Chiral Symmetry, Quark Mass, and Scaling of the Overlap Fermions

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The chiral symmetry relation and scaling of the overlap fermions are studied numerically on the quenched lattices at 3 couplings with about the same physical volume. We find that the generalized Gell-Mann-Oakes-Renner relation is satisfied to better than 1% down to the smallest quark mass at $m_0 a = 0.006$. We also obtain the quark mass from the PCAC relation and the pseudoscalar masses. The renormalization group invariant quark mass is shown to be fairly independent of scale. The π and ρ masses at a fixed m_π/m_ρ ratio indicate small $O(a^2)$ corrections. It is found that the critical slowing down sets in abruptly at a very small quark mass close to those of the physical u and d quarks.

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Recent advances in chiral fermion formulation on the lattice hold great promise in implementing chiral fermions for QCD at finite lattice spacing [1]. There are distinct advantages over the previous formulations. For example, the Wilson fermion breaks chiral symmetry at finite lattice spacing a and, therefore, the task of extrapolating the Monte Carlo results to the continuum and chiral limits requires fine tuning and is often difficult. In this case, one could not expect low energy theorems to be reproduced at finite lattice spacing. Similarly, the staggered fermion can be formulated only with four flavors with an $U(1)$ subgroup of the flavor nonsinglet chiral symmetry. At finite lattice spacing where the numerical calculations are carried out, the flavor symmetry is broken. Furthermore, the anomalous chiral Ward identity does not hold for these fermions unless at the continuum limit. This makes the analysis of anomaly on the lattice rather unclear. There is no unambiguous identification of the fermion zero modes with the topology of the background gauge field. These difficulties due to the coupling of chiral symmetry with the continuum limit have rendered the studies of low energy phenomenology of QCD on the lattice unsettling.

The picture has been altered dramatically with the advent of Neuberger's overlap fermion [2] which is derived from the overlap formalism [3]. All of the above-mentioned impediments can be avoided pending pristine numerical simulation. It is shown to have correct anomaly and exact chiral symmetry on the lattice [3–5], and there are no order a artifacts [6]. The overlap fermion has a compact form in four dimensions and is easily employed to derive low energy theorems, chiral symmetry relations, and anomaly at finite lattice spacing. In this Letter, we shall study the overlap fermion numerically. We test chiral symmetry via the Gell-Mann-Oakes-Renner relation at finite lattice spacing and check the scaling behavior of the π and ρ masses. The preliminary results were reported earlier [7]. We also obtain the quark mass from the chiral Ward identity and verify that it is free from additive renormalization and the renormalization group invariant quark mass is indeed independent of scale.

Neuberger's Dirac operator has the following form for the massive case [8]:

$$D(m_0) = 1 + \frac{m_0 a}{2} + \left(1 - \frac{m_0 a}{2}\right)\gamma_5 \epsilon(H), \quad (1)$$

where $\epsilon(H) = H/\sqrt{H^2}$ is the matrix sign function of H which we take to be the Hermitian Wilson-Dirac operator, i.e., $H = \gamma_5 D_w$. Here D_w is the usual Wilson fermion operator, except with a negative mass parameter $-\rho = 1/2\kappa - 4$ in which $\kappa_c < \kappa < 0.25$. We take $\kappa = 0.19$ in our calculation which corresponds to $\rho = 1.368$. The massless operator $D(0)$ is shown [9] to satisfy the Ginsparg-Wilson relation [10] $\{\gamma_5, D(0)\} = D(0)\gamma_5 D(0)$. The bare mass parameter m_0 is proportional to the quark mass without additive constant which we shall verify.

