New one-flavor hybrid Monte Carlo simulation method for lattice fermions with γ_5 hermiticity

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ABSTRACT

We propose a new method for Hybrid Monte Carlo (HMC) simulations with odd numbers of dynamical fermions on the lattice. It employs a different approach from polynomial or rational HMC. In this method, γ_5 hermiticity of the lattice Dirac operators is crucial and it can be applied to Wilson, domain-wall, and overlap fermions. We compare HMC simulations with two degenerate flavors and $(1 + 1)$ degenerate flavors using optimal domain-wall fermions. The ratio of the efficiency, (number of accepted trajectories)/(simulation time), is about $3 : 2$. The relation between pseudofermion action of chirally symmetric lattice fermions in four-dimensional (overlap) and five-dimensional (domain-wall) representation are also analyzed.

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1. Introduction

In hybrid Monte Carlo simulations [1], the positive-definiteness of the action is essential to consider it as the statistical weight. When a lattice Dirac operator D is given, a positive-definite action of two degenerate flavors is easily constructed by using the hermitian conjugate of D, namely $D^\dagger D$. The major difference of two-flavor simulations and $(2 + 1)$-flavor simulations is that one cannot easily write down the pseudofermion action for the one-flavor sector. Polynomial or rational HMC methods [2,3], which approximates the square root of $D^\dagger D$, are mostly used for odd flavor simulations.

In this Letter, we provide a pseudofermion action for the one-flavor sector of the lattice fermions with γ_5 hermiticity without invoking the square root approximation for $D^\dagger D$. The main idea is very simple. For any lattice Dirac operators D with γ_5 hermiticity, $P_+ D P_+$ and $P_-(1/D)P_-$ are hermitian, and one can construct a one-flavor pseudofermion action using these. The resultant action has the same determinant as D without any approximations. The non-trivial parts are to first check the positive-definiteness of the pseudofermion action and the discussion of how to obtain the pseudofermion action when there are mass preconditioners like the one in Hasenbusch method.

The construction of the Letter is as follows. In Sections 2–5, the application to Wilson fermions, Wilson fermions with mass preconditioner, domain-wall type fermions and overlap fermions are demonstrated, respectively. In Section 6, the relation between the pseudofermion action in four- and five-dimensional representations are presented. Numerical results are given in Section 7, while a summary and conclusion are provided in Section 8.

2. Wilson fermions

In this section, we derive a pseudofermion action which will yield the same determinant as the Wilson–Dirac operator,

$$
\begin{aligned}
D_W(m) &= (W + m)\mathbf{1} + \sum_\mu t_\mu \gamma_\mu \\
&= \begin{pmatrix} (W + m)\mathbf{1}_{2\times2} & \sum_\mu t_\mu \sigma_\mu \\ \sum_\mu t_\mu \sigma_\mu^\dagger & (W + m)\mathbf{1}_{2\times2} \end{pmatrix},
\end{aligned} \tag{1}
$$

where

$$
W = -\frac{1}{2}\sum_\mu \left[U_\mu(x)\delta_{x+\hat\mu,y} + U_\mu^\dagger(x-\mu)\delta_{x-\hat\mu,y} \right] + 4,
$$

$$
t_\mu = \frac{1}{2}\left[U_\mu(x)\delta_{x+\hat\mu,y} - U_\mu^\dagger(x-\mu)\delta_{x-\hat\mu,y} \right],
$$

$$
\gamma_\mu = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu^\dagger & 0 \end{pmatrix}, \quad \sigma_\mu = (i\mathbf{1}_{2\times2}, \sigma_i),
$$

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$\mathbf{1}_{2\times 2}$ is two-by-two unit matrix and σ_i $(i = 1, 2, 3)$ are Pauli matrices. Throughout this work, we use chiral basis for gamma matrices. To get positive-definite pseudofermion action, we use a determinant relation which is valid for general matrix,

$$\det D_W(m) \cdot \det\big(P'_- D_W(m)^{-1} P'^{\dagger}_-\big) = \det\big(P'_+ D_W(m) P'^{\dagger}_+\big) \qquad (2)$$

where $P'_{+/-}$ are the projectors which reduce two chiral components into one chiral sector, $P'_+ = (1\ \ 0)$, $P'_- = (0\ \ 1)$. The operators $(P'_- D_W(m)^{-1} P'^{\dagger}_-)$ and $(P'_+ D_W(m) P'^{\dagger}_+)$ are hermitian due to γ_5 symmetry. When the inverse of $(W + m)$ is well-defined, the determinant of (1) is written as

$$\det D_W(m) = \det\big(P'_+ D_W(m) P'^{\dagger}_+\big) \cdot \det\left(\frac{1}{P'_- D_W(m)^{-1} P'^{\dagger}_-}\right)$$

$$= \det(W + m)^2 \det W_H(m), \qquad (3)$$

such that $W_H(m)$ is the Schur complement of $D_W(m)$, i.e.,

$$W_H(m) = \frac{1}{P'_- D_W^{-1} P'^{\dagger}_-}$$

$$= (W + m)\mathbf{1}_{2\times 2} - \sum_{\mu,\nu} t_\mu \frac{1}{W + m} t_\nu \sigma^{\dagger}_\mu \sigma_\nu. \qquad (4)$$

Thus, the pseudofermion action for one-flavor Wilson fermions can be written as

$$S_{\text{PF}} = \Phi^{\dagger}_1 (W + m)^{-2} \Phi_1 + \Phi^{\dagger}_2 \big(W_H(m)\big)^{-1} \Phi_2$$

$$= \Phi^{\dagger}_1 (W + m)^{-2} \Phi_1 - \Phi^{\dagger}_2 P'_- H_W(m)^{-1} P'^{\dagger}_- \Phi_2 \qquad (5)$$

where $H_W(m) = \gamma_5 D_W(m)$, Φ_1 is a pseudofermion field without a Dirac index, and Φ_2 is a pseudofermion field with two spinor components.

The positive-definiteness of the operator $W_H(m)$ are discussed as follows. We note that for any background gauge field, the eigenvalues of W and $(\sigma \cdot t)$ satisfy the inequalities[1]: $0 \leqslant \lambda(W) \leqslant 8$, and $|\lambda(\sigma \cdot t)| \leqslant 4$. It then follows that $W_H(m)$ is positive-definite for $m > 4$. Now, consider decreasing m from 4 to a smaller value. If the operator $W_H(m)$ is not positive for some m, e.g. m', then there must exist values of m at which $\det(W_H(m))$ is zero or singular in the region $m' < m < 4$. Among these values, if we denote the largest one as m_{cr}, then for $m > m_{cr}$, the positive-definiteness of $W_H(m)$ is assured.

The value m_{cr} corresponds to the opposite sign of the smallest eigenvalue of W. To see this, we use a relation,[2]

$$\lambda_{\min}(W) \leqslant \text{Re}\big(\lambda\big(D_W(0)\big)\big) \leqslant \lambda_{\max}(W). \qquad (6)$$

From this relation, one can see that the value of m which makes $\det(W_H(m))$ singular (i.e. $\det(W + m) = 0$) is larger than the value of m which satisfies $\det(D_W(m)) = \det(W_H(m)) = 0$. There are no values of m which satisfy $\det(W_H(m)) = 0$ or $\det(W_H(m)) = \pm\infty$ above that. The condition for the positive-definiteness of $W_H(m)$ can then be written as

$$m_{cr} = m^*_0 \quad \text{s.t.} \quad \det\big(W + m^*_i\big) = 0, \quad m^*_0 > m^*_1 > m^*_2 > \cdots,$$

$$\phi^{\dagger} W_H(m)\phi > 0 \quad \text{for any } \phi \text{ and for } m > m_{cr}. \qquad (7)$$

The smallest mass one can use in the one-flavor method here is restricted by this bound. But it can be relaxed by using Hasenbusch's preconditioner as discussed in the next section.

