I derive the overlap Dirac operator starting from the overlap formalism, discuss the numerical hurdles in dealing with this operator and present ways to overcome them.

1. Introduction

The overlap Dirac operator, derived from the overlap formalism for the special case of vector gauge theories, is a way to realize exact chiral symmetry on the lattice. Exact chiral symmetry on the lattice does come at a price—numerical implementation of the overlap Dirac operator is significantly more expensive than Wilson or staggered operator. In spite of this numerical hurdle, we already have several physics results in quenched gauge theories using the overlap Dirac operator:

(i) Evidence for spontaneous chiral symmetry breaking at zero temperature.
(ii) Evidence for chiral symmetry breaking in the deconfined phase possibly due to a dilute gas of instanton and anti-instanton.
(iii) Evidence for a diverging chiral condensate in the two dimensional U(1) case.
(iv) A study of exact zero modes of overlap fermions in the adjoint representation lend some support to the existence of fractional topological charge.

In this talk, I shall derive the overlap Dirac operator starting from the overlap formalism, discuss the numerical hurdles in dealing with this operator and present ways to overcome them.

2. The Overlap formalism

The determinant of the chiral Dirac Operator \( C = \sigma_{\mu} (\partial_{\mu} + iA_{\mu}) \) can be realized on the lattice as an overlap of two many body states, namely:

\[
\text{det} C = \langle 0 - |0+ \rangle, \quad (1)
\]

where \(|0\pm >\) are many body ground states of \(a^{\dagger}H(m)a\) and \(a^{\dagger}\gamma_{5}a\) respectively. The \(a^{\dagger}\) and \(a\) are canonical fermion creation and destruction operators and \(\gamma_{5}H(m)\) is a massive Dirac operator on the lattice with the mass set to a value less than zero. One choice is the Wilson Dirac operator, \(H(m) = H_{w}(m)\). This realization of the chiral Dirac operator is natural since \(C\) is an operator that maps two different spaces, namely spinors under the \((0,1/2)\) representation to \((1/2,0)\) representation.
Therefore $C$ does not have an eigenvalue problem and the determinant of $C$ is a map between the highest form in the two spaces connected by the operator $C$.

Clearly, the overlap formula does not fix the phase of $|0+\rangle$ since it is only defined as an eigenvector of a Hamiltonian and this is how it should be since the chiral determinant is a map between two different spaces. The details involved in the phase choice and possible gauge breaking is the subject of chiral gauge theories.

For vector gauge theories, we want $\det CC^\dagger = |\langle 0^- | 0+\rangle|^2$ and the phase choice does not matter indicating a trivial cancelation of anomalies.

Computing the overlap of two many body states seems like an insurmountable numerical task in four dimensional theories since one has to diagonalize $H_w$, form the many body state from the negative energy single particle states and compute the overlap by computing a determinant of a dense matrix, half the size of $H_w$. But there is an elegant solution to circumvent these steps by directly dealing with the many body states and this is the overlap Dirac operator.

The massless overlap Dirac operator

$$D_o = \frac{1}{2} \left[ 1 + \gamma_5 \epsilon(H_w) \right]$$  \hspace{1cm} (2)

is derived from the overlap formalism as follows. Let $U$ be the unitary matrix that diagonalizes $H_w$:

$$H_w U = U \lambda; \quad U = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix}; \quad \epsilon(H_w) \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} = \begin{pmatrix} \alpha & -\gamma \\ \beta & -\delta \end{pmatrix}$$  \hspace{1cm} (3)

Using $\det U = \det \alpha / \det \delta$, we derive

$$|\langle 0^- | 0+\rangle|^2 = \det \delta \det \delta^\dagger = \det \delta \det \alpha \det U^\dagger = \det \begin{pmatrix} \alpha & 0 \\ 0 & \delta \end{pmatrix} U^\dagger$$

$$= \det \frac{1}{2} \left\{ \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} + \begin{pmatrix} \alpha & -\gamma \\ -\beta & -\delta \end{pmatrix} \right\} U^\dagger$$

$$= \det \frac{1}{2} \left\{ \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \alpha & -\gamma \\ \beta & -\delta \end{pmatrix} \right\} U^\dagger$$

$$= \det \frac{1}{2} \left[ U + \gamma_5 \epsilon(H_w) U \right] U^\dagger = \det \frac{1}{2} \left[ 1 + \gamma_5 \epsilon(H_w) \right]$$  \hspace{1cm} (4)

It is not immediately clear as to how it helps numerically since one will have to deal with $\epsilon(H_w)$ without having to diagonalize $H_w$. There are two possible approaches. One approach is to use Gegenbauer polynomials to represent $\sqrt{H_w^2}$.

