Exact local fermionic zero modes

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Abstract

We introduce a simple method to find localized exact fermionic zero modes for any local fermionic action. The zero modes are attached to specific local gauge configurations. Examples are provided for staggered and Wilson fermion actions in 2-6 dimensions, at finite and infinite lattice volumes, and for abelian and non-abelian gauge groups. One of our concrete results is that a finite density of almost zero modes must occur in quenched four dimensional lattice gauge theory simulations that use traditional methods. This density is exponentially suppressed in the gauge coupling constant.

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I. INTRODUCTION

Lattice fermions in interaction with background gauge fields have a tendency to produce localized fermionic approximate zero modes. Since the zero modes are localized, the influence of gauge fields far away from the center of the zero mode is small and should be well approximated by a mean-field, uniform configuration. One would guess then that what causes the zero mode is a certain local structure in the gauge configuration. In this paper we show how one can easily test whether a given local gauge configuration will have an exact zero mode at finite or infinite lattice size. We also show that one can get approximate zero modes in this way, using the variational principle. Inverting the logic, we show how one can find local gauge structures that bind fermionic (approximate) zero modes to them.

There are two main classes of fermionic lattice zero modes: relatively large ones that should scale and have a physical effect in the continuum limit and very local ones, whose size shrinks to zero on continuum scales and therefore are lattice artifacts. The lattice artifact zero modes are a serious impediment to practical simulations in the quenched approximation [1] and to the implementation of exact chirality on the lattice using the overlap Dirac operator [2].

A better understanding of the fermionic zero modes is important in both cases: we want to see their effects clearly when these are genuine continuum effects [3] and would like to suppress them when they are lattice artifacts. There is a difference between the roles the approximate zero modes which are lattice artifacts play in the traditional context and in the overlap context. In a traditional quenched QCD calculation the lattice artifacts can become an unsurmountable problem because their effect on fermion propagators can be spuriously large and there is no natural prescription for how to handle these non-universal effects. In the context of the overlap however, the problem is less severe because there is a well defined natural procedure to deal with these lattice artifacts. The problem is now only of a numerical nature, since the evaluation of the sign function for numerically tiny arguments is computationally costly. Strictly speaking, exact zero modes are not a major difficulty in either framework. Still, when trying to understand the origin of the approximate fermionic zero modes, it is best to start analytical work from exact ones.

II. THE BASIC IDEA

Let $S$ denote a cluster comprising of a finite local collection of sites $s$ and let the gauge field configuration have $U_{\mu}(x) \equiv 1$ on all links outside the cluster. Let $V_S$ be the subspace of the space $V$ of fermion fields $\psi$ with $\psi(x) = 0$ for $x \notin S$. Let $D_f$ be the appropriate sparse matrix realization of the free lattice Dirac operator with uniform link variables $U_{\mu}(x) \equiv 1$. Let us assume that $G_f = D_f^{-1}$ exists. The total Dirac operator, $D$, maps $V$ into $V$ and is given by

$$D = L + D_f$$

(1)

$L$ maps the entire $V$ into $V_S$. Consider now the operator
\[ R = 1 + LG_f \]  

(2)

It naturally defines a restricted operator \( R_S \) from \( V_S \) to \( V_S \).

The equation \( D\psi = 0 \) has a solution in \( V \) if and only if there is a \( \phi \in V_S \) such that \( R_S\phi = 0 \). (At infinite volume this solution will be normalizable if the decay of \( G_f \) is fast enough.) The main point is that \( R_S \) is a small matrix if the cluster is small.

The proof of the above assertion is easy: If \( \psi \) is a zero mode of \( D \) define \( \phi = L\psi \); clearly, \( \phi \in V_S \) and \( L(1+G_fL)\psi = 0 \). If \( \phi \in V_S \) obeys \( R_S\phi = 0 \), define \( \psi = -G_f\phi \). Since \( \phi = -LG_f\phi \), we also have \( L\psi = \phi \) implying \( D\psi = 0 \).