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[1] Throughout this work, $\lambda(X)$ means any one of the eigenvalues of an operator X.
[2] The proof of this relation is given in Appendices A–D.

2.1. Generating pseudofermion fields

To generate the pseudofermion field Φ_2 from a Gaussian random noise field Ξ_2, we need to take the square root of $W_H(m)$, i.e., $\Phi_2 = \sqrt{W_H(m)}\Xi_2$. This can be approximated by using the rational function of $W_H(m)$,

$$\Phi_2 = f_{\text{app}}\big(W_H(m)\big)$$

$$\overset{\text{def}}{=} \left(p_0 + \sum_{l=1}^{N_{\text{app}}} \frac{p_l}{(q_l + W + m)\mathbf{1}_{2\times 2} - \sum_{\mu,\nu} t_\mu \frac{1}{W+m} t_\nu \sigma^{\dagger}_\mu \sigma_\nu}\right)\Xi_2$$

$$\simeq \sqrt{W_H(m)}\Xi_2, \qquad (8)$$

where p_0, p_l and q_l are expressed in terms of Jacobian elliptic functions. At first glance, the operations in (8) look formidable. However, since $W_H(m)$ is the Schur complement of $D_W(m)$, the inversion of the operator within the summation, in Eq. (8) can be obtained by the inversions of the operator $(D_W(m) + q_l P_-)$, i.e.,

$$\begin{pmatrix} 0 \\ \Phi_2 \end{pmatrix} = P_- \left(p_0 + \sum_{l=1}^{N_{\text{app}}} p_l \big(D_W(m) + q_l P_-\big)^{-1}\right)\begin{pmatrix} 0 \\ \Xi_2 \end{pmatrix}. \qquad (9)$$

Note that one cannot apply the multi-shift solver in Eq. (9), since P_- does not commute with $D_W(m)$. However, for a given N_{app} number of inversions, the total number of iterations in the solver can be reduced by using the same idea as the chronological inversion method [4]. When one solves a set of linear equations $(D_W(m) + q_l P_+)\eta_l = \Xi_2$ $(1 \leqslant l \leqslant N_{\text{app}})$ with a given Ξ_2 serially from smaller l by using the iterative method, one can set a better initial guess $\eta^{(0)}_l$ for the iterative method to solve $(D_W(m) + P_+)\eta_l = \Xi_2$ $(2 \leqslant l)$ by using a linear combination of the solutions η_j $(j < l)$ which have already been calculated i.e. $\eta^{(0)}_l = \sum_{j<l} c_{lj}\eta_j$. The coefficients c_{lj} are determined according to the prescription written in Ref. [4].

In this one-flavor method, generating pseudofermions using the approximation given by Eq. (8) makes the simulation not exact. However, without using higher degrees of the approximation, one can make the algorithm exact by adding an accept/reject step after generating the pseudofermion field. In the exact algorithm, the pseudofermion field should be produced according to a probability distribution proportional to $e^{-\phi^{\dagger} \frac{1}{W_H(m)} \phi}$. This is obtained by multiplying the operator $\sqrt{W_H(m)}$ to a Gaussian noise field Ξ. In practice, however, the operator one uses in the simulation is approximated by $f_{\text{app}}(W_H(m))$ rather than $\sqrt{W_H(m)}$. This leads to a probability distribution that is proportional to $e^{-\phi^{\dagger} \frac{1}{f_{\text{app}}(W_H(m))^2} \phi}$. To adjust the difference, one can add an accept/reject step for ϕ with the probability $e^{-\phi^{\dagger}(\frac{1}{W_H(m)} - \frac{1}{f_{\text{app}}(W_H(m))^2})\phi}$. This factor should be smaller than 1 and can be enforced by choosing $f_{\text{app}}(x) > \sqrt{x}$ for the whole eigenvalue region of $W_H(m)$. The discussion using eigenvectors is given in Appendices A–D.

3. Wilson fermions with the Hasenbusch method

The idea of the Hasenbusch method [5] is to factorize the determinant $\det(D_W(m_1))$ into a product of determinants,

$$\det D_W(m_1) = \det\big(D_W(m_1)/D_W(m_2)\big) \cdot \det\big(D_W(m_2)\big) \qquad (10)$$

and the pseudofermion force coming from $\det(D_W(m_1)/D_W(m_2))$ is updated less frequently than the one coming from $\det(D_W(m_2))$ in the molecular dynamics steps. The parameter m_2 is chosen such that the simulation cost is reduced. Furthermore, as already

mentioned, in the one-flavor method for Wilson fermions presented here, the factorization of the determinant allows us to use a smaller fermion mass in the simulation. For the second factor $\det(D_W(m_2))$, the same argument as in Section 2 can be applied. Here, we assume that $m_1 < m_2$ and that m_2 is large enough such that the positive-definiteness of $W_H(m_2)$ is always assured.

Now, we consider how to treat the first factor $\det(D_W(m_1)/D_W(m_2))$. Naively, one might consider the pseudofermion action like,

$$\phi_1^\dagger \left(\frac{W+m_2}{W+m_1}\right)^2 \phi_1 + \phi_2^\dagger \left(W_H(m_2)\frac{1}{W_H(m_1)}\right)\phi_2 \tag{11}$$

but the second term is not hermitian in general, because $W_H(m_1)W_H(m_2) \neq W_H(m_2)W_H(m_1)$ for $m_1 \neq m_2$. To remedy this situation, we rewrite the determinant $\det(D_W(m_1))/(D_W(m_2))$ by using an operator which has different masses for the chirality plus and chirality minus sector, i.e.,

$$\left[\det\left(\frac{D_W(m_1)}{D_W(m_2)}\right)\right]^{-1}$$
$$= \det\left((D_W(0) + P_+ m_1 + P_- m_2)\frac{1}{D_W(m_1)}\right)$$
$$\cdot \det\left(D_W(m_2)\frac{1}{D_W(0) + P_+ m_1 + P_- m_2}\right). \tag{12}$$

One may note that the first and the second factor on the right-hand side are the same as the determinant of,

$$1 + (m_2 - m_1)P'_- \frac{1}{D_W(m_1)}P'^{\dagger}_-,$$
$$1 + (m_2 - m_1)P'_+ \frac{1}{D_W(0) + m_1 P_+ + m_2 P_-}P'^{\dagger}_+, \tag{13}$$

respectively. Then, the pseudofermion action is written as

$$S_{\text{PF}} = \Phi_3^\dagger \Phi_3 + \Phi_4^\dagger \Phi_4 + (m_2 - m_1)\Phi_3^\dagger P'_- \frac{1}{D_W(m_1)}P'^{\dagger}_- \Phi_3$$
$$+ (m_2 - m_1)\Phi_4^\dagger P'_+ \frac{1}{D_W(0) + m_1 P_+ + m_2 P_-}P'^{\dagger}_+ \Phi_4 \tag{14}$$

where Φ_3 and Φ_4 are pseudofermion fields with two spinor components.

