Lattice QCD simulations with clover quarks

Hideo Matsufuru

High Energy Accelerator Research Organization (KEK),
Oho 1-1, Tsukuba 305-0801, Japan

Email: hideo.matsufuru@kek.jp
WWW: http://www.rcnp.osaka-u.ac.jp/~matufuru/

2 April 2012, Ver.1.3.1

Abstract

This is an implementation note for developing a code of the hybrid Monte Carlo algorithm for clover quark action.

Contents

1 Clover fermion action

1.1 Fermion operator

In lattice QCD, the gauge field is represented with a link variable, which is a complex 3×3 matrix belonging to SU(3) group. The link variable on a site x is

$$U_\mu(x) \simeq \exp[iaA_\mu(x + a\hat{\mu}/2)] \in \mathrm{SU}(3) \tag{1.1}$$

where $\hat{\mu}$ is an unit vector in μ-th direction. Throughout this note, we set $a = 1$. We do not consider the case of anisotropic lattices in the following.

The clover fermion is an $O(a)$-improved version of the Wilson quark action. Let us start with the quark action very close to the continuum action, in which the lattice constant a is introduced to make the quantities dimensionless. In the path integral formalism, a field is an integral veriable, and thus the physics is invariant with respect to the change of it. Starting from the Wilson action, let us consider the transformation

$$\psi_c = \left[1 - \frac{ra}{4}(\not{D} - m_c)\right]\psi \tag{1.2}$$

$$\bar{\psi}_c = \bar{\psi}\left[1 - \frac{ra}{4}(\not{D} - m_c)\right]. \tag{1.3}$$

Note that the fields ψ and $\bar{\psi}$ are independent variables, and thus can be subject to different transformations.

$$\mathcal{L} = \bar{\psi}\left[\not{D} + (m_c + \frac{r}{2}am_c^2) - \frac{ra}{2}\ \not{D}^2\right]\psi. \tag{1.4}$$

Since $\not{D}^2 = D^2 + \frac{1}{2}\sigma_{\mu\nu}F_{\mu\nu}$, where $\sigma_{\mu\nu} = -\frac{i}{2}[\gamma_\mu, \gamma_\nu]$ and $F_{\mu\nu} = i[D_\mu, D_\nu]$,

$$\mathcal{L} = \bar{\psi}\left[\not{D} + m - \frac{ra}{2}(D^2 + \frac{1}{2}\sigma_{\mu\nu}F_{\mu\nu})\right]\psi. \tag{1.5}$$

The bare quark mass $m = (m_c + \frac{r}{2}am_c^2)$ plays just an input parameter of the theory. The first term of the $O(a)$ term is the Wilson term, and the second term is called the clover term. Thus discretizing the Eq. (1.5), one can eliminate the $O(a)$ error brought by the Wilson term while keeping the doublers diappear. The above equation is at the tree level, and the with interaction the coefficient of the clover term is in general renormalized. Thus the clover coefficient, c_{SW}, is multiplied to the clover term.

in the above notation, $\sigma_{\mu\nu}$ and $F_{\mu\nu}$ are Hermitian. It is however convenient to use slightly modified notations, where $\bar{\sigma}_{\mu\nu} = \frac{1}{2}[\gamma_\mu, \gamma_\nu]$ and $\bar{F}_{\mu\nu} = [D_\mu, D_\nu]$ so that $\sigma_{\mu\nu}F_{\mu\nu} = \bar{\sigma}_{\mu\nu}\bar{F}_{\mu\nu}$ for numeircal implementation. $\sigma_{\mu\nu}$ and $F_{\mu\nu}$ are anti-hermitian.

With standard discretization, the clover quark action is written as [4]

$$S_Q = \frac{1}{2\kappa}\sum_{x,y}\bar{\psi}(x)D(x,y)\psi(y), \tag{1.6}$$

$$D(x,y) = \delta_{x,y} - \kappa\sum_\mu\left\{(1-\gamma_\mu)U_\mu(x)\delta_{x+\hat{\mu},y} + (1+\gamma_\mu)U_\mu^\dagger(x-\hat{\mu})\delta_{x-\hat{\mu},y}\right\}$$
$$-\kappa c_{SW}\frac{1}{2}\sum_{\mu\nu}\bar{\sigma}_{\mu\nu}\bar{F}_{\mu\nu}. \tag{1.7}$$

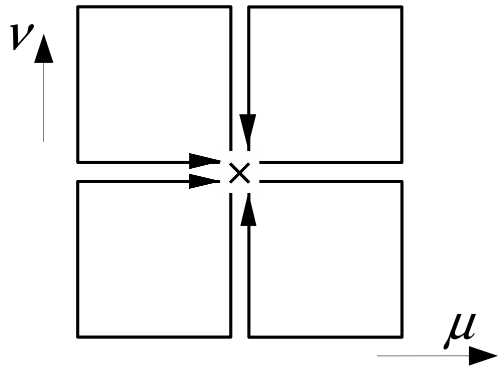

Figure 1: The clover construction of the field strength.

We employed the hopping parameter representation in which the hopping parameter, $\kappa = 1/2(4 + am_0)$, is used as an input parameter instead of a bare quark mass m_0.

The field strength, $F_{\mu\nu}$ is represented as

$$\bar{F}_{\mu\nu} = \frac{1}{4}\left[\mathcal{F}_{\mu\nu}(x)\right]_A \tag{1.8}$$

$$\begin{aligned}\mathcal{F}_{\mu\nu}(x) = \; & U_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x) \\ & - U_\mu(x)U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu}) \\ & + U_\nu(x)U^\dagger_\mu(x-\hat{\mu}+\hat{\nu})U^\dagger_\nu(x-\mu)U_\mu(x-\mu) \\ & - U^\dagger_\nu(x-\hat{\nu})U^\dagger_\mu(x-\hat{\mu}-\hat{\nu})U_\nu(x-\hat{\mu}-\hat{\nu})U_\mu(x-\hat{\mu})\end{aligned} \tag{1.9}$$

where $[\ldots]_A$ means the anti-hermitian operation[1], *i.e.*, $[F]_A = (F - F^\dagger)/2$. This construction is represented as Figure 1.

Since the anticommuting Grassmann fields are difficult to treat numerically, first one integrates out them explicitly:

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp(-\bar{\psi}D[U]\psi) = \det D[U]. \tag{1.10}$$

Due to so-called γ_5-hermiticity, $D^\dagger = \gamma_5 D \gamma_5$, $\det D$ is real. For $\kappa < 1/8$, $\det D > 0$ is also proved. Then

$$\det D[U] = \sqrt{\det Q[U]}, \tag{1.11}$$

where

$$Q = D^\dagger D = H^2 \tag{1.12}$$

is hermitian and positive definite. $H = \gamma_5 D$ is hermitian: $H^\dagger = H$.

Let us consider the case with two degenerate flavors. Introducing a bosonic field ϕ (called pseudofermion field),

$$\det[D^\dagger(m)D(m)] = \int \mathcal{D}\phi^\dagger\mathcal{D}\phi \int \mathcal{D}\bar{\phi}\mathcal{D}\phi \exp[-S_{PF}], \tag{1.13}$$

[1] We have decided not to enforce the field strength traceless, while it is a property of the adjoint representation. This is for simplifying HMC force construction.

$$S_{PF} = \phi^\dagger [D^\dagger(m)D(m)]^{-1}\phi. \tag{1.14}$$

This is a starting point action in constructing the HMC algorithm. In the above equations, the bare quark mass (or equivalently the hopping parameter) is exhibited as a preparation to the multi-mass preconditioning mentioned below.