There are several numerical approaches to approximate the sign function $\epsilon(z)$ [11–14]. We adopt the optimal rational approximation [13] with a ratio of polynomials of degree 12 in the Remez algorithm. We find the error to the approximation of $\epsilon(z)$ to be within 10^{-5} in the range $[0.02, 2]$ of the argument z. In the range $[0.0005, 0.02]$, the error can be as large as 1%. To improve the accuracy of $\epsilon(H)$ and hence the chiral symmetry property, the smallest 10 to 20 eigenvalues of H^2 with eigenvalues of $|H|$ less than 0.04 are projected out for exact evaluation of the sign function from these eigenstates [13]. This has the added benefit of reducing the number of iterations for the multimass conjugate gradient inversion of $H^2 + c_i$ in the inner loop by a factor of 3.5 or so. We checked the unitarity of the matrix $V = \gamma_5 \epsilon(H)$. For $Vx = b$, we find $|x^\dagger x - b^\dagger b| \sim 10^{-9}$. Since V is unitary we exploit the identity $(1 + V^\dagger)(1 + V) = 2 + V + V^\dagger$ in order to use the conjugate gradient algorithm on the Hermitian matrix $V + V^\dagger$ instead of $V^\dagger V$ which has a higher condition number. Furthermore, since $[V + V^\dagger, \gamma_5] = 0$, one can use a chiral source, i.e., $\gamma_5 b = \pm b$ to save one matrix multiplication [15] per iteration. In the present study, we consider three lattices: $6^3 \times 12$ at $\beta = 5.7$, $8^3 \times 16$ at $\beta = 5.85$, and $10^3 \times 20$ at $\beta = 6.0$, which have about the same physical volume. With residuals at 10^{-7}, the inner loop takes typically ~200–250 iterations and is almost independent of the lattice volume. The outer loop takes ~40–110 iterations from the small to large lattice volumes. Even for topological sectors with charge $Q \neq 0$, we find the critical slowing down is much milder than that of the Wilson fermion and we found no exceptional configurations. The critical slowing down sets in quite abruptly when $m_0 a < 0.006$ for the sector with topology. This is already very close to the physical u and d masses. For comparison, to obtain the same pion mass as in the present study at $m_0 a = 0.006$, it would take ~600 conjugate gradient iterations to converge to a comparable residue for the Wilson fermion at $\beta = 6.0$ on a $16^3 \times 24$ lattice. This shows that the propagator for the overlap fermion is about 50× more costly to calculate than that of the Wilson fermion for these small quark masses.

The lattice chiral symmetry is reflected in the generalized Gell-Mann-Oakes-Renner (GOR) relation

$$m_0 a \int d^4x \, \langle \pi(x)\pi(0)\rangle = 2\langle\bar{\psi}\psi\rangle \,. \tag{2}$$

Since it is satisfied for each quark mass, lattice volume and spacing, configuration by configuration, and for each source [15,16], it serves as an economic test of chiral symmetry. Here $\pi(x) = \bar{\psi}\gamma_5(\tau/2)\psi$ is the pion interpolation field and the quark propagator is the external one with $D_c^{-1} = (1 - m_0 a/2)^{-1}[D^{-1}(m_0) - 1/2]$ [8,17]. Alternatively, one can use the bilinears $(1 - m_0 a/2)^{-1}\bar{\psi}\Gamma(1 - D/2)\psi$ for the operators and D^{-1} as the propagator. We utilize this relation in Eq. (2) as a check of the numerical implementation of the Neuberger operator. We find that for the lattices we consider the GOR relation is satisfied very well (to within 10^{-3}) all the way down to the smallest mass $m_0 a = 2 \times 10^{-4}$ for the $Q = 0$ sector. For the $Q \neq 0$ sector, the presence of zero modes demands higher precision for the approximation of $\epsilon(H)$.

For example, we show in Fig. 1 the ratio of the right to left side of Eq. (2) for a typical configuration with topology on the $6^3 \times 12$ lattice at $\beta = 5.7$ as a function of the quark mass $m_0 a$. When only 10 smallest eigenmodes of H^2 are projected, we see that the ratio deviates from one for small quark masses. For the smallest mass $m_0 a = 0.006$, it may deviate as much as 16%. The situation is considerably improved when 20 smallest eigenmodes are included where the deviation is reduced to 1%. Our result with the overlap is appreciably better than the domain-wall fermion case when the size of the fifth dimension is limited to $L_s = 10$ to 48 [18] with $8^3 \times 32$ lattice and the same β at 5.7. In the latter case, the ratio deviates from unity by ~55% for $L_s = 10$ and ~15% for $L_s = 48$ at the quark mass $m_f a = 0.02$. Comparing the calculated pion mass [19] and neglecting the volume difference, this quark mass corresponds to $m_0 a \sim 0.07$ in our study where the

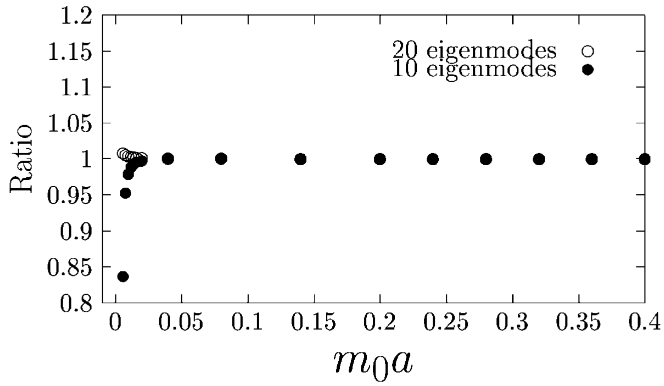

FIG. 1. Ratio of the right to left side of Eq. (2) for a configuration with topology. The symbols ● (○) indicate the case with projection of 10 (20) smallest eigenmodes.

deviation is less than 10^{-3}. Even at a quark mass 12 times smaller, i.e., $m_0 a = 0.006$, the deviation is only at the 1% level in the overlap case.

