Estimating domain wall fermion chiral symmetry breaking

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The effects of explicit chiral symmetry breaking for domain wall fermions resulting from the finite size of the fifth dimension are discussed. The relation between the eigenfunctions of the five-dimensional transfer matrix and the residual mass are be reviewed and their effect on the operator mixing appearing in the calculation of B_K is estimated.

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1. Introduction

The development of methods for treating lattice fermions which preserve the chiral symmetries present in the continuum theory represents a major advance, permitting familiar quantities such as B_K to be studied with improved precision and new quantities, such as CP violation in K meson decays, to be treated using lattice methods for essentially the first time [1, 2, 3]. These methods require significantly more computer resources than the standard Wilson or staggered formulations.

Calculations using the five-dimensional, domain wall fermion (DWF) formulation are more demanding by approximately a factor of L_s, the extent of the lattice in the fifth dimension. The precision of the resulting chiral symmetry depends on the separation between the left- and right-handed light degrees of freedom which are bound to the four dimensional boundaries $s = 0$ and $s = L_s - 1$, where s is the fifth-dimensional coordinate. For finite L_s, propagation between these two boundaries is possible and introduces a residual breaking of chiral symmetry. Given the strong motivation to use a relatively small value of L_s to reduce computational cost, it is important to be able to estimate the size of these residual chiral symmetry breaking effects and their dependence on L_s. This chiral symmetry breaking propagation across the fifth-dimension of the DWF lattice can be conveniently investigated by using the transfer matrix formalism, developed for the case of domain wall fermions in Ref. [4].

2. DWF transfer matrix

Lüscher's original discussion of the Wilson fermion transfer matrix has been exploited to analyze lattice chiral fermions in Refs. [5, 4]. The case of DWF has been thoroughly treated in Ref. [4]. One first defines a matrix $\mathscr{T}$ which, like the Wilson Dirac operator, acts on four-dimensional Dirac wave-functions (for a $L^3 \times T$ lattice with three colors and a single flavor, this is an $L^3 \times T \times 12$-dimensional space):

$$\mathscr{T} = \begin{pmatrix} B^{-1} & B^{-1}C \\ C^\dagger B^{-1} & C^\dagger B^{-1}C + B, \end{pmatrix} \equiv e^{-H_T} \tag{2.1}$$

where

$$B_{n,m} = (5-M)\delta_{n,m} - \frac{1}{2}\sum_\mu [\delta_{n+\hat{\mu},m}U_{n,\mu} + \delta_{n-\mu,m}U^\dagger_{m,\mu}] \quad \text{and} \tag{2.2}$$

$$C_{n,m} = \frac{1}{2}\sum_\mu [\delta_{n+\hat{\mu},m}U_{n,\mu} - \delta_{n-\mu,m}U^\dagger_{m,\mu}]\sigma_\mu \tag{2.3}$$

This matrix can then be used to construct a "second-quantized" transfer matrix T with acts on a $2^{L^3 \times T \times 12}$-dimensional Fock space:

$$T = e^{-\sum_{n,m} q^\dagger(x_n)(H_T)_{n,m}q(x_m)}. \tag{2.4}$$

Here $q(x_n)$ is the quantized lattice fermion field, a function of space and time. Continuing to describe the results of Ref. [4], we can use this matrix to reproduce the usual discrete DWF path integral that is evaluated numerically in a lattice calculation ($L_s > s \geq s' \geq 0$):

$$\int d[\Psi(x,s)]d[\overline{\Psi}(x,s)]\,e^{-S_F}\,\Psi(x_n,s)\overline{\Psi}(x_{n'},s') = Z\,\text{tr}\Big\{T^{L_s-s}q(x_n)T^{s-s'}q(x_{n'})^\dagger T^{s'}\mathscr{O}(m_f)\Big\}. \tag{2.5}$$

Here, to be concrete, we examine the case of the calculation of a 5-dimensional fermion propagator. This expression is valid even before an average over gauge fields is performed. The Grassmann variables Ψ and $\overline{\Psi}$ correspond to the five-dimensional DWF fields and the operator $\mathscr{O}(m_f)$ represents the m_f-dependent boundary conditions imposed on the DWF path integral:

$$\mathscr{O}(m_f) = \prod_n (\hat{c}_n \hat{c}_n^\dagger + m_f \hat{c}_n^\dagger \hat{c}_n)(\hat{d}_n \hat{d}_n^\dagger + m_f \hat{d}_n^\dagger \hat{d}_n), \tag{2.6}$$

where $\hat{c}_n$ and $\hat{d}_n^\dagger$ are the right and left-handed components of $q(x_n)$. When $m_f = 0$, $\mathscr{O}(m_f = 0)$ projects onto a "surface" vacuum state $|0_S\rangle$ which is annihilated by $\hat{c}_n$ and $\hat{d}_n$.