The Hasenbusch acceleration (multi-mass preconditioning) is applied by introducing a preconditioning field with heavier quark mass,

$$\begin{aligned} \det[D^\dagger(m)D(m)] &= \det[D^\dagger(m')D(m')]\det[D(m')^{\dagger-1}D^\dagger(m)D(m)D(m')^{-1}] & (1.15)\\ &= \int \mathcal{D}\bar{\phi}_1\mathcal{D}\phi_1\mathcal{D}\bar{\phi}_2\mathcal{D}\phi_2 \exp\left[-S_{PF}^{(1)} - S_{PF}^{(2)}\right], & (1.16) \end{aligned}$$

$$\begin{aligned} S_{PF}^{(1)} &= \phi_1^\dagger [D^\dagger(m')D(m')]^{-1}\phi_1, & (1.17)\\ S_{PF}^{(2)} &= \phi_2^\dagger \left\{D(m')[D(m)^\dagger D(m)]^{-1}D^\dagger(m')\right\}\phi_2, & (1.18) \end{aligned}$$

where m' is a mass of the preconditioner. Here we restrict ourselves to the case of single preconditioner.

1.2 HMC force

By differentiating the Hamiltonian $\mathcal{H}$ by simulation time τ,

$$\frac{d\mathcal{H}}{d\tau} = \sum_{\mu,x} \mathrm{Tr}\left[\frac{dP_\mu(x)}{d\tau}P_\mu(x) + iP_\mu(x)R_\mu(x)\right], \tag{1.19}$$

where the force $R_\mu(x)$ satisfying

$$\frac{dS}{d\tau} = \sum \mathrm{Tr}[iP_\mu(x)R_\mu(x)] \tag{1.20}$$

is anti-hermitian and traceless. The evolution of $P_\mu(x)$ is

$$\begin{aligned} iP_\mu(x) &\to iP_\mu(x) + \Delta\tau R_\mu(x),\\ U_\mu(x) &\to \exp[\Delta\tau \cdot iP_\mu(x)]U_\mu(x). & (1.21) \end{aligned}$$

We consider the Hasenbusch preconditioned version, Eq.(1.16), since the unpreconditioned action is the same as the first term of the preconditioned one, Eq.(1.17). Let us start with the preconditioner,

$$S_{PF}^{(1)} = \phi^\dagger[D^\dagger(m)D(m)]^{-1}\phi = \phi^\dagger Q(m)^{-1}\phi. \tag{1.22}$$

Since $\frac{dQ^{-1}}{d\tau} = -Q^{-1}\frac{dQ}{d\tau}Q^{-1}$,

$$\begin{aligned} \frac{d}{d\tau}S_{PF}^{(1)} &= -\psi^\dagger \frac{d}{d\tau}[D^\dagger(m)D(m)]\psi\\ &= -\psi^\dagger\left[\dot{H}(m)H(m) + H^\dagger(m)\dot{H}(m)\right]\psi,\\ &= -\left\{[H(m)\psi]^\dagger \dot{H}(m)\psi + h.c.\right\}, & (1.23) \end{aligned}$$

where $\psi = Q(m)^{-1}\phi$.

Since the clover operator is composed of the Wilson kernel (D_W) and the clover term (D_SW), $R_\mu(x)$ has two parts:

$$R_\mu(x) = R_\mu^W(x) + R_\mu^{SW}(x). \tag{1.24}$$

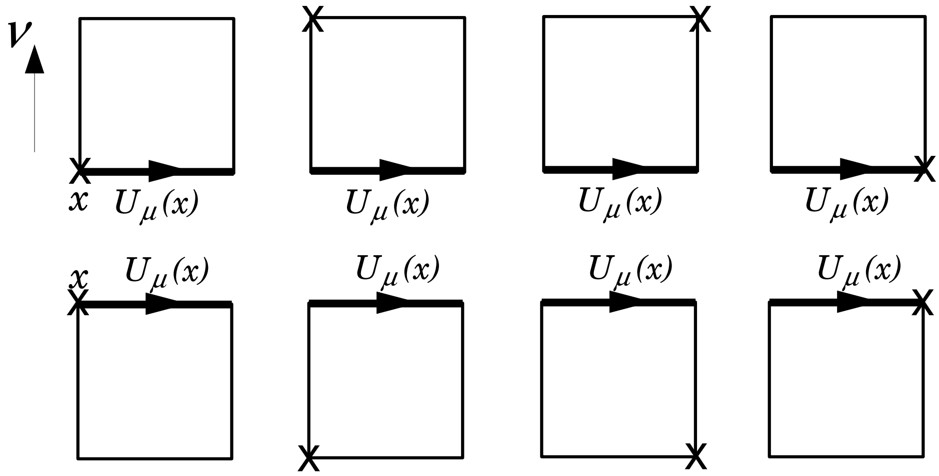

Figure 2: Contribution to the force from the clover term to update the link variable $U_\mu(x)$. The crosses represent the pseudofermion field.

Force of the Wilson kernel:
The derivative of hermitian Wilson kernel is calculated as follows. For general vectors ζ and η,

$$\begin{aligned}
\zeta^\dagger \frac{dH_W}{d\tau}\eta &= -\kappa\cdot\zeta^\dagger(x)\sum_{x,\mu}\{\gamma_5(1-\gamma_\mu)iP_\mu(x)U_\mu(x)\eta(x+\hat\mu) \\
&\qquad -\gamma_5(1+\gamma_\mu)U_\mu^\dagger(x-\hat\mu)iP_\mu(x-\hat\mu)\eta(x-\hat\mu)\Big\} \\
&= -\kappa\sum_{x,\mu} iP_\mu(x)_{ab}\Big\{\zeta^\dagger(x)_b[\gamma_5(1-\gamma_\mu)U_\mu(x)\eta(x+\hat\mu)]_a \\
&\qquad -[\gamma_5(1+\gamma_\mu)U_\mu(x)\zeta(x+\hat\mu)]_b^\dagger\eta(x)]_a\Big\} \\
&= -\kappa\sum_{x,\mu} iP_\mu(x)_{ab}\Big\{\zeta^\dagger(x)_b[T_{+\mu}\eta(x)]_a - [T_{-\mu}^\dagger\zeta(x)]_b^\dagger\eta(x)_a\Big\}, \qquad (1.25)
\end{aligned}$$

where in the last line we defined $T_{+\mu}\eta(x)\equiv\gamma_5(1-\gamma_\mu)U_\mu(x)\eta(x+\hat\mu)$ and $T_{-\mu}^\dagger\eta(x)\equiv\gamma_5(1+\gamma_\mu)U_\mu(x)\eta(x+\hat\mu)$. Thus let us define

$$\bar R_\mu^W[\zeta,\eta](x)_{ab} = -\kappa\Big[\zeta^\dagger(x)_b[T_{+\mu}\eta(x)]_a - [T_{-\mu}^\dagger\zeta(x)]_b^\dagger\eta(x)_a\Big]_{AT}. \qquad (1.26)$$