The condition for the positive-definiteness is given as follows. When $m_1 = m_2$, the operators in Eq. (13) are the identity operators and their positive-definiteness is trivial. When one decreases m_1 with m_2 fixed, the positive-definiteness will be lost only if either of the determinants in Eq. (12) becomes zero or singular. Thus, up to the largest m_1 which satisfies $\det(D_W(0) + m_1 P_+ + m_2 P_-) = 0$, the positive-definiteness of the operators in Eq. (13) are assured. Note that this mass value is smaller than the limit given in Eq. (7). This can be seen by using the eigenvalue relation which is similar to Eq. (6),

$$\lambda_{\min}(W + m_1) \leqslant \text{Re}\big(\lambda\big(D_W(0) + m_1 P_+ + m_2 P_-\big)\big)$$
$$\leqslant \lambda_{\max}(W + m_2). \tag{15}$$

The largest m_1 which yields $\det(D_W(0) + m_1 P_+ + m_2 P_-) = 0$ is larger than the largest m which yields $\det D_W(m) = 0$. This can be understood from

$$\gamma_5\big(D_W(0) + m_1 P_+ + m_2 P_-\big) = H_W\left(\frac{m_1 + m_2}{2}\right) + \frac{m_1 - m_2}{2} \tag{16}$$

and the properties of spectral flows of $H_W(m)$ [6]. Moreover, for some gauge configurations, $\det(D_W(m))$ may not be zero for any value of m. But there must exist m_1 which satisfies $\det(D_W(0) + m_1 P_+ + m_2 P_-) = 0$ for any gauge configurations.

4. Domain-wall fermions

The domain-wall type fermion operator [7] can be expressed as,

$$\mathcal{D}_{\text{dwf}}(m) = \boldsymbol{\omega} D_W(-m_0)\big(1 + cL(m)\big) + \big(1 - L(m)\big) \tag{17}$$

with $L(m) = P_+ L_+(m) + P_- L_-(m)$ such that,

$$L_+(m)_{s,s'} = \begin{cases} \delta_{s',s-1}, & 1 < s \leqslant N_s, \\ -m\delta_{s',N_s}, & s = 1, \end{cases}$$
$$L_-(m)_{s,s'} = \begin{cases} \delta_{s',s+1}, & 1 \leqslant s < N_s, \\ -m\delta_{s',1}, & s = N_s, \end{cases} \tag{18}$$

where m is the (bare) fermion mass, and $m_0 \in (0, 2)$ is a parameter called the "domain-wall height". The label s is the coordinate in the fifth dimension. Throughout this work, we assume that the number of sites in the fifth dimension N_s is even. The constant c and the diagonal matrix $\boldsymbol{\omega} = \text{diag}\{\omega_s\}$ specify the type of domain-wall fermion. The operator $\mathcal{D}_{\text{dwf}}(m)$ is the conventional domain-wall fermion for $c = 0$ and $\omega_s = 1$. It becomes an optimal domain-wall fermion when $c = 1$ and ω_s's are tuned such that maximal chiral symmetry is obtained.

To obtain the pseudofermion action for one-flavor, we modify the operator $\mathcal{D}_{\text{dwf}}(m)$ by multiplying $1/(1 + cL)$ from the right.

$$\mathcal{D}'_{\text{dwf}}(m) \overset{\text{def}}{=} \mathcal{D}_{\text{dwf}}(m)/(1 + cL) = \boldsymbol{\omega} D_W(-m_0) + M(m, c) \tag{19}$$

with

$$M(m, c) = \frac{1 - L(m)}{1 + cL(m)}$$
$$= \frac{1 - L_+(m)}{1 + cL_+(m)}P_+ + \frac{1 - L_-(m)}{1 + cL_-(m)}P_-$$
$$= M_+(m, c)P_+ + M_-(m, c)P_-. \tag{20}$$

In the following, we suppress the argument c of $M_\pm(m, c)$ for simplicity. Using the Schur decomposition, the determinant of the operator $\mathcal{D}'_{\text{dwf}}(m)$ can be written as

$$\det \mathcal{D}'_{\text{dwf}}(m) = \det\big[\boldsymbol{\omega}(W - m_0) + M_+(m)\big]^2 \det \mathcal{W}_H(m)$$
$$= \det\big[\boldsymbol{\omega}(W - m_0) + M_-(m)\big]^2 \det \overline{\mathcal{W}}_H(m), \tag{21}$$

where

$$\mathcal{W}_H(m) = R_5\bigg(\big[\boldsymbol{\omega}(W - m_0) + M_-(m)\big]\mathbf{1}_{2\times2}$$
$$- t_\mu \frac{1}{\boldsymbol{\omega}(W - m_0) + M_+(m)}t_\nu \sigma_\mu^\dagger \sigma_\nu\bigg), \tag{22}$$

$$\overline{\mathcal{W}}_H(m) = R_5\bigg(\big[\boldsymbol{\omega}(W - m_0) + M_+(m)\big]\mathbf{1}_{2\times2}$$
$$- t_\mu \frac{1}{\boldsymbol{\omega}(W - m_0) + M_-(m)}t_\nu \sigma_\mu \sigma_\nu^\dagger\bigg). \tag{23}$$

Here R_5 is the reflection operator in the fifth dimension, $(R_5)_{s,s'} = \delta_{s,N_s+s'-1}$, which is introduced such that $\mathcal{W}_H(m)$ and $\overline{\mathcal{W}}_H(m)$ are hermitian. For optimal domain-wall fermions, one still can choose ω_s's which maintain maximal chiral symmetry and satisfies $\omega_{N_s+1-s} = \omega_s$. After incorporating the contributions of the Pauli–Villars fields, the fermion determinant for domain-wall fermions becomes,

$$\frac{\det \mathcal{D}_{\text{dwf}}(m)}{\det \mathcal{D}_{\text{dwf}}(1)} = \frac{\det[\boldsymbol{\omega}(W - m_0) + M_+(m)]^2 \det \mathcal{W}_H(m)}{\det[\boldsymbol{\omega}(W - m_0) + M_+(1)]^2 \det \overline{\mathcal{W}}_H(1)}. \quad (24)$$

In principle, one can use a pseudofermion action like,

$$S_{\text{PF}}^{(\text{separate})}$$

$$= \Phi_1^\dagger \big[\boldsymbol{\omega}(W - m_0) + M_+(1) \big] \frac{1}{[\boldsymbol{\omega}(W - m_0) + M_+(m)]^2}$$

$$\times \big[\boldsymbol{\omega}(W - m_0) + M_+(1) \big] \Phi_1 + \Phi_2^\dagger \frac{1}{\mathcal{W}_H(m)} \Phi_2$$

$$+ \Phi_3^\dagger \overline{\mathcal{W}}_H(1) \Phi_3. \quad (25)$$

But it is known that in the two-flavor simulation of domain-wall fermions, it is effective when a pseudofermion action uses a single set of pseudofermion field to estimate both the light fermion and Pauli–Villars terms [8]. Then, we use the same technique used in Hasenbusch method for Wilson fermions, i.e., to use a lattice Dirac operator which has different masses on chirality plus and chirality minus sectors.

