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Adams, David Henry

[General bounds on the Wilson-Dirac operator](#) Physical Review D, 2003; 68(6):065009

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<http://link.aps.org/doi/10.1103/PhysRevD.68.065009>

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20<sup>th</sup> May 2013

<http://hdl.handle.net/2440/55595>

## General bounds on the Wilson-Dirac operator

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(Received 9 May 2003; published 11 September 2003)

Lower bounds on the magnitude of the spectrum of the Hermitian Wilson-Dirac operator  $H(m)$  have previously been derived for  $0 < m < 2$  when the lattice gauge field satisfies a certain smoothness condition. In this paper lower bounds are derived for  $2p - 2 < m < 2p$  for general  $p = 1, 2, \dots, d$  where  $d$  is the spacetime dimension. The bounds can alternatively be viewed as localization bounds on the real spectrum of the usual Wilson-Dirac operator. They are needed for the rigorous evaluation of the classical continuum limit of the axial anomaly and the index of the overlap Dirac operator at general values of  $m$ , and provide information on the topological phase structure of overlap fermions. They are also useful for understanding the instanton size dependence of the real spectrum of the Wilson-Dirac operator in an instanton background.

DOI: 10.1103/PhysRevD.68.065009

PACS number(s): 11.15.Ha

### I. INTRODUCTION

It is well known from numerical studies (see, e.g., [1,2]) that in smooth gauge backgrounds in  $d$  dimensions the real eigenvalues of the Wilson-Dirac operator are localized around the values  $0, 2, 4, \dots, 2d$  (in units of the inverse lattice spacing, and with Wilson parameter  $r = 1$ ). In this paper we give an analytic derivation of this numerical observation. Our smoothness condition is the “admissibility condition” of [3,4]:

$$\|1 - U(p)\| \leq \epsilon \quad \forall \text{ plaquette } p. \quad (1.1)$$

Since the plaquette variable has the expansion  $U(p) = 1 - a^2 F_{\mu\nu}(x) + O(a^3)$  in powers of the lattice spacing  $a$ , Eq. (1.1) can be regarded as an approximate smoothness requirement on the curvature of the lattice gauge field. If  $U$  is the lattice transcript of a smooth continuum gauge field then Eq. (1.1) is automatically satisfied for any  $\epsilon > 0$  when the lattice is sufficiently fine.

In fermionic definitions of the topological charge of lattice gauge fields the low-lying real eigenmodes of the Wilson-Dirac operator  $D_w$  are interpreted as would-be zero modes, while the other real eigenmodes are interpreted as would-be doubler modes. This interpretation relies on the real eigenvalues being localized as described above, which is not the case in general for arbitrary rough gauge fields. The localization result for the real spectrum of  $D_w$  derived in this paper provides a specific analytic criterion under which the localization is guaranteed. It is also of interest in connection with the overlap fermion formulation on the lattice [5,6]. This is because a real eigenmode for the Wilson-Dirac operator is equivalent to a zero mode for the Hermitian Wilson-Dirac operator with negative mass parameter:

$$D_w \psi = \frac{m}{a} \psi \Leftrightarrow H(m) \psi \equiv \gamma_5 (a D_w - m) \psi = 0. \quad (1.2)$$

Localization of the real eigenvalues of  $D_w$  around  $0, 2, \dots, 2d$  (in units of  $1/a$ ) is therefore equivalent to the absence of zero modes for  $H(m)$ , i.e., to the existence of nonzero lower bounds on  $|H(m)|$ , when  $m$  is away from these values. This implies a topological phase structure for the overlap Dirac operator [6]  $D_{\text{ov}} = (1/a)[1 + \gamma_5 H(m)/|H(m)|]$ , since the index of  $D_{\text{ov}}$  (a well-defined integer) is locally independent of  $m$  but can jump at the values for which  $H(m)$  has zero mode(s). The topological phase structure of  $D_{\text{ov}}$  has previously been studied in Refs. [7,8]. The bounds derived in this paper lead to analytic information on the topological phases which complements the numerical results of those papers.

Furthermore, a nonzero lower bound on  $|H(m)|$  allows the locality of the overlap Dirac operator and its smooth dependence gauge field to be analytically established [3] (see also [9]). The general bounds derived in this paper allow the unnatural restriction  $0 < m < 2$  on the results of [3] to be removed. These bounds are also required for the rigorous evaluation of the classical continuum limits of the axial anomaly and index of the overlap Dirac operator [10,11].<sup>1</sup> As a final application we will discuss qualitative implications of the bounds for the instanton size dependence of the real spectrum of the Wilson-Dirac operator in an instanton background.

The paper is organized as follows. In Sec. II the previously derived lower bounds on  $|H(m)|$  are summarized and the new general bounds are formulated. The new bounds are derived in Sec. III. The derivation is rather technical and not very illuminating, so in Sec. IV we supplement it with a heuristic argument which provides a clearer intuitive understanding of why the bounds exist. The heuristic considerations are further developed to give an analytic explanation of properties of the spectral flow of  $H(m)$  previously observed in numerical studies. In Sec. V the above-mentioned applications of the bounds are discussed, and the results of the paper are summarized in Sec. VI. A generalization of the

<sup>1</sup>Other evaluations of the classical continuum limit of the axial anomaly [less rigorous, and not using a lower bound on  $|H(m)|$ ] have been given in [12–15].

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FIG. 1. Illustration of the intervals (2.3) (with  $\delta_k \equiv \sqrt{1-c_k\epsilon}$ ) in the dimension  $d=4$  case. The bounds (2.2) imply that the real eigenvalues of  $D_w$  lie in these intervals.

bounds from the standard case of Wilson parameter  $r=1$  to general values  $r>0$  is given in the Appendix.

## II. SUMMARY OF PREVIOUS BOUNDS AND FORMULATION OF THE NEW BOUNDS

For  $m \leq 0$  and  $m \geq 2d$  ( $d = \text{spacetime dimension}$ ) it is well known that  $|H(m)| \geq |m|$  and  $|H(m)| \geq m - 2d$ , respectively; see, e.g., [5,17,2]. (We review these bounds and generalize them to arbitrary values of the Wilson parameter  $r$  in the Appendix.) By Eq. (1.2) this implies that the real eigenvalues of  $D_w$  (in units of  $1/a$ ) must lie in the interval  $[0, 2d]$ .

In [3,4] lower bounds of the form

$$|H(m)| \geq \sqrt{1-c_1\epsilon} - |1-m| \quad (2.1)$$

were derived when the lattice gauge field satisfies the smoothness condition (1.1). The currently sharpest bound has  $c_1 = 6(2+\sqrt{2}) \approx 20.5$  in four dimensions [4] and generalizes to  $c_1 = (2+\sqrt{2})d(d-1)/2$  in  $d$  dimensions. Clearly, Eq. (2.1) can be a nontrivial lower bound only if  $\epsilon < 1/c_1$  and  $|1-m| < \sqrt{1-c_1\epsilon}$ . The latter implies  $0 < m < 2$ . Lower bounds on  $|H(m)|$  in the ‘‘doubler regions’’  $2 < m < 4$ ,  $4 < m < 6, \dots, 2d-2 < m < 2d$  have so far been missing.

Note that by Eq. (1.2), the existence of a nontrivial lower bound on  $|H(m)|$  for  $|1-m| < \sqrt{1-c_1\epsilon}$  is equivalent to the Wilson-Dirac operator  $D_w$ , having no real eigenvalues in the open interval  $[1-\sqrt{1-c_1\epsilon}, 1+\sqrt{1-c_1\epsilon}]$ . To extend this to a general localization result for the real eigenvalues of  $D_w$  existence of lower bounds on  $|H(m)|$  for  $k-1 < m < k+1$ ,  $k=1,3,\dots,2d-1$ , needs to be established.