From Eq. (1.23), setting $\eta=\psi$ and $\zeta=H(m)\psi$,

$$R_\mu^W(x)_{ab} = -\bar R_\mu^W[\zeta,\eta](x)_{ab} - \bar R_\mu^W[\eta,\zeta](x)_{ab} \qquad (1.27)$$

Force of the clover term:
The clover term contributtion is also written as

$$R_\mu^{SW}(x)_{ab} = -\bar R_\mu^{SW}[\zeta,\eta](x)_{ab} - \bar R_\mu^{SW}[\eta,\zeta](x)_{ab} \qquad (1.28)$$

with $\eta = \psi$ and $\zeta = H(m)\psi$, and

$$\bar{R}_\mu^{SW}[\zeta, \eta](x) = -\frac{\kappa \cdot c_{SW}}{4} \sum_{j=1}^{8} \left[R_\mu^{SW(j)}(x) \right]_{AT}, \tag{1.29}$$

where taking $\bar{\eta} = \gamma_5 \bar{\sigma}_{\mu\nu} \eta(x)$, each contribution depicted in Figure 2 is written as[2]

$$\begin{aligned}
R_\mu^{SW(1)}(x)_{ab} &= \sum_\nu [\zeta^\dagger(x)]_b [U_\mu(x) V_{\mu,+\nu}^\dagger(x) \bar{\eta}(x)]_a, & (1.30)\\
R_\mu^{SW(2)}(x)_{ab} &= \sum_\nu [\zeta^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)]_b [V_{\nu,+\mu}(x) \bar{\eta}(x+\hat{\nu})]_a, & (1.31)\\
R_\mu^{SW(3)}(x)_{ab} &= \sum_\nu [\zeta^\dagger(x+\hat{\mu}+\hat{\nu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)]_b [U_\mu(x) U_\nu(x+\hat{\mu}) \bar{\eta}(x+\hat{\mu}+\hat{\nu})]_a, & (1.32)\\
R_\mu^{SW(4)}(x)_{ab} &= \sum_\nu [\zeta^\dagger(x+\hat{\mu}) V_{\mu,+\nu}^\dagger(x)]_b [U_\mu(x) \bar{\eta}(x+\hat{\mu})]_a, & (1.33)\\
R_\mu^{SW(5)}(x)_{ab} &= -\sum_\nu [\zeta^\dagger(x)]_b [U_\mu(x) V_{\mu,-\nu}^\dagger(x) \bar{\eta}(x)]_a, & (1.34)\\
R_\mu^{SW(6)}(x)_{ab} &= -\sum_\nu [\zeta^\dagger(x-\hat{\nu}) U_\nu(x-\hat{\nu})]_b [V_{\nu,+\mu}^\dagger(x-\hat{\nu}) \bar{\eta}(x-\hat{\nu})]_a, & (1.35)\\
R_\mu^{SW(7)}(x)_{ab} &= -\sum_\nu [\zeta^\dagger(x-\hat{\nu}+\hat{\mu}) U_\mu^\dagger(x-\hat{\nu}) U_\nu(x-\hat{\nu})]_b & \\
&\qquad \times [U_\mu(x) U_\nu^\dagger(x+\hat{\mu}-\hat{\nu}) \bar{\eta}(x+\hat{\mu}-\hat{\nu})]_a, & (1.36)\\
R_\mu^{SW(8)}(x)_{ab} &= -\sum_\nu [\zeta^\dagger(x+\hat{\mu}) V_{\mu,-\nu}^\dagger(x)]_b [U_\mu(x) \bar{\eta}(x+\hat{\mu})]_a. & (1.37)
\end{aligned}$$

Force of preconditioned clover kernel:
For the preconditioned dynamical fermion, Eq. (1.18), the force is similarly obtained.

$$\begin{aligned}
\frac{d}{d\tau} S_{PF}^{(2)} &= \phi_2^\dagger \left\{ \dot{D}(m') Q(m)^{-1} D^\dagger(m') - D(m') Q(m)^{-1} D^\dagger(m) \dot{D}(m) Q(m)^{-1} D^\dagger(m') + h.c. \right\} \phi_2 \\
&= \left\{ \phi_2^\dagger \dot{D}(m') \psi_2 - [D(m)\psi_2]^\dagger \dot{D}(m) \psi_2 + h.c. \right\}, \qquad (1.38)
\end{aligned}$$

where $\psi_2 = Q(m)^{-1} D^\dagger(m') \phi_2$, and hence setting $\eta = \psi_2$ and $\zeta = 2\kappa' D(m)\psi_2 - 2\kappa\phi_2$, the same formulae (1.27) and (1.28) apply.

1.3 Even-odd preconditioning

Since the quark solver is most time consuming part of the simulations, it is quite important to improved the solver algorithm. In the case of clover quark operator, the even-odd preconditioning efficiently works. By decomposing the lattice sites into even and odd sites, the clover quark operator is expressed as

$$D = \begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix} = \begin{pmatrix} 1 - f_{ee} & M_{eo} \\ M_{oe} & 1 - f_{oo} \end{pmatrix} \tag{1.39}$$

[2] The above expressions, $R_\mu^{SW(2)}$, $R_\mu^{SW(3)}$, $R_\mu^{SW(6)}$, and $R_\mu^{SW(7)}$ were modified from the ver.1.1, to adjust to the stout smearing recursion formula.

where M_{ee} and M_{oo} are composed of only the nearest neighbor interaction, and D_{ee} and D_{oo} are without inter-site interaction in which f_{ee} and f_{oo} concern the clover term. The linear equation to be solved is

$$\begin{pmatrix} D_{ee} & D_{eo} \\ D_{oe} & D_{oo} \end{pmatrix} \begin{pmatrix} x_e \\ x_o \end{pmatrix} = \begin{pmatrix} b_e \\ b_o \end{pmatrix}. \tag{1.40}$$

This leads to the equation for the even part,

$$(D_{ee} - M_{eo} D_{oo}^{-1} M_{oe}) = b'_e \equiv b_e - d_{eo} D_{oo}^{-1} b_o. \tag{1.41}$$

Once this equation is solved, the odd part of the solution is easily obtained as

$$x_o = D_{oo}^{-1}(b_o - D_{oe} x_e). \tag{1.42}$$

Eq. (1.41) works as an incomplete LU precondioner, leading to better convergence than the original equation. In addition, the size of operation vectors is halved.

However, in the case of clover quark operator, the clover term makes the D_{oo}^{-1} operation much involved compared to the Wilson operator.

2 Stout smearing

In this section, we describe implementation of the stout smearing [11]. While the following construction mainly based on APE-type smearing, only small change is needed for fat link [12] and HYP smearing [13].

In the following, notation follows Ref. [11] as much as possible.

