Lattice QCD with Ginsparg-Wilson fermions

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Lattice QCD using fermions whose Dirac operator obeys the Ginsparg-Wilson relation, is perhaps the best known formulation of QCD with a finite cutoff. It reproduces all the low energy QCD phenomenology associated with chiral symmetry at finite lattice spacings. In particular it explains the origin of massless pions due to spontaneous chiral symmetry breaking and leads to new ways to approach the $U(1)$ problem on the lattice. Here we show these results in the path integral formulation and derive for the first time in lattice QCD a known formal continuum relation between the chiral condensate and the topological susceptibility. This relation leads to predictions for the critical behavior of the topological susceptibility near the phase transition and can now be checked in Monte-Carlo simulations even at finite lattice spacings.

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I. INTRODUCTION

Formulating QCD non-perturbatively is important for understanding the low energy phenomenology of hadronic physics. The only such formulation that is known at present is through the lattice regularization. However, until now fermions have been a major obstacle. The main reason has been that chiral symmetry is easily broken on the lattice. Since two of the main features of low energy QCD, namely the spontaneous breaking of chiral symmetry and the anomaly, are intimately connected with chiral symmetry, one hardly uses the lattice discretization to discuss the low energy phenomenology of QCD. Even if such a discussion was carried out, one usually needs to invoke continuum limits before the formulation can actually be argued to reproduce all the low energy properties of QCD.

At finite lattice spacings it is usually unclear as to how chiral symmetry is realized and what properties of QCD are lost. For example with Wilson fermions [1], since chiral symmetry is explicitly broken, there is no reason to expect massless pions unless one tunes a mass parameter to a critical point. Further, the critical point appears to describe spontaneous breaking of parity and flavor symmetry [2]. Thus the soft pion theorems of QCD will not be reproduced at finite lattice spacings. If instead one starts with staggered fermions [3], one can only formulate four flavors of QCD in the Lagrangian formulation. In this case a $U(1)$ subgroup of the flavor non-singlet chiral symmetry is exact on the lattice. However, the flavor symmetry gets broken at finite lattice spacings which again is expected to be restored only in the continuum limit.

The anomalous breaking of the flavor singlet chiral symmetry is expected to give the $\eta'$ particle its mass. With both Wilson and staggered fermions, discussions involving the anomaly have new complications. Since the lattice regularization breaks the anomalous chiral symmetry along with other chiral symmetries, the effects of the anomaly cannot be easily isolated. The simple continuum discussion in terms of the zero modes of the Dirac operator and topology of the gauge fields breaks down. All this indicates that both Wilson and staggered fermion formulations are not ideal for a description of low energy QCD phenomenology at finite lattice spacings.

A long time ago Ginsparg and Wilson [4] showed that if the Dirac operator, $D$, obeyed the relation

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D,$$

where $a$ is the lattice spacing, then the theory would have a remnant chiral symmetry up to contact terms. An year ago Hasenfratz noticed that the fixed point action of QCD obeyed the Ginsparg-Wilson relation [5] and hence a series of interesting results [6,7] about renormalization and lattice index theorems followed. The new massless fermion formulations motivated by the overlap [8] also obeyed the Ginsparg Wilson relation. It seemed that there was more to the relation than was appreciated in the past. Recently Lüscher showed that there is an exact chiral symmetry on the lattice [9] due to the Ginsparg-Wilson relation, since the Nielsen-Ninomiya theorem [10] is not applicable. As a result, for the first time, we can write down a formulation of QCD with the right internal symmetries of the theory at finite lattice spacings. Thus in this formulation the role of the continuum limit is merely to renormalize some multiplicative constants and suppress finite lattice artifacts which do not change the internal symmetry structure of the theory. This leads to the most elegant non-perturbative formulation of QCD.

In this paper we review the main features of the above observations. We use the exact chiral symmetry that arises due to the Ginsparg-Wilson relation to derive the essential physics of low energy QCD in the path integral formulation. For the first time we are able to discuss the physics of chiral symmetry breaking relevant to QCD with any number of flavors, the associated pion physics and the essential ingredients of the $U(1)$ problem, all directly at finite lattice spacings without much effort. In particular we derive a chiral condensate of the theory which reflects the breaking of chiral symmetry. For two
or more flavors we reproduce the Goldstone’s theorem if the chiral symmetry is spontaneously broken. Further, since the Ginsparg-Wilson relation allows for the breaking of the anomalous chiral symmetry through exact zero modes of the Dirac operator like in the continuum, we can easily discuss a solution to the $U(1)$ problem. By introducing an explicit quark mass we can derive a well known continuum relation, between the chiral condensate and the topological susceptibility, in lattice QCD. The problems associated with the quenched approximation can be traced to the violation of this relation. Near the chiral phase transition at finite temperatures, this relation also leads to predictions for the critical behavior of the topological susceptibility which have not been appreciated before. These predictions can be verified in Monte-Carlo simulations.