Using the Schur decomposition of $[\mathcal{D}_{\text{dwf}}(1) - (M_+(1) - M_+(m))P_+]$, we obtain the relation

$$\det\big[\boldsymbol{\omega}(W - m_0) + M_+(m)\big]^2 \cdot \det\big[\mathcal{W}_H(m) + \Delta_-(m)\big]$$

$$= \det\big[\boldsymbol{\omega}(W - m_0) + M_-(1)\big]^2 \cdot \det\big[\overline{\mathcal{W}}_H(1) - \Delta_+(m)\big], \quad (26)$$

where

$$\big[\Delta_+(m)\big]_{s,s'} = \big[R_5\big(M_+(1) - M_+(m)\big)\big]_{s,s'},$$

$$\big[\Delta_-(m)\big]_{s,s'} = \big[R_5\big(M_-(1) - M_-(m)\big)\big]_{s,s'}. \quad (27)$$

The properties of these matrices are given in Appendices A–D. Using (26), we can write the inverse of (24) as

$$\det\left[1 + \Delta_-(m) \frac{1}{\mathcal{W}_H(m)} \right] \cdot \det\left[1 + \Delta_+(m) \frac{1}{\overline{\mathcal{W}}_H(1) - \Delta_+(m)} \right], \quad (28)$$

and it can be used to construct the pseudofermion action. Using (B.6), we can simplify (28) to

$$\det \mathcal{A} \cdot \det \mathcal{B} \quad (29)$$

where,

$$\mathcal{A} \overset{\text{def}}{=} \left(1 + g'(m, 1, c)(v^\dagger R_5)_s \left[\frac{1}{\mathcal{W}_H(m)} \right]_{s,s'} (R_5 v)_{s'} \right),$$

$$\mathcal{B} \overset{\text{def}}{=} \left(1 + g'(m, 1, c)(v^\dagger)_s \left[\frac{1}{\overline{\mathcal{W}}_H(1) - \Delta_+(m)} \right]_{s,s'} v_{s'} \right). \quad (30)$$

The constant g' and vector v are given in Eq. (B.6) and (B.4). In the following, the arguments of g' are suppressed for simplicity ($g' = g'(m, 1, c)$). Note that the five-dimensional matrix in Eq. (28) is reduced to a four-dimensional matrix in this expression. Thus we can write the pseudofermion action for one-flavor domain-wall fermions as

$$S_{\text{PF}} = \Phi_1^\dagger \mathcal{A} \Phi_1 + \Phi_2^\dagger \mathcal{B} \Phi_2$$

$$= \Phi_1^\dagger \Phi_1 - g' \Phi_1^\dagger P_-'(v^\dagger R_5)_s \left[\frac{1}{\gamma_5 R_5 \mathcal{D}_{\text{dwf}}'(m)} \right]_{s,s'}$$

$$\times (R_5 v)_{s'} P_-'^\dagger \Phi_1 + \Phi_2^\dagger \Phi_2 + g' \Phi_2^\dagger P_+'(v^\dagger)_s$$

$$\times \left[\frac{1}{\gamma_5 R_5 \mathcal{D}_{\text{dwf}}'(1) - \Delta_+(m)P_+} \right]_{s,s'} v_{s'} P_+'^\dagger \Phi_2 \quad (31)$$

where Φ_1 and Φ_2 are the pseudofermion fields (on the four-dimensional lattice) with two spinor components.

Now we assert that the operators in (29) are positive-definite for $0 < m \leqslant 1$. At $m = 1$, they are equal to the identity operator, and thus are positive-definite. As m is decreased, the operators in (29) will cease to be positive-definite only if either of the determinants in (29) becomes zero or singular. Using $[W, \frac{1}{\sqrt{\boldsymbol{\omega}}} M_-(1) \frac{1}{\sqrt{\boldsymbol{\omega}}}] = [W, \frac{1}{\sqrt{\boldsymbol{\omega}}} M_+(m) \frac{1}{\sqrt{\boldsymbol{\omega}}}] = 0$, and the fact that the eigenvalues of $\frac{1}{\sqrt{\boldsymbol{\omega}}} M_-(1) \frac{1}{\sqrt{\boldsymbol{\omega}}}$ and $\frac{1}{\sqrt{\boldsymbol{\omega}}} M_+(m) \frac{1}{\sqrt{\boldsymbol{\omega}}}$ are not real[3] for $0 < m \leqslant 1$. We immediately see that $(\boldsymbol{\omega}(W - m_0) + M_-(1))$ and $(\boldsymbol{\omega}(W - m_0) + M_+(m))$ cannot have a zero eigenvalue for $0 < m \leqslant 1$. Thus the operators in (29) are well-defined for $0 < m \leqslant 1$. Furthermore, since (28) is equal to the determinant of the four-dimensional Dirac operator with the approximation for the sign function of $H_{\text{kernel}} = \gamma_5 D_W (2 + (1 - c)D_W)^{-1}$, the determinant cannot be zero and it follows that the operators in (29) are positive-definite for $0 < m \leqslant 1$.

4.1. Generating pseudofermion field

We now discuss how to approximate the inverse square root of the operators $\widehat{\mathcal{A}}$ and $\widehat{\mathcal{B}}$ when one generates the pseudofermion fields Φ_1 and Φ_2 from the Gaussian noise. Focusing on Eq. (35), we start from the inverse relation of five-dimensional operators,

$$\big[(\overline{\mathcal{W}}_H(m) + \alpha \widehat{\Delta}_+) / (\overline{\mathcal{W}}_H(m) + \beta \widehat{\Delta}_+) \big]^{-1}$$

$$= (\overline{\mathcal{W}}_H(m) + \beta \widehat{\Delta}_+) / (\overline{\mathcal{W}}_H(m) + \alpha \widehat{\Delta}_+), \quad (32)$$

$$\left(1 + (\beta - \alpha) \widehat{\Delta}_+ \frac{1}{\overline{\mathcal{W}}_H(m) + \beta \widehat{\Delta}_+} \right)^{-1}$$

$$= 1 + (\alpha - \beta) \widehat{\Delta}_+ \frac{1}{\overline{\mathcal{W}}_H(m) + \alpha \widehat{\Delta}_+}. \quad (33)$$

Multiplying by $S^\dagger$ from the left and S from the right, one obtains

$$\left(1 + (\beta - \alpha) g' \, \text{diag}(0, \ldots, 0, 1) \widehat{S}^\dagger \frac{1}{\overline{\mathcal{W}}_H(m) + \beta \widehat{\Delta}_+} \widehat{S} \right)^{-1}$$

$$= 1 + (\alpha - \beta) g' \, \text{diag}(0, \ldots, 0, 1) \widehat{S}^\dagger \frac{1}{\overline{\mathcal{W}}_H(m) + \alpha \widehat{\Delta}_+} \widehat{S} \overset{\text{def}}{=} \mathcal{M}. \quad (34)$$

Here, $\mathcal{M}_{ss'} = 0$ for $s < s'$. Then, the relation, Eq. (34), also holds for the sub-block $(s, s') = (N_s, N_s)$,

$$\left(1 + (\beta - \alpha) g' v^\dagger \frac{1}{\overline{\mathcal{W}}_H(m) + \beta \widehat{\Delta}_+} v \right)^{-1}$$

$$= 1 + (\alpha - \beta) g' v^\dagger \frac{1}{\overline{\mathcal{W}}_H(m) + \alpha \widehat{\Delta}_+} v. \quad (35)$$

One can obtain a similar equation for $\mathcal{W}_H(m)$ and Δ_-.

