Improving the locality of the overlap Dirac operator via approximate solutions of the Ginsparg-Wilson relation

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We determine a free field hypercubic lattice Dirac operator which is optimally close to satisfying the Ginsparg-Wilson relation. Inserting this operator into the overlap formula, we show that the analytic locality bound on the resulting overlap Dirac operator is substantially stronger than in the standard case. The improvement generally persists in gauge backgrounds when the plaquette variables are all close to unity.

The overlap Dirac operator provides a formulation of lattice QCD with exactly massless quarks. Actually there are many overlap operators: for each choice of ultra-local lattice Dirac operator \( D \) an overlap Dirac operator \( D_{ov} \), is obtained by inserting \( D \) into the overlap formula:

\[
D_{ov} = \frac{m}{a} (1 + A(A^* A)^{-1/2}) \, , \quad A \equiv D - \frac{m}{a}
\]  

(1)

Here \( a \) is the lattice spacing and \( m \) is a parameter which controls topological properties of \( D_{ov} \) and the number of fermion species described by the corresponding lattice fermion action. In the standard overlap operator, \( D \) is taken to be the Wilson-Dirac operator \( D_w \).

The locality issue for \( D_{ov} \) is nontrivial due to the inverse square root \((A^* A)^{-1/2}\) in (1), which also causes difficulties for numerical implementation. To ensure that the lattice theory is in the right universality class to reproduce continuum physics, \( D_{ov} \) should be exponentially-local. An exponential-locality bound was derived in [2]:

\[
|| (A^* A)^{-1/2} (x,y) || \leq K e^{-\theta |x-y|/a}
\]

(2)

where \( |x-y| \equiv \sum_\mu |x_\mu - y_\mu| \). Set \( l \) to be the maximum distance in units of lattice spacing between lattice sites coupled by \( D \) as measured by this norm (e.g. \( l = 1 \) for the Wilson-Dirac operator). Then the decay constant in (2) is

\[
\tilde{\theta} = \theta / 2l
\]

(3)

with \( \theta \) determined by the condition number \( C \):

\[
\theta = \log \left( \frac{\sqrt{C} + 1}{\sqrt{C} - 1} \right) \, , \quad C = \frac{\lambda_{\max} (A^* A)}{\lambda_{\min} (A^* A)}
\]

(4)

\( \lambda_{\max} \) (\( \lambda_{\min} \)) are the maximum (minimum) eigenvalues. Moreover \( K = \lambda_{\min} (A^* A)^{-1/2} \) (this and [3]–[4] were not written out explicitly in [2] but follow easily from the formulae derived there).

To obtain a locality bound independent of the gauge field, gauge field-independent bounds \( 0 < u \leq A^* A \leq v < \infty \) are required; then \( \lambda_{\min} \) and \( \lambda_{\max} \) can be replaced by \( u \) and \( v \), respectively, in the preceding. An upper bound \( v \) can easily be derived via triangle inequalities. However, to get a nonzero lower bound \( u \) some restriction on the lattice gauge fields is generally required, since gauge backgrounds in which \( A \) has zero-modes do exist in general (reflecting topological properties of \( D_{ov} \)). In the standard Wilson-Dirac case this can be done by imposing an admissibility condition [2,3,4]:

\[
|| 1 - U(p) || \leq \epsilon \quad \forall \text{plaqquete } p.
\]

(5)

The currently sharpest lower bound is \( 1 - 6(2 + \sqrt{2}) \epsilon \leq A^*_w A_w \) (in 4 dimensions and with \( m = 1 \)).

In [5] the possibility of improving locality and convergence properties of the overlap Dirac operator by taking the input \( D \) to be an approximate solution of the Ginsparg-Wilson (GW) relation [6] was pointed out. This is based on the observation that if \( D \) is an exact GW solution, i.e.
\( \gamma_5 D + D \gamma_5 = \frac{m}{a} D \gamma_5 D \), then the overlap formula simply gives this operator back again: \( D_{ov} = D \). (To see this, note that the GW relation is equivalent to \( A^* A = \left( \frac{m}{a} \right)^2 \) where \( A \equiv D - \frac{m}{a} \cdot \).) It is known that ultra-local operators cannot exactly satisfy the GW relation [7]; but approximate solutions are possible, and for these the preceding observation implies \( D_{ov} \approx D \), indicating that \( D_{ov} \) is “close to being ultra-local”. This heuristic reasoning needs to be treated with caution though, because if \( D \) is very close to satisfying the GW relation then it must be “almost non-ultralocal”. In this note we attempt to get a more precise analytic understanding of the situation by considering the improvement that can be achieved in the locality bound [2]. If \( D \) is an approximate GW solution, i.e. \( A^* A \approx \left( \frac{m}{a} \right)^2 \), then \( \lambda_{\text{min}} \approx \lambda_{\text{max}} \approx \left( \frac{m}{a} \right)^2 \), hence the condition number \( C \) is close to unity and consequently the parameter \( \theta \) in Table 1 is very large. However, the effect of the the increase in \( \theta \) in the decay constant [3] must be at least partly offset by an increase in \( l \), since the closer \( D \) is to satisfying the GW relation the longer its range must be. Therefore, to improve the locality bound on the overlap Dirac operator, we are led to look for short range approximate solutions to the GW relation to use as input in the overlap formula.

