PROCEEDINGS OF SCIENCE

$O(a^2)$ improvement of the overlap-Dirac operator

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We construct an $O(a^2)$-improved overlap-Dirac operator by designing an improved overlap kernel, based on the Symanzik improvement program. Field rotation terms are also identified to improve off-shell amplitudes for both massless and massive fermions. We check the free dispersion relation and propagator, and show that improved results become to close to the continuum ones at low momentum region. We test the effect of improvement on the full-QCD gauge configuration and find that the relativistic dispersion relation is satisfied within a few percent error up to $m_q a \approx 0.5$.

The XXVII International Symposium on Lattice Field Theory
July 26-31, 2009
Peking University, Beijing, China

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PoS(LAT2009)082

1. Introduction

Discretization effect is one of the most significant sources of the systematic error in lattice QCD calculations. The improvement of lattice action and operators have therefore been extensively studied since the early days of lattice field theory. The most well-known and widely used example is the clover fermion action [1], which removes the $O(a)$ error in the Wilson's original lattice fermion action. According to the Symanzik's improvement program [2], it adds a dimension-five operator to the lattice action to cancel the source of error of $O(a)$ present in the Wilson fermion action. A non-perturbative method to tune the parameter in the action has also been established later [3]. For further improvement, one has to add dimension-six and dimension-seven operators consecutively, as discussed in [4], for instance. These highly improved lattice actions are not so popular in the current lattice QCD simulations, since the action contains many terms with parameters to be tuned.

One of the reasons for the difficulty of designing highly improved lattice fermion operator is that the number of operators to be considered is large because of the explicit violation of the chiral symmetry in the Wilson fermion action. Indeed, the $O(a)$ term appears because of the chiral symmetry violation, while the chirally symmetric lattice actions do not have this contribution from the beginning as one cannot write down the relevant operator of dimension-five while preserving chiral symmetry. The same argument applies at $O(a^{2m+1})$ in general (for m a positive integer). In other words, if one starts the improvement program from chirally symmetric lattice actions, the first error one encounters is $O(a^2)$, and once it is removed, the next is $O(a^4)$. Therefore, the effect of improvement is much more dramatic than in the case of the improvement of the Wilson fermion. In fact, the $O(a^2)$-improvement of the staggered fermion has been worked out and used in numerical simulations [5]. It uses this property of chirally symmetric lattice fermion action. When used for heavy quarks, one can greatly accelerate the convergence to the continuum limit.

In this work we consider the $O(a^2)$-improvement of the overlap fermion [6]. The overlap fermion preserves exact chiral symmetry through the Ginsparg-Wilson relation [7]. Although the numerical cost is high in the practical use of the overlap fermion, dynamical fermion simulations have already been performed by the JLQCD and TWQCD collaborations, from which many interesting physics results have been obtained thanks to its excellent chiral property (for a recent summary, see [8]).

The improvement can be achieved by two steps, *i.e.* improvement of the action and the field rotation. Since the form of the overlap fermion is largely restricted by the Ginsparg-Wilson relation, improvement of the lattice action is done by modifying the kernel operator to be used to construct the overlap operator. To be explicit, we use the fermion action of Eguchi-Kawamoto [9] and Hamber-Wu [10], which is called the D34 action in the convention of [4]. Once we remove the Lorentz-violating discretization effects of $O(a^2)$ by this choice of the kernel operator, remaining errors can be removed by field rotations.

2. Formulation of the improved operator

The overlap operator in the massive case is defined by

$$D_{\rm ov}(m_q) = \left(1 - \frac{am_q}{2\rho}\right) D_{\rm ov} + m_q, \tag{2.1}$$

where the massless operator $D_{\rm ov}$ is given by

$$D_{\rm ov} = \frac{\rho}{a}\left(1+\frac{X}{\sqrt{X^\dagger X}}\right), \qquad X = D_{\rm w} - \frac{\rho}{a}. \tag{2.2}$$

The parameter ρ controls the large negative mass of the overlap kernel. The conventional choice for the kernel operator is that of the Wilson fermion $D_{\rm w}$, which is

$$D_{\rm w} = \sum_\mu (\gamma_\mu \nabla_\mu - \frac{1}{2} a \Delta_\mu) \sim \not{D} - \frac{a}{2} D^2 + O(a^2). \tag{2.3}$$

Near the continuum limit, it reduces to the continuum Dirac operator $\not{D}$ plus the $O(a)$ error coming from the Wilson term. ∇_μ and Δ_μ are first- and second-order covariant lattice derivatives, respectively.

