The chiral limit in lattice QCD

Hidenori Fukaya (for JLQCD collaboration)
Theoretical Physics Laboratory, RIKEN
Wako, Saitama 351-0198, Japan
E-mail: hfukaya@riken.jp

It has been a big challenge for lattice QCD to simulate dynamical quarks near the chiral limit. Theoretically, it is well-known that the naive chiral symmetry cannot be realized on the lattice (the Nielsen-Ninomiya theorem). Also practically, the computational cost rapidly grows as the quark mass is reduced. The JLQCD collaboration started a project to perform simulations with exact but modified chiral symmetry using the the overlap-Dirac operator and the topology conserving action. The latter is helpful to reduce the numerical cost of the dynamical quarks. Our simulation of two-flavor QCD has been successful to reduce the sea quark mass down to a few MeV.

Keywords: lattice QCD, chiral symmetry

1. Introduction

Lattice QCD, has been successful to analyze the low-energy dynamics of mesons and baryons. Non-perturbative quantities, such as the hadron spectrum, matrix elements, the chiral phase transition etc. have been investigated by large-scale calculations often using supercomputers.

The lattice regularization, however, violates some important symmetries that the continuum theory has. For instance, the translational invariance is violated except for its discrete subgroup. The chiral symmetry, one of the most important symmetries of QCD, is also difficult to realize on the lattice. This is known as the fermion-doubling problem that any chiral Dirac operator must have unphysical poles.\(^1,2\) In order to eliminate the doubler modes, one has to give up the chiral symmetry, or to employ complicated Dirac operators satisfying the Ginsparg-Wilson relation,\(^3-8\) for which the locality is less obvious and more importantly much larger numerical cost is required compared to the explicitly local (the so-called ultra-local) Dirac operators. Most of the previous QCD simulations with the dynamical quarks were, therefore, limited to those with the Dirac operator which explicitly breaks
the chiral symmetry. Moreover, the sea quark mass in such simulations were much larger than the physical values. Their results may contain systematic effects due to additive quark mass renormalization, unwanted operator mixings with opposite chirality, additional symmetry breaking terms in the chiral perturbation theory, chiral extrapolation from rather heavy quark masses, and so on.

The JLQCD collaboration started a new project to simulate QCD near the chiral limit. It uses a new supercomputer system installed at KEK in early 2006. We employ the overlap-Dirac operator, which satisfies the Ginsparg-Wilson relation and thus realizes the exact chiral symmetry. In order to avoid gauge configurations that are too rough and the topology is not well-defined, we use the Iwasaki action combined with the topology conserving action for the gauge part of the action. It turned out that keeping topology is also helpful to reduce numerical costs of the dynamical overlap fermions. On a $16^3 \times 32$ lattice with the lattice spacing $a \sim 0.11$–0.12 fm, we have simulated two-flavor QCD with the quark mass down to $\sim 3$ MeV, which is even smaller than the physical up and down quark masses.

We found that the locality of the overlap-Dirac operator is good enough compared to the QCD scale (See Ref. [15]). The preliminary results from the project have been reported in Refs. [16–18].

The outline of this article is as follows. In Sec. 2, We give a brief review about how the exact chiral symmetry and its topological properties can be realized on the lattice. The results of numerical simulations are reported in Sec. 3. Since our simulations are limited in a fixed topological sector on a fixed volume lattice $\sim 2^3 \times 4$ fm$^4$, the effects from finite volume and topology could be significant after reaching the chiral limit. We discuss this in Sec. 4. Summary and discussion are given in Sec. 5.

2. Chiral symmetry and topology

The difficulty of chiral symmetry on the lattice is summarized by the Nielsen-Ninomiya theorem: any local Dirac operator which satisfies $D \gamma_5 + \gamma_5 D = 0$ must have unphysical poles. One can easily see this in free fermions. By the discretization, the continuum Dirac operator in the momentum space, $D = i\gamma_\mu p_\mu$, is replaced by the lattice counterpart

$$D^{\text{naive}} = \frac{\gamma_\mu}{2}(\partial_\mu + \partial^*_\mu) \sim i\gamma_\mu \sin(ap_\mu).$$

(1)

It has unphysical poles at $p_\mu = \pi/a$. Here, $\partial_\mu$ and $\partial^*_\mu$ denote the forward and backward subtraction, respectively. Wilson’s prescription to avoid
the unphysical poles is to add a higher derivative term
\[ D_W = \frac{\gamma_\mu}{2} (\partial_\mu + \partial_\mu^*) - \frac{a}{2} \partial_\mu \partial_\mu^* \sim \gamma_\mu \sin(ap_\mu) + \frac{2}{a} \sum_\mu \sin^2(p_\mu a/2). \] (2)

This additional term, known as the Wilson term, gives the doublers a mass of the cut-off scale and let them decoupled from the theory. but it explicitly breaks the chiral symmetry. Since the Wilson term contains the covariant derivative, the eigenvalue distribution of the Dirac operator is largely deformed from the continuum limit. As a result, one loses the identification of the zero-modes, and thus the clear definition of the quark mass.