Most of the results that we derive already appear in [9]. However, we have included them for the coherent presentation of our work, and as far as we know this is the first time the results have been derived in the path integral formulation based on the symmetry discovered by Lüscher [9]. This makes the re-derivations sufficiently different and perhaps more transparent. Our presentation of the $U(1)$ problem and its consequences are new. We have tried to keep the derivations simple and easily accessible to readers familiar with field theory.

II. CHIRAL SYMMETRY

Let us begin by reviewing the exact lattice chiral symmetry, discovered by Lüscher [9], that arises due to the Ginsparg-Wilson relation. The partition function of lattice QCD is given by

$$Z = \int [dU] e^{-\frac{S_G[U]}{\kappa}} \int [d\bar{\Psi}] [d\Psi] e^{-S_F[\bar{\Psi}, \Psi]} ,$$

where $S_G[U]$ is some lattice gauge action and $g^2$ is the bare gauge coupling. The fermionic action is given by

$$S_F[\bar{\Psi}, \Psi] = -a^4 \sum_{x,y} \bar{\Psi}(x) D_{x,y} \Psi(y),$$

where we assume that $D$ obeys eq.(1). We have suppressed color and flavor indices for convenience. The action is invariant under the infinitesimal chiral transformations of the form

$$\delta \Psi = e\gamma_5(1 - a\frac{1}{2}D)\Psi, \quad \delta \bar{\Psi} = e\bar{\Psi}(1 - a\frac{1}{2}D)\gamma_5 .$$

However, the measure is not invariant under these transformations. In fact if $(\langle d[\Psi]|d[\bar{\Psi}]\rangle)$ is the measure,

$$\delta \langle d[\phi] \rangle = c a \tau(\gamma_5 D)|d[\phi]| = -2\epsilon N_f(n_+ - n_-)|d[\phi]| ,$$

where $N_f$ is the number of quark flavors [9]. This means that the flavor-singlet chiral transformation suffers an anomaly on the lattice like in the continuum. Further like in the continuum the anomaly arises only due to a non-zero index of $D$ which is given by $(n_+ - n_-)$, where $n_+$ are the number of zero modes of $D$ which are also simultaneous eigenstates of $\gamma_5$ with eigenvalue $\pm 1$. We will explain the origin of eq.(4) later. The flavored chiral transformations are obtained in the usual way by including a traceless flavor matrix in the transformations of eq.(6). The flavored transformations are exact symmetries of the theory. Thus chiral symmetry and the anomaly emerge exactly like in the continuum, however all the above arguments are being made on a finite lattice.

A natural candidate for the chiral condensate emerges like in the continuum. Starting from the definition of the (unnormalized) expectation value, $\langle \Psi \gamma_5 \Psi \rangle$ and performing a change of integration variables by an infinitesimal chiral transformation, it is easy to show that

$$\langle \Psi \gamma_5 \Psi \rangle = \langle \Psi \gamma_5 \Psi \rangle + 2\epsilon \langle \Psi(1 - \frac{1}{2}aD)\Psi \rangle .$$

This means that if the theory has an exact chiral symmetry then

$$\langle \Psi(1 - \frac{1}{2}aD)\Psi \rangle = 0 .$$

When the theory contains more than one flavor, the above relation strictly holds at finite volumes. This is because there exist flavored (chiral) symmetries that are not broken by any anomalies. The only way the chiral condensate could be non-zero, is due to spontaneous breaking of chiral symmetry which is a subtle feature of the thermodynamic limit. To see this one has to add a small mass term to the Dirac operator and break the symmetry explicitly. If the symmetry is spontaneously broken then the condensate would be non-zero when the thermodynamic limit is taken before the explicit symmetry breaking mass is set to zero. In the case of a single flavor, the only chiral symmetry of the action is broken by the measure and $\langle \Psi(1 - \frac{1}{2}aD)\Psi \rangle \neq 0$ even in finite volumes.

