} & \dots & D_{12,cs}^{-1}(n|m_0) & \dots & D_{12,11}^{-1} & D_{12,12}^{-1} \end{pmatrix} \begin{pmatrix} 0 \\ \dots \\ 0 \\ 1_{idx=cs,x=m_0} \\ 0 \\ \dots \\ 0 \end{pmatrix} \quad (172)$$

and  $\sum_n O(m|n)D^{-1}(n|m_0)_{c,s}$  as a vector  $\vec{v}(m)$  can be written as

$$\begin{pmatrix} OD_{1,cs}^{-1}(m) \\ OD_{2,cs}^{-1}(m) \\ \dots \\ OD_{11,cs}^{-1}(m) \\ OD_{12,cs_2}^{-1}(m) \end{pmatrix} = \begin{pmatrix} O_{1,1} & O_{1,2} & \dots & O_{1,11} & O_{1,12} \\ O_{2,1} & O_{2,2} & \dots & O_{2,11} & O_{2,12} \\ O_{3,1} & O_{3,2} & \dots & O_{3,11} & O_{3,12} \\ \dots & \dots & \dots & \dots & \dots \\ O_{10,1} & O_{10,2} & \dots & O_{10,11} & O_{10,12} \\ O_{11,1} & O_{11,2} & \dots & O_{11,11} & O_{11,12} \\ O_{12,1} & O_{12,2} & \dots & O_{12,11} & O_{12,12} \end{pmatrix} \begin{pmatrix} D_{1,cs}^{-1} \\ D_{2,cs}^{-1} \\ \dots \\ D_{11,cs}^{-1} \\ D_{12,cs_2}^{-1} \end{pmatrix} \quad (173)$$

And the trace is just

$$\sum_{i=1}^{12} (OD^{-1})_{i,i}(n) \quad (174)$$

Also, note that, the  $D$  and  $\psi$  are scaled.

Now, we can consider the physical meaning of  $J_G$ . Using

$$F_{0i} = E^i, \quad F_{ij} = 2c\epsilon_{ijk}B_i \quad (175)$$

therefor

$$\begin{aligned} \mathbf{j} &= (x, y, 0) \times (\mathbf{E} \times \mathbf{B}) \\ \mathbf{j} &= (x, y, 0) \times ((F_{01}, F_{02}, F_{03}), F_{23}, F_{31}, F_{12}) \\ j_z &= -2c(xF_{01}F_{12} + yF_{02}F_{12} - xF_{03}F_{23} + yF_{03}F_{13}) \end{aligned} \quad (176)$$

### 8.1.8 The Current density and Charge density

In the case of exponential  $\sigma^{12}$  term, it is interesting to also measure

$$J_{12} = -i\kappa \langle \bar{\psi} \gamma_4 \sigma^{12} \psi \rangle \quad (177)$$

Also the currents defined as

$$J_\mu = \langle \bar{\psi} \gamma_\mu \psi \rangle \quad (178)$$

is measured, such that

$$\begin{aligned} J_x &= \langle \bar{\psi} (\gamma_1 + y \Omega \gamma_4) \psi \rangle \\ J_y &= \langle \bar{\psi} (\gamma_2 - x \Omega \gamma_4) \psi \rangle \\ J_z &= \langle \bar{\psi} \gamma_3 \psi \rangle \\ J_\tau &= \langle \bar{\psi} \gamma_4 \psi \rangle \end{aligned} \quad (179)$$

we also measure the

$$\begin{aligned} J_1 &= \langle \bar{\psi} \gamma_1 \psi \rangle \\ J_2 &= \langle \bar{\psi} \gamma_2 \psi \rangle \end{aligned} \quad (180)$$

and the chiral charge density

$$n_5 = a^3 \langle \bar{\psi} \gamma_4 \gamma_5 \psi \rangle \quad (181)$$

### 8.1.9 The Topological Density

The topological charge is defined as (**This might has to be modified in the rotating frame!**)

$$\begin{aligned} Q &= \frac{1}{32\pi^2} a^4 \sum_n \epsilon_{\mu\nu\rho\sigma} \text{tr} [C_{\mu\nu}(n) C_{\rho\sigma}(n)] \\ C_{\mu\nu}(n) &= \text{Im} [U_{\mu\nu}(n)] \end{aligned} \quad (182)$$