A natural arena in which to look for such operators is the class of hypercubic operators. These are the lattice Dirac operators which couple sites within the same lattice hypercube. For such operators the parameter \( l \) in [4] equals the spacetime dimension \( d \), so in 4 dimensions an increase in \( \theta \) by more than a factor of 4 is required in order to achieve a locality bound that is stronger than the one for the standard overlap operator. We begin by considering the free field case. Define the hermitian operators \( S_\mu = \frac{1}{2i} (T_{+\mu} - T_{-\mu}) \) and \( C_\nu = \frac{1}{2} (T_{+\nu} + T_{-\nu}) \) where \( T_{+\mu} \) (\( T_{-\mu} \)) are the usual forward (backward) parallel transport operators. Then a general free field hypercubic operator can be written in terms of the free field \( S_\mu \)'s and \( C_\nu \)'s as [8]

\[
D = \frac{1}{a} (\gamma^\mu \rho_\mu + \lambda)
\]

\[
- i \gamma_5 \rho_\mu = S_\mu \sum_{p=1}^{d} 2^p \kappa_p \sum_{v_1 \prec \cdots \prec v_p, v_1 \neq \mu \neq v_j} C_{v_1} \cdots C_{v_p}
\]

and \( \lambda = \sum_{p=0}^{d} 2^p \lambda_p \sum_{v_1 \prec \cdots \prec v_p} C_{v_1} \cdots C_{v_p} \) Here \( \kappa_1, \ldots, \kappa_d \) and \( \lambda_0, \ldots, \lambda_d \) are coupling parameters; they are the most general couplings allowed by the lattice symmetries. The requirements of correct formal continuum limit \( (D \to \gamma^\mu \partial_\mu) \) and vanishing bare mass are equivalent to the constraints \( \sum_{p=1}^{d} 2^p \frac{d-1}{p} \kappa_p = 1 \) and \( \sum_{p=0}^{d} 2^p \frac{d}{p} \lambda_p = 0 \). These can be used to eliminate \( \kappa_1 \) and \( \lambda_0 \); then \( D \) contains \( 2d - 1 \) free parameters \( \kappa_2, \ldots, \kappa_d; \lambda_1, \ldots, \lambda_d \). (The Wilson-Dirac operator, which contains just one free parameter –the Wilson parameter \( r \)– is obtained by setting \( \kappa_1 = 1/2, \lambda_0 = dr, \lambda_1 = -r/2 \) and \( \kappa_p = \lambda_p = 0 \) for \( p \geq 2 \)).

A number of free field hypercubic operators which approximately satisfy the GW relation are already known and have been discussed in [5]; the truncation of the standard overlap operator, the truncated Fixed Point (FP) operator (the FP operator is a GW solution which is known explicitly only in the free field case [4]), and the “GW-improved” operator obtained by inserting the truncated FP operator into the overlap formula and then truncating again. However, one can attempt to do better still by considering the condition number [4] as a function \( C = C(\kappa_2, \ldots, \kappa_d; \lambda_1, \ldots, \lambda_d) \) on the parameter space of free field hypercubic operators and finding the point(s) at which \( C \) has a minimum. We did this numerically, using the expression

\[
C = \max_k \{ A^* A(k) \} / \min_k \{ A^* A(k) \}
\]

where \( A^* A(k) \) is the free field momentum representation of \( A^* A \). For concreteness we fix the spacetime dimension to be \( d = 4 \) and set \( m = 1 \) in [4], i.e. \( aA = aD - 1 \). The lattice spacing \( a \) drops out in the expression for \( C \). When calculating a minimum of \( C(\kappa_2, \ldots, \lambda_4) \) numerically one must specify an initial point (actually two initial points for our Mathematica calculation). We tried various choices of starting points corresponding to the truncated FP operator and other free field hypercubic operators considered in [5]. In each case the the numerical calculation converged to the same minimum of \( C(\kappa_2, \ldots, \lambda_4) \) at the point in parameter space listed in the last column of Table 1. Thus we have found a new free field
Table 2
The coupling parameters of the new “optimal” free field hypercubic operator. For comparison the parameters of the truncated FP operator are also listed.

|         | Trunc. FP | Optimal |
|---------|-----------|---------|
| $\kappa_2$ | 0.03208   | 0.03230 |
| $\kappa_3$ | 0.01106   | 0.01107 |
| $\kappa_4$ | 0.00475   | 0.00613 |
| $\lambda_1$ | -0.06076  | -0.06191 |
| $\lambda_2$ | -0.03004  | -0.03027 |
| $\lambda_3$ | -0.01597  | -0.01576 |
| $\lambda_4$ | -0.00843  | -0.00778 |

In Table 2 we list $\lambda_{\text{min}}$, $\lambda_{\text{max}}$ and the condition number $C$ for the new operator, as well as the decay constant $\theta$ in the locality bound (2) for the corresponding overlap Dirac operator, and compare with the values for other operators. The $\theta$ for the new operator is significantly larger than for the previously considered free field hypercubic operators, and is larger than the Wilson-Dirac $\tilde{\theta}$ by more than a factor of 3.