Our aim in this paper is to generalize Eq. (2.1) to bounds of the following form:

$$|H(m)| \geq \sqrt{1-c_k\epsilon} - |k-m|, \quad k=1,3,5,\dots,2d-1. \quad (2.2)$$

For given  $m \in ]k-1, k+1[$ , this lower bound is nontrivial when  $\epsilon$  in the smoothness condition (1.1) is chosen such that  $\epsilon < [1-(k-m)^2]/c_k$ . On the other hand, if we require only  $\epsilon < 1/c_k$  for all  $k$  then the bound is nontrivial for all values of  $m$  except those lying in one of the following intervals:

$$\begin{aligned} & [0, 1-\sqrt{1-c_1\epsilon}], \\ & [k+\sqrt{1-c_k\epsilon}, k+2-\sqrt{1-c_{k+2}\epsilon}], \quad k=1,3,\dots,2d-1, \\ & [2d-1+\sqrt{1-c_{2d-1}\epsilon}, 2d] \end{aligned} \quad (2.3)$$

illustrated in Fig. 1. In this case the real eigenvalues of  $D_w$  (in units of  $1/a$ ) must lie in these intervals. Clearly, when  $\epsilon$  is small these intervals are localized around the values  $0, 2, 4, \dots, 2d$ . More specifically, we see that the real eigenvalues of  $D_w$  are guaranteed to lie in the intervals  $[0, \delta]$ ,  $[2p-\delta, 2p+\delta]$  ( $p=1,2,\dots,d-1$ ),  $[2d-\delta, 2d]$  when  $\epsilon < [1$

$-(1-\delta)^2]/c_k$  for all  $k=1,3,\dots,2d-1$ . This is the advertised localization result for the real spectrum of  $D_w$ . Explicit values for the  $c_k$ 's will be determined in the next section.

## III. DERIVATION OF THE BOUNDS

The Wilson-Dirac operator  $D_w$  with general Wilson parameter  $r$  is given by

$$aD_w(r) = \sum_{\mu} \gamma^{\mu} \frac{1}{2} (T_{+\mu} - T_{-\mu}) + r \left( 1 - \frac{1}{2} (T_{+\mu} + T_{-\mu}) \right), \quad (3.1)$$

where  $T_{\pm\mu}$  are the forward/backward parallel transporters  $[(T_{+\mu})_{xy} = U_{\mu}(x) \delta_{x,y-\hat{\mu}}, (T_{\pm\mu})^* = (T_{\pm\mu})^{-1} = T_{\mp\mu}]$ .  $D_w$  is an operator on the lattice spinor fields living on a hypercubic lattice on an even  $d$ -dimensional Euclidean spacetime and taking values in some unitary representation of the (unspecified) gauge group. The spacetime may be either the infinite volume  $\mathbf{R}^d$  or a finite volume  $d$ -torus  $T^d$ . In the former case the (completion of the) space of spinor fields is an infinite-dimensional Hilbert space, while in the latter case it is simply a finite-dimensional complex vector space with inner product. In the following,  $\|\cdot\|$  denotes the operator norm. Clearly,  $\|T_{\pm\mu}\| = 1$ , so  $D_w$  is bounded. A well-known, important consequence of Eq. (1.1) is

$$\|[T_{\pm\mu}, T_{\pm\nu}]\| \leq \epsilon, \quad \|[T_{\pm\mu}, T_{\mp\nu}]\| \leq \epsilon. \quad (3.2)$$

It is useful to define the Hermitian operators

$$\begin{aligned} S_{\mu} &= \frac{1}{2i} (T_{+\mu} - T_{-\mu}), & C_{\mu} &= \frac{1}{2} (T_{+\mu} + T_{-\mu}), \\ R_{\mu} &= 1 - C_{\mu}. \end{aligned} \quad (3.3)$$

These have bounds  $-1 \leq S_{\mu} \leq 1$ ,  $-1 \leq C_{\mu} \leq 1$ ,  $0 \leq R_{\mu} \leq 2$  and satisfy (in any gauge background) the following identities:

$$[S_{\mu}, C_{\mu}] = 0, \quad [S_{\mu}, R_{\mu}] = 0, \quad (3.4)$$

$$S_{\mu}^2 + C_{\mu}^2 = 1, \quad S_{\mu}^2 = R_{\mu}(2 - R_{\mu}). \quad (3.5)$$

The Wilson-Dirac operator can then be written as

$$D_w(r) = \frac{1}{a} \sum_{\mu} i \gamma^{\mu} S_{\mu} + r R_{\mu}. \quad (3.6)$$

For later use we also note the relations

$$R_{\mu} = \frac{1}{2} \nabla_{\mu}^* \nabla_{\mu}, \quad 2 - R_{\mu} = \frac{1}{2} (2 + \nabla_{\mu})^* (2 + \nabla_{\mu}), \quad (3.7)$$

where  $\nabla_{\mu} = T_{+\mu} - 1$ .

The Hermitian Wilson-Dirac operator (normalized by  $1/a$ ) is given by

$$H(m,r) = \gamma_5[aD_w(r) - rm]. \quad (3.8)$$

$|H(m,r)| = \sqrt{H(m,r)^2}$  is defined via spectral theory. In the following we set  $r=1$  and consider  $H(m) = H(m,1)$ ; the case of general  $r$  is dealt with in the Appendix.

To derive the desired bounds (2.2) it suffices to show the following:

$$H(k)^2 \geq 1 - c_k \epsilon, \quad k = 1, 3, \dots, 2d-1. \quad (3.9)$$

Indeed, the eigenvalues  $\lambda(m)$  of  $H(m)$  satisfy  $|d\lambda/dm| \leq 1$  [16,4], implying  $|H(m')| \geq |H(m)| - |m - m'|$  (an alternative derivation of this was also given in the first paper of [3]), and this together with Eq. (3.9) implies the bounds (2.2).

To derive bounds of the form (3.9) we use Eqs. (3.5)–(3.7) to express  $H(m)^2$  as follows:

$$\begin{aligned} H(m)^2 &= (aD_w^* - m)(aD_w - m) \\ &= 1 + \chi(m) + E', \end{aligned} \quad (3.10)$$

where

$$\chi(m) = \sum_{\mu} S_{\mu}^2 + \left(-m + \sum_{\mu} R_{\mu}\right)^2 - 1 \quad (3.11)$$

$$= \sum_{\mu \neq \nu} R_{\mu} R_{\nu} - 2(m-1) \sum_{\mu} R_{\mu} + m^2 - 1 \quad (3.12)$$

and

$$E' = \sum_{\mu \neq \nu} \gamma^{\mu} \gamma^{\nu} \frac{1}{2} [S_{\mu}, S_{\nu}] + i \gamma^{\mu} [S_{\mu}, C_{\nu}]. \quad (3.13)$$

Using Eq. (3.2) and triangle inequalities a bound on  $E'$  of the form

$$\|E'\| \leq c' \epsilon \quad (3.14)$$

can be obtained. The value for  $c'$  obtained in [4] in the four-dimensional case is  $c' = 6(1 + \sqrt{2}) \approx 14.5$  and generalizes to  $c' = (1 + \sqrt{2})d(d-1)/2$  in  $d$  dimensions.

To complete the derivation of Eq. (3.9) we need to show that  $\chi(k)$  can be written in the form

$$\begin{aligned} \chi(k) &= P(k) + E(k), \quad P(k) \geq 0, \quad \|E(k)\| \leq c''_k \epsilon \quad \text{for } k \\ &= 1, 3, \dots, 2d-1. \end{aligned} \quad (3.15)$$

It then follows from Eq. (3.10) that Eq. (3.9) is satisfied with  $c_k = c''_k + c'$ .

It is easy to derive a decomposition and bound (3.15) in the  $k=1$  case [3,4]. In this case Eq. (3.12) reduces to

$$\chi(1) = \sum_{\mu \neq \nu} R_{\mu} R_{\nu}. \quad (3.16)$$

Using Eq. (3.7) one finds  $R_{\mu} R_{\nu} = 1/2 \nabla_{\mu}^* \nabla_{\nu} R_{\nu} = 1/2 \nabla_{\mu}^* R_{\nu} \nabla_{\mu} + 1/2 \nabla_{\mu}^* [\nabla_{\mu}, R_{\nu}] = P_{\mu\nu} + E_{\mu\nu}$  where  $P_{\mu\nu} = 1/2 \nabla_{\mu}^* R_{\nu} \nabla_{\mu} \geq 0$  and  $\|E_{\mu\nu}\| \leq \epsilon$ , leading to  $\chi(1) = P(1) + E(1)$  with  $P(1) \geq 0$  and  $\|E(1)\| \leq d(d-1)\epsilon$  in  $d$  dimensions [3]. A more subtle decomposition  $\chi(1) = P(1) + E(1)$  was derived in [4] for which  $\|E(1)\| \leq 1/2d(d-1)\epsilon$ . In this way the  $k=1$  bound (2.1) was obtained with  $c_1 = c''_1 + c' = 6 + 6(1 + \sqrt{2}) \approx 20.5$  in four dimensions [4].