The above observations can be easily extended to the case that \( R_S^\dagger R_S \) has a small eigenvalue \( \eta \). Then, one gets a variational upper bound for the lowest eigenvalue of \( D^\dagger D \). If there are several linearly independent small eigenvalue eigenstates of \( R_S \) then we have bounds on several of the lowest eigenvalues of \( D^\dagger D \). For a single state \( \phi \in V_S \) satisfying

\[ R_S^\dagger R_S\phi = \eta\phi \]  

(3)

we make the variational ansatz

\[ \psi = -G_f\phi \]  

(4)

and find

\[ \lambda_{\min}(D^\dagger D) \leq \eta \frac{\phi^\dagger\phi}{\phi^\dagger D^\dagger D_f\phi} \]  

(5)

### III. “FLUXON” CONFIGURATION WITH STAGGERED FERMIONS

This is an example that was partially analyzed before [4]. The gauge configuration consists of making all links that go out into the positive directions of a fixed site be \(-1\). All other links are set to unity. This configuration was called a “fluxon” in the past. It is a local minimum of the single plaquette action with gauge groups \( U(1) \) or \( SU(2) \) and with both a fundamental and an adjoint term. For \( SU(2) \) it is known that there is a crossover along the Wilson line which is related to an end point of a transition line in the extended fundamental-adjoint plane [4]. The transition across that line can be argued to be related to a condensation of fluxons. At weak coupling there is a finite and calculable density of local fluxons.

We first consider naive fermions in a single fluxon background. In \( d \) dimensions we shall find, at infinite volume, several degenerate normalizable fermionic zero modes. The decay of the zero modes is power-like, since the fermionic theory is massless.

In \( d \) dimensions the \( \gamma_\mu \) matrices are \( 2^{d_2}\times 2^{d_2} \), where \( d_2 \) is the integer part of \( \frac{d}{2} \). A simple calculation produces the following \((d+1)2^{d_2}\times (d+1)2^{d_2} \) \( R_S \) matrix:

\[ R_S = \begin{pmatrix} 1 - \frac{1}{d} \gamma \gamma^T & 0 \\ 0 & 0 \end{pmatrix} \]  

(6)

Here we introduced a \( 2^{d_2}d \times 2^{d_2} \) matrix \( \gamma \) and the \( 2^{d_2} \times 2^{d_2}d \) matrix \( \gamma^T \).
\[ \gamma = \begin{pmatrix} \gamma_1 \\ \gamma_2 \\ \vdots \\ \gamma_d \end{pmatrix}, \quad \gamma^T = (\gamma_1 \gamma_2 \ldots \gamma_d) \tag{7} \]

The most evident zero mode (normalizable for \( d \geq 3 \)) is given by choosing

\[ \phi = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \chi \end{pmatrix} \tag{8} \]

Each entry above has \( 2d^2 \) components. We then find \( 2d^2 \)-fold degenerate zero modes given by (up to normalization factors):

\[ \psi_0(x) = -\int \frac{d^d p}{(2\pi)^d} \frac{\sin px}{\sum_\mu \gamma_\mu \sin p_\mu} \chi \tag{9} \]

This class of zero modes has been found previously in [4]. Our more detailed study here shows that there are more zero modes: Choose \( \phi' \)

\[ \phi' = \begin{pmatrix} \gamma_1' \\ \gamma_2' \\ \vdots \\ \gamma_d' \\ 0 \end{pmatrix} \tag{10} \]

It is easy to check that

\[ (1 - \frac{1}{d} \gamma \gamma^T) \phi' = 0 \tag{11} \]

The new zero modes of \( D \) are

\[ \psi'_0(x) = i\delta_{x,0}' x + \frac{1}{2} \int \frac{d^d p}{(2\pi)^d} \sin px \frac{1}{\sum_\mu \sin^2 p_\mu} \left[ \sum_{\mu \neq \nu} \gamma_\mu \gamma_\nu \sin(p_\mu - p_\nu) + \sum_\mu \sin 2p_\mu \right] \chi' \tag{12} \]

In four dimensions for example, we have found 8 zero modes. There are no other zero modes. Each set of four zero modes maps into itself under the action of \( \gamma_5 \). One can easily decompose each set of 4 zero modes into 2 of positive chirality and 2 of negative chirality. One naive lattice fermion should represent 16 continuum fermions. The fluxon configuration background breaks the continuum flavor symmetry because there are half as many zero modes as expected continuum fermions.

