The overlap Dirac operator as a continued fraction

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We use a continued fraction expansion of the sign–function in order to obtain a five dimensional formulation of the overlap lattice Dirac operator. Within this formulation the inverse of the overlap operator can be calculated by a single Krylov space method and nested conjugate gradient procedures are avoided. We point out that the five dimensional linear system can be made well conditioned using equivalence transformations on the continued fractions.

1 Introduction

Let us start with noting the overlap Dirac operator $D$ describing chirally symmetric fermions on the lattice [1],

$$D = \frac{1}{2} \left( 1 + \gamma_5 \text{sign} \left( H(-m) \right) \right), \quad (1)$$

where $H(-m)$ is a hermitian Dirac operator with a negative mass parameter $-m$ of the order of the cut-off of the lattice theory, $m \sim O(a)$. A bare quark mass $\mu$ is most conveniently introduced as $D(\mu) = (1 - \mu)D + \mu$. In order to calculate efficiently the sign–function in eq.(1) one can use a rational approximation $\text{sign}(x) \approx R_{n,m}(x)$ where $R_{n,m}$ is a (nondegenerate and irreducible) rational function with algebraic polynomials of order $n$ and $m$ as numerator and denominator, respectively. Rational approximations usually converge much faster with their degree than polynomial approximations, but of course for our specific application it might still be much more expensive to apply the low degree denominator of the rational function than to apply a high order polynomial. However, noting that a rational function can be written as a partial fraction by matching poles and residues, i.e., $R_{n,m}(x) \sim x \sum_k c_k/(x^2 + q_k)$, one can use a multi–shift linear system solver where the convergence is governed by the smallest of the shifts $q_k$. The overall cost is therefore roughly equivalent to one inversion of $H^2$. 

In order to do physics we need to compute inverses of the overlap operator $D(\mu)$ to obtain propagators, fermionic forces for Hybrid Monte Carlo, etc. If we consider the multi–shift linear system above, we realise that the inversion of $D(\mu)$ leads to a two–level nested linear system solution, which is rather cumbersome and forbidding. It is well known how this can be avoided by introducing a continued fraction representation of the rational approximation and auxiliary fields, the non–linear system $D(\mu)\psi = \chi$ can be unfolded into a set of systems linear in $H$. The auxiliary fields can be interpreted as fields living in a fictitious fifth dimension and in this way the nested 4D Krylov space problem reduces to finding a solution in a single 5D Krylov space. One can also regard the auxiliary fields as additional fermion flavours which, when integrated out, generate an effective Dirac operator equivalent to $D(\mu)$.

2 Matrix representation of the sign–function

Consider a rational approximation to the sign–function and expand it as a continued fraction,

$$R_{2n+1,2n}(x) = \alpha_0 x + \frac{\alpha_1}{x + \frac{\cdots}{\cdots + \frac{\alpha_{2n}}{x}}}.$$  \hfill (2)

If we rewrite the linear system

$$\left(\alpha_0 x + \frac{\alpha_1}{x + \frac{\cdots}{\cdots + \frac{\alpha_{2n}}{x}}}\right) \psi = \chi$$ \hfill (3)

using appropriate auxiliary fields $\phi_1, \phi_2, \ldots, \phi_{2n}$ we obtain the system

$$\begin{pmatrix}
  \alpha_0 x & \sqrt{\alpha_1} & \cdots & \sqrt{\alpha_{2n}} \\
  \sqrt{\alpha_1} & -x & \sqrt{\alpha_2} & \cdots \\
  \vdots & \ddots & \ddots & \ddots \\
  \sqrt{\alpha_{2n}} & \cdots & -x & \sqrt{\alpha_{2n}} \\
\end{pmatrix}
\begin{pmatrix}
  \psi \\
  \phi_1 \\
  \phi_2 \\
  \vdots \\
  \phi_{2n-1} \\
  \phi_{2n} \\
\end{pmatrix}
= \begin{pmatrix}
  \chi \\
  0 \\
  0 \\
  \vdots \\
  0 \\
  0 \\
\end{pmatrix}. \hfill (4)
$$

By performing explicitly a Schur decomposition of the matrix it is easy to see that the inverse of eq.(2) is just the $(1, 1)$–component of the Schur complement.