2.1 Smeared link

$$C_\mu(x) = \sum_{\nu\neq\mu} \rho_{\mu\nu} \left[U_\nu(x) U_\mu(x+\hat{\nu}) U_\nu^\dagger(x+\hat{\mu}) + U_\nu^\dagger(x-\hat{\nu}) U_\mu(x-\hat{\nu}) U_\nu(x-\hat{\nu}+\hat{\mu}) \right] \quad (2.1)$$

$$Q_\mu(x) = -i \left[\Omega_\mu(x)\right]_{AT} = \frac{i}{2}[\Omega_\mu^\dagger(x) - \Omega_\mu(x)] - \frac{i}{2N}\mathrm{Tr}[\Omega_\mu^\dagger(x) - \Omega_\mu(x)], \quad (2.2)$$

$$\Omega_\mu(x) = C_\mu(x) U_\mu^\dagger(x) \qquad \text{(no summation over } \mu) \quad (2.3)$$

$$U_\mu^{(k)}(x) = \exp\left[iQ_\mu^{(k-1)}(x) \right] U_\mu^{(k-1)}(x) \quad (2.4)$$

$$U \equiv U^{(0)} \to U^{(1)} \to U^{(2)} \to \cdots \to U^{(n)} \equiv \tilde{U}. \quad (2.5)$$

In practical code, it is convenient to treat $iQ_\mu(x)$ as a variable.

2.2 Representation for SU(3)

$\exp(iQ)$, where Q is hermitian and traceless matrix. Cayley-Hamiltonian theorem:

$$Q^3 - c_1 Q - c_0 I = 0, \quad (2.6)$$

where

$$c_0 = \det Q = \frac{1}{3}\mathrm{Tr}(Q^3) = \frac{i}{3}\mathrm{Tr}[(iQ)^3], \quad (2.7)$$

$$c_1 = \frac{1}{2}\mathrm{Tr}(Q^2) = -\frac{1}{2}\mathrm{Tr}[(iQ)^2] \geq 0. \quad (2.8)$$

$$(2.9)$$

The Hermiticity of Q requires $27c_0^2 - 4c_1 \leq 0$.

$$-c_0^{max} \leq c_0 \leq c_0^{max}, \qquad c_0^{max} = 2\left(\frac{c_1}{3}\right)^{3/2} \quad (2.10)$$

c_1 is also restricted as $0 \leq c_1^{max}$ due to the definition of Q (see the paper [11]).

$$\exp(iQ) = f_0 I + f_1 Q + f_2 Q^2 = f_0 I - i f_1 (iQ) - f_2 (iQ)^2. \quad (2.11)$$

Three complex valued scalar coefficients $f_j = f_j(c_0, c_1)$ are basis independent. f_j are represented as follows (for derivation see Ref. [11]).

$$f_j = \frac{h_j}{9u^2 - w^2}, \quad (2.12)$$

$$
\begin{aligned}
h_0 &= (u^2 - w^2)e^{2iu} + e^{-iu}[8u^2\cos(w) + 2iu(3u^2 + w^2)\xi_0], && (2.13)\\
h_1 &= 2ue^{2iu} - e^{-iu}[2u\cos(w) - i(3u^2 - w^2)\xi_0], && (2.14)\\
h_2 &= e^{2iu} - e^{-iu}[\cos(w) + 3iu\xi_0], && (2.15)
\end{aligned}
$$

where

$$
\begin{aligned}
u &= \sqrt{c_1/3}\cdot\cos(\theta/3), && (2.16)\\
w &= \sqrt{c_1}\cdot\sin(\theta/3), && (2.17)\\
\theta &= \arccos(c_0/c_0^{max}) && (2.18)\\
\xi_0(w) &= \frac{\sin w}{w}. && (2.19)
\end{aligned}
$$

Stable evaluation of ξ_0 requires some care.

2.3 HMC force

In HMC evolution, the following Hamiltonian is conserved:

$$
\mathcal{H} = \frac{1}{2}\mathrm{Tr}\left[P_\mu(x)^2\right] + S[U,\phi]. \quad (2.20)
$$

By differentiating with respect to ficticious time,

$$
\frac{d}{d\tau}\mathcal{H} = \mathrm{Tr}\left[\frac{dP_\mu(x)}{d\tau}P_\mu(x)\right] + \frac{d}{d\tau}S[U,\phi], \quad (2.21)
$$

$$
\frac{d}{d\tau}S[U,\phi] = \frac{dU^{ab}}{d\tau}\frac{\partial S[U,\phi]}{\partial U^{ab}} + \frac{dU^{\dagger ab}}{d\tau}\frac{\partial S[U,\phi]}{\partial U^{\dagger ab}} = 2\mathrm{ReTr}\left[iP_\mu(x)U_\mu(x)\Sigma_\mu(x)\right], \quad (2.22)
$$

where

$$
\Sigma_\mu(x)_{ab} = \frac{\partial S[U,\phi]}{\partial U^{ba}}. \quad (2.23)
$$

Defining the force field $R_\mu(x)$ with

$$
\frac{d}{d\tau}S[U,\phi] \equiv \sum_{x,\mu}\mathrm{Tr}\left[iP_\mu(x)R_\mu(x)\right], \quad (2.24)
$$

$$
R_\mu(x) = 2[U_\mu(x)\Sigma_\mu(x)]_{AT}, \quad (2.25)
$$

Hamilton equation reads

$$
\frac{d}{d\tau}iP_\mu(x) = R_\mu(x), \qquad \frac{d}{d\tau}U_\mu(x) = iP_\mu(x)U_\mu(x). \quad (2.26)
$$

For the stout smearing, HMC force can be calculated recursively.

$$
\frac{d}{d\tau}S^{(k)}_{stout}[\tilde{U}] = \sum_{x,\mu}2\mathrm{ReTr}\left[\Sigma^{(k)}_\mu(x)\frac{d}{d\tau}U^{(k)}_\mu(x)\right], \quad (2.27)
$$

$$
\frac{d}{d\tau}U^{(k)}_\mu(x) = \frac{d}{d\tau}\left[e^{iQ^{(k-1)}_\mu(x)}\cdot U^{(k-1)}_\mu(x)\right] \quad (2.28)
$$

Since the right hand side of Eq. (2.28) is expressed in terms of $U_\mu^{(k)}$, recursion formula

$$\begin{aligned}\mathrm{ReTr}\left[\Sigma_\mu^{(k)}(x)\frac{d}{d\tau}U_\mu^{(k)}(x)\right] &= \mathrm{ReTr}\left[\Sigma_\mu^{(k-1)}(x)\frac{d}{d\tau}U_\mu^{(k-1)}(x)\right] = \cdots \\ &= \mathrm{ReTr}\left[\Sigma_\mu^{(0)}(x)\frac{d}{d\tau}U_\mu^{(0)}(x)\right] = \mathrm{ReTr}\left[iP_\mu(x)U_\mu(x)\Sigma_\mu^{(0)}(x)\right] \qquad (2.29)\end{aligned}$$

In the following, variables with (k) and $(k-1)$ are denoted with and without $'$, respectively.