III. PIONS AND THE U(1) PROBLEM

In the presence of a mass term we can derive the modified relation

$$(1 + am)[(D + m)\gamma_5 + \gamma_5(D + m)] = m(2 + am)\gamma_5 + a(D + m)\gamma_5(D + m) ,$$

using the Ginsparg-Wilson relation. To see the origin of massless pions when the chiral symmetry is spontaneously broken, let us look at the zero momentum pion correlation function $G_{ab}(p = 0)$, which is given by

$$G_{ab} = \frac{1}{\Omega} \sum_{x,y} \langle \Psi i\tau^a \gamma_5 \Psi(x) \bar{\Psi} i\tau^b \gamma_5 \bar{\Psi}(y) \rangle .$$
where $\Omega a^4$ is the space-time volume, $\tau^{a,b}$ are the $N_f^2 - 1$ hermitian, traceless flavor matrices. Doing the Grassmann integral the above correlator can be rewritten as

$$G_{ab} = \frac{1}{\Omega a^8} \langle \text{tr} \left( \frac{1}{D + m} \tau^a \gamma_5 \frac{1}{D + m} \tau^b \gamma_5 \right) \rangle,$$

$$= \delta_{ab} \frac{1}{\Omega a^8} \langle \text{tr} \left( \frac{1}{D + m} \gamma_5 \frac{1}{D + m} \gamma_5 \right) \rangle,$$

where we have absorbed the fermion determinant in the path integral measure along with the Boltzmann weight due to spontaneous chiral symmetry breaking. In both these cases, if $G_{ab}$ must remain non-singular, the singular piece in the first term must cancel with a corresponding piece in the second term. This requires

$$\lim_{m \to 0} G_{ab} = \delta_{ab} \frac{1}{ma^4} \langle \bar{\Psi} [1 - \frac{1}{2} aD] \Psi \rangle.$$

If chiral symmetry is spontaneously broken the right hand side is singular in the chiral limit, if $\langle \bar{\Psi} [1 - \frac{1}{2} aD] \Psi \rangle \neq 0$. This is expected to be true in finite volumes for one flavor QCD due to the anomaly, and infinite volumes for two or more flavor QCD due to spontaneous chiral symmetry breaking. In both these cases, $G_{00}$ remains non-singular, which only enter through the fermion determinant. Thus in the quenched limit the left hand side is independent of the mass and number of fermion flavors, which only enter through the fermion determinant, exactly like in the continuum. This is because we can use eq.(8) and eq.(5) to show that

$$\text{tr} \left( \frac{1}{D + m} \gamma_5 \right) = \frac{2N_f}{m(2 + am)} (n_+ - n_-)$$

(15)

is even on a finite lattice. Thus we get

$$G_{00} = \frac{(1 + am)}{m(1 + am/2)} \langle \bar{\Psi} [1 - \frac{1}{2} aD] \Psi \rangle,$$

$$- \frac{(2N_f)^2}{m^4(2 + am)^2} \frac{1}{\Omega} \langle (n_+ - n_-)^2 \rangle.$$  (16)

This relation can be used to obtain new insight on the $U(1)$ problem. A solution to the $U(1)$ problem requires $G_{00}$ to remain non-singular in the chiral limit. It is clear that the first term on the right hand side is singular in the chiral limit, if $\langle \bar{\Psi} [1 - \frac{1}{2} aD] \Psi \rangle \neq 0$. This is expected to be true in finite volumes for one flavor QCD due to the anomaly, and infinite volumes for two or more flavor QCD due to spontaneous chiral symmetry breaking. In both these cases, $G_{00}$ must remain non-singular, the singular piece in the first term must cancel with a corresponding piece in the second term. This requires

$$\frac{1}{\Omega} \langle (n_+ - n_-)^2 \rangle = \frac{m}{N_f} \langle \bar{\Psi} [1 - \frac{1}{2} aD] \Psi \rangle,$$

(17)

at the leading order in the chiral limit. Thus we see that the solution to the $U(1)$ problem requires a connection between the lattice topological susceptibility defined using the index of the lattice Dirac operator, and the chiral condensate in the chiral limit. Such a connection is known in the literature in the context of effective models [12] and the large $N_c$ limit [13]. However, now the same result emerges directly from lattice QCD.

At finite volumes in the one flavor case, eq.(17) is easy to understand since only sectors with unit topological charge contribute to both sides of the equation. However, if one takes the infinite volume limit before taking the chiral limit, the relation is somewhat surprising. In this limit, the chiral condensate is expected to get contributions from a non-zero density of small eigenvalues of the Dirac operator. This is the content of the Banks-Casher formula [14] and will be derived later in the present context. The exact zero modes of the Dirac operator on the other hand are expected to be suppressed with the volume. Thus it is unclear why the topological susceptibility, which is related to exact zero modes on the lattice, is also related to the density of approximate zero modes as eq.(17) requires. Another interesting consequence of the equation is that the topological susceptibility goes linearly to zero with the mass, independent of the number of flavors, if chiral symmetry is spontaneously broken. This appears to be a consequence of the fact that the thermodynamic limit and the chiral limit do not commute [12].