For the square root of a general positive-definite operator A, the rational approximation can be used.

$$\sqrt{A} \sim p_0 + \sum_{i=1}^{n} \frac{p_i}{q_i + A}. \quad (36)$$

In the case of $\mathcal{A}$, one has to calculate

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[3] The eigenvalues of $L_\pm(m)$ are $(m)^{1/N_s} \exp(i\pi(2k + 1)/N_s)$ with integer k, $0 \leqslant k \leqslant (N_s - 1)$. Then, the eigenvalues of $M(m)$ are not real for $c \neq -1$.

$$\phi_1 = \left(1 + g'v^\dagger R_5 \left[\frac{1}{\mathcal{W}_H(m)}\right] R_5 v\right)^{-\frac{1}{2}} \Xi_1$$

$$= \left(1 - g'v^\dagger R_5 \left[\frac{1}{\mathcal{W}_H(m) + \Delta_-}\right] R_5 v\right)^{\frac{1}{2}} \Xi_1. \tag{37}$$

Each term of the summation in Eq. (36) is

$$\frac{p_i}{q_i + 1 - g'v^\dagger R_5 \frac{1}{\mathcal{W}_H(m)+\Delta_-} R_5 v}$$

$$= \frac{p_i}{1 + q_i}\left[1 + \frac{1}{1+q_i} g'v^\dagger R_5 \frac{1}{\mathcal{W}_H(m) + \frac{q_i}{1+q_i}\Delta_-} R_5 v\right] \tag{38}$$

$$= \frac{p_i}{1+q_i} + \frac{p_i}{(1+q_i)^2} g'v^\dagger R_5 \frac{1}{\mathcal{W}_H(m) + \frac{q_i}{1+q_i}\Delta_-} R_5 v \tag{39}$$

$$= \frac{p_i}{1+q_i} + \hat{p}_i g'v^\dagger R_5 \frac{1}{\mathcal{W}_H(m) + \hat{q}_i\Delta_-} R_5 v. \tag{40}$$

Then, to obtain ϕ_1 one needs to calculate

$$\sqrt{\frac{1}{\mathcal{A}}}\Xi_1 \sim \hat{p}_0 \Xi_1 + \sum_i^n \hat{p}_i g'v^\dagger R_5 \frac{1}{\mathcal{W}_H(m) + \hat{q}_i\Delta_-} R_5 v \Xi_1 \tag{41}$$

with,

$$\hat{p}_0 = p_0 + \sum_i^n \frac{p_i}{1+q_i}, \qquad \hat{p}_i = \frac{p_i}{(1+q_i)^2}, \qquad \hat{q}_i = \frac{q_i}{1+q_i}. \tag{42}$$

The same method can be used for the operator $\mathcal{B}$.

5. Overlap fermions

In this section, we construct the pseudofermion action for one-flavor overlap fermions [9],

$$D_{ov}(m) = 1 + m + (1-m)\gamma_5 \operatorname{sign}\big(H_W(-m_0)\big). \tag{43}$$

This operator satisfies Ginsparg–Wilson Relation (GWR) [10],

$$D_{ov}(m)^\dagger D_{ov}(m)$$
$$= (1-m^2)\big(D_{ov}(0)^\dagger + D_{ov}(0)\big) + 4m^2$$
$$= 2(1-m^2)\big(P_+ D_{ov}(0)P_+ + P_- D_{ov}(0)P_-\big) + 4m^2. \tag{44}$$

The overlap fermion also possesses γ_5 hermiticity, and so the application is similar to Wilson fermions. We begin by breaking this operator into its chiral components.

$$D_{ov}(m) = \begin{pmatrix} P'_+ D_{ov}(m)P'^\dagger_+ & P'_+ D_{ov}(m)P'^\dagger_- \\ P'_- D_{ov}(m)P'^\dagger_+ & P'_- D_{ov}(m)P'^\dagger_- \end{pmatrix}$$
$$\stackrel{\text{def}}{=} \begin{pmatrix} D_{++}(m) & D_{+-}(m) \\ D_{-+}(m) & D_{--}(m) \end{pmatrix}. \tag{45}$$

The determinant is written as,

$$\det\big(D_{ov}(m)\big)$$
$$= \det\big(D_{++}(m)\big)\det\left(D_{--}(m) - D_{-+}(m)\frac{1}{D_{++}(m)}D_{+-}(m)\right). \tag{46}$$

By using GWR, one can show that the operators on the right-hand side are positive-definite for $0 < m \leqslant 1$, provided that $D_{ov}(m)$ itself is well defined. The pseudofermion action is written as

$$\phi_1^\dagger \frac{1}{D_{++}(m)}\phi_1 + \phi_2^\dagger P'_- \frac{1}{D_{ov}(m)}P'^\dagger_- \phi_2. \tag{47}$$

Practically, one has to use a reflection/refraction [11] or topology fixing term [12] to treat or avoid singularities in $D_{ov}(m)$ related to the topological change.

The authors of [13] proposed a simulation method for one-flavor with overlap fermions. We now highlight the differences between their work and our work. In Ref. [13], the authors use GWR, and factorize $\det D_{ov}(m)^\dagger D_{ov}(m)$ into two parts.

$$\det D_{ov}(m)^\dagger D_{ov}(m)$$
$$= \det P'_+ D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_+ \cdot \det P'_- D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_- \tag{48}$$

The difference of the first factor and second factor of the right-hand side comes from the topological zero-mode of $D_{ov}(m)$. Then, the one-flavor determinant is written as

$$\det D_{ov}(m)$$
$$= \det P'_+ D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_+ \cdot m^{(N_+ - N_-)}$$
$$= \det P'_- D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_- \cdot m^{(N_- - N_+)}. \tag{49}$$

Here, $N_{+/-}$ are the numbers of topological zero-modes with a definite chirality. By using GWR, one obtains the relation between these operators and Schur complement,

$$P'_- D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_-$$
$$= D_{--}(m)\left(D_{--}(m) - D_{-+}(m)\frac{1}{D_{++}(m)}D_{+-}(m)\right). \tag{50}$$

In other words, in Eq. (46), the determinant is factorized as,

$$\det\big(D_{ov}(m)\big)$$
$$= \det\big(D_{++}(m)\big)\cdot \det\left(\frac{P'_- D_{ov}(m)^\dagger D_{ov}(m)P'^\dagger_-}{D_{--}(m)}\right)$$
$$= \det\big(D_{++}(m)\big)\cdot \det\left(\frac{2(1+m)D_{--}(m) - 4m}{D_{--}(m)}\right). \tag{51}$$

Later, we show that the second factor corresponds to the $\mathcal{A}$ term in Eq. (31). Due to the cancellation between the numerator and the denominator, the force for the $\mathcal{A}$ term in HMC is smaller than that of the $\mathcal{B}$ term.