$$\begin{aligned}\frac{d}{d\tau}e^{iQ_\mu(x)} &= \frac{d}{d\tau}\left(f_0 + f_1 Q + f_2 Q^2\right) \\ &= \frac{df_0}{d\tau} + \frac{df_1}{d\tau} + \frac{df_2}{d\tau} + f_1\frac{dQ}{d\tau} + f_2\frac{dQ}{d\tau}Q + f_2 Q\frac{dQ}{d\tau} \qquad (2.30)\end{aligned}$$

f_j depends on τ via u and w,

$$\frac{df_j}{d\tau} = \frac{\partial f_j}{\partial u}\frac{du}{d\tau} + \frac{\partial f_j}{\partial w}\frac{dw}{d\tau}, \qquad (2.31)$$

and u and w via c_0 and c_1 as

$$\frac{du}{d\tau} = \frac{\partial u}{\partial c_0}\frac{dc_0}{d\tau} + \frac{\partial u}{\partial c_1}\frac{dc_1}{d\tau}, \qquad \frac{dw}{d\tau} = \frac{\partial w}{\partial c_0}\frac{dc_0}{d\tau} + \frac{\partial w}{\partial c_1}\frac{dc_1}{d\tau}. \qquad (2.32)$$

Then using the expressions for c_0 and c_1 with Q lead to

$$\begin{aligned}\frac{dc_0}{d\tau} &= \frac{1}{3}\frac{d}{d\tau}\mathrm{Tr}(Q^3) = \mathrm{Tr}\left(Q^2\frac{dQ}{d\tau}\right), \\ \frac{dc_1}{d\tau} &= \frac{1}{2}\frac{d}{d\tau}\mathrm{Tr}(Q^2) = \mathrm{Tr}\left(Q\frac{dQ}{d\tau}\right). \qquad (2.33)\end{aligned}$$

By explicit calculation,

$$\begin{aligned}\frac{\partial u}{\partial c_0} &= \frac{1}{2(9u^2-w^2)}, \qquad \frac{\partial u}{\partial c_1} = \frac{u}{(9u^2-w^2)}, \\ \frac{\partial w}{\partial c_0} &= \frac{-3u}{2w(9u^2-w^2)}, \qquad \frac{\partial w}{\partial c_1} = \frac{3u^2-w^2}{2w(9u^2-w^2)}, \qquad (2.34)\end{aligned}$$

and then $df_j/d\tau$ is expressed as

$$\frac{df_j}{d\tau} = b_{1j}\mathrm{Tr}\left(Q\frac{dQ}{d\tau}\right) + b_{2j}\mathrm{Tr}\left(Q^2\frac{dQ}{d\tau}\right) \qquad (2.35)$$

by defining

$$\begin{aligned}b_{1j} &= \frac{2ur_j^{(1)} + (3u^2-w^2)r_j^{(2)} - 2(15u^2+w^2)f_j}{2(9u^2-w^2)^2}, \qquad (2.36) \\ b_{2j} &= \frac{r_j^{(1)} - 3ur_j^{(2)} - 24uf_j}{2(9u^2-w^2)^2}, \qquad (2.37)\end{aligned}$$

where

$$r_j^{(1)} = \frac{\partial h_j}{\partial u}, \qquad r_j^{(2)} = \frac{1}{w}\frac{\partial h_j}{\partial w} \qquad (2.38)$$

are explicitly read as

$$\begin{aligned} r_0^{(1)} &= 2[u+i(u^2-w^2)]e^{2iu} \\ &\quad +2e^{-iu}\{4u(2-iu)\cos(w)+[u(3u^2+w^2)+i(9u^2+w^2)]\xi_0(w)\}, && (2.39) \\ r_1^{(1)} &= 2(1+2iu)e^{2iu}+e^{-iu}\{-2(1-iu)\cos(w)+(3u^2-w^2+6iu)\xi_0(w)\}, && (2.40) \\ r_2^{(1)} &= 2ie^{2iu}+ie^{-iu}\{\cos(w)-3(1-iu)\xi_0(w)\}, && (2.41) \\ r_0^{(2)} &= -2e^{2iu}+2iue^{-iu}\{\cos(w)+(1+4iu)\xi_0(w)+3u^2\xi_1(w)\}, && (2.42) \\ r_1^{(2)} &= -ie^{-iu}\{\cos(w)+(1+2iu)\xi_0(w)-3u^2\xi_1(w)\}, && (2.43) \\ r_2^{(2)} &= e^{-iu}\{\xi_0(w)-3iu\xi_1(w)\}, && (2.44) \end{aligned}$$

with

$$\xi_0(w) = \frac{\sin(w)}{w}, \qquad \xi_1(w) = \frac{\cos(w)}{w^2} - \frac{\sin(w)}{w^3}. \tag{2.45}$$

Defining

$$B_i = b_{i0} + b_{i1}Q + b_{i2}Q^2, \tag{2.46}$$

$$\frac{dU'}{d\tau} = e^{iQ}\frac{dU}{d\tau} + \left\{ \mathrm{Tr}\left[Q\frac{dQ}{d\tau}\right]B_1 + \mathrm{Tr}\left[Q^2\frac{dQ}{d\tau}\right]B_2 + f_1\frac{dQ}{d\tau} + f_2\frac{dQ}{d\tau}Q + f_2Q\frac{dQ}{d\tau}\right\}U. \tag{2.47}$$

Thus

$$\mathrm{ReTr}\left(\Sigma'\frac{dU'}{d\tau}\right) = \mathrm{ReTr}\left(\Sigma' e^{iQ}\frac{dU}{d\tau}\right) - \mathrm{ReTr}\left(i\Lambda\frac{d\Omega}{d\tau}\right), \tag{2.48}$$

$$\Lambda = [\Gamma]_{HT} = \frac{1}{2}(\Gamma+\Gamma^\dagger) - \frac{1}{2N_c}\mathrm{Tr}(\Gamma+\Gamma^\dagger), \tag{2.49}$$

$$\Gamma = \mathrm{Tr}(U\Sigma' B_1)Q + \mathrm{Tr}(U\Sigma' B_2)Q^2 + f_1 U\Sigma' + f_2 QU\Sigma' + f_2 U\Sigma' Q. \tag{2.50}$$

For numerical implementation, instead of Λ, $i\Lambda = [i\Gamma]_{AT}$ is a convenient variable. Final expression of $\Sigma_\mu(x)$ is obtained by refering to an explicit form of the smearing scheme. For the APE type smearing,

$$\begin{aligned} \Sigma_\mu(x) &= \Sigma'_\mu(x)\left[f_0 I + f_1 Q_\mu(x) + f_2 Q_\mu^2(x)\right] + iC_\mu^\dagger(x)\Lambda_\mu(x) \\ &\quad + i\sum_{\nu\neq\mu}\Big\{ -\rho_{\nu\mu}U_\nu(x+\hat\mu)U_\mu^\dagger(x+\hat\nu)U_\nu^\dagger(x)\Lambda_\nu(x) \\ &\qquad + \rho_{\nu\mu}\Lambda_\nu(x+\hat\mu)U_\nu(x+\hat\mu)U_\mu^\dagger(x+\hat\nu)U_\nu^\dagger(x) \\ &\qquad - \rho_{\mu\nu}U_\nu(x+\hat\mu)U_\mu^\dagger(x+\hat\nu)\Lambda_\mu(x+\hat\nu)U_\nu^\dagger(x) \\ &\qquad - \rho_{\mu\nu}U_\nu^\dagger(x-\hat\nu+\hat\mu)U_\mu^\dagger(x-\hat\nu)\Lambda_\mu(x-\hat\nu)U_\nu(x-\hat\nu) \\ &\qquad + \rho_{\nu\mu}U_\nu^\dagger(x-\hat\nu+\hat\mu)U_\mu^\dagger(x-\hat\nu)\Lambda_\nu(x-\hat\nu)U_\nu(x-\hat\nu) \\ &\qquad - \rho_{\nu\mu}U_\nu^\dagger(x-\hat\nu+\hat\mu)\Lambda_\nu(x-\hat\nu+\hat\mu)U_\mu^\dagger(x-\hat\nu)U_\nu(x-\hat\nu)\Big\}. \end{aligned} \tag{2.51}$$

2.4 Smeared clover fermion force

The force of the clover fermions, Eqs. (1.27) (1.28) must be changed in accord with the recursion formula (2.29). This is most simply done by multiplying $U_\mu^\dagger(x)$ to $\bar R_\mu^W(x)$ and $\bar R_\mu^{SW}(x)$ without taking antihermitian-traceless operation[3].