Near the continuum limit, the overlap operator with the Wilson kernel becomes

$$D_{\rm ov} = \not{D} - \frac{a}{2\rho}\not{D}^2 + \frac{a^2}{6}\sum_\mu \gamma_\mu D_\mu^3 + \frac{a^2}{2\rho^2}\left(\not{D}^3 - \frac{\rho}{2}\{\not{D}, D^2\}\right) + O(a^3). \tag{2.4}$$

The $O(a)$ term can be simply removed by a field rotation proportional to $D_{\rm ov}$, while the $O(a^2)$ terms, especially the third term of right-hand side which violates the Lorentz symmetry, cannot be removed. The usual overlap operator thus has an $O(a^2)$ discretization error. To remove the Lorentz-violating term, we introduce the improved kernel, which is closer to the continuum limit $D'_{\rm w} \sim \not{D} + O(a^3)$. Then, the overlap operator takes a simple form up to $O(a^4)$ errors:

$$D'_{\rm ov} = \not{D} - \frac{a}{2\rho}\not{D}^2 + \frac{a^2}{2\rho^2}\not{D}^3 - \frac{3a^3}{8\rho^3}\not{D}^4 + O(a^4). \tag{2.5}$$

With this operator we can remove the unwanted terms up to and including the $O(a^3)$ term by a field rotation proportional to $D_{\rm ov}$, and the remaining errors start from $O(a^4)$.

As an improved kernel which has no $O(a)$ and $O(a^2)$ errors, we use the D34 action. Massless D34 action is defined by

$$D_{\rm D34} = \sum_\mu \nabla_\mu \left(1 - ba^2\Delta_\mu\right)\gamma_\mu + \sum_\mu ca^3 \Delta_\mu^2. \tag{2.6}$$

In order to remove the $O(a^2)$ error at tree level, b = 1/6. The parameter c is an arbitrary parameter to control the mass of doublers. We take c = 1/6 in the following. For the free case, this action has no $O(a)$ and $O(a^2)$ error, but it is no longer the case once the gauge interaction is turned on. In particular, the $O(a)$ term may arise as radiative corrections, and one has to add another term to cancel it. The explicit form of this action on the lattice is

$$\begin{aligned} aD_{\rm D34} = {} & 4\delta_{x,y} - \frac{2}{3}\sum_\mu \left[(1-\gamma_\mu)U_{\mu,x}\delta_{x+\mu,y} + (1+\gamma_\mu)U^\dagger_{\mu,x-\mu}\delta_{x-\mu,y}\right] \\ & + \frac{1}{12}\sum_\mu \left[(2-\gamma_\mu)U_{\mu,x}U_{\mu,x+\mu}\delta_{x+2\mu,y} + (2+\gamma_\mu)U^\dagger_{\mu,x-\mu}U^\dagger_{\mu,x-2\mu}\delta_{x-2\mu,y}\right]. \end{aligned} \tag{2.7}$$

We now consider the field rotation to remove the remaining discretization effects. Starting from the continuum action, $\int d^4x\ \bar{\psi}_c(x)(\not{D}+m_q)\psi_c(x)$ with fermion fields ψ_c and $\bar{\psi}_c$, one may define a rotation

$$\psi_c = \Omega_c \psi \qquad \bar{\psi}_c = \bar{\psi}\bar{\Omega}_c, \tag{2.8}$$

which produces the action $\int d^4x\ \bar{\psi}(x)D'_{\rm ov}(m_q)\psi(x)$ corresponding to (2.5). Namely, the rotation satisfy the relation $D'_{\rm ov}(m_q) = \bar{\Omega}_c(\not{D}+m_q)\Omega_c$. So far, the rotation matrices Ω_c and $\bar{\Omega}_c$ are written in terms of the continuum operator $\not{D}$. Note that a field rotation does not affect spectral quantities, as far as the Jacobian of the transformation is taken into account. The Jacobian may affect the renormalization of the gauge coupling at the quantum level but does not matter at the classical level.