Another definition is

$$\begin{aligned} Q &= \frac{1}{32\pi^2} a^4 \sum_n \epsilon_{\mu\nu\rho\sigma} \text{tr} [C_{\mu\nu}^{clover}(n) C_{\rho\sigma}^{clover}(n)] \\ C_{\mu\nu}^{clover}(n) &= \frac{1}{4} \text{Im} [U_{\mu,\nu}(n) + U_{\nu,-\mu}(n) + U_{-\mu,-\nu}(n) + U_{-\nu,\mu}(n)] \end{aligned} \quad (183)$$

Note for both  $C_{\mu\nu}$  and  $C_{\mu\nu}^{clover}$ , one have  $C_{\mu\nu} = -C_{\nu\mu}$ , alone with  $\epsilon_{\mu\nu\rho\sigma}$ , it doubles the term. Therefor

$$\sum \epsilon_{\mu\nu\rho\sigma} \text{tr} [C_{\mu\nu}(n) C_{\rho\sigma}(n)] = 8 (\text{tr} [C_{12}(n) C_{34}(n)] - \text{tr} [C_{13}(n) C_{24}(n)] + \text{tr} [C_{14}(n) C_{23}(n)]) \quad (184)$$

### 8.1.10 The Polyakov loop

Polyakov loop is measured straight forwardly.

### 8.1.11 The Chiral Condensate

The Chiral condensate can be calculate by Grassman number integral

$$\langle \bar{u}u \rangle = \text{tr}[D_u^{-1}] \quad (185)$$

We are using two degenerate fermions, so

$$\langle \bar{\psi}\psi \rangle = \text{tr}[D^{-1}] = a^{-4} \frac{1}{m + \frac{4}{a}} \text{tr} [\hat{D}^{-1}] = a^{-4} \times 2a\kappa \text{tr} [\hat{D}^{-1}] = 2a^{-3}\kappa \text{tr} [\hat{D}^{-1}] \quad (186)$$

## 8.2 Sample Producer

In HMC, the most time-consuming operation is  $(DD^\dagger)^{-1}\phi$ , which need to solve the Wilson-Dirac equation, a matrix equation  $\mathbf{b} = A\mathbf{x}$ , where  $A = DD^\dagger$  is a matrix depending on the gauge field and acting on the pseudo-fermion field.

At the same time, applying machine learning algorithms to physics problems has gained more and more attentions. The machine learning algorithms has been applied to solve partial differential equations [18]. In Ref. [19], deep learning is applied to map between potential and energy bypassing the need to solve the Schrödinger equation, in other words, the Schrödinger equation is implicitly solved by the network. So, it is reasonable to ask whether the machine learning can also help to solve the Wilson-Dirac equation? For example, is it possible to train the network to output eigenvectors by inputting a gauge field, or even better output  $\mathbf{x}$  by inputting a gauge field and a pseudo-fermion field  $\mathbf{b}$ ?

## 8.3 Data Analyse

We write the data analyse code based on Ref. [20] in Mathematica.

### 8.3.1 What is autocorrelation

The problem to address is that, the configurations generated are not statistically independent. So one need to take the relations between configurations into account.

To consider the relation between two sets, correlation functions are used, assuming two sets  $a_{\alpha,\beta}$ , assume  $a_{\alpha,\beta} - \bar{a}_{\alpha,\beta}$  is a normal distribution.

$$\langle (a_\alpha - \bar{a}_\alpha)(a_\beta - \bar{a}_\beta) \rangle = \frac{1}{N^2} \sum_{i,j} \Gamma_{\alpha\beta}(j-i) \quad (187)$$

and

$$C_{\alpha\beta} = \sum_{t=-\infty}^{\infty} \Gamma_{\alpha\beta}(t) \quad (188)$$

**Note that,  $C_{\alpha\alpha}(0) = N\langle\delta_\alpha^2\rangle$  is the standard error.**

For one single observable, one can define a correlation of a set of itself with delayed Markov time as

$$\tau_\alpha = \frac{1}{2\Gamma_{\alpha\alpha}(0)} \sum_{t=-\infty}^{\infty} \Gamma_{\alpha\alpha}(t) \quad (189)$$

For a purely exponential behaviour,  $\Gamma_{\alpha\beta}(t) \sim \exp(-|t|/\tau)$ . Generally, we can estimate  $2\tau_\alpha$  as an interval such that two configurations are effectively independent [20].