Typically one need to go to a high order polynomial and this method is not expected to efficient. The other approach is to use the rational approximation where one approximates $\epsilon(H_w)$ as a sum of poles

$$\epsilon(H_w) = c_0 + \sum_{i=1}^n \frac{c_i H_w}{H_w^2 + d_i}$$  \hspace{1cm} (5)
Using the method of multiple masses, one action of $\epsilon(H_w)$ on a vector can be realized by a single conjugate gradient algorithm independent of the number of poles. This makes it numerically quite attractive.

3. Spectrum of the quenched $H_w$

$\epsilon(H_w)$ is discontinuous at the zero of $H_w$. Approximations have to be good up to lowest eigenvalue of $H_w$ and this can be a problem if $H_w$ has very small eigenvalues. The density of the spectrum of $H_w(m)$, $\rho(\lambda)$, in a quenched ensemble has a non-zero $\rho(0)$ at any fixed lattice coupling at the values of $m$ that are relevant ($m < m_c$). This numerical result has support from an analytical argument where one shows that small defects can already give rise to a gapless spectrum.

One can also show that a change in gauge field topology necessitates zero eigenvalues at any mass. To see this, let us assume we have a gauge field configuration that has zero topology. Then $H_w(m)$ has an equal number of + and - eigenvalues. Consider evolving from this configuration to another gauge field configuration that has non-zero topology. This configuration has a spectrum where the number of + and - eigenvalues of $H_w(m)$ are not equal. The spectrum as a function of the evolution has one configuration in the path where $H_w(m)$ has a zero eigenvalue. In a discrete evolution scheme the exact zero will be avoided but one can have arbitrarily small eigenvalues.

Therefore one will have to live with very small eigenvalues of $H_w(m)$ or its variants. Numerical techniques that deal with $\epsilon(H_w)$ will have to project out a few small eigenvectors and treat them exactly. On a finite lattice and at a fixed lattice spacing, the number of eigenvalues below a fixed number $\lambda_{\text{min}}$ will grow with volume since $\rho(0)$ is finite. This would mean that one has to project out more eigenvalues as one increases the volume and/or go to a larger number of poles in the rational approximation. It is useful to compare the overlap formalism with the related method used to realize chiral symmetry on the lattice, namely domain wall fermions. This is a five dimensional realization and the effective overlap Dirac operator is obtained by setting $H = H_d = \log(T_w)$ where $T_w$ is the transfer matrix in the fifth direction. The low lying spectrum of $H_d$ is completely governed by the low lying spectrum of $H_w$ and hence the problems caused by a finite $\rho(0)$ exist for domain wall fermions. In practice one works with a finite extent in the fifth direction ($L_s$) and this amounts to an approximation of the $\epsilon(H_w)$ by $\tanh(\frac{1}{2}L_s H_d)$. Clearly, small eigenvalues are not taken care of properly at a finite $L_s$ and one will have to go to larger $L_s$ as one increases the lattice volume at a fixed lattice spacing. Current simulations using domain wall fermions seem to indicate a significant effect due to finite $L_s$. One can avoid this by projecting out small eigenvalues and treating them exactly in the domain wall formalism.

Each action of $\epsilon(H_w)$ requires a Conjugate Gradient type algorithm and therefore the solution to the equation of the form $D_\psi(m) \psi = b$ requires nested Conjugate Gradient. Is it numerically much more involved than domain wall fermions since it only involves one inversion of a higher dimensional operator? One can write down a
five dimensional operator from which one gets the required four dimensional overlap Dirac operator by integrating out all but one fermion degree of freedom. An analysis of the condition numbers shows that the the five dimensional inversion is no less expensive that two nested conjugate gradients. In the nested case, it is easy to see that the condition number is proportional to the product of the condition number of $H_w$ and the fermion mass, $\mu$. This also turns out to be the case for the five dimensional version and for the conventional domain wall fermions. This shows that it is practical to work directly with the four dimensional operator.

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