When one performs a HMC simulation with a topological fixing term, it is apparent that using the pseudofermion action with the factorization in Eq. (49) is more effective than the factorization in Eq. (51). For the five-dimensional representation Eq. (31), using only the $\mathcal{B}$ term and choosing the fermion mass parameter m' to satisfy $(1-m') = (1-m^2)/m$, one can perform the HMC simulation respecting the factorization in Eq. (49).

6. The relation of the pseudofermion action with four- and five-dimensional representations

The ratio of determinants, Eq. (24), is equivalent to the determinant of the effective four-dimensional operator,

$$D_{4d}(m) = \frac{1}{2}(1+m) + \frac{1}{2}(1-m)\gamma_5 f\big(H_{kernel}(-m_0)\big), \tag{52}$$

where the function $f(x)$ is polar or a rational function which approximates the sign function. The form of the function f is determined by ω. The operator H_{kernel} is defined as,

$$H_{kernel}(-m_0) = \gamma_5 \frac{D_W(-m_0)}{2 - (1-c)D_W(-m_0)}. \tag{53}$$

By using the Schur decomposition, the one-flavor pseudofermion action is written as

Table 1
Comparison of HMC efficiency for the 2-flavor and $(1+1)$-flavor QCD with optimal domain-wall quarks. The step size for the gauge field $\Delta\tau_{\text{Gauge}}$ is 0.007(0.010) for $m = 0.019(0.038)$. While the step size $\Delta\tau_{\text{PF}}$ for $(1+1)$-flavor pseudofermions is 0.14(0.20) for $m = 0.019(0.038)$, which is 4 times larger than that for the 2-flavor case. Here, $N_{\text{Iter}}^{(\text{HB})}$, $N_{\text{Iter}}^{(\text{MD})}$, and $N_{\text{Iter}}^{(\text{Total})}$ are the average CG iterations for one trajectory (for generating initial pseudofermion fields, molecular dynamics, and their sum respectively).

m	N_{f}	$N_{\text{Iter}}^{(\text{HB})}/10^3$	$N_{\text{Iter}}^{(\text{MD})}/10^3$	$N_{\text{Iter}}^{(\text{Total})}/10^3$	Acceptance	Acceptance/$N_{\text{Iter}}^{(\text{Total})}$
0.019	$1+1$	75(1)	260(1)	345(1)	0.88(3)	$2.6(1) \times 10^{-6}$
	2	0.6(1)	239(2)	240(2)	0.90(3)	$3.8(2) \times 10^{-6}$
0.038	$1+1$	54(1)	125(1)	179(1)	0.90(3)	$5.0(2) \times 10^{-6}$
	2	0.6(1)	112(1)	113(1)	0.91(3)	$8.0(3) \times 10^{-6}$

$$\Phi_1^\dagger P' \frac{1}{D_{4d}(m)} P'^\dagger_- \Phi_1 + \Phi_2^\dagger \frac{1}{P'_+ D_{4d}(m) P'^\dagger_+} \Phi_2. \tag{54}$$

Examining two cases, $c = 0$ and $c = 1$, we show that the five-dimensional expression Eq. (31) reproduces Eq. (54). This equivalence is not only of theoretical value, but aids in practical simulations. When one generates ϕ_1 and ϕ_2, from Eq. (31), one has to know the eigenvalue spectrum of $\mathcal{A}$ and $\mathcal{B}$, a priori, in order to apply the rational approximation for the square root function. However, in the four-dimensional case, the spectrum is already known.

Case 1: $c = 0$

In this case, the propagator of the five-dimensional fermion at the boundary $s = 1$ or N_s yields the propagator of the four-dimension fermion [14],

$$D_{ch} + m \stackrel{\text{def}}{=} \frac{(1-m)D_{4d}}{1 - D_{4d}} = \frac{1 + \gamma_5 f(H_{\text{kernel}}(-m_0))}{1 - \gamma_5 f(H_{\text{kernel}}(-m_0))} + m, \tag{55}$$

$$\frac{1}{D_{ch} + m} = B \frac{1}{\mathcal{D}_{\text{dwf}}(m)} R_5 B^\dagger. \tag{56}$$

Here, B is defined as

$$B_s = P_- \delta_{1,s} + P_+ \delta_{N_s,s}. \tag{57}$$

This relation holds only for $c = 0$. Note that this operator satisfies chiral symmetry $D_{ch}\gamma_5 + \gamma_5 D_{ch} = 0$ in the limit $N_s \to \infty$, in which $f(x)$ becomes the sign function. From Eqs. (55) and (56),

$$P_- \left(\frac{1}{D_{4d}(m)} \right) P_- = P_- + (1-m) P_- \left[\frac{1}{\mathcal{D}_{\text{dwf}}(m)} \right]_{s=1, s'=N_s} P_-. \tag{58}$$

After incorporating the pseudofermion field, the left-hand side becomes the first term of Eq. (54). The right-hand side equals to the $\mathcal{A}$ term of Eq. (31) by substituting $g' = (1-m)$ and $v^\dagger = (0, \ldots, 0, 1)$.

Next, consider the $\mathcal{B}$ term. By using Eq. (35), one obtains,

$$1 + (1-m)v^\dagger \frac{1}{\overline{\mathcal{W}}_H(1) - \Delta_+(m)} v$$

$$= \left[1 - (1-m)v^\dagger \frac{1}{\overline{\mathcal{W}}_H(1)} v \right]^{-1}$$

$$= \left[1 - (1-m)P'_+ \frac{1}{D_{ch} + 1} P'^\dagger_+ \right]^{-1} = \left[P'_+ D_{4d} P'^\dagger_+ \right]^{-1} \tag{59}$$

where we used the relation $D_{4d}(m) = (D_{ch} + m)/(D_{ch} + 1)$.

Case 2: $c = 1$

In this case, there are relations for D_{4d} and five-dimensional operators [15],

$$\left[B\mathcal{D}_{\text{dwf}}(m)^{-1} \mathcal{D}_{\text{dwf}}(1) B^\dagger \right] = D_{4d}(m)^{-1}, \tag{60}$$

$$\left[B\mathcal{D}_{\text{dwf}}(1)^{-1} \mathcal{D}_{\text{dwf}}(m) B^\dagger \right] = D_{4d}(m). \tag{61}$$

By using the relations,

$$B(1 + cL(m))^{-1} = \frac{\sqrt{\lambda_c}}{1 + c^4 m} \left(P_+ v^\dagger + P_- v^\dagger R_5 \right), \tag{62}$$

$$\Delta(m)(1 + cL(m))B^\dagger = g(m, 1, c)\sqrt{\lambda_c}(P_+ v + P_- R_5 v), \tag{63}$$

one can show that Eq. (60), Eq. (61) and projector $P_{+/-}$ reproduce the operators in Eq. (30).