The rational function can also be mapped into a so–called simple continued fraction: \footnote{Note that since polynomial approximations can also be expanded into continued fractions all our considerations apply to them as well.}

$\frac{\alpha_0 x + \frac{\alpha_1}{x + \frac{\cdots}{\cdots + \frac{\alpha_{2n}}{x}}}}{}$. \hfill (3)
The overlap Dirac operator as a continued fraction

\[ R_{2n+1,2n}(x) = \beta_0 x + \frac{1}{\beta_1 x + \frac{1}{\beta_2 x + \cdots + \frac{1}{\beta_{2n} x}}} \]  

which leads to a different matrix

\[
\begin{pmatrix}
\beta_0 x & 1 & \\
1 & -\beta_1 x & 1 \\
& 1 & \beta_2 x \\
& & \ddots \\
& & -\beta_{2n-1} x & 1 \\
& & & 1 & \beta_{2n} x
\end{pmatrix},
\]

and we find that the \( \alpha \)'s and \( \beta \)'s are related through

\[
\beta_0 = \alpha_0, \beta_1 = \frac{1}{\alpha_1}, \ldots, \beta_i = \frac{1}{\alpha_i \beta_{i-1}}, \ldots,
\]

\[
\alpha_0 = \beta_0, \alpha_1 = \frac{1}{\beta_1}, \ldots, \alpha_i = \frac{1}{\beta_{i-1} \beta_i}, \ldots.
\]

In order to understand the relation between different continued fraction representations of the same rational function in detail we need to take a closer look at the properties of continued fractions (see e.g. [1, 5]).

3 Continued fractions

A generic (truncated) continued fraction \( \frac{A_n}{B_n} \) is conveniently written as

\[
\frac{A_n}{B_n} = \beta_0 + \frac{\alpha_1}{\beta_1 + \frac{\alpha_2}{\beta_2 + \cdots + \frac{\alpha_n}{\beta_n}}}
\]

Simple continued fractions have the property \( \alpha_i = 1, i = 1, \ldots, n \) and one usually writes

\[
\frac{A_n}{B_n} = [\beta_0; \beta_1, \beta_2, \ldots, \beta_n].
\]

Continued fractions are widely used in many areas of physics and mathematics, in particular also in number theory. Finite continued fractions provide an alternative representation of rational numbers and form the basis of rational approximation theory. Infinite continued fractions on the other hand can be used to represent irrational numbers. Some numbers have beautiful continued fraction expansions while others have very mysterious ones. Let us quickly note a few examples for our amusement:
\[ \phi = [1; 1, 1, 1, 1, \ldots], \]
\[ \sqrt{2} = [1; 2, 2, 2, 2, \ldots], \]
\[ e = [2; 1, 2, 1, 4, 1, 1, 6, 1, 1, 8, 1, 1, 10, 1, \ldots], \]
\[ \pi = [3; 7, 15, 1, 292, 1, 1, 2, 1, 3, 1, \ldots], \]

where \( \phi = \frac{1}{2}(1 + \sqrt{5}) \) is the golden mean. It is interesting to note that there is no regular pattern known for \( \pi \), and it is not known why this is so.

Evaluation of continued fractions can be done through forward or backward recurrence algorithms, and the former makes use of the intimate relation between continued fractions and the coupled two term relations

\[
A_{i} = \beta_i A_{i-1} + \alpha_i A_{i-2}, \quad i = 1, 2, 3, \ldots, \quad (11)
\]
\[
B_{i} = \beta_i B_{i-1} + \alpha_i B_{i-2}, \quad i = 1, 2, 3, \ldots, \quad (13)
\]

which can equivalently be written as an iterative matrix equation,

\[
\begin{pmatrix} A_i \\ B_i \end{pmatrix} = \begin{pmatrix} A_{i-1} & A_{i-2} \\ B_{i-1} & B_{i-2} \end{pmatrix} \begin{pmatrix} \beta_i \\ \alpha_i \end{pmatrix}. \quad (14)
\]

There is also an interesting connection between continued fractions, Moebius transformations and the corresponding unimodular matrices.