Our goal now is to derive a decomposition and bound (3.15) for  $\chi(k)$  in the case of general  $k = 1, 3, \dots, 2d-1$ . Setting

$$R_{\mu}^{(0)} = 2 - R_{\mu} \quad \text{and} \quad R_{\mu}^{(1)} = R_{\mu}, \quad (3.17)$$

we begin by noting the identity

$$\chi(m) = \bar{\chi}(m) + \bar{\chi}(m)_{\text{rev}}, \quad (3.18)$$

where

$$\begin{aligned} \bar{\chi}(m) &= \frac{1}{2^{d+\Gamma}} \sum_{q_1, \dots, q_d=0,1} \{[m - 2(q_1 + \dots + q_d)]^2 - 1\} \\ &\quad \times R_1^{(q_1)} R_2^{(q_2)} \dots R_d^{(q_d)}. \end{aligned} \quad (3.19)$$

$\bar{\chi}(m)_{\text{rev}}$  is defined by replacing  $R_1^{(q_1)} R_2^{(q_2)} \dots R_d^{(q_d)}$  by  $R_d^{(q_d)} \dots R_2^{(q_2)} R_1^{(q_1)}$  in Eq. (3.19). The key feature of this expression is that, unlike the original expression (3.12), it is a sum of monomials in the positive operators  $R_{\mu}$  and  $2 - R_{\nu}$  (recall that  $0 \leq R_{\mu} \leq 2$ ) with *positive coefficients* when  $m$  is an odd integer (in particular when  $m = k = 1, 3, \dots, 2d-1$ ). As we will see shortly, this provides for a decomposition  $\chi(k) = P(k) + E(k)$  of the form required in Eq. (3.15).

To derive Eq. (3.18), consider the expansion of  $\bar{\chi}(m)$  in powers of the  $R_{\mu}$ 's:

$$\begin{aligned} \bar{\chi} &= \alpha_0 + \alpha_1 \sum_{\mu} R_{\mu} + \dots + \alpha_p \sum_{\mu_1 < \dots < \mu_p} R_{\mu_1} \dots R_{\mu_p} + \dots \\ &\quad + \alpha_d R_1 R_2 \dots R_d. \end{aligned} \quad (3.20)$$

The expansion of  $\bar{\chi}(m)_{\text{rev}}$  is identical except that the ordering of the  $R_{\mu}$ 's is reversed. In light of Eq. (3.12), to derive Eq. (3.18) it suffices to show that

$$\begin{aligned} \alpha_0 &= \frac{1}{2} (m^2 - 1), \quad \alpha_1 = -(m-1), \quad \alpha_2 = 1, \\ &\quad \text{and } \alpha_p = 0 \quad \text{for } p \geq 3. \end{aligned} \quad (3.21)$$

Let us focus on the term of order  $p$  in Eq. (3.20). It gets contributions from the terms in Eq. (3.19) with  $q_1 + \dots + q_d \leq p$ . The terms with  $q_1 + \dots + q_d = s$  are

$$\begin{aligned} &\frac{1}{2^{d+\Gamma}} [(m-2s)^2 - 1] \sum_{\nu_1 < \dots < \nu_s} (2 - R_{\nu_1}) \dots (2 - R_{\nu_{s-1}}) R_{\nu_s} \\ &\quad \times (2 - R_{\nu_{s+1}}) \dots (2 - R_{\nu_{s-1}}) R_{\nu_s} (2 - R_{\nu_{s+1}}) \dots (2 - R_d). \end{aligned} \quad (3.22)$$

For  $s \leq p$  the contribution of this to the  $\alpha_p$  term in Eq. (3.20) is

$$\frac{1}{2^{d+1}} [(m-2s)^2 - 1] (-1)^{p-s} 2^{d-p} \binom{p}{s} \sum_{\mu_1 < \dots < \mu_p} R_{\mu_1} \dots R_{\mu_p} \quad (3.23)$$

(the binomial coefficient  $\binom{p}{s}$  appears because it is the number of ways to pick  $s$  distinct elements from a set of  $p$  elements). It follows that

$$\alpha_p = \frac{1}{2^{p+1}} \sum_{s=0}^p [(m-2s)^2 - 1] \binom{p}{s} (-1)^{p-s}. \quad (3.24)$$

From this we find  $\alpha_0 = 1/2(m^2 - 1)$ ,  $\alpha_1 = -(m - 1)$ , and  $\alpha_2 = 1$  as claimed in Eq. (3.21). In the  $p \geq 3$  case we calculate

$$\begin{aligned} \alpha_p &= \frac{1}{2^{p+1}} \sum_{s=0}^p (4s^2 - 4ms + m^2 - 1) \binom{p}{s} (-1)^{p-s} \\ &= \frac{1}{2^{p+1}} \left( 4p(p-1) \sum_{s=0}^{p-2} \binom{p-2}{s} (-1)^{p-2-s} + 4(m-1)p \right. \\ &\quad \left. \times \sum_{s=0}^{p-1} \binom{p-1}{s} (-1)^{p-1-s} + (m^2 - 1) \sum_{s=0}^p \binom{p}{s} (-1)^{p-s} \right) \\ &= 0 \end{aligned} \quad (3.25)$$

(each sum vanishes since  $\sum_{s=0}^{p-2} \binom{p-2}{s} (-1)^{p-2-s} = (1 - 1)^{p-2}$ , etc.). This completes the derivation of Eq. (3.21), thereby establishing Eq. (3.18).

We now show how Eqs. (3.18), (3.19) lead to a decomposition  $\chi(k) = P(k) + E(k)$  of the form (3.15). The operator product  $R_1^{(q_1)} \dots R_d^{(q_d)}$  in Eq. (3.19) decomposes into a positive piece and a piece involving commutators as follows. Setting

$$\nabla_\mu^{(0)} = 2 + \nabla_\mu = T_{+\mu} + 1 \quad \text{and} \quad \nabla_\mu^{(1)} = \nabla_\mu = T_{+\mu} - 1, \quad (3.26)$$

then  $\|\nabla_\mu^{(q)}\| \leq 2$  for  $q = 0, 1$  and, by Eqs. (3.7) and (3.17),

$$R_\mu^{(q)} = \frac{1}{2} (\nabla_\mu^{(q)}) * \nabla_\mu^{(q)}. \quad (3.27)$$

Using this and the commutator relations  $[O, O_1 \dots O_p] = \sum_{s=1}^p O_1 \dots O_{s-1} [O, O_s] O_{s+1} \dots O_p$  we obtain

$$R_1^{(q_1)} \dots R_d^{(q_d)} = P^{(q_1, \dots, q_d)} + E^{(q_1, \dots, q_d)} \quad (3.28)$$

with

$$P^{(q_1, \dots, q_d)} = \frac{1}{2^d} (\nabla_d^{(q_d)} \dots \nabla_1^{(q_1)}) * \nabla_d^{(q_d)} \dots \nabla_1^{(q_1)}, \quad (3.29)$$

$$E^{(q_1, \dots, q_d)}$$

$$\begin{aligned} &= \sum_{p=1}^{d-1} \frac{1}{2^p} (\nabla_p^{(q_p)} \dots \nabla_1^{(q_1)}) * \left( \sum_{s=p}^d R_p^{(q_p)} \dots R_{s-1}^{(q_{s-1})} \right. \\ &\quad \left. \times [\nabla_p^{(q_p)}, R_s^{(q_s)}] R_{s+1}^{(q_{s+1})} \dots R_d^{(q_d)} \nabla_{p-1}^{(q_{p-1})} \dots \nabla_1^{(q_1)} \right). \end{aligned} \quad (3.30)$$

Clearly,  $P^{(q_1, \dots, q_d)} \geq 0$ . Furthermore, the bounds  $\|\nabla_\mu^{(q_\mu)}\|, \|R_\mu^{(q_\mu)}\| \leq 2$  and, by Eq. (3.2),  $\|[\nabla_\mu^{(q_\mu)}, R_\nu^{(q_\nu)}]\| \leq \epsilon$ , together with triangle inequalities, lead to the bound

$$\|E^{(q_1, \dots, q_d)}\| \leq c \epsilon, \quad (3.31)$$

where

$$c = \sum_{p=1}^{d-1} \sum_{s=p}^d 2^{d-p-1} 2^{p-1} = 2^{d-3} (d-1)(d+2). \quad (3.32)$$