7. Numerical tests

We compare the efficiency of the HMC simulation for two-flavor and $(1+1)$-flavor QCD with domain-wall type fermion with $c = 1$ and $\omega_s = 1$, on a $12^3 \times 24 \times 16(N_s)$ lattice. For the gluon action, we use Iwasaki gauge action at $\beta = 2.30$. In the molecular dynamics, we use the Omelyan integrator [16], and the Sexton–Weingarten method [17]. The pseudofermion action for the two-flavor simulation is the one with even–odd preconditioning which is described in Ref. [18]. The time step for the gauge field, $(\Delta\tau_{\text{Gauge}})$, is the same for both two-flavor and $(1+1)$-flavor cases, while the time step $(\Delta\tau_{\text{PF}})$ for the pseudofermion fields in the $(1+1)$-flavor case is four times larger than that for the two-flavor case. The acceptance rate is roughly the same for both cases. We use conjugate gradient (CG) with mixed precision for the inversion of the quark matrix (with even–odd preconditioning). The length of each trajectory is set to two. After discarding 300 trajectories for thermalization, we accumulate 100 trajectories for the comparison of efficiency. Our results are given in Table 1. We see that the acceptance rate is almost the same for $(1+1)$-flavor and two-flavor simulations. If the auto-correlation time is the same, then the efficiency of HMC can be estimated by the total acceptance divided by the CG iteration number, and the efficiency ratio for two-flavor and $(1+1)$-flavor is about $3 : 2$.

From this study, one can speculate the performance of $(2+1)$-flavor simulations with two degenerate light flavors with bare mass $m = 0.019$ and a single heavy flavor with bare mass $m = 0.038$. Assume that one set the step size of light flavor as 0.025 and the step size of heavy flavor as 0.125 which is about two third of the value used in the study above to compensate the increase of total force due to the increase of flavors, while keeping the same trajectory length. Then, the total number of CG iterations in the molecular dynamics steps become 340 and 200 for light and heavy flavor, respectively. By including CG iterations in the heatbath part, it takes about 600 CG iterations in total for one sweep. Thus, the $(2+1)$-flavor simulation take 2.5 times more CG iterations than two-flavor simulations.

8. Concluding remarks

In this work, we presented one-flavor method for HMC. The largest difference of the method presented here from polynomial and rational HMC is that the pseudofermion action yields the one-flavor determinant without any approximations. Then the extra accept/reject step with noisy estimator, which is commonly used in polynomial or rational HMC to make the algorithm exact, is not needed. For the overlap fermion, the difference from the method

in Ref [13] is that this can be used even if GWR is not exact. For the lattice fermions with γ_5 symmetry, it is always possible to construct real (hermitian) pseudofermion action, but one has to careful about the positive-definiteness, since it depends on the type of lattice fermions used. For chirally symmetric fermions like domain-wall/overlap fermions, positive-definiteness is assured in the entire mass parameter region which can be used in two-flavor simulations. On the other hand, for Wilson fermions, there exist a bound for the smallest mass where the positive-definiteness is assured. If the bound is larger than the mass value which is intended to use, one has to add Hasenbusch mass preconditioner then one can push the mass smaller. Comparison between two-flavor and $(1 + 1)$-flavor using domain-wall type fermion HMC simulation shows that one can increase the step size of $(1 + 1)$-flavor simulation while keeping same acceptance ratio. The reason might be that for $(1 + 1)$-simulation it is effectively the same as using four-dimensional operator and the force from the bulk mode is completely cancelled between the light fermion and Pauli–Villars field, while for the two-flavor pseudofermion action used in the comparison in this work, the cancellation was done only partly. The bottle neck of this method is generating pseudofermion field from Gaussian noise and it should be tuned and improved. Not only HMC itself, one can use these pseudofermion action for reweighting method, for example, to adjust the strange quark mass or to see the effects due to the difference of up down sea quark mass by using existing configurations. This approach for one-flavor simulation should be investigated further numerically and theoretically.

Acknowledgements

Appendix A. The eigenvalue relation

We prove a relation between "eigenvalues of the real part" and "the real part of the eigenvalues" for a general matrix M.

$$\lambda_{\min}\big(\mathrm{Re}[M]\big) \leqslant \mathrm{Re}\big[\lambda(M)\big] \leqslant \lambda_{\max}\big(\mathrm{Re}[M]\big), \tag{A.1}$$

where $\lambda(M)$ can be any one of the eigenvalues of M, $\mathrm{Re}[M]$ is the real part of M, $\mathrm{Re}[M] \overset{\text{def}}{=} (M+M^\dagger)/2$, $\lambda_{\min}(\mathrm{Re}[M])$ and $\lambda_{\min}(\mathrm{Re}[M])$ are the smallest and the largest eigenvalue of $\mathrm{Re}[M]$, respectively.

Proof. The eigenvectors ϕ_i of $\mathrm{Re}[M]$ form an orthonormal basis,

$$\mathrm{Re}[M]\phi_i = h_i\phi_i, \qquad (\phi_i, \phi_j) = \delta_{i,j}. \tag{A.2}$$

Here, $(\ ,\ )$ means the inner product.

The eigenvectors ψ_i of M can be expressed in terms of the ϕ_i's as,

$$M\psi_i = \lambda_i\psi_i, \quad \psi_i = \sum_l c_l^{(i)}\phi_l. \tag{A.3}$$

Here, we set $(\psi_i, \psi_i) = 1$. This yields $\sum_l |c_l^{(i)}|^2 = 1$. The inner product of ψ_i and $M\psi_i$ gives the eigenvalue λ_i,

$$\lambda_i = (\psi_i, M\psi_i). \tag{A.4}$$

Then, we divide M into the real part $\mathrm{Re}[M]$ and the imaginary part $\mathrm{Im}[M] \overset{\text{def}}{=} (M - M^\dagger)/2$, and substitute these into Eq. (A.4),

$$\lambda_i = \big(\psi_i, \mathrm{Re}[M]\psi_i\big) + \big(\psi_i, \mathrm{Im}[M]\psi_i\big). \tag{A.5}$$

After taking the real part of this equation, only the first term remains,

$$\mathrm{Re}(\lambda_i) = \big(\psi_i, \mathrm{Re}[M]\psi_i\big). \tag{A.6}$$

By substituting Eq. (A.3) into the right-hand side of this equation, one obtains

$$\big(\psi_i, \mathrm{Re}[M]\psi_i\big) = \sum_{k,l}\big(c_k^{(i)}\big)^* c_l^{(i)}\big(\phi_k, \mathrm{Re}[M]\phi_l\big) = \sum_l |c_l^{(i)}|^2 h_l. \tag{A.7}$$

This is equal to or larger than smallest eigenvalue of $\mathrm{Re}[M]$,

$$\sum_l |c_l^{(i)}|^2 h_l - \lambda_{\min}\big(\mathrm{Re}[M]\big) = \sum_l |c_l^{(i)}|^2\big(h_l - \lambda_{\min}\big(\mathrm{Re}[M]\big)\big) \geqslant 0. \tag{A.8}$$

Thus, by using Eqs. (A.6)–(A.8), it is proven that $\mathrm{Re}[\lambda(M)]$ cannot be smaller than $\lambda_{\min}(\mathrm{Re}[M])$,

$$\lambda_{\min}\big(\mathrm{Re}[M]\big) \leqslant \mathrm{Re}\big[\lambda(M)\big]. \tag{A.9}$$

The other inequality in Eq. (A.1), $\mathrm{Re}[\lambda(M)] < \lambda_{\max}(\mathrm{Re}[M])$, can be proven in a similar way. □

Appendix B. Eigenvalues and eigenvectors of matrix $\Delta_\pm(m)$

Here, we derive the eigenvectors and the eigenvalues of $\Delta_+(m)$ defined in Eq. (27). We work explicitly on $N_s = 4$. After obtaining the answers for $N_s = 4$, to convert the answers for general N_s is straightforward.