Neuberger’s overlap-Dirac operator\(^6,7\) is defined by
\[ D = \frac{1}{\bar{a}} \left( 1 + \gamma_5 \frac{a H_W}{\sqrt{a^2 H_W^2}} \right), \quad \bar{a} = \frac{a}{1 + s}, \quad a H_W = \gamma_5 (a D_W - 1 - s), \] (3)
where a constant \( s \) is taken in a range \( 0 < s < 1 \). It satisfies the Ginsparg-Wilson relation,\(^8\) \( \gamma_5 D + D \gamma_5 = \bar{a} D \gamma_5 D \), and the fermion action \( S_F = \sum_x \bar{\psi}(x) D \psi(x) \), is exactly invariant under the chiral rotation,\(^9\)
\[ \psi \rightarrow e^{i\alpha \gamma_5} \psi, \quad \bar{\psi} \rightarrow e^{i\alpha \gamma_5}, \quad \gamma_5 = \gamma_5 (1 - \bar{a} D), \] (4)
at finite lattice spacings. Since \( |\gamma_5 \frac{a H_W}{\sqrt{a^2 H_W^2}}|^2 = 1 \), the eigenvalues of the overlap Dirac operator are distributed on a circle with a radius \((1 + s)/a\). Note that this circle exactly passes the origin where we can count the number of the chiral zero-modes (all the zero-modes commute with \( \gamma_5 \)), and the quark mass can be simply defined by just adding \( m \) to \( D \). Because of the relation\(^20\)
\[ n_+ - n_- = \frac{1}{2} \text{Tr} \gamma_5 / 2, \] (5)
where \( n_\pm \) denotes the number of zero-modes with \( \pm \) chirality, and the perturbative expansion of \( \gamma_5 \),\(^21,22\)
\[ \gamma_5(x, x)/2 = \frac{1}{32\pi^2} \text{Tr} \epsilon_{\mu \nu \rho \sigma} F_{\mu \nu}(x) F_{\rho \sigma}(x) + O(a^2), \] (6)
one can identify the index \( n_+ - n_- \) as the topological charge.

One should note, however, that Eq.(3) is ill-defined when \( H_W \) has zero-modes. From Eq.(5),
\[ Q \equiv n_+ - n_- = \frac{1}{2} \text{Tr} \gamma_5 / 2 = \frac{1}{2} \text{Tr} \gamma_5 (1 - \bar{a} D) / 2 = \frac{1}{2} \text{Tr} \frac{H_W}{\sqrt{H_W}}, \] (7)
one can see that the topological charge \( Q \) changes when the eigenvalue of \( H_W \) crosses zero. In other words, the equation \( H_W = 0 \) forms the topology boundaries in the configuration space. On the topology boundaries,
$H_W = 0$, the overlap-Dirac operator is not smooth and its locality is not obvious. Near zero-modes of $H_W$ also cause practical problems that the numerical cost of approximating $1/\sqrt{H_W^2}$ increases as the inverse of the lowest eigenvalue and the discontinuity of $D$ requires a huge extra numerical cost for the dynamical quarks.

In order to achieve $H_W \neq 0$ at a finite lattice spacing (note that $H_W \neq 0$ is automatically satisfied in $a \rightarrow 0$ limit), which is known as the admissibility condition, a transparent way is to add extra fields which produces a determinant, to the theory. It is nothing but the determinant of two-flavor Wilson fermions and twisted-mass ghosts with a twisted mass $m_t$. Both of the additional fields have a cut-off scale mass and do not affect the low-energy physics. With this determinant, the overlap-Dirac operator $D$ is smooth, and its locality is guaranteed. Furthermore, the numerical costs are largely reduced. Since this determinant does not allow the topology change during the hybrid Monte Carlo updates, we call it the topology conserving action.