Here,  $\Gamma_{\alpha\beta}(t)$  is **autocorrelation**.

### 8.3.2 How to calculate autocorrelation, and how to use it to obtain the interval

Considering, we have already obtained a set of measurements by using configurations generated with Markov chain  $\{a_\alpha^{i,r}\}$ , where  $\alpha$  indicating different observables,  $r = 1 \rightarrow R$  indicating different replicas (usually, different replicas are obtained by running multi-times starting from same parameters, or running parallelly starting from same parameters), and  $i = 1 \rightarrow N_r$  is index of each value in the replica.

Assume we measured  $a_\alpha^{i,r}$ , and want to obtain  $F = f(a_\alpha)$ .

In Ref. [20], a biased estimator is used such that

$$\begin{aligned} N &= \sum_r^R N_r, \\ \bar{a}_\alpha^r &= \frac{1}{N_r} \sum_i a_\alpha^{i,r} \\ \bar{\bar{a}}_\alpha &= \frac{1}{N} \sum_r^R N_r \bar{a}_\alpha^r \\ \bar{F} &= \frac{1}{N} \sum_r^R N_r f(\bar{a}_\alpha^r), \\ \bar{\bar{F}} &= f(\bar{\bar{a}}_\alpha) \end{aligned} \tag{190}$$

and

$$F_{mean} = \begin{cases} \bar{\bar{F}}, & R = 1 \\ \frac{R\bar{F} - \bar{\bar{F}}}{R-1}, & R \geq 2 \end{cases} \tag{191}$$

The error is related to a correlation

$$\bar{\bar{\Gamma}}_{\alpha\beta}(t) = \frac{1}{N - Rt} \sum_{r=1}^R \sum_{i=1}^{N_r-t} (a_\alpha^{i,r} - \bar{\bar{a}}_\alpha) (a_\beta^{i+t,r} - \bar{\bar{a}}_\beta) \tag{192}$$

at first we need to project it onto single variable, for this purpose, we need to calculate gradient as

$$\begin{aligned} h_\alpha &= \sqrt{\frac{\Gamma_{\alpha\alpha}(0)}{N}}, \\ \bar{\bar{f}}_\alpha &\approx \frac{1}{2h_\alpha} (f(\bar{\bar{a}}_1, \bar{\bar{a}}_2, \dots, \bar{\bar{a}}_\alpha + h_\alpha, \dots) - f(\bar{\bar{a}}_1, \bar{\bar{a}}_2, \dots, \bar{\bar{a}}_\alpha - h_\alpha, \dots)) \end{aligned} \tag{193}$$

and

$$\bar{\bar{\Gamma}}_F(t) = \sum_{\alpha\beta} \bar{f}_\alpha \bar{f}_\beta \bar{\bar{\Gamma}}_{\alpha\beta}(t) \quad (194)$$

then the sum from  $t = -\infty \rightarrow \infty$  is approximated as

$$\bar{\bar{C}}_F(W) = \bar{\bar{\Gamma}}_F(0) + 2 \sum_{t=1}^W \bar{\bar{\Gamma}}_F(t) \quad (195)$$

By definition, if window  $W$  is known, then

$$\bar{\tau}_{int}(W) = \frac{\bar{\bar{C}}_F(W)}{2\bar{\bar{C}}_F(0)} \quad (196)$$

To get  $\tau$  one need to use a factor  $S$  to fit the exponential, assuming

$$2\bar{\tau}_{int}(W) = \sum_{t=-\infty}^{\infty} \exp\left(-\frac{S|t|}{\bar{\tau}(W)}\right) \quad (197)$$

with  $S$  as a constant usually  $S = 1 \rightarrow 2$ .

Then one can let  $\bar{\tau}(W) = S\tau_{int}(W)$ , and calculate

$$g(W) = \exp\left(-\frac{W}{\bar{\tau}(W)}\right) - \frac{\bar{\tau}(W)}{\sqrt{WN}} \quad (198)$$

and fix  $W$  as the first index such that  $g(W) < 0$  change sign.

Once  $W$  is obtained, one can calculate  $2\bar{\tau}_{int}(W)$  which is the Markov time separation such that two configurations can be considered as independent. Also, the error estimate is

$$\delta_F^2 = \frac{\bar{\bar{C}}(W)}{N} \quad (199)$$

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