[3] This is temporary setting. For performance reason, the formulae should be changed in accord with the recursion formula in near future.

3 HYP smearing

3.1 General form of HYP smearing

The HYP smearing was introduced in Ref. [13]. It was applied to HMC update algorithm in Ref. [14], in the form of normalized-HYP defined in the following. BMW collaboration has used the stout-HYP smearing and call it HEX smearing [15].

The HYP smearing is composed of consecutive smearing and projection as

$$\begin{aligned}
C^{(1)}_{\mu;\nu\rho}(x) &= \frac{\alpha_3}{2}\sum_{\pm\sigma\neq\mu,\nu,\rho} U_\sigma(x)U_\mu(x+\hat{\sigma})U^\dagger_\sigma(x+\hat{\mu}) &(3.1)\\
V^{(1)}_{\mu;\nu\rho}(x) &= P[\alpha_3; C^{(1)}_{\mu;\nu\rho}(x), U_\mu(x)] &(3.2)\\
C^{(2)}_{\mu;\nu}(x) &= \frac{\alpha_2}{4}\sum_{\pm\rho\neq\mu,\nu} V^{(1)}_{\rho;\mu\nu}(x)V^{(1)}_{\mu;\nu\rho}(x+\hat{\rho})V^{(1)\dagger}_{\rho;\mu\nu}(x+\hat{\mu}) &(3.3)\\
V^{(2)}_{\mu;\nu}(x) &= P[\alpha_2; C^{(2)}_{\mu;\nu}(x), U_\mu(x)] &(3.4)\\
C^{(3)}_{\mu}(x) &= \frac{\alpha_1}{6}\sum_{\pm\nu\neq\mu} V^{(2)}_{\nu;\mu}(x)V^{(2)}_{\mu;\nu}(x+\hat{\nu})V^{(2)\dagger}_{\nu;\mu}(x+\hat{\mu}) &(3.5)\\
V_\mu(x) &= P[\alpha_1; C^{(3)}_\mu(x), U_\mu(x)] &(3.6)
\end{aligned}$$

where the indices after semicolon is the excluded directions. $P\left[\alpha; C, U\right]$ represents a projection of C to SU(N). The following three kinds of projection operators are frequently used.

Maximum SU(N) projection:

$$\Omega_\mu(x) = (1-\alpha)U_\mu(x) + C_\mu(x), \tag{3.7}$$

$$P\left[\alpha; C_\mu(x), U_\mu(x)\right] = \max_{V\in SU(N)} \mathrm{ReTr}(V\Omega^\dagger). \tag{3.8}$$

Unitary normalization (how is it called?):

$$V = \Omega(\Omega^\dagger\Omega)^{-1/2} \tag{3.9}$$

Stout projection:

$$P\left[\alpha; C_\mu(x), U_\mu(x)\right] = \exp\left([C_\mu(x)U^\dagger_\mu(x)]_{AT}\right)U_\mu(x). \tag{3.10}$$

Using the same notation as the last section,

$$\begin{aligned}
P\left[\alpha; C_\mu(x), U_\mu(x)\right] &= \exp\left[iQ_\mu(x)\right]U_\mu(x), &(3.11)\\
iQ_\mu(x) &= [\Omega_\mu(x)]_{AT}, \qquad \Omega_\mu(x) = C_\mu(x)U^\dagger_\mu(x) &(3.12)
\end{aligned}$$

HYP smearing with these projections are sometimes called projected-HYP, normalized-HYP, and stout-HYP, respectively.

3.2 HMC force of stout-HYP smearing

The force of stout-HYP smeared fermion operator can be obtained recursively just as same as the stout-APE smearing derived in the last section.

3rd to 2nd level recursion:

$$V_\mu(x) = \exp\left[iQ_\mu^{(3)}(x)\right] U_\mu(x), \tag{3.13}$$

$$iQ_\mu^{(3)}(x) = \left[C_\mu^{(3)}(x)U_\mu^\dagger(x)\right]_{AT} \tag{3.14}$$

$$C_\mu^{(3)}(x) = \frac{\alpha_1}{6}\sum_{\nu\neq\mu}\Big[\, V_{\nu;\mu}^{(2)}(x)V_{\mu;\nu}^{(2)}(x+\hat\nu)V_{\nu;\mu}^{(2)\dagger}(x+\hat\mu) + V_{\nu;\mu}^{(2)\dagger}(x-\hat\nu)V_{\mu;\nu}^{(2)}(x-\hat\nu)V_{\nu;\mu}^{(2)}(x-\hat\nu+\hat\mu)\Big] \tag{3.15}$$

where $\alpha_3' = \alpha_3/6$. The recursion formula reads

$$\sum_{x,\mu}\mathrm{ReTr}\left(\Sigma_\mu'(x)\frac{dV_\mu(x)}{d\tau}\right) = \sum_{x,\mu}\mathrm{ReTr}\left(\Xi_\mu^{(3)}(x)\frac{dU_\mu(x)}{d\tau} + \sum_{\nu\neq\mu}\Sigma_{\mu;\nu}^{(3)}(x)\frac{dV_{\mu;\nu}^{(2)}(x)}{d\tau}\right) \tag{3.16}$$

$$\Xi_\mu^{(3)}(x) = \Sigma_\mu'(x)e^{iQ_\mu^{(3)}(x)} + C_\mu^{(3)\dagger}(x)i\Lambda_\mu^{(3)}(x) \tag{3.17}$$