The reversed product  $R_d^{(q_d)} \dots R_1^{(q_1)}$  has an analogous decomposition  $P_{\text{rev}}^{(q_1, \dots, q_d)} + E_{\text{rev}}^{(q_1, \dots, q_d)}$  with identical bounds. Consequently, by Eqs. (3.18), (3.19) we get the decomposition

$$\chi(m) = P(m) + E(m), \quad (3.33)$$

where  $P(m)$  and  $E(m)$  are given by Eq. (3.19) with  $R_1^{(q_1)} \dots R_d^{(q_d)}$  replaced by  $P^{(q_1, \dots, q_d)} + P_{\text{rev}}^{(q_1, \dots, q_d)}$  and  $E^{(q_1, \dots, q_d)} + E_{\text{rev}}^{(q_1, \dots, q_d)}$ , respectively. The coefficient in the summand in Eq. (3.19) is  $\geq 0$  when  $m$  is an odd integer; hence  $P(k) \geq 0$  for odd  $k$  and in particular for  $k = 1, 3, \dots, 2d - 1$  as required in Eq. (3.15). Furthermore, from Eqs. (3.31), (3.32), we get the bound

$$\|E(k)\| \leq c_k'' \epsilon \quad (3.34)$$

with

$$\begin{aligned} c_k'' &= 2c \left( \frac{1}{2^d} \sum_{q_1, \dots, q_d=0,1} [(k - 2(q_1 + \dots + q_d))^2 - 1] \right) \\ &= \frac{2c}{2^d} \sum_{p=0}^d \binom{d}{p} [(k - 2p)^2 - 1] \\ &= 2^{d-3} (d-1)(d+2) [(k-d)^2 - 1 + d] \quad (d \geq 2). \end{aligned} \quad (3.35)$$

Thus we have established the existence of a decomposition and bound (3.15) for  $\chi(k)$  for general  $k = 1, 3, \dots, 2d - 1$ . By our previous discussion this implies the existence of the desired bounds (2.2). We remark that Eq. (3.35) is invariant under  $k \rightarrow 2d - k$ . This is as expected in light of the well-known fact that a lower bound on  $|H(m)|$  is also a lower bound on  $|H(2d - m)|$  (see the Appendix).

The bound (3.34), (3.35) is rather weak. For example, in the  $d = 4$  case it is

$$c_k''(d=4) = 36[(k-4)^2 - 1] + 144, \quad (3.36)$$

giving in the  $k=1$  case  $c_1''=432$ , which is much larger than the values  $c_1''=12$  and  $c_1''=6$  obtained in [3] and [4], respectively. Note, however, that for the applications discussed in this paper it suffices simply to show the existence of bounds of the form (2.2) without necessarily finding sharp ones. The largeness of  $c_k''$  in the above bound is due to the large number of terms in the expression (3.19) for  $\tilde{\chi}(m)$ . In practice, it is often possible to simplify this expression such that a sharper bound (i.e., smaller  $c_k''$ ) can be derived. We discuss this in the  $d=4$  case in the following.

In the remainder of this section we specialize to dimension  $d=4$  and consider  $\chi(k)$  for  $k=1,3,5,7$ . We wish to simplify the expression (3.18), (3.19) for  $\chi(k)$  in order to get bounds with smaller  $c_k''$ . In order to have the decomposition  $\chi(k) = P(k) + E(k)$ , the simplified expression must continue to be a sum of monomials in the positive operators  $R_\mu$ ,  $(2 - R_\nu)$  with positive coefficients. In the  $k=1$  case Eq. (3.18) simplifies to  $\chi(1) = \sum_{\mu \neq \nu} R_\mu R_\nu$  [recall Eq. (3.16)] from which the previously discussed bounds with  $c_1''=12$  [3] and  $c_1''=6$  [4] can be derived. In the  $k=7$  case  $\tilde{\chi}(7)$  reduces to  $\sum_{\mu < \nu} (2 - R_\mu)(2 - R_\nu)$ , leading to

$$\chi(7) = \sum_{\mu \neq \nu} (2 - R_\mu)(2 - R_\nu). \quad (3.37)$$

Arguments analogous to the ones in [3] and [4] lead to bounds with  $c_7''=c_1''=12$  and  $c_7''=c_1''=6$ , respectively. Turning now to the  $k=3$  case, Eq. (3.19) gives

$$\begin{aligned} \tilde{\chi}(3) &= \frac{1}{4}(2 - R_1)(2 - R_2)(2 - R_3)(2 - R_4) + \frac{3}{4}R_1R_2R_3R_4 \\ &+ \frac{1}{4}[(2 - R_1)R_2R_3R_4 + R_1(2 - R_2)R_3R_4 \\ &+ R_1R_2(2 - R_3)R_4 + R_1R_2R_3(2 - R_4)]. \end{aligned} \quad (3.38)$$

In this case there does not appear to be a major simplification with the required properties. In fact, it is quite easy to show that  $\chi(3)$  cannot be written as a sum of monomials of order  $\leq 3$  in  $R_\mu$ ,  $(2 - R_\nu)$  with positive coefficients (we leave this as an exercise for the reader). Minor simplifications are possible though, for example,

$$\begin{aligned} \tilde{\chi}(3) &= \frac{1}{4}[(2 - R_1)(2 - R_2)(2 - R_3)(2 - R_4) + R_1R_2R_3 \\ &\times (2 - R_4)] + \frac{1}{2}(R_1R_2R_4 + R_1R_3R_4 + R_2R_3R_4). \end{aligned} \quad (3.39)$$

$\tilde{\chi}(3)_{\text{rev}}$  simplifies analogously. Estimates of the kind used to derive Eqs. (3.31), (3.32) show that the decomposition  $P(3) + E(3)$  of the resulting expression for  $\chi(3)$  satisfies  $\|E(3)\| \leq c_3''\epsilon$  with  $c_3''=42$ . This is considerably smaller than the value  $c_3''=144$  provided by Eq. (3.36). It is plausible that

a bound with even smaller  $c_3''$  can be derived, e.g., by an extension of the arguments of [4], but we will not pursue this here. Finally, in the  $k=5$  case analogous arguments lead (as expected) to a bound with  $c_5''=c_3''=42$  (we omit the details).

#### IV. HEURISTIC CONSIDERATIONS

In this section we present a heuristic argument which provides a clearer intuitive understanding of why bounds of the form derived in the previous section should hold. We go on to heuristically derive certain properties of the spectral flow of  $H(m)$  previously observed in numerical studies (e.g., [1,17]).

Consider a ‘‘near zero mode’’ for  $H(m)$ :

$$H(m)^2 \psi \approx 0. \quad (4.1)$$

If  $\epsilon$  in the smoothness condition (1.1) is small then  $E' \approx 0$  in Eq. (3.10), and Eq. (4.1) becomes (recall  $C_\mu = 1 - R_\mu$ )

$$\left[ \sum_{\mu} S_{\mu}^2 + \left( -m + \sum_{\mu} (1 - C_{\mu}) \right)^2 \right] \psi \approx 0. \quad (4.2)$$

Since  $S_{\mu}^2 \geq 0$  it follows that  $S_{\mu} \psi \approx 0$  for  $\mu = 1, \dots, 2d$  and consequently, by Eq. (3.5),  $C_{\mu}^2 \psi = (1 - S_{\mu}^2) \psi \approx \psi$ , which implies that  $C_{\mu} \psi \approx (-1)^{j_{\mu}} \psi$  for  $j_{\mu} = 0$  or  $1$ . Then Eq. (4.2) reduces to

$$\begin{aligned} 0 &\approx \left( -m + \sum_{\mu} (1 - C_{\mu}) \right)^2 \\ &\approx \left( -m + \sum_{\mu} [1 - (-1)^{j_{\mu}}] \right)^2 \psi, \end{aligned} \quad (4.3)$$

which implies that

$$m \approx \sum_{\mu} [1 - (-1)^{j_{\mu}}]. \quad (4.4)$$

Thus we see heuristically that when  $\epsilon$  is small the only values of  $m$  for which  $H(m)$  can have ‘‘near zero modes’’ are  $m = 0, 2, 4, \dots, 2d$ . This makes plausible the result of the previous section, namely, that when  $m$  is away from these values a nonzero lower bound on  $|H(m)|$  should exist.

In fact the above heuristic approach can be further developed to get an alternative rigorous derivation of the bounds (2.2) [18]. However, the argument is technically more complicated than the one in Sec. III and does not lead to sharper bounds, so we do not present it here.