The relation described by eq.(17) is valid only in the full theory of QCD where fermions can be created and destroyed in the vacuum. In the quenched limit the left hand side is independent of the mass and number of fermion flavors, which only enter through the fermion determinant. Thus in the quenched theory the flavor-singlet pion correlator will show divergences in the chiral limit, since the singular pieces between the two terms in eq.(16) do not cancel. The form of these singularities have been predicted using chiral perturbation theory...
IV. CRITICAL BEHAVIOR OF ZERO MODES

We can extend the above analysis to finite temperatures. It is clear that eq.(17) will be valid at non-zero temperatures in the phase where chiral symmetry remains broken and if the flavor singlet pseudo-scalar correlator is free of infra-red divergences. It is usually believed that for two massless flavors, infra-red divergences arise at the chiral transition $T_c$, only due to diverging correlation lengths in the pseudo-scalar isovector(the pions) channel and the scalar isocalar channel(the sigma). This leads to the $O(4)$ critical behavior which is second order \[ O(4) \] If this is true, the flavor singlet correlator given in eq.(16), must be free of infra-red singularities even at $T_c$. The chiral condensate is the order parameter of the phase transition and at $T_c$ has a critical behavior given by

$$\langle \Psi [1 - \frac{1}{2} a D] \Psi \rangle \sim m^{\frac{1}{2}}$$

(18)

where $\delta = 4.82 \pm 0.05$ \[ \delta \] is an $O(4)$ critical exponent. The cancellation of the singular pieces in the right hand side of eq.(18) leads to

$$\frac{1}{\Omega} \langle (n_+ - n_-)^2 \rangle \sim m^{1 + \frac{1}{2}}$$

(19)

at $T_c$. This critical behavior of the topological susceptibility has been ignored in the literature and can form a useful consistency check of $O(4)$ critical behavior.

For $T > T_c$, the topological susceptibility need not be related to the chiral condensate since in this phase both terms in the eq.(14) are finite in the chiral limit. However, if we assume that the thermodynamic and the chiral limits commute in the chirally symmetric phase, then for two or more flavors we can also predict

$$\frac{1}{\Omega} \langle (n_+ - n_-)^2 \rangle \sim \begin{cases} m & T < T_c \\ m^{N_f} & T > T_c \end{cases}$$

(20)

The prediction for $T > T_c$, is easily derivable from general considerations \[ T_c \]. This behavior is consistent with what we know about the phase transition. For example, with three or more flavors the transition is expected to be first order. This is reflected in the dramatic change in the small mass dependence of the topological susceptibility. The change in the two flavor theory is smaller and matches with the prediction of eq.(13) for a second order transition.

It is useful to look for the above critical behavior of the topological susceptibility in any study of the QCD phase transition, since it reflects the interesting interplay between the chiral symmetry and the $U(1)$ anomaly. It has been appreciated that this interplay is important in determining the order of the phase transition for two light flavors \[ \text{[14]} \]. In particular if the anomalous $U(1)$ is small for some dynamical reason, the fluctuations from new degrees of freedom can make the transition first order. On the other hand if the symmetry is broken by a large amount then the phase transition is expected to be in the $O(4)$ universality class.

The fermionic definition of the topological susceptibility, used in the above analysis can in principle be measured on the lattice since it involves calculating zero modes of the Dirac operator in a realistic simulation. In the staggered fermion formulation, which is most suited for studying the chiral phase transition, zero modes are shifted due to finite lattice spacing effects \[ \text{[20]} \]. Such effects distort the critical behavior of zero modes, and one needs to invoke the continuum limit to see the effects of the anomalous symmetry emerge at the QCD phase transition \[ \text{[24,23]} \]. However, approaching the continuum limit is quite difficult. On the contrary, there is evidence \[ \text{[22]} \] that with Ginsparg-Wilson fermions the continuum limit is not necessary to see the zero modes that are responsible for the anomalous symmetry breaking. Thus the above critical behavior should emerge even at finite lattice spacings.