3. Lattice simulation

We generate the gauge configurations of two-flavor QCD according to the Boltzmann weight

$$\exp(-\beta S_G) \det((1 - \bar{a}m/2)D + m)^2 \det H_W^2/(H_W^2 + m_t^2),$$

where $\beta S_G$ denotes the Iwasaki gauge action with the coupling $\beta = 2.3$ and 2.35, and $(1 - \bar{a}m/2)D + m$ is an expression of the massive overlap fermion. We take $\bar{a} = a/1.6$ and $am_t = 0.2$ for all the simulations. On a $16^3 \times 32$ lattice, we have performed $O(1000)$ trajectories of the hybrid Monte Carlo updates in the $Q = 0$ topological sector. The lattice spacing is estimated to be $a \sim 0.11-0.12$ fm from the Sommer scale $r_0 (= 0.49$ fm). Details are seen in Refs. [16–18]

The new supercomputer system at KEK and some algorithmic improvements enable us to reduce the quark mass down to $ma = 0.002(\sim 3$ MeV), which is even less than the physical value. In fact, we observe that the numerical cost, or the number of multiplication of $D_W$, does not depend too strongly on the sea quark mass $m$. However, we note that this insensitivity to $m$ indicates that the lowest eigenvalue of $D$ is larger than the quark mass, due to the finite volume effects, as discussed in the next section.
Fig. 1. Chiral extrapolation of pseudo-scalar (left) and vector meson masses (right).

Meson masses are evaluated from the correlation functions measured with smeared source and local sink operators. Figure 1 shows the chiral extrapolation of the pion and the vector meson masses. The pion mass agrees well with the leading ChPT formula,

\[ m_\pi^2 \propto m_\Sigma/F_\pi^2, \]

where the bare quark mass needs no additive renormalization, owing to the exact chiral symmetry. With our present statistics, we find no significant deviation from a simple linear fit

\[ m_\pi^2 = b_{PS} m_\pi, \quad m_V = a_V + b_V m_\pi^2, \]  

(10)

which gives \( \chi^2/\text{dof} \lesssim 1.0 \). With this linear fit, we obtain \( a = 0.1312(23) \text{ fm} \) using the \( \rho \) meson mass as an input. This is consistent with the estimate from \( r_0 \) within 10% accuracy.

4. Finite \( V \) and fixed \( Q \) effects

Since our simulations are done on a fixed volume lattice (\( \sim 1.8 \times 2 \text{ fm}^4 \)) in a fixed topological sector, any observable may systematic errors due to the finite volume and fixed topology. Although the simplest solution to eliminate these errors is to go to larger volumes, we can take an alternative way that we treat finite \( V \) and \( Q \) effects using an effective theory.

The chiral perturbation theory (ChPT)\(^{25,26} \) and the chiral Random Matrix theory (ChRMT)\(^{27} \) are valid in estimating the finite \( V \) effects on pions, especially when the quark mass is so small that the pion Compton wavelength is larger than the lattice size. This set-up is known as the \( \epsilon \)-regime. In the \( \epsilon \)-regime, ChRMT describes the eigenvalue spectrum of the Dirac operator with the chiral condensate \( \Sigma \) as an unique parameter. The pion correlator in the \( \epsilon \)-regime is no more exponential but quadratic function of \( t \), of which curvature depends on the pion decay constant \( F_\pi \).

We compare our numerical result at the lightest quark mass with the
prediction of ChRMT and ChPT. The left panel of Fig.2 shows the cumulative eigenvalue distribution of the overlap Dirac operator, from which we extract the chiral condensate as $\Sigma = (251(7)(11) \text{ MeV})^3$, where the errors are statistical and an estimate of the higher order effects in the $\epsilon$-expansion. This value is consistent with earlier works\textsuperscript{31,32} which are done with heavier quark masses. The right panel shows the pion correlator and the quadratic fit curve, which gives $F_\pi = 86(7) \text{ MeV}$. Note that this value is obtained near the chiral limit without doing any chiral extrapolations.

5. Summary and discussion

The QCD simulation in the chiral regime is feasible with the exact chiral symmetry respected. The topology conserving action is very helpful to reduce the numerical cost of the dynamical overlap quarks. We can reduce the sea quark mass to the physical up and down quark masses or even lower. Near the chiral limit, the finite $V$ and fixed $Q$ effects are important since the pion is sensitive to these effects. Through the chiral perturbation theory or the chiral Random Matrix Theory, these effects can even be used to extract the low energy constants, such as the chiral condensate and the pion decay constant. To extend our lattice size is, however, important to confirm them in the future works.