We now proceed to study the spectral flow of  $H(m)$ . For this it is useful to introduce the operators  $\mathcal{T}_{\mu}$  defined by<sup>2</sup>

$$(\mathcal{T}_{\mu})_{xy} = \gamma_5 \gamma^{\mu} (-1)^{n_{\mu}} \delta_{xy} \quad (n_{\mu} = x_{\mu}/a \in \mathbf{Z}). \quad (4.5)$$

<sup>2</sup>These have proved useful in previous lattice fermion contexts; see, e.g., [13] and the references therein.

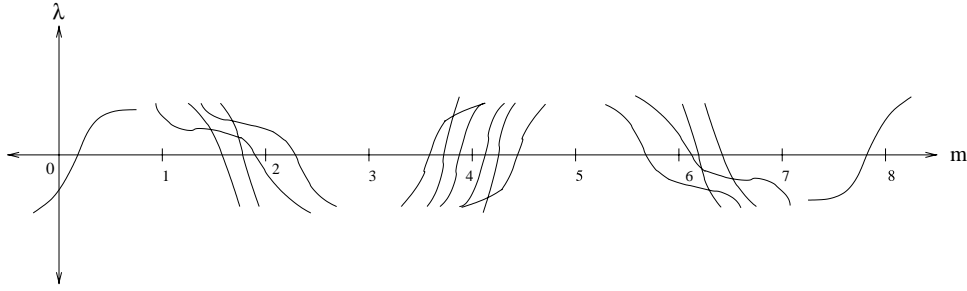


FIG. 2. Illustration of the spectral flow associated with a typical eigenvector family of  $H(m)$  of the kind discussed in the text in dimension  $d=4$ : A crossing near  $m=0$  with + sign is associated with four crossings near  $m=2$  with - sign, six crossings near  $m=4$  with + sign, four crossings near  $m=6$  with - sign, and one crossing near  $m=8$  with + sign.

These have the following properties:  $\mathcal{T}_\mu^2 = -1$ ,  $\mathcal{T}_\mu \mathcal{T}_\nu = -\mathcal{T}_\nu \mathcal{T}_\mu$  for  $\mu \neq \nu$ ,  $[\mathcal{T}_\mu, \gamma^5 S_\nu] = 0$ ,  $C_\mu \mathcal{T}_\mu = -\mathcal{T}_\mu C_\mu$ ,  $[\mathcal{T}_\mu, C_\mu] = 0$  for  $\mu \neq \nu$ , and  $\mathcal{T}_\mu \gamma_5 = -\gamma_5 \mathcal{T}_\mu$ . Using these we find

$$H(m)\mathcal{T}_\mu = -\mathcal{T}_\mu[H(m) + 2\gamma_5 C_\mu] \quad (\text{no sum over } \mu). \quad (4.6)$$

By Eq. (3.2)  $[H(m), C_\mu] \approx 0$  when  $\epsilon$  is small, so the eigenspaces of  $H(m)$  can be decomposed into approximate eigenspaces for the  $C_\mu$ 's. That is, for eigenvectors  $\psi(m)$  of  $H(m)$  with  $H(m)\psi = \lambda(m)\psi(m)$  we can assume that  $C_\mu\psi(m) \approx c_\mu\psi(m)$ . The eigenvalues  $c_\mu$  are independent of  $m$  since  $C_\mu$  is independent of  $m$  and has a discrete spectrum. Then, by Eq. (4.6),

$$\begin{aligned} H(m)\mathcal{T}_\mu\psi(m) \\ = -\mathcal{T}_\mu H(m - 2c_\mu)\psi(m) \quad (\text{no sum over } \mu) \end{aligned} \quad (4.7)$$

Set  $\psi_\mu(m) := \mathcal{T}_\mu\psi(m - 2c_\mu)$ . It follows from Eq. (4.7) that  $\psi_\mu(m)$  is an approximate eigenvector for  $H(m)$  with eigenvalue  $\approx -\lambda(m - 2c_\mu)$ . Similarly, we find

$$\begin{aligned} H(m)\psi_{\mu_1 \dots \mu_p}(m) \\ \approx (-1)^p \lambda[m - 2(c_{\mu_1} + \dots + c_{\mu_p})] \psi_{\mu_1 \dots \mu_p}(m), \end{aligned} \quad (4.8)$$

where  $\psi_{\mu_1 \dots \mu_p}(m) := \mathcal{T}_{\mu_1} \dots \mathcal{T}_{\mu_p} \psi[m - 2(c_{\mu_1} + \dots + c_{\mu_p})]$ , when the  $\mu_j$ 's are all mutually distinct.

Now, if  $\lambda(m)$  crosses zero near  $m=0$  then by our previous argument [recall Eq. (4.4)]  $c_\mu \approx (-1)^{j_\mu}$  with  $\sum_\mu (1 - (-1)^{j_\mu}) \approx 0$ , i.e.  $c_\mu \approx 1$  for all  $\mu$ , and Eq. (4.8) becomes

$$H(m)\psi_{\mu_1 \dots \mu_p}(m) \approx (-1)^p \lambda(m - 2p) \psi_{\mu_1 \dots \mu_p}(m), \quad (4.9)$$

i.e.,  $\psi_{\mu_1 \dots \mu_p}(m)$  is an approximate eigenvector for  $H(m)$  whose approximate eigenvalue  $\lambda(-1)^p \lambda(m - 2p)$  crosses zero near  $m=2p$ . Furthermore, the sign of the crossing is  $(-1)^p$  relative to the sign of the crossing of zero by  $\lambda(m)$  near  $m=0$ . We note the following. (i) If  $\{\mu_1, \dots, \mu_p\} \neq \{\nu_1, \dots, \nu_p\}$  then  $\psi_{\mu_1 \dots \mu_p}(m)$  and  $\psi_{\nu_1 \dots \nu_p}(m)$  are approxi-

mately orthogonal since they are approximate eigenvectors for the  $C_\mu$ 's with different eigenvalues. (ii)  $\psi_{\mu_1 \dots \mu_p}(m)$  is unchanged up to a sign under a change of ordering of the  $\mu_j$ 's (since  $\mathcal{T}_\mu \mathcal{T}_\nu = -\mathcal{T}_\nu \mathcal{T}_\mu$  for  $\mu \neq \nu$ ). Hence we can assume that the  $\mu_j$ 's are ordered so that  $\mu_1 < \dots < \mu_p$ . (iii) If  $\tilde{\psi}(m)$  is an eigenvector for  $H(m)$  whose eigenvalue  $\tilde{\lambda}(m)$  crosses zero at some value  $m_0$  then by Eq. (4.4)  $m_0 \approx \sum_\mu [1 - (-1)^{j_\mu}]$  where  $C_\mu \tilde{\psi}(m) \approx (-1)^{j_\mu} \tilde{\psi}(m)$  for  $j_\mu = 0$  or 1. Any such eigenvector arises in the way described above, i.e.,  $\tilde{\psi}(m) = \psi_{\mu_1 \dots \mu_p}(m) = \mathcal{T}_{\mu_1} \dots \mathcal{T}_{\mu_p} \psi(m - 2p)$ . Indeed, we set  $\psi(m) = (-1)^p \mathcal{T}_{\mu_1} \dots \mathcal{T}_{\mu_p} \tilde{\psi}(m + 2p)$  with the  $\mu_j$ 's being the  $\mu$ 's for which  $j_\mu = 1$ . Then by Eq. (4.8)  $\psi(m)$  is an approximate eigenvector for  $H(m)$  whose eigenvalue  $\lambda(m)$  is  $\approx 0$  at some value of  $m$  near zero. (To see this, recall  $\mathcal{T}_\mu^2 = -1$ .) Thus we have heuristically established the following. The eigenvectors of  $H(m)$  whose eigenvalues cross zero at some value of  $m$  can be naturally grouped into sets of  $2^d$  elements. One of the eigenvectors  $\psi(m)$  has an eigenvalue  $\lambda(m)$  crossing zero near  $m=0$  with crossing sign  $\pm$ . There are  $d$  eigenvectors  $\psi_d(m)$  with eigenvalues crossing zero near  $m=2$  with sign  $\mp$ , and more generally  $d!/[p!(d-p)!]$  eigenvectors  $\psi_{\mu_1 \dots \mu_p}(m)$ ,  $\mu_1 < \dots < \mu_p$ , with eigenvalues crossing zero near  $m=2p$  with crossing sign  $\mp(-1)^p$  for  $p=1, 2, \dots, d$ . This is precisely the spectral flow property of  $H(m)$  found in numerical studies in two and four dimensions [1,17]. An illustration of the spectral flow associated with one such family in the  $d=4$  case is given in Fig. 2. The Hermitian Wilson-Dirac operator in any gauge background  $U$  has the well-known property  $H(U, m) = -H(-U, 2d - m)$ , so that  $H(m) = OH(U, 2d - m)O^{-1}$  for a certain unitary operator  $O$  (see, e.g., [2,17]).<sup>3</sup> Hence if  $\lambda(m)$  is an eigenvalue for  $H(m)$  then  $-\lambda(m)$  is an eigenvalue for  $H(2d - m)$ . This property must be manifested in the eigenvalues of the family of eigenvectors of  $H(m)$  discussed above, and is also illustrated in Fig. 2. Combining this spectral property of  $H(m)$  with the fact that the index of the overlap Dirac operator equals  $-1/2$  times the spectral asymmetry of  $H(m)$  [5,6], an immediate consequence is the relation  $\text{index}[D_{\text{ov}}(m)] = -\text{index}[D_{\text{ov}}(2d - m)]$  which was emphasized in [7].