Consider now staggered fermions; they are treated by block diagonalizing the naive fermion system. When we decouple the four dimensional naive fermions into four staggered fermions, each will have two zero modes. In the continuum limit each staggered fermion should reproduce four flavors. With only two zero modes for a staggered fermion it is again clear that the fluxons are nonperturbative contributors to lattice flavor symmetry breaking.
IV. “FLUXON” CONFIGURATION WITH WILSON FERMIONS

The zero modes we found above were localized only by power decays. To get light quarks with Wilson fermions the mass parameter has to be given negative values. The free propagator is now massive, decaying exponentially. We use the same technique to look for negative mass values where fluxons can produce exact, exponentially localized, fermionic zero modes.

We work in dimension \( d \) larger or equal to 2. The matrix \( R_S \) now becomes:

\[
R_S = 1 + \begin{pmatrix}
(1 + \gamma_1)G_f(0, \hat{1}) & \cdots & (1 + \gamma_1)G_f(0, \hat{d}) & (1 + \gamma_1)G_f(0, 0) \\
\vdots & \ddots & \vdots & \vdots \\
(1 + \gamma_d)G_f(0, \hat{1}) & \cdots & (1 + \gamma_d)G_f(0, \hat{d}) & (1 + \gamma_d)G_f(0, 0) \\
\sum_{\mu}(1 - \gamma_{\mu})G_f(\hat{\mu}, \hat{1}) & \cdots & \sum_{\mu}(1 - \gamma_{\mu})G_f(\hat{\mu}, \hat{d}) & \sum_{\mu}(1 - \gamma_{\mu})G_f(\hat{\mu}, 0)
\end{pmatrix}
\]  

(13)

To search for zero modes we calculate the determinant of \( R_S \). It inherits reality from the determinant of \( D \). By working out explicitly the cases \( d = 2, 3, 4, 5, 6 \) we arrive at a formula for general \( d \). We have not derived the formula for arbitrary \( d \), so we present it as a conjecture.

\[
\det R_S = \left[ 1 + \frac{d - 1}{d}[x(m + d) - 1]^2 + 2[x(m + d) - 1] + d(d - 1)xy \right]^{2^{d_2}}
\]  

(14)

The parameters \( x \) and \( y \) are defined by fermionic propagators:

\[
x = \int \frac{d^d p}{(2\pi)^d} \frac{b(p)}{b^2(p) + s^2(p)} , \quad y = \int \frac{d^d p}{(2\pi)^d} \frac{\cos p_1[2\sin^2 p_2 - b(p)\cos p_2]}{b^2(p) + s^2(p)} , \quad b(p) = m + d - \sum_{\mu}\cos p_\mu \quad , \quad s^2(p) = \sum_{\mu}\sin^2 p_\mu
\]  

(15)

When there are zero modes, they will be \( 2^{d_2} \)-fold degenerate (at least for \( d = 2, 3, 4, 5, 6 \)).

It is a simple matter now to search for an \( m \) for which there are zero modes. We start from \( m = 0 \) and search going towards negative values. The first mass values which gives zero modes is listed below. As far as simulations go, only the region \(-2 < m < 0\) is of interest.

For \( d = 4 \) the first zero is at \( m = -2.87982 \), for \( d = 3 \) the first zero is at \( m = -1.940553 \), and for \( d = 2 \) the first zero is at \( m = -0.90096 \). So, in four dimensions the fluxon is not of great importance, but in two dimensions it is. Note that the fermions do not react to the fluxon as they would to an instanton in the continuum as reflected by the zero-mode degeneracy we find.

V. A SMALL TWO DIMENSIONAL INSTANTON

We now turn to analyze a small two dimensional instanton. It is described by four plaquettes making up a square, with each plaquette carrying \( \frac{\pi}{2} \) units of angular flux.