Numerical simulations are performed on Hitachi SR11000 and IBM System Blue Gene Solution at High Energy Accelerator Research Organization (KEK) under a support of its Large Scale Simulation Program (No. 06-13). This work is supported in part by the Grant-in-Aid of the Ministry of Education (No. 18840045).

References

1. H. B. Nielsen and M. Ninomiya, Nucl. Phys. B 185, 20 (1981) [Erratum-ibid. B 195, 541 (1982)].
2. H. B. Nielsen and M. Ninomiya, Nucl. Phys. B 193, 173 (1981).
3. D. B. Kaplan, Phys. Lett. B 288, 342 (1992) [arXiv:hep-lat/9206013].
4. Y. Shamir, Nucl. Phys. B 406, 90 (1993) [arXiv:hep-lat/9303005].
5. V. Furman and Y. Shamir, Nucl. Phys. B 439, 54 (1995) [arXiv:hep-lat/9405004].
6. H. Neuberger, Phys. Lett. B 417, 141 (1998) [arXiv:hep-lat/9707022].
7. H. Neuberger, Phys. Lett. B 427, 353 (1998) [arXiv:hep-lat/9801031].
8. P. H. Ginsparg and K. G. Wilson, Phys. Rev. D 25, 2649 (1982).
9. M. Luscher, Phys. Lett. B 428, 342 (1998) [arXiv:hep-lat/9802011].
10. Y. Iwasaki, Nucl. Phys. B 258, 141 (1985).
11. Y. Iwasaki and T. Yoshie, Phys. Lett. B 143, 449 (1984).
12. P. M. Vranas, arXiv:hep-lat/0001006.
13. T. Izubuchi and C. Dawson [RBC Collaboration], Nucl. Phys. Proc. Suppl. 106, 748 (2002).
14. H. Fukaya, S. Hashimoto, K. I. Ishikawa, T. Kaneko, H. Matsufuru, T. Onogi and N. Yamada [JLQCD Collaboration], Phys. Rev. D 74, 094505 (2006) [arXiv:hep-lat/0607020].
15. N. Yamada et al. [JLQCD Collaboration], arXiv:hep-lat/0609073.
16. H. Fukaya et al. [JLQCD Collaboration], arXiv:hep-lat/0702003.
17. T. Kaneko et al. [JLQCD Collaboration], arXiv:hep-lat/0610036.
18. H. Matsufuru et al. [JLQCD Collaboration], PoS LAT2006, 031 (2006) [arXiv:hep-lat/0610026].
19. K. G. Wilson, “Quarks And Strings On A Lattice,” New Phenomena In Subnuclear Physics. Part A. Plenum Press, New York, 1977.
20. P. Hasenfratz, V. Laliena and F. Niedermayer, Phys. Lett. B 427, 125 (1998) [arXiv:hep-lat/9801021].
21. Y. Kikukawa and A. Yamada, Phys. Lett. B 448, 265 (1999) [arXiv:hep-lat/9806013].
22. D. H. Adams, Annals Phys. 296, 131 (2002) [arXiv:hep-lat/0112003].
23. P. Hernandez, K. Jansen and M. Luscher, Nucl. Phys. B 552, 363 (1999) [arXiv:hep-lat/9808010].
24. M. Luscher, Nucl. Phys. B 568, 162 (2000) [arXiv:hep-lat/0004009].
25. J. Gasser and H. Leutwyler, Phys. Lett. B 188, 477 (1987).
26. P. H. Damgaard, M. C. Diamantini, P. Hernandez and K. Jansen, Nucl. Phys. B 629, 445 (2002) [arXiv:hep-lat/0112016].
27. P. H. Damgaard and S. M. Nishigaki, Phys. Rev. D 63, 045012 (2001) [arXiv:hep-th/0006111].
28. Z. Fodor, S. D. Katz and K. K. Szabo, JHEP 0408, 003 (2004) [arXiv:hep-lat/0311010].
29. N. Cundy, J. van den Eshof, A. Frommer, S. Krieg, T. Lippert and K. Schafer, Comput. Phys. Commun. 165, 221 (2005) [arXiv:hep-lat/0405003].
30. M. Hasenbusch, Phys. Lett. B 519, 177 (2001) [arXiv:hep-lat/0107019].
31. T. DeGrand, Z. Liu and S. Schaefer, Phys. Rev. D 74, 094504 (2006) [Erratum-ibid. D 74, 099904 (2006)] [arXiv:hep-lat/0608019].
32. C. B. Lang, P. Majumdar and W. Ortner, arXiv:hep-lat/0611010.