The average of u and d quark masses in the modified minimal subtraction ($\overline{\text{MS}}$) scheme at the renormalization scale μ is obtained from the axial Ward identity $Z_A \partial_\mu A_\mu = 2Z_S^{-1} m_0 Z_P P$ via the ratio of the matrix elements

$$\begin{aligned} m_q^{\overline{\text{MS}}}(\mu) &= Z_S^{-1}(\mu) m_0 \\ &= \lim_{t\to\infty} \frac{Z_A(\mu)}{Z_P(\mu)} \frac{\sum_{\vec{x}}\langle 0|\nabla_t A_4(x)|\pi(0)\rangle}{2\sum_{\vec{x}}\langle 0|P(x)|\pi(0)\rangle} \,, \end{aligned} \tag{3}$$

where $A_\mu = \bar{\psi} i\gamma_\mu\gamma_5(\tau/2)\psi$ and $P = \bar{\psi} i\gamma_5(\tau/2)\psi$. We first note that since $Z_S = Z_P$ for the overlap fermion, they drop out from the equation between the second and third terms in Eq. (3). As a result, Z_A can be determined by the axial Ward identity nonperturbatively. With our Monte Carlo data, we find $Z_A = 1.05(5)$, 1.12(5), and 1.25(1) for $\beta = 5.7$, 5.85, and 6.0 which is approaching the tree-level value of $\rho = 1.368$ [15,20] with weaker coupling. These are somewhat smaller than the resummed cactus diagram of one-loop calculation [21] of Z_A which are 1.67, 1.66, and 1.65, respectively [22] when the tree-level factor of $\rho = 1.368$ is included. To determine the renormalized quark mass $m_q^{\overline{\text{MS}}} a$ with Eq. (3), we assume that the ratio Z_A/Z_P is better determined in perturbation than Z_A and Z_P individually. Using the ratio Z_A/Z_P from the perturbative calculation at $\mu = 1/a$ [21,22], $m_q^{\overline{\text{MS}}} a$ is defined in Eq. (3) and plotted in Fig. 2 against the bare mass $m_0 a$ for the three lattices.

We first observe that the renormalized quark mass does not have an additive part due to the lattice chiral symmetry.

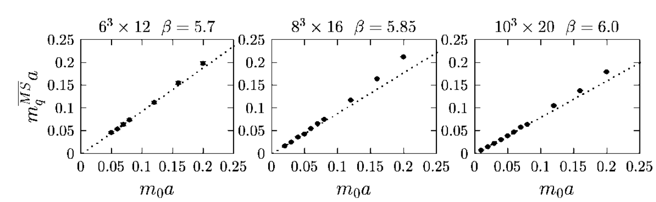

FIG. 2. Renormalized quark mass vs the bare quark mass on the three lattices.

The linear fit including the smallest 5, 7, and 8 quark masses for $\beta = 5.7$, 5.85, and 6.0, respectively, shows that the intercepts are of the order of 10^{-3} and are consistent with zero. This is a distinct advantage over the Wilson fermion whose quark mass is subject to additive renormalization which depends on the gauge configuration. From the slope we can determine the nonperturbative Z_S^{-1} which are 0.95(5), 0.89(5), and 0.80(1) for $\beta = 5.7$, 5.85, and 6.0. The renormalization group invariant quark mass is defined as the integration constant of the evolution equation such that

$$m_q^{RGI} = \Delta Z_S(\mu) m_q^{\overline{\rm MS}}(\mu) = \Delta Z_S(\mu) Z_S^{-1}(\mu) m_0 , \quad (4)$$