The natural arithmetic operation for continued fractions is inversion and the corresponding rule is particularly simple:

\[
[\beta_0; \beta_1, \ldots]^{-1} = \begin{cases} 
0; \beta_0, \beta_1, \ldots & \text{if } \beta_0 \neq 0, \\
[\beta_1; \beta_2, \ldots] & \text{if } \beta_0 = 0.
\end{cases} \quad (15)
\]

It is also helpful to write down the rule for the multiplication of a continued fraction by a constant \( c \),

\[
c \cdot [\beta_0; \beta_1, \ldots, \beta_n] = [c \cdot \beta_0; \frac{c}{c} \beta_1, c \cdot \beta_2, \frac{c}{c} \beta_3, c \cdot \beta_4, \ldots]. \quad (16)
\]

Most important for our purpose, however, is the equivalence transformation of a continued fraction which is stated in the following theorem:

**Theorem 1.** Two continued fractions \( \beta_0 + \frac{\alpha_1}{\beta_1} + \ldots + \frac{\alpha_n}{\beta_n} \) and \( \beta'_0 + \frac{\alpha'_1}{\beta'_1} + \ldots + \frac{\alpha'_n}{\beta'_n} \) are equivalent iff there exists a sequence of non-zero constants \( c_n \) with \( c_0 = 1 \) such that

\[
\begin{align*}
\alpha'_i &= c_i c_{i-1} \alpha_i, \quad i = 1, 2, 3, \ldots, n, \\
\beta'_i &= c_i \beta_i, \quad i = 0, 1, 2, \ldots, n.
\end{align*}
\]

The theorem is easily seen to hold true by explicitly writing out the full continued fraction,
The overlap Dirac operator as a continued fraction

\[
\beta_0 + \frac{\alpha_1}{\beta_1 + \frac{\alpha_2}{\beta_2 + \frac{\alpha_3}{\beta_3 + \cdots}}} = \beta_0 + \frac{c_1\alpha_1}{c_1\beta_1 + \frac{c_2\alpha_2}{c_2\beta_2 + \frac{c_3\alpha_3}{c_3\beta_3 + \cdots}}}
\]  

(19)

and it is also clear that in terms of approximants we simply have

\[
\frac{A_n}{B_n} = \frac{c_1c_2\cdots c_n\alpha_n}{c_1c_2\cdots c_n\beta_n}
\]

So we find that a given rational function corresponds to an equivalence class of continued fractions and the class is parametrised by the (non-zero) coefficients \(c_i\). While the equivalence transformation itself appears to be rather trivial, and indeed leaves the value of the continued fraction invariant, it affects the spectrum of the corresponding matrix representation [3].

In the analytic theory of continued fractions one considers continued fractions of the form

\[
\beta_0(z) + \frac{\alpha_1(z)}{\beta_1(z) + \frac{\alpha_2(z)}{\beta_2(z) + \frac{\alpha_3(z)}{\beta_3(z) + \cdots}}} = \beta_0 + \frac{c_1\alpha_1(z)}{c_1\beta_1(z) + \frac{c_2\alpha_2(z)}{c_2\beta_2(z) + \frac{c_3\alpha_3(z)}{c_3\beta_3(z) + \cdots}}}
\]

(20)

i.e., the coefficients are functions of a complex variable \(z\). So-called \(J\)-fractions are of the special form

\[
[r_1z + s_1, r_2z + s_2, r_3z + s_3, \ldots]
\]

(21)

where \(r_i, s_i\) are complex numbers with \(r_i \neq 0\). One can show that the \(n\)-th approximant of a \(J\)-fraction is an element of \(R_{n-1,n}\). Conversely, let

\[
P_{n-1}(z) = p_1z^{n-1} + p_2z^{n-2} + \ldots + p_n ,
\]

\[
Q_n(z) = q_0z^n + q_1z^{n-1} + \ldots + q_n ,
\]

(22, 23)

then we have

\[
\frac{P_{n-1}(z)}{Q_n(z)} = [r_1z + s_1, r_2z + s_2, \ldots, r_nz + s_n]
\]

(24)

where \(r_i, s_i\) are uniquely determined by \(p_i, q_i\). We can now replace \(z\) by \(-z\), apply an appropriate equivalence transformation and, using the fact that \(P_{n-1}(z)/Q_n(z)\) is odd, we find \(s_i = 0\) from uniqueness. Therefore we can always write

\[
z\frac{P_{n-1}(z^2)}{Q_n(z^2)} = [k_1z, k_2z, k_3z, \ldots, k_mz],
\]

(25)

where \(m = 2n - 1\) or \(m = 2n\) according as \(Q_n(0) = 0\) or \(Q_n(0) \neq 0\).