There are several choices of the rotations to identify the continuum Dirac operator as the improved overlap operator up to neglected higher order terms. Since the higher powers of the overlap operator, such as $D^2_{\rm ov}$, in the lattice action is computationally expensive in practical simulations, we arrange the field rotation so that they vanish in the lattice action. Our choice of the field rotation is

$$\Omega_c = 1 - \frac{a}{2\rho}\not{D} + \frac{a^2}{2\rho^2}\not{D}^2 - \frac{3a^3}{8\rho^3}\not{D}^3 - \frac{m_q a^2}{4\rho^2}(\not{D}-m_q)\left(1-\frac{a}{2\rho}\not{D}\right), \qquad \bar{\Omega}_c = 1. \tag{2.9}$$

With this choice, the massive improved operator takes a simple form

$$D'_{\rm ov}(m_q) = \left(1 - \frac{a}{2\rho}M(m_q,\rho)\right)D'_{\rm ov} + M(m_q,\rho) \tag{2.10}$$

with $M(m_q,\rho) = m_q\left(1+\frac{m_q^2 a^2}{4\rho^2}\right)$. It means that one can simply use the conventional overlap operator in the numerical simulation except that the kernel is improved. Since the rotation operator is proportional to $\not{D}$, the on-shell quantities are unchanged, and off-shell amplitudes are obtained by undoing the rotation. To do so, the lattice version of the rotation is given by

$$\Omega_L = 1 - \frac{a}{2\rho}D'_{\rm ov} + \frac{a^2}{4\rho^2}D'^2_{\rm ov} + \frac{a^3}{8\rho^3}D'^3_{\rm ov} - \frac{m_q a^2}{4\rho^2}(D'_{\rm ov}-m_q) - \frac{m_q^2 a^3}{8\rho^3}D'_{\rm ov}, \qquad \bar{\Omega}_L = 1, \tag{2.11}$$

where Ω_L and $\bar{\Omega}_L$ are the same as Ω_c and $\bar{\Omega}_c$ up to the $O(a^3)$ terms. The off-shell improved propagator is then constructed as $\Omega_L D'^{-1}_{\rm ov}(m_q)\bar{\Omega}_L = (\not{D}+m_q)^{-1} + O(a^4)$ [1], which does not require additional inversion of the overlap operator.

3. Relations at the tree level

Here, we compare the improved overlap fermion action with the unimproved one at the tree level. We consider the dispersion relation

$$E(\vec{p}) = \sqrt{\vec{p}^2 + m_q^2} + O(a^n), \tag{3.1}$$

[1] We note that this construction of the rotation has an apparent problem that the manifest chiral symmetry of the form $\gamma_5 S_F(x,y) + S_F(x,y)\gamma_5 = 0$ is lost. We will discuss on a modification of the lattice action to satisfy this condition in future publications.

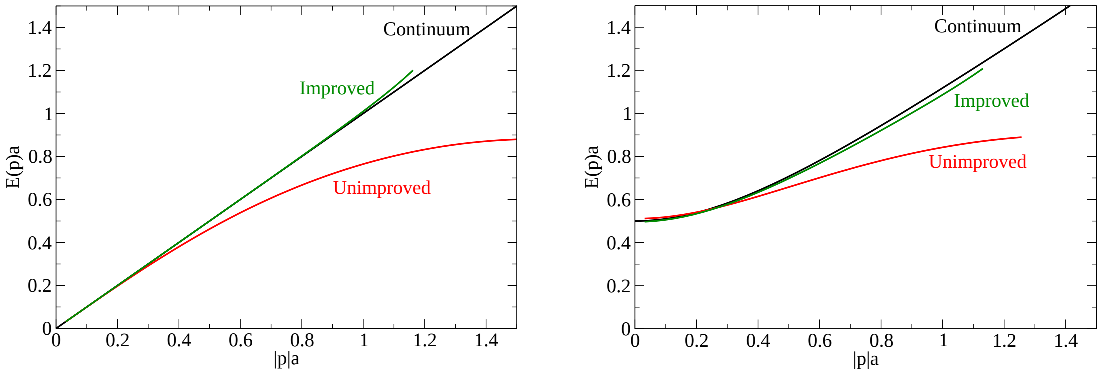

Figure 1: Dispersion relation with the Wilson (unimproved) and with the improved kernels. Left shows the