We can analyze the large L_s behavior of Eq. 2.5 by introducing a new Fock space basis using the eigenfunctions of H_T: $H_T \psi_k^\pm = \pm E_k^\pm \psi_k^\pm$ and expressing the original fermionic operator $q(x_n)$ as:

$$q(x_n) = \sum_k \psi_k^+(x_n) \hat{o}_k + \sum_k \psi_k^-(x_n) \hat{p}_k^\dagger. \tag{2.7}$$

Using these operators and dropping an over-all factor, the transfer matrix of Eq. 2.4 becomes:

$$T = e^{-(\sum_k E_k^+ \hat{o}_k^\dagger \hat{o}_k + \sum_k E_k^- \hat{p}_k^\dagger \hat{p}_k)} \tag{2.8}$$

It is now easy to discuss the large-s behavior of the transfer matrix T^s:

$$T^s \approx |0_T\rangle\langle 0_T| + \sum_k e^{-sE_k^+} \hat{o}_k^\dagger |0_T\rangle\langle 0_T| \hat{o}_k + \sum_k e^{-sE_k^-} \hat{p}_k^\dagger |0_T\rangle\langle 0_T| \hat{p}_k + \ldots. \tag{2.9}$$

Here the "transfer matrix" vacuum $|0_T\rangle$ is annihilated by $\hat{o}_k$ and $\hat{p}_k$. In the limit of large s, T^s will simply project onto $|0_T\rangle$. The next leading corrections in Eq. 2.9 come by occupying one of the fermionic states corresponding to eigenvectors of H_T with eigenvalue $E_k^\pm$ close to zero.

While there are few exact results regarding those eigenfunction of the operator H_T with small eigenvalues, it is likely that they fall into two classes [6, 7, 8, 9]: the first is possibly rare, localized states with eigenvalues approaching zero while the second is more numerous de-localized or extended states whose eigenvalues lie above a mobility edge λ_c, $E_k^\pm \geq \lambda_c$ [9].

3. Residual mass

We can now combine Eq. 2.9 with this assumed eigenspectrum of H_T to estimate the dependence of residual DWF chiral symmetry breaking on L_s. We start by examining a general matrix element of a product of "physical" 4-dimension fermion fields which is best represented by a product of operators containing right-handed and left-handed fermion fields, evaluated on the $s = L_s - 1$ and $s = 0$ boundaries: O_R and O_L respectively. Generalizing Eq. 2.5 and, for simplicity, setting $m_f = 0$ we find:

$$\langle O_R O_L\rangle = \langle 0_S|O_R T^{L_s} O_L|0_S\rangle \approx \langle 0_S|O_R \Big\{ |0_T\rangle\langle 0_T| + \sum_k e^{-L_s E_k^+} \hat{o}_k^\dagger |0_T\rangle\langle 0_T| \hat{o}_k$$

$$+ \sum_k e^{-L_s E_k^-} \hat{p}_k^\dagger |0_T\rangle\langle 0_T| \hat{p}_k + \ldots \Big\} O_L|0_S\rangle. \tag{3.1}$$

Here the leading term, the projection operator $|0_T\rangle\langle 0_T|$, divides the Greens function into two independent factors demonstrating the separate, flavored chiral symmetry of the left- and right-handed

fermions. The first correction permits quark number ± 1 exchanges between these two otherwise independent sectors. This suggests that the second and third terms in Eq. 3.1 should be interpreted at low energies as the residual mass operator $m_{\text{res}}\overline{\psi}\psi$ expressed in this 5-dimensional language.