Table 2
$\lambda_{\text{min}}(A^* A)$, $\lambda_{\text{max}}(A^* A)$, $C$ and $\tilde{\theta}$ for the free field Wilson-Dirac operator, the truncated FP and its GW-improved version, and the new “optimal” hypercubic operator.

|        | $\lambda_{\text{min}}$ | $\lambda_{\text{max}}$ | $C$ | $\theta$ |
|--------|-------------------------|-------------------------|-----|---------|
| Wilson-Dirac | 1                        | 49                       | 49  | 0.14    |
| Trunc. FP | 0.919                   | 1.023                    | 1.113 | 0.45   |
| GW-improved | 0.932                   | 1.032                    | 1.107 | 0.46   |
| Optimal   | 0.938                   | 1.005                    | 1.072 | 0.51   |

The coupling parameters of the new “optimal” free field hypercubic operator are also presented in Table 2. The values for the truncated FP operator are also listed for comparison. The parameters are defined as $\lambda_{\text{min}}, \lambda_{\text{max}}$, and the condition number $C$. The decay constant $\theta$ in the locality bound (2) is also provided for the corresponding overlap Dirac operator, and compared with the values for other operators. The $\theta$ for the new operator is significantly larger than for the previously considered free field hypercubic operators, and is larger than the Wilson-Dirac $\tilde{\theta}$ by more than a factor of 3.

Gauged hypercubic operators can be built up in various ways from free field operators. We now point out that if the free field operator is a good approximate GW solution then the same is generally true for the gauged operator when the gauge field satisfies the admissibility condition (6) with small $\epsilon$. General ultra-local gauged lattice Dirac operators are polynomials in the parallel transporters $T_{\pm \mu}$. Since these can be expressed in terms of the $S_{\mu}$, $C_{\nu}$ defined earlier, $A^* A = A^* A(S_{\mu}, C_{\nu})$. Inserting the spectral decompositions $S_{\mu} = \sum_{\alpha} s_{\mu \alpha} P_{\mu \alpha}$, $C_{\nu} = \sum_{\beta} c_{\nu \beta} P_{\nu \beta}$ (where $P_{\mu \alpha}$, $Q_{\nu \beta}$ are the projections onto the eigenspaces with eigenvalues $s_{\mu \alpha}$, $c_{\nu \beta}$, respectively), and using the fact that in any gauge background $s_{\mu \alpha}$, $c_{\nu \beta} \in [-1, 1]$, one can make a connection with $A^* A_{\text{free}}$ and derive bounds

$$\lambda_{\text{min}, f} - \lambda_{\text{min}, f}(C_f - 1)K_- O(\epsilon) \leq A^* A$$

$$\leq \lambda_{\text{max}, f} + \lambda_{\text{min}, f}(C_f - 1)K_- O(\epsilon)$$

(7)

(the derivation will be given elsewhere) where the subscript “f” refers to the free field quantities. Here $K_- = \sum_{|\psi|=1} |\langle \psi, O_\sigma \psi \rangle|$ where $O_{\alpha_1 \ldots \beta_4} = P_{1\alpha_1} \cdots Q_{4\beta_4}$ and the sum is restricted to the $\sigma = \{\alpha_1, \ldots, \beta_4\}$ for which $\langle \psi, O_\sigma \psi \rangle$ is negative. Since $\sum_{\sigma(\psi)} |\langle \psi, O_\sigma \psi \rangle| + \sum_{\sigma(-)} |\langle \psi, O_\sigma \psi \rangle| = 1$ for all unit norm $\psi$, and $|\langle \psi, O_\sigma \psi \rangle| \leq 1 \forall \sigma$, we can expect $K_-$ to be of order 1 in typical gauge backgrounds. Then, if the free field operator is a good approximate GW solution (i.e. $C_f \approx 1$), the terms with $K_-$ are very small in (7). The bounds then imply that the condition number of the gauged operator is close to the free field condition number when $\epsilon$ is small. Finally we mention that hypercubic and other short range lattice Dirac operators which are reasonable approximate GW solutions in equilibrium gauge backgrounds have already been found in numerical work; see (10) and the ref.’s therein.

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