Using the matrix $M_+(m, c)$, i.e.,

$$M_+(m, c) = (\mathbf{1} - L_+)(\mathbf{1} + cL_+)^{-1} = \frac{1 + \frac{1}{c}}{1 + cL_+} - \frac{\mathbf{1}}{c}, \tag{B.1}$$

the matrix $\Delta_+(m_1, m_2) \overset{\text{def}}{=} R_5[M_+(m_2) - M_-(m_1)]$ is written as,

$$\Delta_+(m_1, m_2) = R_5 \frac{1 + \frac{1}{c}}{1 + c^4 m_2}\begin{pmatrix} 1 & c^3 m_2 & -c^2 m_2 & c m_2 \\ -c & 1 & c^3 m_2 & -c^2 m_2 \\ c^2 & -c & 1 & c^3 m_2 \\ -c^3 & c^2 & -c & 1 \end{pmatrix}$$
$$- R_5 \frac{1 + \frac{1}{c}}{1 + c^4 m_1}\begin{pmatrix} 1 & c^3 m_1 & -c^2 m_1 & c m_1 \\ -c & 1 & c^3 m_1 & -c^2 m_1 \\ c^2 & -c & 1 & c^3 m_1 \\ -c^3 & c^2 & -c & 1 \end{pmatrix}$$
$$= g(m_1, m_2, c)\, Q\,(c).$$

Here, $g(m_1, m_2, c)$ and $Q\,(c)$ are defined as,

$$g(m_1, m_2, c) = \frac{(1 + c)(m_2 - m_1)}{(1 + c^4 m_1)(1 + c^4 m_2)},$$
$$Q = \begin{pmatrix} c^6 & -c^5 & c^4 & -c^3 \\ -c^5 & c^4 & -c^3 & c^2 \\ c^4 & -c^3 & c^2 & -c \\ -c^3 & c^2 & -c & 1 \end{pmatrix}. \tag{B.2}$$

The matrix $\Delta_+(m)$ in Eq. (27) is given by $\Delta_+(m) = \Delta_+(m, 1)$.

Eigenvalues and eigenvectors of Q are,

$$Q u_i = 0 \quad (i = 1, 2, 3),$$
$$Q v = \lambda_c v \quad \text{with } \lambda_c = c^6 + c^4 + c^2 + 1, \tag{B.3}$$
$$u_1 = \begin{pmatrix} 1 \\ c \\ 0 \\ 0 \end{pmatrix}, \qquad u_2 = \begin{pmatrix} 0 \\ 1 \\ c \\ 0 \end{pmatrix}, \qquad u_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ c \end{pmatrix},$$

$$v = \frac{1}{\sqrt{c^6 + c^4 + c^2 + 1}} \begin{pmatrix} -c^3 \\ c^2 \\ -c \\ 1 \end{pmatrix}. \tag{B.4}$$

Define unitary matrix S as

$$S = (u'_1 \quad u'_2 \quad u'_3 \quad v). \tag{B.5}$$

Here, u'_1, u'_2 and u'_3 are the vectors made by orthonormalization of u_1, u_2 and u_3. Then, $\Delta_+(m_1, m_2)$ is written as,

$$\begin{aligned} \Delta_+(m_1, m_2) &= g(m_1, m_2, c) S \, \mathrm{diag}(0, 0, 0, \lambda_c) S^\dagger \\ &= g'(m_1, m_2, c) S \, \mathrm{diag}(0, 0, 0, 1) S^\dagger, \end{aligned} \tag{B.6}$$

with $g'(m_1, m_2, c) = \lambda_c g(m_1, m_2, c)$.

The similar relation for $\Delta_-(m_1, m_2) = R_5 [M_-(m_2) - M_-(m_1)]$ is given by multiplying R_5 from left and right to this equation.

Appendix C. Exactness — Point of view with eigenvalues

Consider the eigenvalues and eigenvectors of the operator W_H

$$W_H \psi_i = h_i \psi_i. \tag{C.1}$$

The Gaussian noise field Ξ, and pseudo fermion field ϕ, are expressed as linear combination of the eigenvectors ψ_i

$$\Xi = \sum_i b_i \psi_i, \qquad \phi = \sum_i c_i \psi_i. \tag{C.2}$$

The path integral of ϕ is written as the product of integral w.r.t the coefficient c_i

$$\int d\phi^\dagger d\phi \, e^{-\phi^\dagger \frac{1}{W_H} \phi} = \int \prod_i dc_i^* dc_i \, e^{-\sum_i c_i^* \frac{1}{h_i} c_i}. \tag{C.3}$$

When b_i has a distribution $e^{-b_i^* b_i}$, one can make the distribution proportional to $e^{-c_i^* \frac{1}{h_i} c_i}$ by multiplying by $\sqrt{h_i}$, $c_i = \sqrt{h_i} b_i$.

On the other hand, constructing $c_i = f_{\mathrm{app}}(h_i) b_i$, the distribution become $e^{-c_i^* \frac{1}{f_{\mathrm{app}}(h_i)^2} c_i}$.

The difference can be adjusted by accept/reject step with the probability

$$e^{-c_i^* (\frac{1}{h_i} - \frac{1}{f_{\mathrm{app}}(h_i)^2}) c_i}. \tag{C.4}$$

To take this factor as a probability, this must be less than one, i.e., $f_{\mathrm{app}}(h_i) \geqslant \sqrt{h_i}$. This condition is understood that $e^{-c_i^* \frac{1}{f_{\mathrm{app}}(h_i)^2} c_i}$ has a slightly broader distribution than $e^{-c_i^* \frac{1}{\sqrt{h_i}} c_i}$, and the accept/reject step makes the distribution narrow by suppressing larger c_i.

Appendix D. Linear algebra

Here, we remind the readers some relations of linear algebra.

- Schur Decomposition

$$\begin{aligned} \begin{pmatrix} A & B \\ C & D \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ CA^{-1} & 1 \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{pmatrix} \begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 1 & BD^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} 1 & 0 \\ D^{-1}C & 1 \end{pmatrix}. \end{aligned} \tag{D.1}$$

- The Inversion of an Schur Complement

$$\begin{pmatrix} 0 \\ y \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} w \\ x \end{pmatrix} \Rightarrow y = (D - CA^{-1}B)x. \tag{D.2}$$

- Project-and-reduce Operator $P'_\pm$ in General γ-matrix Representations with Eigenvector $\phi_\pm$ of $P_\pm$

$$P_\pm \phi_\pm = \phi_\pm, \tag{D.3}$$

$$P_\pm \phi_\mp = 0, \tag{D.4}$$

$$P'_\pm V = (\phi_\pm, V), \quad V \text{ is a general vector.} \tag{D.5}$$

- The Determinant of an Operator with Projector $P_\pm$

$$\det P'_+ M P'^\dagger_+ = \det(P_+ M + P_-) = \det(M P_+ + P_-), \tag{D.6}$$

$$\begin{aligned} \det(M P_+ + P_-) &= \det\big(M(P_+ + M^{-1} P_-)\big) \\ &= \det(M) \det\big(P_+ + M^{-1} P_-\big) \\ &= \det(M) \det\big(P'_- M^{-1} P'^\dagger_-\big). \end{aligned} \tag{D.7}$$

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