where $\Delta Z_S(\mu)$ is the evolution factor which nullifies the scale dependence of $m_q(\mu)$ in a specific scheme. Using the four-loop calculation of $\Delta Z_S(\mu)$ in the $\overline{\rm MS}$ scheme [23], we obtain the product of $\Delta Z_S(\mu) Z_S^{-1}(\mu)$ which should be scale invariant. The results from the 3 lattices give 1.12(1), 1.17(6), and 1.14(5) for $\beta = 5.7$, 5.85, and 6.0. They are indeed independent of scale within errors. From the pion mass fit to be discussed later, we determine $m_0 = 6.8(5)$ MeV from the physical pion mass on the $\beta = 6.0$ lattice. This gives $m_q^{RGI} = 7.6(6)$ MeV for the average of u and d quark masses, which in turn gives $m_q^{\overline{\rm MS}}(\mu = 2\text{ GeV}) = 5.5(5)$ MeV. The lattice scale is set by the Sommer scale r_0 as derived from the static quark potential [24]. We should point out that this quark mass should not be taken literally, since the volume is quite small. The primary purpose of the present study is to verify that the quark mass extracted from the overlap fermion action does not have additive renormalization and that m_q^{RGI} is indeed scale invariant.

Next we look at hadron masses. The results for the π, ρ, and nucleon masses on the $10^3 \times 20$ lattice at $\beta = 6.0$ are given in Fig. 3. They are obtained by a single exponential fit with covariance matrix.

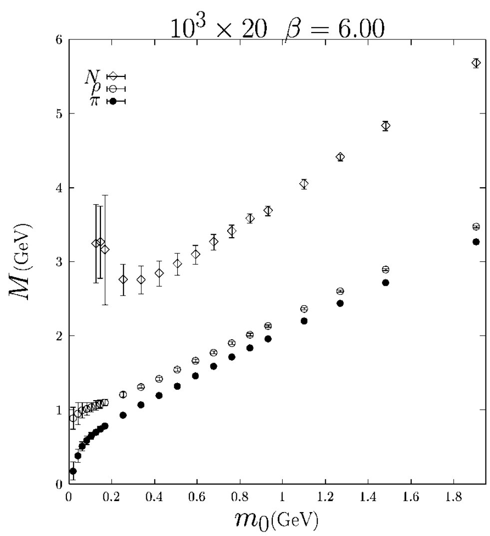

FIG. 3. Masses of π, ρ, and N on the $10^3 \times 20$ lattice at $\beta = 6.0$ vs m_0. The Sommer scale r_0 is used for conversion to physical units.

We see clearly that the nucleon mass suffers from the finite volume effect when m_0 is smaller than 0.4 GeV. Although the ρ and π masses appear not affected as much, there is the worry that the finite volume effect is present when one considers the pion mass behavior as a function of the quark mass m_0. Here we shall concentrate on the region $L > 1/m_\pi$ where the chiral perturbation analysis is expected to apply. Plotted in Fig. 4 are the pseudoscalar meson mass squared ($m_P^2 a^2$) as a function of $m_0 a$ for the three lattices for those pseudoscalar mesons whose Compton wavelengths are less than the respective lattice size.

We fit them with a form suggested by the quenched chiral perturbation theory [25]

$$m_P^2 a^2 = 2 A m_0 a^2 \{1 - \delta \ln(2 A m_0 / \Lambda_\chi^2)\} + 4 B m_0^2 . \quad (5)$$

We find that for Λ_χ in between 0.6 and 1.4 GeV, the chiral-log δ for the $\beta = 6.0$ case is in the range of 0.20(3) to 0.37(14), which is slightly larger than that obtained in the Wilson fermion [26]. The fit is stable with reasonably small χ^2 (χ^2/d.o.f. = 0.35) and is fairly insensitive to the range of the fitted quark masses shown in Fig. 4. The solid curves represent those fitted with Eq. (5) for $\Lambda_\chi = 1.0$ GeV. On the other hand, the fit for $\beta = 5.85$ and 5.7 lattices shows that δ is consistent with zero [the typical value ranges from 0.03(26) to $-0.29(21)$] and the result is more sensitive to the range of quark masses that are fitted, although χ^2/d.o.f. is $\sim$0.1. At this stage, we cannot draw a definite conclusion from these inconsistent results, except to point out that perhaps this is due to the finite volume effect. After all, the physical volumes of the lattices we use are quite small ($L \sim 1$ fm). Another possibility is