<sup>3</sup>For  $O$  to exist the number of lattice sites along each edge of  $T^d$  must be even.

## V. APPLICATIONS OF THE BOUNDS

We have already seen in Sec. II how the general bounds (2.2) lead to a localization result on the real spectrum of the Wilson-Dirac operator, thus providing an analytic understanding of the numerical results for the real spectrum in “smooth” gauge backgrounds. In this section we discuss applications of the bounds to overlap fermions [6]. The general bounds allow analytic results on the overlap Dirac operator  $D_{\text{ov}}$  which were previously derived for the  $0 < m < 2$  to be extended to the general  $m$  case ( $m \neq 0, 2, 4, \dots, 2d$ ). Although  $0 < m < 2$  is the physically relevant case (i.e., the case where  $D_{\text{ov}}$  is free from spurious fermion species) this restriction appears quite unnatural and it is of some theoretical interest to know the properties of  $D_{\text{ov}}$  in the regions  $2p < m < 2p + 2$ ,  $p = 1, 2, \dots, d$ , where the extra fermion species are present.

### A. Locality and smooth gauge field dependence of the overlap Dirac operator

With the bounds (2.2) the arguments of Ref. [3] for the locality of  $D_{\text{ov}}$  and its smooth dependence on the lattice gauge field carry over unchanged from the  $0 < m < 2$  case to the  $k - 1 < m < k + 1$  case ( $k = 1, 3, \dots, 2d - 1$ ) after choosing  $\epsilon < [1 - (k - m)^2]/c_k$  so that the lower bound on  $|H(m)|$  is greater than zero. The size of the exponential decay constant in the locality bound for  $D_{\text{ov}}$  depends on the size of  $c_k$ , but for the existence of the locality bound it is enough to know that Eq. (2.2) holds for a specific value of  $c_k$ , which is independent of the lattice gauge field.

### B. Evaluation of the classical continuum limit of the axial anomaly and index of the overlap Dirac operator

The rigorous evaluation of the classical continuum limit of the axial anomaly<sup>4</sup> and the index of the overlap Dirac operator at general values of  $m$  requires the existence of a nontrivial lower bound on  $|H(m)|$  when the lattice is sufficiently fine [10,11]. We claimed in [10,11] that such bounds exist and promised to provide them in a forthcoming paper. The present paper delivers on that promise. Again, the actual values of the  $c_k$ 's do not matter: The lattice transcript of a smooth continuum gauge field automatically satisfies the smoothness condition (1.1) for any  $\epsilon > 0$  when the lattice is sufficiently fine (see [11] for the rigorous justification of this point), so all that matters for the classical continuum limit calculations is that the bounds hold for some choice of  $c_k$ 's which are independent of the gauge field and lattice spacing.

### C. Topological phase structure of the overlap Dirac operator

In the finite volume  $d$ -torus case the index of  $D_{\text{ov}}$   $= (1/a)[1 + \gamma_5 H(m)/|H(m)|]$  is a well-defined integer; it is

<sup>4</sup>It may sound contradictory to speak of the “classical” continuum limit of a purely quantum quantity such as the axial anomaly, so let us explain the meaning: “Classical” refers to the fact that one considers the  $a \rightarrow 0$  limit of the axial anomaly with the lattice gauge field given by the lattice transcript of a *smooth continuum gauge field*. See [10,11] for the details.

locally constant in  $m$  but may jump at the values at which  $H(m)$  has zero mode(s). Thus  $D_{\text{ov}}$  has different topological phases and the value of  $m$  should be chosen so that  $D_{\text{ov}}$  is in the “correct” phase. This issue has previously been studied both analytically and numerically in [7] and numerically in [8]. However, the analytic arguments in [7] are problematic since they involve treating topologically nontrivial fields as perturbations of the trivial gauge field  $U = 1$ . On the other hand, the bounds (2.2) provide rigorous nonperturbative insight into the topological phase structure when the lattice gauge fields are required to satisfy the smoothness condition (1.1) with  $\epsilon < 1/c_k$  for all  $k = 1, 3, \dots, 2d - 1$ : they imply that there are distinct topological phases for  $D_{\text{ov}}$ , with each phase characterized by  $m$  being in one of the open intervals  $]k - \sqrt{1 - c_k \epsilon}, k + \sqrt{1 - c_k \epsilon}[$ . The result of [11] states that for  $SU(N)$  gauge fields on the  $d$ -torus ( $d = 2n, n > 1$ ), or  $U(1)$  gauge fields on the two-torus,  $\text{index}(D_{\text{ov}})$  coincides with the index of the continuum Dirac operator in the classical continuum limit provided  $0 < m < 2$ .<sup>5</sup> This indicates that the “proper” topological phase for  $D_{\text{ov}}$  is the one where  $m$  is in the interval  $]1 - \sqrt{1 - c_1 \epsilon}, 1 + \sqrt{1 - c_1 \epsilon}[$ . We denote  $\text{index}(D_{\text{ov}})$  by  $Q$  when  $D_{\text{ov}}$  is in this phase. A complete description of the topological phases for  $D_{\text{ov}}$  when the smoothness condition (1.1) is imposed is now as follows. For  $m \leq 0$ ,  $D_{\text{ov}}$  is in a topologically trivial phase [i.e.,  $\text{index}(D_{\text{ov}}) = 0$  in any gauge background] [5]. For  $0 < m \leq 1 - \sqrt{1 - c_1 \epsilon}$ ,  $D_{\text{ov}}$  is not in a distinct topological phase:  $\text{index}(D_{\text{ov}})$  can be any value from 0 to  $Q$  depending on the background gauge field. In a given gauge background, as  $m$  is increased from 0 to  $1 - \sqrt{1 - c_1 \epsilon}$ , the total spectral flow of  $H(m)$  is  $Q$ . This is due to the well-known fact that at each crossing of zero by an eigenvalue of  $H(m)$  the index of  $D_{\text{ov}}$  changes by  $\mp 1$  depending on the sign of the crossing. For  $1 - \sqrt{1 - c_1 \epsilon} < m < 1 + \sqrt{1 - c_1 \epsilon}$ ,  $D_{\text{ov}}$  is in the “proper” topological phase where  $\text{index}(D_{\text{ov}}) = Q$ . For  $1 + \sqrt{1 - c_1 \epsilon} \leq m \leq 3 - \sqrt{1 - c_3 \epsilon}$ ,  $D_{\text{ov}}$  is no longer in a distinct topological phase and the spectral flow of  $H(m)$  as  $m$  increases through this region is  $-dQ$ . For  $3 - \sqrt{1 - c_3 \epsilon} < m < 3 + \sqrt{1 - c_3 \epsilon}$ ,  $D_{\text{ov}}$  is in another distinct topological phase with  $\text{index}(D_{\text{ov}}) = (1 - d)Q$ . The pattern continues as  $m$  increases: For  $k - \sqrt{1 - c_k \epsilon} < m < k + \sqrt{1 - c_k \epsilon}$ ,  $D_{\text{ov}}$  is in a distinct topological phase with  $\text{index}(D_{\text{ov}}) = (\sum_{p=0}^{(k-1)/2} (-1)^p \binom{d}{p})Q$ . Then, as  $m$  increases from  $k + \sqrt{1 - c_k \epsilon}$  to  $k + 2 - \sqrt{1 - c_{k+2} \epsilon}$ ,  $D_{\text{ov}}$  is no longer in a distinct topological phase, and the spectral flow of  $H(m)$  through this region is  $(-1)^{(k+1)/2} \binom{d}{(k+1)/2} Q$ . Finally, after  $m$  has increased to  $2d$  we have  $\text{index}(D_{\text{ov}}) = (\sum_{p=0}^d (-1)^p \binom{d}{p})Q = (1 - 1)^d Q = 0$  and  $D_{\text{ov}}$  is back in a topologically trivial phase, in which it remains for all  $m \geq 2d$ .