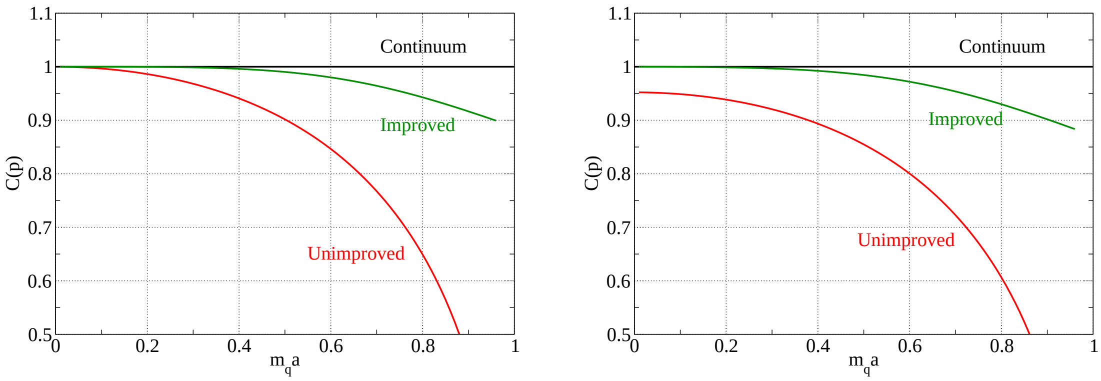

Figure 2: Effective speed of light for the $\mathbf{p} = (0,0,0)$ (left) and $\mathbf{p} = (2\pi/L,0,0)$ (right). The lattice volume $L = 16$ is assumed; $2\pi/L \simeq 0.39$.

which contains the lattice artifact of $O(a^n)$. The power n is 2 for the Wilson kernel while it should be 4 for the improved kernel. Figure 1 shows $E(\vec{p})$ for massless (left) and massive (right) cases. We can see that the improved operator certainly gives the dispersion relation close to the continuum one. To see more quantitatively, in Figure 2 we show the effective speed of light defined by

$$c(\vec{p})^2 = \frac{E(\vec{p})^2 - E(\vec{0})^2}{\vec{p}^2}, \tag{3.2}$$

for $\vec{p} = (0,0,0)$ (left panel) and $\vec{p} = (2\pi/L,0,0)$ at L = 16 (right panel). The results are shown as a function of $m_q a$. These plots imply that improved operator indeed very well reproduces the continuum dispersion relation with only a few per cent errors up to $m_q a \sim 0.5$. while the unimproved operator shows much larger deviation already very close to $m_q a = 0$.

We also look at the off-shell amplitude (or the quark propagator) at the tree level. We parameterize the quark propagator $S_F(p)$ as $S_F(p) = F_1(p)\not{p} + F_2(p) m_q$ after the appropriate rotation Ω_L. We extract $F_1(p)$ and $F_2(p)$ through

$$F_1(p) = \frac{1}{4}\frac{p^2+m_q^2}{p^2}\mathrm{tr}[i\not{p}S_F(p)] = 1 + O(a^n) \tag{3.3}$$

$$F_2(p) = \frac{1}{4}\frac{p^2+m_q^2}{m^2}\mathrm{tr}[m_q S_F(p)] = 1 + O(a^n). \tag{3.4}$$