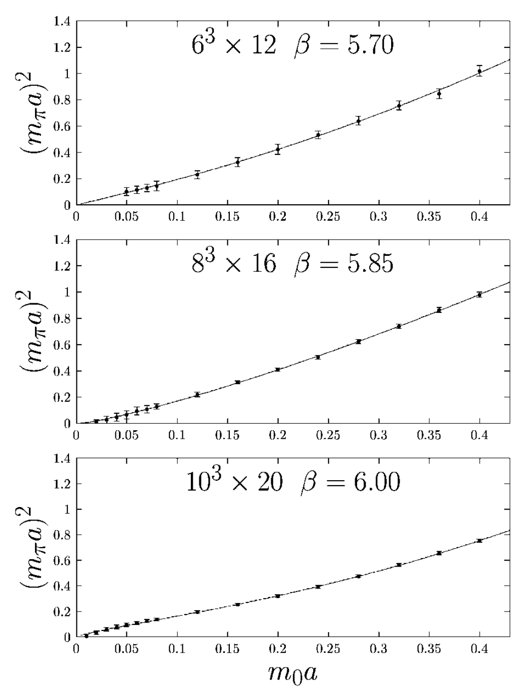

FIG. 4. Pion mass squared as a function of the bare quark mass on the three lattices. The lines are fits to Eq. (5) with $\Lambda_\chi = 1.0$ GeV.

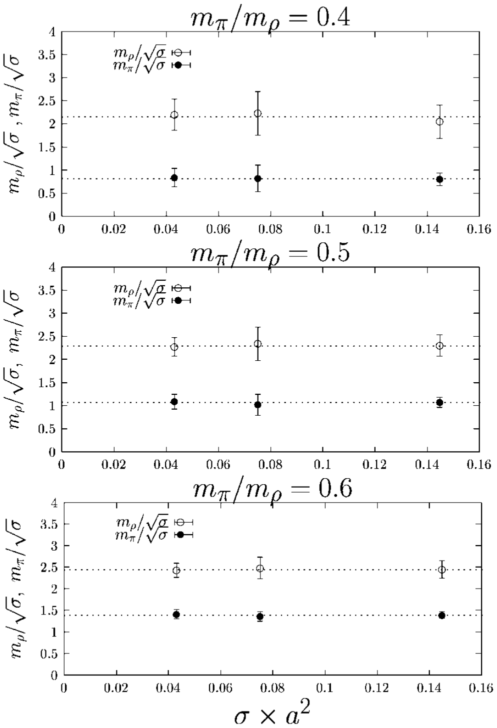

FIG. 5. Pion and rho masses in units of $\sqrt{\sigma}$ on the three lattices are plotted against σa^2. They are given at three different m_π/m_ρ ratios. The dotted lines are fits with a constant.

that the smaller quark mass cases may already fall into the finite size scaling region where the pion mass may have a different behavior than prescribed in Eq. (5). This is more so for β at 5.7 and 5.85 than for β at 6.0 as evidenced from the chiral behavior of the quark condensate $\langle\bar{\psi}\psi\rangle$ [7] and will be studied elsewhere.

Finally, we examine the scaling of ρ and π masses. Since $m_\pi^2 a^2$ and $m_\rho a$ are fairly linear in $m_0 a$, we fit them with $m_\rho a = A + B m_0 a$ and $m_\pi^2 a^2 = C m_0 a + D m_0^2 a^2$ for simplicity. The fits are decent with $\chi^2/\text{d.o.f.} < 1$ for the three lattices and the full range of quark masses in Fig. 4. From the fits of $m_\rho a$ and $m_\pi^2 a^2$, we determine m_0 for which the ratio of $m_\pi/m_\rho = 0.4$, 0.5, 0.6, and plot in Fig. 5 the corresponding m_ρ and m_π in units of $\sqrt{\sigma}$ as a function of σa^2, where σ is the string tension. The errors on the vector and pseudoscalar masses are determined from interpolating the data from the neighboring quark masses. It is known that the overlap operator does not have $O(a)$ artifacts [6]. It appears from Fig. 5 that even the $O(a^2)$ errors are small.

To conclude, we find that when the matrix sign function $\epsilon(H)$ in the overlap fermion is well approximated, the promised chiral symmetry at finite lattice spacing and the scaling of the renormalization group invariant quark mass and hadron masses are manifested in the present numerical calculation. One drawback of the overlap fermion is the large numerical overhead in the present algorithm. But, the stake of being able to implement chiral symmetry at finite lattice spacing is high. Furthermore, the unexpected feature of being able to push the critical slowing down to close to the physical u and d quark masses has the advantage of being able to study the correct chiral behavior. The nice scaling result is encouraging for controlling the continuum extrapolation and may afford the possibility of working at relatively large lattice spacings. For the moment, the study is limited to small volumes. As long as one can extend it to large volumes, it appears that one will be at a stage of putting all the systematic errors under control at least for the quenched approximation.

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