The above description of the topological phase structure of  $D_{\text{ov}}$  is compatible with the results of previous numerical studies in two and four dimensions [7,8]. To put the above analytical argument on a completely rigorous footing, a

<sup>5</sup>This was shown in [11] in the case of the four-torus, but the argument generalizes straightforwardly to the general  $d = 2n$ -torus.



rigorous derivation of the heuristic result of Sec. IV for the spectral flow of  $H(m)$  is required. This remains as a problem for future work. We note, however, that further evidence for the validity of this description comes from the result of [11], which states that *in the classical continuum limit*

$$\text{index}(D_{\text{ov}}) = \begin{cases} \left( \sum_{p=0}^{(k-1)/2} (-1)^p \binom{p}{d} \right) Q & \text{for } k-1 < m < k+1 \quad (k=1,3,\dots,2d-1), \\ 0 & \text{for } m \leq 0 \text{ and } m \geq 2d, \end{cases}$$

where  $Q$  is the index of the continuum Dirac operator.

A generalization of the overlap Dirac operator has been presented in [19] and it would also be of interest to establish the topological phase structure of this operator. For this, bounds on the generalized Hermitian Wilson-Dirac operator for general  $m$  are needed. A bound has already been derived in [20] for  $0 < m < 2$  by a generalization of the argument of [4]. It is plausible that bounds for general  $m$  can be derived by a generalization of the argument in the present paper. We leave this as a potential topic for future work.

**D. Instanton size dependence of the real spectrum of the Wilson-Dirac operator in an instanton background**

Approximate instantons on the lattice can be obtained either through a cooling procedure [21] or by taking an appropriate lattice transcript of a continuum instanton field [22,17]. We will focus on the latter case. In this case numerical studies have shown that the real eigenvalues of  $D_w$  are well localized around  $0,2,\dots,2d$  [or, equivalently, the crossings of zero by eigenvalues of  $H(m)$  occur close to these values] when the instanton is large at the scale of the lattice spacing, but become delocalized as the instanton size is decreased [17]. The standard explanation of this is that instantons which are small at the scale of the lattice spacing are not slowly varying at this scale in the region in which they are localized, so their lattice transcripts are “rough” in this region. On the other hand, large instantons *are* slowly varying, so their lattice transcripts are “smooth.” The bounds (2.2) can be used to give a more precise version of this intuitive explanation as follows. A continuum instanton field centered at  $x^{(0)}$  has the form [23]

$$A_\mu(x) = 2 \eta_\alpha^{\mu\nu} \frac{x_\nu - x_\nu^{(0)}}{|x - x^{(0)}|^2 + \rho^2} t^\alpha, \quad (5.1)$$

where  $\eta_\alpha^{\mu\nu}$  is the ’t Hooft symbol,  $t^\alpha$  are generators of the SU(2) subgroup, and the parameter  $\rho$  specifies the size of the instanton. Its curvature is

$$F_{\mu\nu}(x) = -4 \eta_\alpha^{\mu\nu} \frac{\rho^2}{(|x - x^{(0)}|^2 + \rho^2)^2} t^\alpha. \quad (5.2)$$

When putting the instanton on the lattice with periodic boundary conditions it is important to transform (5.1) to a singular gauge before taking the lattice transcript (and the lattice volume must also be sufficiently large that the singular gauge instanton is close to vanishing at the boundary

[22,17].  $\|F_{\mu\nu}(x)\|$  is not affected by this though, since it is gauge invariant. From Eq. (5.2) we see that  $\|F_{\mu\nu}(x)\|$  diverges at  $x^{(0)}$  in the limit of small instanton size  $\rho$ . Hence for small  $\rho$  the lattice transcribed field generally violates the smoothness condition (1.1) since  $\|1 - U(p)\| = \|a^2 F_{\mu\nu}(x) + O(a^3)\|$  becomes large for plaquettes  $p$  close to  $x^{(0)}$ . [This is assuming there is no special cancellation between  $a^2 F_{\mu\nu}(x)$  and the  $O(a^3)$  term; generically there is no reason to expect such a cancellation to occur, and in particular when the lattice spacing is small  $a^2 F_{\mu\nu}(x)$  will dominate the  $O(a^3)$  term.] Then the localization result of Sec. II for the real spectrum of  $D_w$  breaks down.<sup>6</sup>

On the other hand, from Eq. (5.2) we get a bound

$$\|F_{\mu\nu}(x)\| \leq \frac{4 \|\eta_\alpha^{\mu\nu} t^\alpha\|}{\rho^2} \quad (5.3)$$

showing that  $\|F_{\mu\nu}(x)\|$  vanishes uniformly in the limit of large  $\rho$ . Consequently, for large  $\rho$  the smoothness condition (1.1) will be satisfied generically on sufficiently fine lattices, thereby guaranteeing localization of the real spectrum of  $D_w$  according to the result of Sec. II.

These considerations can be extended to more general gauge fields describing a collection of topologically charged “lumps” (e.g., instanton–anti-instanton configurations, multi-instantons, instanton gases). The topological charge of a lump is given by

$$Q_{\text{lump}} = \frac{1}{32\pi^2} \int_{\text{lump}} d^4x \epsilon_{\mu\nu\sigma\rho} \text{tr} F_{\mu\nu}(x) F_{\sigma\rho}(x) \approx \pm 1. \quad (5.4)$$

If the lump size is small then  $\|F_{\mu\nu}(x)\|$  must be large in the lump region in order that the magnitude of the integral in Eq. (5.4) can be  $\approx 1$ . The smaller the lump is, the larger  $\|F_{\mu\nu}(x)\|$  must be in the lump region. This generically leads to violation of the smoothness condition (1.1), as before. On the other hand, if the lump size is large,  $\|F_{\mu\nu}(x)\|$  is not

<sup>6</sup>More precisely, the assumptions under which the localization was derived break down. This does not necessarily imply that the localization result itself must break down, although it is not surprising that it should do so. We can turn things around and interpret the numerical results for the delocalization of the real spectrum in small instanton backgrounds as indicating that, in general, a smoothness requirement of the form (1.1) is not only sufficient but also a necessary requirement for the real spectrum of  $D_w$  to be localized.

forced to be large in any particular region. Generically, we can expect  $\|F_{\mu\nu}(x)\|$  to decrease with increasing lump size, and to vanish in the large lump limit. Then, by the same argument as before, localization of the real spectrum of  $D_w$  will generically hold in gauge backgrounds describing topological lumps when all the lumps are sufficiently large and the lattice is sufficiently fine.

**VI. SUMMARY**

We have derived general lower bounds on the magnitude of the spectrum of the Hermitian Wilson-Dirac operator:

$$|H(m)| \geq \sqrt{1 - c_k \epsilon} - |k - m| \quad \text{for } k = 1, 3, \dots, 2d - 1,$$

where  $\epsilon$  is the constraining parameter in the smoothness condition (1.1) (and the Wilson parameter is  $r = 1$ ; the generalization to arbitrary  $r > 0$  is given in the Appendix). Thus we have supplemented the previous bounds for the ‘‘physical’’ case  $k = 1$  [3,4] with bounds for the ‘‘doubler’’ cases  $k = 3, 5, \dots, 2d - 1$ . The bounds were shown to hold with

$$c_k = c' + c''_k,$$

$$c' = (1 + \sqrt{2})d(d - 1)/2,$$

$$c''_k = 2^{d-3}(d - 1)(d + 2)[(k - d)^2 - 1 + d].$$

The bounds are rather weak due to the large size of  $c''_k$ , which is due to the large number of terms in the expression (3.19) for  $\tilde{\chi}(k)$ . In practice, it is often possible to get sharper bounds (i.e., smaller  $c''_k$ ) by considering simplified expressions for  $\tilde{\chi}(k)$ . For example, in dimension  $d = 4$  we saw how such simplifications lead to bounds with  $c''_1 = c''_7 = 12$  and  $c''_3 = c''_5 = 42$ . In the  $k = 1$  case this is the same as the value obtained in [3]. It is plausible that bounds with even smaller  $c''_k$  can be derived by an extension of the arguments of [4] (which gave  $c''_1 = 6$ ) but we did not pursue this. For the applications considered in this paper it suffices simply to show that bounds of the above form exist, without necessarily finding sharp ones.