A relation between this residual mass term and the second and third terms in the operator in curly brackets in Eq. 3.1 can be obtained if we express the operators o_k and p_k in terms of the conventional 4-dimension field $q(x)$, inverting Eq. 2.7:

$$\sum_n m_{\text{res}}\overline{\psi}(x_n)\psi(x_n) \rightarrow \quad m_{\text{res}}\sum_n \Big\{ q_R(x_n)^\dagger|0_T\rangle\langle 0_T|q_L(x_n) - q_R(x_n)|0_T\rangle\langle 0_T|q_L(x_n)^\dagger + \Big\} \quad (3.2)$$

$$\stackrel{?}{\approx} \sum_{n,n'}\sum_k \psi_k^+(x_n)\psi_k^+(y_{n'})^\dagger e^{-L_s E_k^+} \, q_R(x_n)^\dagger|0_T\rangle\langle 0_T|q_L(y_{n'})$$

$$+ \sum_{n,n'}\sum_k \psi_k^-(x_n)^\dagger\psi_k^-(y_{n'}) e^{-L_s E_k^-} \, q_R(x)|0_T\rangle\langle 0_T|q_L(y)^\dagger. \quad (3.3)$$

Here the RHS of Eq. 3.2 is the residual mass term written in the transfer matrix language while the expression in Eq. 3.3 is a rewritten version of the leading order contribution from the second and third terms in Eq. 3.1.

We can justify this relation and estimate m_{res}, if we assume that the quantities $\sum_k \psi_k^\pm(x_n)\psi_k^\pm(y_{n'})$ are localized on the long distance scale at which m_{res} is defined:

$$K_{a,b}(x,y) = \sum_{k,a}\psi_{k,a}^\pm(x)^\dagger\psi_{k,b}^\pm(y)e^{-L_s E_k^\pm} \approx m_{\text{res}}\delta^4(x-y)\delta_{a,b}, \quad (3.4)$$

where a and b are spin-color indices and we assume that the diagonal spin-color structure will appear and any dependence on the label $\pm$ will disappear when a volume and/or gauge average is performed. We can then approximate: $m_{\text{res}} = \frac{1}{12}\int d^4x K_{a,a}(x,y) \approx \frac{1}{12}R^4 K_{a,a}(y,y)$. Were the "radius" R estimates the small region in x that contributes and a sum over the repeated index a is intended. Finally, $K(y,y)$ and hence m_{res} can be determined by integrating over y and using the orthonormality of the eigenfunctions $\psi_{k,a}^\pm(y)$:

$$m_{\text{res}} = \frac{R^4}{12}K_{a,a}(y,y) = \frac{R^4}{12L^4}\int d^4y K_{a,a}(y,y) \quad (3.5)$$

$$= \frac{R^4}{12L^4}\sum_k e^{-L_s E_k^\pm} = R^4\int_o^\infty d\lambda \rho(\lambda)e^{-L_s\lambda} \quad (3.6)$$

$$\sim R_e^4 \rho_e(\lambda_c)\frac{e^{-\lambda_c L_s}}{L_s} + R_l^4 \rho_l(0)\frac{1}{L_s}. \quad (3.7)$$

Here $\rho(\lambda)$ on the RHS of Eq. 3.6 is the density of eigenvalues of H_T per unit space-time volume, color and spin. The final Eq. 3.7 is a generalization of Eq. 3.6 displaying the expected contributions of localized (l) and extended (e) modes with possibly different average sizes R_l and R_e. In this final equation we have also taken the limit of large L_s. This is the "standard" result for the dependence of m_{res} on L_s, although the factor of $1/L_s$ is usually missing from the left-most term.

4. Operator mixing

Having developed a reasonably systematic approach to estimating the size of DWF chiral symmetry breaking, we can now apply this method to a quantity of special interest: the mixing

between the usual O_{LL} operator whose matrix element gives B_K and potentially larger operators whose matrix elements do not vanish in the chiral limit. Here we will examine the case of mixing between O_{LL} and O_{LR} where:

$$O_{LL/LR} = \overline{s}\gamma^{\mu}(1 - \gamma^5)d\overline{s}\gamma^{\mu}(1 \pm \gamma^5)d. \tag{4.1}$$

The mixing between these two operators can be represented by the equation $O_{LL}^{\text{cont}} = Z_{LL,LL}O_{LL} + Z_{LL,LR}O_{LR}$, expressing the continuum operator O_{LL}^{cont} in terms of those defined on the lattice. The mixing term $Z_{LL,RR}$ is required to remove the contribution of the wrong chirality operator O_{LR} that will appear in matrix elements of the lattice operator O_{LL} coming from residual chiral symmetry breaking.