V. DISCUSSION AND CONCLUSIONS

All the above results have been derived without specifying an explicit realization of the the Dirac operator that obeys the Ginsparg-Wilson relation. However, it is important that the Dirac operator does not suffer from doubling, since it is possible to find Dirac operators which obey the Ginsparg-Wilson relation but do not solve the fermion doubling problem. In such cases, the real dynamics of QCD will not be reproduced. The chiral symmetry discussed could be flavored as in staggered fermions. The two known classes of solutions based on the fixed point actions \[ \text{[6,23]} \] and the overlap formulation \[ \text{[8]} \] are expected to solve the doubling problem completely. The proposal by Neuberger has a simple structure based on the four dimensional Wilson like Dirac operator $D_W$, and is given by $a D = 1 + D_W (D_W^* D_W)^{-1/2}$. The important point is that $D_W$ must have an appropriately tuned negative mass term to be in the right phase to produce QCD. Whether such a phase exists is currently being explored. A further effect of the Wilson mass is to renormalize the theory and control leading lattice artifacts.

The Neuberger Dirac operator is also closely related to the Shamir’s variant of the domain wall fermions \[ \text{[25]} \], when the distance between the walls is taken to infinity. It is likely that all the nice properties discussed above will emerge with small violations when the walls are separated by a large but finite separation. This strat-
ergy can be used for practical simulations and still retain the interesting properties of Ginsparg-Wilson fermions. Preliminary tests for QCD have proved that domain wall fermions preserve chiral symmetry properties very well [29]. Presently, these Domain wall fermions are being used to study the QCD phase transition [27]. Preliminary tests seem to indicate the presence of zero modes that break the anomalous $U_A(1)$ symmetry even above the phase transition. This suggests that it should be possible to extend the above discussion of the critical behavior of the topological charge to such a study. This would give a more quantitative grasp of the two flavor QCD phase transition than has been possible before.

The above solutions to the Ginsparg-Wilson relation obey an extra hermiticity property, namely $D^\dagger = \gamma_5 D \gamma_5$. Based on this it is possible to write a formula for the chiral condensate in terms of the eigenvalues of the Dirac operator. It is easy to show that $aD - 1$ is unitary whose eigenvalues can be represented as $-\exp(i\theta)$, $-\pi \leq \theta \leq \pi$. The exact zero modes of $D$ correspond to eigenvalues at $\theta = 0$. Thus

$$\langle \Psi \big| \frac{1}{2} aD \big| \Psi \rangle = \frac{1}{a^2} \int_{-\pi}^{\pi} d\theta \rho(\theta) \frac{1 + \cos(\theta) + i \sin(\theta)}{2(1 - \cos(\theta) - i \sin(\theta) + am)}, \quad (21)$$

where $\rho(\theta)$ is the normalized density of eigenvalues $\int d\theta \rho(\theta) = 4N_fN_c$. Due to the hermiticity of $D$ the eigenvalues come in complex conjugate pairs, so that $\rho(\theta)$ is a symmetric function. In the $m \to 0$ limit it is easy to show that

$$\langle \Psi \big| \frac{1}{2} aD \big| \Psi \rangle = \frac{1}{a^2} \pi \rho(0). \quad (22)$$

This is the Banks Casher formula [14]. In the present context it is easy to see that $\text{tr}(\gamma_5 D)$ gets contribution only from the subspace of eigenvectors of $D$ with eigenvalues $2/a$. However this contribution is also related to $(n_+ - n_-)$ due to the fact that $\text{tr}(\gamma_5) = 0$. This is one way to understand the origin of eq.(3).

Results from simulations using the Dirac operator suggested by Neuberger in the Schwinger model [28] and the domain wall fermions in quenched QCD [29] give clear evidence for divergences in the quenched chiral condensate due to exact zero modes on finite lattices. Such singularities are expected due to the anomaly as discussed above, but have not been seen in realistic simulations involving staggered fermions. This perhaps reflects the fact that the breaking of chiral symmetry in the quenched theory, is represented well by Ginsparg-Wilson fermions even at finite lattice spacings. Thus, quenched lattice QCD with Ginsparg-Wilson fermions may give a more definitive answer to the question about the reliability of the quenched approximation.

In conclusion, we have shown how Ginsparg-Wilson fermions reproduce the low energy physics of QCD at finite lattice spacings. The exact chiral symmetry of the action can in principle be used to derive a host of soft pion theorems even at finite lattice spacings. We have concentrated on the Goldstone's theorem and obtained interesting consequences from a solution to the $U(1)$ problem. We have also suggested how the critical behavior of the topological susceptibility can confirm the second order nature of the QCD phase transition with two massless quarks. If simulations involving Ginsparg-Wilson fermions are feasible it is very likely that the results would reflect physical reality more easily than the conventional fermion formulations.

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