As discussed in Sec. II, the lower bounds on  $|H(m)|$  imply a localization result for the real eigenvalues of the usual Wilson-Dirac operator: the eigenvalues of  $D_w$  (in units of  $1/a$ ) are localized around the values  $0, 2, 4, \dots, 2d$  when  $\epsilon$  is sufficiently small. (A precise formulation of this statement was given in Sec. II.)

The bounds allow previous results on the overlap Dirac operator to be extended from the  $0 < m < 2$  case to general values of  $m$  ( $m \neq 0, 2, \dots, 2d$ ). This includes evaluation of the classical continuum limit of the axial anomaly and index [10,11], and the results of [3] on locality of the overlap Dirac operator and its smooth dependence of the gauge field. The bounds were also seen to imply the existence of topological phases for the overlap Dirac operator when attention is restricted to the space of lattice gauge fields satisfying Eq. (1.1) with  $\epsilon < 1/c_k$  for all  $k$ . A complete description of the

topological phase structure was obtained by combining the bounds with the heuristic result of Sec. IV on the spectral flow properties of  $H(m)$ .

Finally, we pointed out how the bounds can be used to get a more precise understanding of why the real spectrum of the Wilson-Dirac operator in an instanton background is generally localized around  $0, 2, \dots, 2d$  when the instanton size is large but becomes delocalized when the instanton is small at the scale of the lattice spacing. (The argument also applies to more general gauge fields describing a collection of ‘‘topological lumps.’’) Our argument for delocalization of the real spectrum in small instanton backgrounds involved an assumption, namely, that, generically, the smoothness condition (1.1) is not only sufficient but also a *necessary* condition for localization of the spectrum. Numerical studies (e.g., [17]) seem to indicate that this is the case, but it would be interesting if it could be proved analytically. This is relevant for the issue of chiral symmetry breaking in lattice gauge theory since it means that the contribution to the density of near-zero eigenvalues of the Dirac operator from gauge fields describing small topological lumps is reduced on the lattice. Is this reduction an unwanted lattice artifact, or is it a genuinely physical feature revealed by lattice regularization (in the same way that lattice and other regularizations reveal the presence of anomalies that one would not have expected from formal continuum considerations)?

**ACKNOWLEDGMENTS**

Part of this work was done during a visit to the National Center for Theoretical Sciences, Hsinchu, Taiwan. I thank the NCTS, and in particular Ting-Wai Chiu, for kind hospitality and support during the visit, and for stimulating discussions. I also thank Herbert Neuberger for exchanges on bounds during the Chiral '99 workshop, Martin Lüscher for supplying me with the first paper in [3], and Pierre van Baal for useful feedback on the manuscript (including the suggestion to include the figures). Part of the work was also done at Adelaide University where the author was supported by the Australian Research Council. The remainder was done at Leiden University where the author is supported by the Human Potential and Mobility Program of the European Commission (contract HPMF-CT-2002-01716).

**APPENDIX: BOUNDS IN THE CASE OF GENERAL WILSON PARAMETER  $r > 0$**

Using Eqs. (3.6)–(3.8), a simple calculation gives [5]

$$H(m, r)^2 = H(0, r)^2 - 2mr^2 \sum_{\mu} R_{\mu} + r^2 m^2. \quad (\text{A1})$$

It follows that

$$|H(m, r)| \geq rm \quad \text{when } m \leq 0. \quad (\text{A2})$$

It is well known that a lower bound on  $|H(m)|$  is also a lower bound on  $|H(2d - m)|$ ; hence Eq. (A2) implies

$$|H(2d + m, r)| \geq rm \quad \text{when } m \geq 0. \quad (\text{A3})$$

To see this explicitly, write  $H(m,r)$  out according to the definitions (3.1) and (3.8):

$$H(m,r,U) = \gamma_5 \left( rd - rm + \sum_{\mu} \frac{1}{2} [\gamma^{\mu}(T_{+\mu} - T_{-\mu}) - r(T_{+\mu} + T_{-\mu})] \right). \quad (\text{A4})$$

It follows that

$$H(2d-m,r,U) = -\gamma_5 \left( rd - rm + \sum_{\mu} \frac{1}{2} \{ \gamma^{\mu} [(-T_{+\mu}) - (-T_{-\mu})] - r[(-T_{+\mu}) + (-T_{-\mu})] \} \right). \quad (\text{A5})$$

Since  $(T_{+\mu})_{xy} = U_{\mu}(x) \delta_{x,y-\hat{\mu}}$  and  $(T_{-\mu})_{xy} = U_{\mu}(x - \hat{\mu})^{-1} \delta_{x,y+\hat{\mu}}$ , the replacement  $T_{\pm\mu} \rightarrow -T_{\pm\mu}$  is equivalent to  $U \rightarrow -U$ . Hence Eq. (A5) can be written as

$$H(2d-m,r,U) = -H(m,r,-U). \quad (\text{A6})$$

The operator  $R_{\mu}(U) = 1 - 1/2(T_{+\mu} + T_{-\mu})$  remains positive under  $U \rightarrow -U$ , so the argument leading to Eq. (A2) remains valid under this replacement and we get  $|H(2d-m,r,U)| = |H(-m,r,-U)| \geq rm$  for  $m \geq 0$  as claimed in Eq. (A3).

It remains to derive the generalization of the bounds (2.2) in the general  $r$  case. In this case the relations (3.10)–(3.13) become

$$H(m,r)^2 = \sum_{\mu} S_{\mu}^2 + r^2 \left( -m + \sum_{\mu} R_{\mu} \right)^2 + E'(r), \quad (\text{A7})$$

where  $E'(r) = \sum_{\mu \neq \nu} (\gamma^{\mu} \gamma^{\nu})^2 / 2 [S_{\mu}, S_{\nu}] + ir \gamma^{\mu} [S_{\mu}, C_{\nu}]$  has a bound  $\|E'(r)\| \leq c'(r)\epsilon$ . A simple generalization of the argument in [4] shows that this bound is satisfied with

$c'(r) = (1 + r\sqrt{2})d(d-1)/2$ . Following [16,4] we also note that for an eigenvalue  $\lambda(m,r) = \langle \psi(m,r), H(m,r) \psi(m,r) \rangle$  we have  $(d/dm)\lambda(m,r) = -r \langle \psi(m,r), \gamma_5 \psi(m,r) \rangle$  and consequently  $|(d/dm)\lambda(m,r)| \leq r$ , which implies  $|H(m,r)| \geq |H(m',r)| - r|m' - m|$ .

We consider the cases  $r \leq 1$  and  $r \geq 1$  separately. In the former case Eq. (A7) together with Eq. (3.10) gives

$$H(m,r)^2 = r^2 \left[ \sum_{\mu} S_{\mu}^2 + \left( -m + \sum_{\mu} R_{\mu} \right)^2 \right] + (1-r^2) \sum_{\mu} S_{\mu}^2 + E'(r) \geq r^2 [1 + \chi(m)] - c'(r)\epsilon. \quad (\text{A8})$$

This together with Eq. (3.15) gives  $H(k,r)^2 \geq r^2 \{1 - [c_k'' + c'(r)/r^2]\epsilon\}$ , and consequently, setting  $c_k(r) = c_k'' + c'(r)/r^2$ ,

$$|H(m,r)| \geq r \sqrt{1 - c_k(r)\epsilon} - r|k - m|, \quad k = 1, 3, \dots, 2d-1. \quad (\text{A9})$$

In the  $r \geq 1$  case we rewrite Eq. (A7) as

$$H(m,r)^2 = \sum_{\mu} S_{\mu}^2 + \left( -m + \sum_{\mu} R_{\mu} \right)^2 + (r^2 - 1) \left( -m + \sum_{\mu} R_{\mu} \right)^2 + E'(r) \geq 1 + \chi(m) - c'(r)\epsilon, \quad (\text{A10})$$

and it follows from Eq. (3.15) that

$$|H(m,r)| \geq \sqrt{1 - \tilde{c}_k(r)\epsilon} - r|k - m|, \quad k = 1, 3, \dots, 2d-1, \quad (\text{A11})$$

with  $\tilde{c}_k(r) = c_k'' + c'(r)$ .

Note that the bounds (A9) for the  $r < 1$  case and (A11) for the  $r > 1$  case are both weaker than the bound (2.2) for the  $r = 1$  case.

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