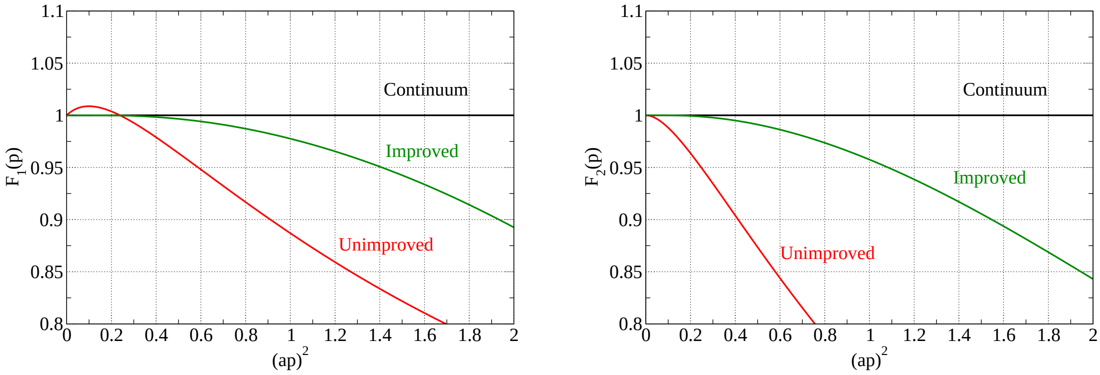

Figure 3: Left panel shows $F_1(p)$ and right panel shows $F_2(p)$ versus $(ap)^2$. The direction of momentum is $p = (1,1,1,1)$

In Figure 3, $F_1(p)$ (left panel) and $F_2(p)$ (right panel) are shown. Since the improved operator has no $O(a^2)$ term, the slope of the curve corresponding to the improved action vanishes near $(ap)^2 = 0$. These plots are shown for $m_q a = 0.5$.

4. Non-perturbative test on a dynamical lattice

We also test the improved overlap fermion action by calculating the meson dispersion relation. We use the gauge configurations including 2+1 flavors of dynamical quarks generated by the JLQCD and TWQCD collaborations [8]. The lattice spacing is about $a \simeq 0.11$ fm, and the lattice size is $16^3 \times 48$. Sea quark masses are $m_{ud}a = 0.015$ and $m_s a = 0.080$.

For the valence quark, we use the improved overlap fermion constructed in this work with $\rho = 1.4$. We calculate the dispersion relation of the pseudo-scalar meson at several different valence quark masses between 0.050 and 0.800 in the lattice unit.

The effective speed of light is shown in Figure 4. We observe large statistical fluctuations for small valence quark masses, as always happens for the correlators with finite momenta. For larger quark mass region, we find that the improved operator indeed gives the value closer to unity. Below $m_q a \approx 0.5$, the deviation of the speed of light from 1 is only a few per cent.

So far, we use the improved kernel as its original form. However, the $O(a)$ and $O(a^2)$ errors in the kernel operator may appear as radiative corrections. We therefore should tune the parameters in the action so that these errors vanish, which is left for future works. Also, we are going to extend the formulation so that the improved action produces off-shell amplitudes that are consistent with the Ginsparg-Wilson relation.

This work is supported in part by the Grant-in-Aid of the Ministry of Education (No. 21674002). Numerical simulations are performed on IBM System Blue Gene Solution at High Energy Accelerator Research Organization (KEK) under a support of its Large Scale Simulation Program (No. 09-05).

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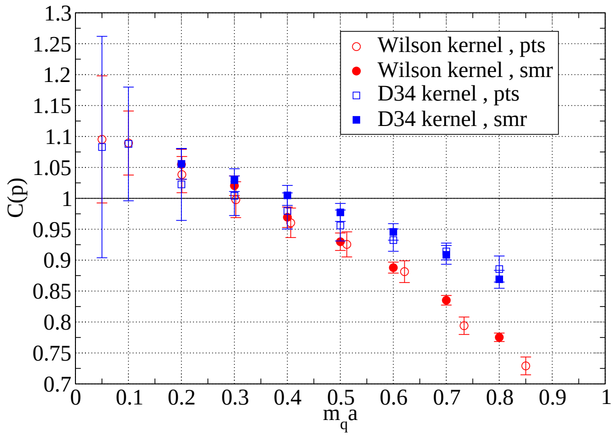

Figure 4: Effective speed of light calculated with the improved and unimproved overlap fermion actions. These are calculated from two smallest momentum $|\mathbf{p}| = 0, 2\pi/L$. The results are shown for the overlap fermion with the Wilson kernel (circles) and with the improved kernel (squared). Open and filled symbols represent the data with a point source and with a smeared source, respectively.

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