4 Application to the overlap operator

We are now in a position to apply our knowledge to find the solution to the equation

\[
\frac{2}{\mu - \mu^*} \gamma_5 D(\mu) \psi = \chi.
\]

Collecting the results from the previous two sections we obtain an equivalence class of five dimensional linear systems
where the $k_i$'s and $n$ are uniquely determined by the given rational approximation to the sign–function, the $c_i$'s parametrise the corresponding equivalence class and $A = \frac{1+\mu}{1-\mu}$. It is now crucial to see how the spectrum of the five dimensional matrix depends on the free parameters $c_i$ as we already emphasised in the last section. While for a generic set of parameters the five dimensional system is usually ill–defined, the condition number can be kept under control with a clever choice of $c_i$'s \[3, 6\] enabling one to optimise the matrix, e.g., for fast inversions. As was pointed out in \[3\] the equivalence transformations can be understood as a block Jacobi preconditioning without any computational overhead. The particularly simple structure of the five dimensional operator allows improvements in various directions: one can easily change and optimise the hermitian overlap kernel $H$ or apply various well known preconditioning techniques such as an even–odd or ILU decomposition \[6\].

It is instructive to see that the first auxiliary field disentangles $\gamma_5$ from the sign–function, i.e., $(A \cdot \gamma_5 + \text{sign}(H))\psi = \chi$ maps into

$$
\begin{pmatrix}
A\gamma_5 + k_0H & c_1 \\
c_1 & -c_1^2k_1H & c_1c_2 \\
c_1c_2 & c_2^2k_2H & \ddots \\
\vdots & \vdots & \ddots \\
-c_2^2k_{2n-1}H & c_2c_{2n-1} & c_2^2k_{2n}H
\end{pmatrix}
\begin{pmatrix}
\psi \\
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_{2n-1} \\
\phi_{2n}
\end{pmatrix}
= 
\begin{pmatrix}
\chi \\
0 \\
0 \\
\vdots \\
0 \\
0
\end{pmatrix}
$$

(26)

where we used $\text{sign} = \text{sign}^{-1}$. Additional fields are then only used to generate the sign–function (or its approximation, respectively). We now have two systems which can be easily solved,

$$
\psi = \frac{1}{A}\gamma_5(\chi - c\phi), \quad \phi = \frac{1}{c}\text{sign}(H)\psi,
$$

(27)

yielding recursion relations for $\psi$ and $\phi$,

$$
\psi^{(i+1)} = \frac{1}{A}\gamma_5(\chi - \text{sign}(H)\psi^{(i)}), \quad \phi^{(i+1)} = \frac{1}{A}\text{sign}(H)\gamma_5(\frac{1}{c}\chi - \phi^{(i)}).
$$

(28)

Equivalently, there are recursion relations for the residuals and one can show that

$$
|r_{\psi,\phi}^{(i)}| = \left(\frac{1-\mu}{1+\mu}\right)^i |r_{\psi,\phi}^{(0)}|.
$$

(29)

Of course one can use a similar recursive scheme for the case where $\text{sign}(H)$ is expressed as a continued fraction and one has several auxiliary fields.

Projection of eigenvectors of $H$ close to 0 is a valuable tool to improve approximations to the overlap operator and here it is straightforward to implement. However, we wish to point out that in this formulation it might not be necessary at all. Consider the linear system in the lower right corner,
\[ c_{2n-1}c_{2n}\phi_{2n-1} - c_{2n}^2 k_{2n} H \phi_{2n} = 0. \tag{30} \]

For a typical rational approximation to the sign–function we have \( k_{2n} \gg 1 \) and with the choice \( c_{2n} \approx 1/\sqrt{k_{2n+1}} \ll 1 \). So it turns out that the system in eq. (30) is essentially equivalent to finding eigenvectors of \( H \) close to zero, i.e., the two Krylov spaces possibly have a large overlap. Indeed a truncation in the fifth dimension, i.e., of a given continued fraction, changes the approximation only in the neighbourhood around \( H = 0 \) and therefore provides a natural truncation scheme for approximations of fixed accuracy. It also opens up the possibility of applying successively better approximations to the overlap operator which are ultra–local in five dimensions.

5 Summary and outlook

We have shown how to use a continued fraction expansion of the sign–function in order to obtain a five dimensional formulation of the overlap lattice Dirac operator. We have pointed out that the operator can be made well conditioned using equivalence transformations on the continued fractions. It is now important to investigate in detail strategies to exploit this freedom in practical applications and such a study is under way [6]. If successful, and first results indicate that this is indeed the case, the formulation would provide a valuable alternative for the simulation of dynamical chiral fermions.

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