The calculations are now more involved, but the bottom line is that we find a non-degenerate zero at \( m = -0.39182 \), which certainly is of interest. For this value of \( m \) the free
propagator decays quite fast so the zero mode is quite local. Effects of boundary conditions can be easily investigated by appropriately adjusting $D_f$ and the gauge background. They are more sizable with periodic boundary conditions than with antiperiodic boundary conditions. We have also looked at the dependence on the toron coordinates (zero Fourier modes of the gauge fields $A_\mu(x)$ where the link variables are $U_\mu(x) = e^{iA_\mu(x)}$). Boundary conditions are implemented by choosing specific toron configurations. Finite volume calculations require the replacement of the momentum integrals by the appropriate sums.

VI. FINDING GAUGE CONFIGURATIONS THAT BIND ZERO MODES

Choosing a cluster of sites of certain shape we now view the link variables residing on the links in the cluster as unknowns. For each such gauge field configuration we numerically compute the smallest eigenvalue of $R_S^\dagger R_S$, $\lambda_{\text{min}}(R_S^\dagger R_S)$, using Wilson fermions at some negative value of the mass parameter $m$. Varying the gauge background, and proceeding by steepest descent we can find local minima of $\lambda_{\text{min}}(R_S^\dagger R_S)$ as a function of the link variables. Often, we end up finding the minimum to be zero and then the corresponding gauge field configuration binds a localized exact zero mode. This search for a gauge configuration can be repeated for different starting gauge configurations and different values of the mass parameter. To speed the numerical procedure up we took the free propagators appearing in $R_S$ on a finite periodic lattice of size $8^d$.

Restricting ourselves to $U(1)$ fields, in 3D, on a cluster comprising of four sites that can support a fluxon, we find zero modes only for $m < -1.9$. The minimizing configuration is not a fluxon and it depends upon the gauge configuration we start our steepest descent search from. Nevertheless, always, the Wilson plaquette action of the minimizing configuration is close to the one of a fluxon. As long as we restrict our gauge configurations to having nontrivial links only along the links contained in the cluster, different link configurations are gauge inequivalent. Thus, there are many gauge inequivalent configurations that can produce fermionic zero modes.

In four dimensions the situation is similar for the fluxon type cluster but now we find zero modes only for $m < -2.5$, which is outside of the range of immediate interest.

Our next step is to see what happens when we increase the cluster size. We consider now larger clusters that make up a cube in 3D or a hypercube in 4D. Keeping the gauge fields still in $U(1)$ we find that now we can get zero modes at masses closer to zero. In 3D zero modes are occurring for $m < -1.1$ and in 4D for $m < -1.7$. Thus, a moderate increase in cluster size increases the chances to produce zero modes at Wilson masses relevant to QCD simulations.

Finally we also look at what happens when one goes from the abelian $U(1)$ gauge group to the non-abelian $SU(2)$ gauge group. We find that making the non-abelian gauge group always allows certain gauge configuration to bind zero modes for Wilson masses closer to zero than in the abelian case. Thus, increasing the size of the group also increases the chances to produce zero modes at practically relevant values of the Wilson mass parameter $m$.

The results of our numerical search are summarized in Fig. 1. We plot there on logarithmic scale the minimum of the smallest eigenvalue of $R_S^\dagger R_S$ as a function of the Wilson
mass parameter \( m \), for four different clusters. The 3-link and 4-link clusters in 3D and 4D mentioned in the figure contain 4 sites and 5 sites respectively and can accommodate the fluxon configurations we studied analytically before. The other two clusters we plot results for are the cube in 3D and the hypercube in 4D. For example, we see in the figure that we can get zero modes for \( m < -1.1 \) in 4D if we consider a cluster that makes up a hypercube. Note the sudden decrease in \( \lambda_{\text{min}}(R_S^* R_S) \) as a function of \( m \); it reflects a major change in the minimizing gauge configuration. Thus, for this type of cluster, \( \lambda_{\text{min}}(R_S^* R_S) \) has a non-analytic dependence on the gauge background at some value of \( m \) located inside the range of interest \( -2 < m < 0 \). Whatever the ultimate role of this effect is in a full quenched simulation of QCD is, it cannot be helpful to the hope of recovering a limit that can be described by a local effective Lagrangian of some kind.