$$\begin{aligned}\Sigma_{\mu;\nu}^{(3)}(x) = i\,\frac{\alpha_1}{6}\Big\{ & -V_{\nu;\mu}^{(2)}(x+\hat\mu)V_{\mu;\nu}^{(2)\dagger}(x+\hat\nu)U_\nu^\dagger(x)\Lambda_\nu^{(3)}(x)\\ & -V_{\nu;\mu}^{(2)\dagger}(x-\hat\nu+\hat\mu)U_\mu^\dagger(x-\hat\nu)\Lambda_\mu^{(3)}(x-\hat\nu)V_{\nu;\mu}^{(2)}(x-\hat\nu)\\ & +V_{\nu;\mu}^{(2)\dagger}(x-\hat\nu+\hat\mu)V_{\mu;\nu}^{(2)\dagger}(x-\hat\nu)\Lambda_\nu^{(3)}(x-\hat\nu)U_\nu(x-\hat\nu)\\ & +\Lambda_\nu^{(3)}(x+\hat\mu)U_\nu(x+\hat\mu)V_{\mu;\nu}^{(2)\dagger}(x+\hat\nu)V_{\nu;\mu}^{(2)\dagger}(x)\\ & -V_{\nu;\mu}^{(2)}(x+\hat\mu)U_\mu^\dagger(x+\hat\nu)\Lambda_\mu^{(3)}(x+\hat\nu)V_{\nu;\mu}^{(2)\dagger}(x)\\ & -U_\nu^\dagger(x-\hat\nu+\hat\mu)\Lambda_\nu^{(3)}(x-\hat\nu+\hat\mu)V_{\mu;\nu}^{(2)\dagger}(x-\hat\nu)V_{\nu;\mu}^{(2)}(x-\hat\nu)\Big\}\end{aligned} \tag{3.18}$$

where $i\Lambda_\mu^3(x)$ is determined from Σ_μ', $Q_\mu^{(3)}$, and U_μ using formulae Eqs. (2.49) and (2.50) in the previous section.

2nd to 1st level recursion:

$$V_{\mu;\nu}^{(2)}(x) = \exp\left[iQ_{\mu;\nu}^{(2)}(x)\right] U_\mu(x), \tag{3.19}$$

$$iQ_{\mu;\nu}^{(2)}(x) = \left[C_{\mu;\nu}^{(2)}(x)U_\mu^\dagger(x)\right]_{AT} \tag{3.20}$$

$$C_{\mu;\nu}^{(2)}(x) = \frac{\alpha_2}{4}\sum_{\rho\neq\mu\nu}\Big[\, V_{\rho;\nu\mu}^{(1)}(x)V_{\mu;\nu\rho}^{(1)}(x+\hat\rho)V_{\rho;\nu\mu}^{(1)\dagger}(x+\hat\mu) + V_{\rho;\nu\mu}^{(1)\dagger}(x-\hat\rho)V_{\mu;\nu\rho}^{(1)}(x-\hat\rho)V_{\rho;\nu\mu}^{(1)}(x-\hat\rho+\hat\mu)\Big]. \tag{3.21}$$

The recursion formula reads

$$\sum_{x,\mu,\nu\neq\mu}\mathrm{ReTr}\left(\Sigma_{\mu;\nu}^{(3)}(x)\frac{dV_{\mu;\nu}^{(2)}(x)}{d\tau}\right) = \sum_{x,\mu,\nu\neq\mu}\mathrm{ReTr}\left(\Xi_{\mu;\nu}^{(2)}(x)\frac{dU_\mu(x)}{d\tau} + \sum_{\rho\neq\mu\nu}\Sigma_{\mu;\nu\rho}^{(2)}(x)\frac{dV_{\mu;\nu\rho}^{(1)}(x)}{d\tau}\right) \tag{3.22}$$

$$\Xi^{(2)}_{\mu;\nu}(x) = \Sigma^{(3)}_{\mu;\nu}(x)e^{iQ^{(2)}_{\mu;\nu}(x)} + C^{(2)\dagger}_{\mu;\nu}(x)i\Lambda^{(2)}_{\mu;\nu}(x) \tag{3.23}$$

$$\begin{aligned}\Sigma^{(2)}_{\mu;\nu\rho}(x) = i\,\frac{\alpha_2}{4}\Big\{ & -V^{(1)}_{\rho;\nu\mu}(x+\hat{\mu})V^{(1)\dagger}_{\mu;\nu\rho}(x+\hat{\rho})U^{\dagger}_{\nu}(x)\Lambda^{(2)}_{\rho;\nu}(x) \\ & -V^{(1)\dagger}_{\rho;\nu\mu}(x-\hat{\rho}+\hat{\mu})U^{\dagger}_{\mu}(x-\hat{\rho})\Lambda^{(2)}_{\mu;\nu}(x-\hat{\rho})V^{(1)}_{\rho;\nu\mu}(x-\hat{\rho}) \\ & +V^{(1)\dagger}_{\rho;\nu\mu}(x-\hat{\rho}+\hat{\mu})V^{(1)\dagger}_{\mu;\nu\rho}(x-\hat{\rho})\Lambda^{(2)}_{\rho;\nu}(x-\hat{\rho})U_{\rho}(x-\hat{\rho}) \\ & +\Lambda^{(2)}_{\rho;\nu}(x+\hat{\mu})U_{\rho}(x+\hat{\mu})V^{(1)\dagger}_{\mu;\nu\rho}(x+\hat{\rho})V^{(1)\dagger}_{\rho;\nu\mu}(x) \\ & -V^{(1)}_{\rho;\nu\mu}(x+\hat{\mu})U^{\dagger}_{\mu}(x+\hat{\rho})\Lambda^{(2)}_{\mu;\nu}(x+\hat{\rho})V^{(1)\dagger}_{\rho;\nu\mu}(x) \\ & -U^{\dagger}_{\rho}(x-\hat{\rho}+\hat{\mu})\Lambda^{(2)}_{\rho;\nu}(x-\hat{\rho}+\hat{\mu})V^{(1)\dagger}_{\mu;\nu\rho}(x-\hat{\rho})V^{(1)}_{\rho;\nu\mu}(x-\hat{\rho})\Big\}\end{aligned} \tag{3.24}$$

where $i\Lambda^{(2)}_{\mu;\nu}(x)$ is determined from $\Sigma^{(3)}_{\mu;\nu}$, $Q^{(2)}_{\mu;\nu}$, and U_μ using formulae Eqs. (2.49) and (2.50) in the previous section. Note that while $V^{(1)}_{\mu;\nu\rho} = V^{(1)}_{\mu;\rho\nu}$ holds, $\Sigma^{(2)}_{\mu;\nu\rho} \neq \Sigma^{(2)}_{\mu;\rho\nu}$ because of $\Lambda^{(2)}_{\mu;\nu}$ and $\Lambda^{(2)}_{\rho;\nu}$ in the above equation.

1st level recursion:

$$V^{(1)}_{\mu;\nu\rho}(x) = \exp\left[iQ^{(1)}_{\mu;\nu\rho}(x)\right]U_\mu(x), \tag{3.25}$$

$$iQ^{(1)}_{\mu;\nu\rho}(x) = \left[C^{(1)}_{\mu;\nu\rho}(x)U^{\dagger}_{\mu}(x)\right]_{AT} \tag{3.26}$$

$$\begin{aligned}C^{(1)}_{\mu;\nu\rho}(x) = \frac{\alpha_3}{2}\sum_{\sigma\neq\mu\nu\rho}\Big[& U_\sigma(x)U_\mu(x+\hat{\sigma})U^{\dagger}_{\sigma}(x+\hat{\mu}) \\ & + U^{\dagger}_{\sigma}(x-\hat{\sigma})U_\mu(x-\hat{\sigma})U_\sigma(x-\hat{\sigma}+\hat{\mu})\Big]\end{aligned} \tag{3.27}$$