The mixing coefficient of interest can be computed by evaluating a Greens function far off-shell to avoid innocuous "mixing" caused by low-energy, spontaneous, chiral symmetry breaking:

$$Z_{LL,LR}(\mu) = \frac{1}{128}\prod_{1 \le i \le 4}\left\{\int d^4 x_i\, e^{ip_i \cdot x_i}\right\}\langle 0|\overline{d}_R(x_1)\not{p}_1\gamma^{\mu}\not{p}_2 s_R(x_2)O_{LL}(0)\overline{d}_L(x_3)\not{p}_3\gamma^{\mu}\not{p}_4 s_L(x_4)|0\rangle_{p_i^2 = \mu^2}$$

$$\approx \frac{1}{8}\prod_{1 \le i \le 2}\left\{\int d^4 x_i\, e^{ip_i \cdot x_i}\right\}\langle 0|\overline{d}_R(x_1)\not{p}_1\gamma^{\mu}\not{p}_2 s_R(x_2)\overline{s}_L(0)\gamma^{\mu}d_L(0)|0\rangle_{p_i^2 = \mu^2}. \tag{4.2}$$

In the top part of Eq. 4.2 we show the usual off-shell Greens function that will determine the O_{LR} component present in the O_{LL} operator. This has been simplified in the lower equation by removing the two normal, chirality conserving fermion contractions — a step accurate only at tree level.

We next evaluate the RHS of Eq. 4.2 using the method discussed above. In the transfer matrix language, the expression to be evaluated takes the form

$$Z_{LL,LR}(\mu) \approx \frac{1}{8}\prod_{1 \le i \le 2}\left\{\int d^4 x_i\, e^{ip_i \cdot x_i}\right\}\langle 0_S|q_R^{d\dagger}(x_1)\not{p}_1\gamma^{\mu}\not{p}_2 q_R^s(x_2)T^{L_s}q_L^{s\dagger}(0)\gamma^{\mu}q_L^d(0)|0_S\rangle_{p_i^2 = \mu^2}. \tag{4.3}$$

We can now insert the large-s expansion for T^s of Eq. 2.9 into Eq. 4.3. Clearly the leading order term $|0_T\rangle\langle 0_T|$ does not contribute since the state $|0_T\rangle$ is an $SU(3)_L \times SU(3)_R$ singlet while the operator $q_L^{s\dagger}(0)q_L^d(0)$ transforms as an $(8,1)$ under this group. Likewise the contribution from a single state of the sort represented by the second and third terms in Eq. 2.9 corresponds to the $(3,1)$ representation and hence also vanishes.

Thus, we must go to the next term in the large s expansion of T^s, one containing two filled eigenstates of H_T. This would suggest a double suppression of order m_{res}^2. However, since two flavors of quarks are involved, there may be a larger contribution from a gauge configuration that supports a single localized mode with near-zero eigenvalue of H_T [10]. While such a mode is suppressed (it will appear infrequently in the gauge average and must be located near the position of the weak operator) if this mode can be used twice, once for the s quark and once for the d quark, only a single suppression factor will be involved. However, this is not possible here: the product $q_L^{s\dagger}(0)q_L^d(0)$ has quark number zero while the pairs $\hat{o}_k^s\hat{o}_k^d$ and $\hat{p}_k^s\hat{p}_k^d$ have quark number ± 2.

Thus, a non-zero contribution to the leading term in Eq. 4.3, requires two independent eigen-functions ψ_k^+ and $\psi_{k'}^-$ for the s and $\overline{d}$ quarks respectively. Carrying out a heuristic estimate, similar

to that in Eqs. 3.4-3.7, gives:

$$Z_{LL,RR} \approx \int_0^\infty d\lambda^+ d\lambda^- e^{-s(\lambda^+ + \lambda^-)} \left\{ R_e^8 \rho_{ee}(\lambda^+, \lambda^-) + R_e^4 R_l^4 \rho_{el}(\lambda^+, \lambda^-) + R_l^8 \rho_{ll}(\lambda^+, \lambda^-) \right\}$$

$$\approx \left\{ R_e^4 \rho_e(\lambda_c) \frac{e^{-\lambda_c L_s}}{L_s} + R_l^4 \rho_l(0) \frac{1}{L_s} \right\}^2 = m_{\text{res}}^2. \tag{4.4}$$

where, for example, $\rho_{ll}(\lambda^+, \lambda^-)$ is the joint distribution of localized, positive and negative energy modes with eigenvalues λ^+ and λ^-. One obtains the lower line of Eq. 4.4 by approximating these joint densities by products of single eigenvalue densities and taking the limit of large L_s.

5. Conclusion

Using the transfer matrix formalism of Furman and Shamir we have made rough estimates of the large L_s behavior of the DWF residual mass and the chiral symmetry violating mixing of the four-Fermi operators which contribute to a calculation of $K^0 - \overline{K}^0$ mixing. We find that this operator mixing, which changes chirality by two units, is doubly suppressed, behaving as m_{res}^2.

Acknowledgments

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