VII. HOW TO AVOID ZERO MODES

We found that a cluster of SU(2) gauge fields as small as a hypercube can give rise to zero modes for Wilson fermions at masses close enough to zero to be relevant to practical simulations. These simulations can be with traditional fermions, or with overlap fermions. In both cases the presence of fermionic zero modes is a problem for quenched simulations; this problem has a practical solution in the overlap case, but they are still costly to handle because they need to be individually identified and projected out \( \mathbb{R} \).

Our construction directly and explicitly shows that the number of fermionic zero modes is proportional to the lattice volume, because the wave functions are explicitly known to decay exponentially, and the clusters are small and can be well separated. The rate of decay of the zero mode wave functions is given by the distance of \( m \) from the nearest even non-negative integer. The pure gauge action for the clusters is exponentially suppressed and it is possible that the density of the associated zero modes be so small that in a practical simulation volume there would be a small chance to even produce one such mode. On the other hand, we know that small modes in numbers proportional to the lattice volume do occur for quenched gauge field configurations. To be sure, we have not established that the particular clusters we investigate here are responsible for all the small modes one sees in typical QCD simulations. But, in principle, we have established that there is a finite density of fermionic zero modes, and that this density is exponentially suppressed in the gauge coupling constant, consistent with numerical findings \( \mathbb{R} \). Clearly, in four dimensions, a crucial question is how this suppression relates to the standard asymptotic freedom formula for a density of dimension four. We hope to come back to this point in the future.

It would be nice to be able to avoid these unphysical zero modes. One can do that by changing the pure gauge action so that the density of the zero modes be further reduced. This has been argued to work to some extent \( \mathbb{R} \). Another way would be, in accordance with the exact bound \( \mathbb{S} \), to make the local field strength close to zero. This could be achieved, for example, by replacing all links by APE smeared ones \( \mathbb{F} \). However, this decouples the fermions from higher momentum modes of the gauge field and makes it somewhat unclear whether we are still dealing with a single scale problem, rather than a two scale problem, where the fermions couple to gauge fields only at the lower scale.

Another possibility, suggested in \( \mathbb{G} \), is to APE smear only the links that enter into
FIG. 1. Plot of $\lambda_{\min}(R_3^1 R_S)$ as a function of mass for four different SU(2) clusters. Two of them are in 3D and two of them are in 4D.
the Wilson mass term, but not those that are coupled to the Dirac $\gamma$-matrices. In practice, implementing this last alternative would roughly quadruple the time it takes to calculate the action of the Wilson Dirac operator on a fermion field, because the projector structure of the $1 \pm \gamma_\mu$ terms is lost and the fermions now interact with two kinds of gauge fields.\footnote{We thank Urs Heller for correcting our original erroneous statement at this point.}

With our methods it is easy to obtain a rough estimate of the effect on the zero modes this latter possibility will have. We simply replace the links entering the Wilson mass term by unity, leaving the links entering the other terms in the Wilson Dirac operator free to change. This clearly is inconsistent in terms of the entire gauge background, but is very easy to implement. We find that this replacement of the Wilson mass term chases the fermionic zero modes away from negative mass values too close to zero. This is an encouraging sign, and the idea deserves further investigation.

\section*{VIII. CONCLUSIONS}

In this paper we have devised a simple way to look for approximate and exact fermionic zero modes on the lattice and for the gauge configurations that bind them. The fermionic zero modes are bound to local gauge configurations and are exponentially localized. In a real quenched simulation they will come at a finite density making the quenched approximation in principle unusable when traditional fermions and a traditional gauge action are employed and one wants realistically light quarks to emerge in the continuum. Our method makes it obvious that such fermion zero modes will occur with a finite probability per unit Euclidean four volume. We hope to use this technique in the reverse, namely, as a method to efficiently search for ways to ameliorate the practical problems posed by fermionic almost zero modes in the overlap context.

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