The recursion formula reads

$$\begin{aligned}&\sum_{x,\mu,\nu\neq\mu,\rho\neq\mu\nu}\mathrm{ReTr}\left(\Sigma^{(2)}_{\mu;\nu\rho}(x)\frac{dV^{(1)}_{\mu;\nu\rho}(x)}{d\tau}\right) \\ &= \sum_{x,\mu,\nu\neq\mu,\rho\neq\mu\nu}\mathrm{ReTr}\left(\Xi^{(1)}_{\mu;\nu\rho}(x)\frac{dU_\mu(x)}{d\tau} + \sum_{\sigma\neq\mu\nu\rho}\Sigma^{(1)}_{\mu;\nu\rho\sigma}(x)\frac{dU_\mu(x)}{d\tau}\right)\end{aligned} \tag{3.28}$$

$$\Xi^{(1)}_{\mu}(x) = \Sigma^{(2)}_{\mu;\nu\rho}(x)e^{iQ^{(1)}_{\mu;\nu\rho}(x)} + C^{(1)\dagger}_{\mu;\nu\rho}(x)i\Lambda^{(1)}_{\mu;\nu\rho}(x) \tag{3.29}$$

$$\begin{aligned}\Sigma^{(1)}_{\mu;\nu\rho\sigma}(x) = i\,\frac{\alpha_3}{2}\Big\{ & -U_\sigma(x+\hat{\mu})U^{(1)\dagger}_{\mu}(x+\hat{\rho})U^{\dagger}_{\sigma}(x)\Lambda^{(1)}_{\sigma;\nu\rho}(x) \\ & -U^{\dagger}_{\sigma}(x-\hat{\sigma}+\hat{\mu})U^{\dagger}_{\mu}(x-\hat{\sigma})\Lambda^{(1)}_{\mu;\nu\rho}(x-\hat{\sigma})U_\sigma(x-\hat{\sigma}) \\ & +U^{\dagger}_{\sigma}(x-\hat{\sigma}+\hat{\mu})U^{\dagger}_{\sigma}(x-\hat{\sigma})\Lambda^{(1)}_{\sigma;\nu\rho}(x-\hat{\sigma})U_\sigma(x-\hat{\sigma}) \\ & +\Lambda^{(1)}_{\sigma;\nu\rho}(x+\hat{\mu})U_\sigma(x+\hat{\mu})U^{\dagger}_{\mu}(x+\hat{\rho})U^{\dagger}_{\sigma}(x) \\ & -U_\sigma(x+\hat{\mu})U^{\dagger}_{\mu}(x+\hat{\sigma})\Lambda^{(1)}_{\mu;\nu\rho}(x+\hat{\sigma})U^{(1)\dagger}_{\sigma}(x) \\ & -U^{\dagger}_{\sigma}(x-\hat{\sigma}+\hat{\mu})\Lambda^{(1)}_{\sigma;\nu\rho}(x-\hat{\sigma}+\hat{\mu})U^{\dagger}_{\mu}(x-\hat{\sigma})U_\sigma(x-\hat{\sigma})\Big\}\end{aligned} \tag{3.30}$$

where $i\Lambda^{(1)}_{\mu;\nu\rho}(x)$ is determined from $\Sigma^{(2)}_{\mu;\nu\rho}$, $Q^{(1)}_{\mu;\nu\rho}$, and U_μ using formulae Eqs. (2.49) and (2.50) in the previous section. Note that $\Lambda^{(1)}_{\mu;\nu\rho} \neq \Lambda^{(1)}_{\mu;\rho\nu}$ because of $\Sigma^{(2)}_{\mu;\nu\rho} \neq \Sigma^{(2)}_{\mu;\rho\nu}$.

All level recursion formula Now combining all the three levels of recursion together, we arrive at

$$\sum_{x,\mu} \mathrm{ReTr}\left(\Sigma'_\mu(x)\frac{dV_\mu(x)}{d\tau}\right) = \sum_{x,\mu} \mathrm{ReTr}\left(\Sigma_\mu(x)\frac{dU_\mu(x)}{d\tau}\right), \tag{3.31}$$

$$\Sigma_\mu(x) = \Xi^{(3)}_\mu(x) + \sum_{\nu\neq\mu}\left[\Xi^{(2)}_{\mu;\nu}(x) + \sum_{\rho\neq\mu\nu}\left(\Xi^{(1)}_{\mu;\nu\rho}(x) + \sum_{\sigma\neq\mu\nu\rho}\Sigma^{(1)}_{\mu;\nu\rho\sigma}(x)\right)\right]. \tag{3.32}$$

A Notation of γ-matrices

We use the hermitian representation of the Euclidean γ matrices which satisfy

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}, \qquad \gamma_\mu^\dagger = \gamma_\mu, \tag{1.1}$$

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4. \tag{1.2}$$

The tensor components are defined as

$$\sigma_{\mu\nu} = -\frac{i}{2}[\gamma_\mu, \gamma_\nu]. \tag{1.3}$$

Dirac representation:

$$\gamma_j = \begin{pmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{pmatrix}, \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \gamma_5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \tag{1.4}$$

where σ_j are 2×2 Pauli matrices and I is the unit matrix.

Chiral representation:

$$\gamma_j = \begin{pmatrix} 0 & -i\sigma_j \\ i\sigma_j & 0 \end{pmatrix}, \gamma_4 = \begin{pmatrix} 0 & -I \\ -I & 0 \end{pmatrix}, \gamma_5 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{1.5}$$

References

[1] K. Symanzik, Nucl. Phys. B **226** (1983) 187; Nucl. Phys. B **226** (1983) 205.

[2] For a review, see M. Luscher, "Chiral gauge theories revisited," arXiv:hep-th/0102028.

[3] A. Ukawa [CP-PACS and JLQCD Collaborations], Nucl. Phys. Proc. Suppl. **106** (2002) 195.

[4] B. Sheikholeslami and R. Wohlert, Nucl. Phys. B **259** (1985) 572.

[5] M. Luscher, JHEP **0305** (2003) 052 [arXiv:hep-lat/0304007].

[6] M. Luscher, Comput. Phys. Commun. **165** (2005) 199 [arXiv:hep-lat/0409106].

[7] The International Lattice DataGrid, `http://www.lqcd.org/ildg/`.

[8] M. Hasenbusch, Phys. Lett. B **519** (2001) 177 [arXiv:hep-lat/0107019].

[9] J. C. Sexton and D. H. Weingarten, Nucl. Phys. B **380** (1992) 665.

[10] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *NUMERICAL RECIPES in FORTRAN, 2nd ed.* (Cambridge Univ. Press, 1986,1992).

[11] C. Morningstar and M. J. Peardon, Phys. Rev. D **69** (2004) 054501 [arXiv:hep-lat/0311018].

[12] T. Blum *et al.*, Phys. Rev. D **55** (1997) 1133 [arXiv:hep-lat/9609036].

[13] A. Hasenfratz and F. Knechtli, Phys. Rev. D **64** (2001) 034504 [arXiv:hep-lat/0103029].

[14] A. Hasenfratz, R. Hoffmann and S. Schaefer, JHEP **0705** (2007) 029 [arXiv:hep-lat/0702028].

[15] S. Durr *et al.*, JHEP **1108** (2011) 148 [arXiv:1011.2711 [hep-lat]].