Efficient computation of low-lying eigenmodes of non-Hermitian Wilson-Dirac type matrices

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A polynomial transformation for non-Hermitian matrices is presented, which provides access to wedge-shaped spectral windows. For Wilson-Dirac type matrices this procedure not only allows the determination of the physically interesting low-lying eigenmodes but also provides a substantial acceleration of the eigenmode algorithm employed.

1. Introduction

The spectra of Wilson-Dirac type matrices $M$ have an elliptic shape, with the real parts of the eigenvalues being positive. Since the large eigenmodes correspond to the doublers, only the small ones should contain physics.

Employing the Arnoldi algorithm, the straightforward approach to the described eigenproblem is to ask the algorithm for the eigenmodes of smallest modulus. By introducing shifts along the real axis ($M + \sigma I$), the part of the spectrum to be found by the algorithm can be influenced.

On the other hand we observe that the Arnoldi algorithm converges much faster when asking for eigenmodes of largest modulus or largest real part of ($-M + \sigma I$) instead, where on a quenched $4^4$ ($8^4$) lattice a gain factor of about 2 (5) in CPU time can be achieved. The disadvantage of this approach is that the computed eigenmodes are not as 'low-lying' as before (in general their imaginary parts are larger). This problem can be cured by a modified approach, which will be described in the following.

2. The polynomial transformation $p_{\sigma,n}$

In order to focus the search for large eigenmodes of ($-M + \sigma I$) on the ones close to the real axis (i.e. on low-lying eigenmodes of $M$), we propose to determine the eigenmodes of largest real parts of

$$p_{\sigma,n}(D) = (D + \sigma I)^n ,$$

with $D$ defined through $M = I - \kappa D$. Using $D$ is only a matter of notation, one could as well work with $p(M) = (-M + \sigma I)^n$.\footnote{For polynomial acceleration of eigenmode algorithms, see e.g. [2]}

For the standard Wilson-Dirac matrix, $D$ can be even-odd preconditioned. The polynomial transformation then takes the form

$$p_{\sigma,n}(D_{eo}D_{oe}) = (D_{eo}D_{oe} + \sigma I)^n ,$$

where $e$ and $o$ stand for even and odd respectively.

The spectral windows amenable to $p_{\sigma,n}$ can be identified by determining those complex numbers, $a$, which are mapped into $S = \{ a \in \mathbb{C} | \text{real}(p_{\sigma,n}(a)) \geq c \}$, where $c$ depends on the number of eigenmodes to be determined. This is illustrated in Fig. (1). The curves enclose the complex numbers belonging to $S$, with their shape being fixed by $\sigma$ and $n$. With respect to the eigenmode algorithm, $S$ represents the regions of sensitivity, i.e. the algorithm is capable to find eigenmodes lying inside the wedge-like regions $S$.

3. Results

The spectral windows of the standard and the clover improved Wilson-Dirac matrix amenable to $p_{\sigma,n}$ are displayed in Fig. (2).

The left frame shows that the computed eigenmodes are indeed enclosed by the curves defined

[1] For polynomial acceleration of eigenmode algorithms, see e.g. [2]
through $S$ and that they are close to the real axis, i.e. low-lying.

Furthermore the second frame illustrates that with too large an exponent $n$, physically uninteresting eigenmodes with large imaginary parts will be computed by the algorithm.

Finally the right frame demonstrates that preconditioning can help to substantially reduce $n$ without changing the interesting window of sensitivity, as the curves cutting the real axis nearly coincide.

In Fig. (3) further such examples are given. The left frame shows 200 eigenmodes as found on a quenched $8^4$ lattice. The right frame compares, for a full QCD $16^3 \times 32$ lattice, the eigenmodes found for the exponents $n = 1$ and $n = 24$. The plotted curves enclose the regions of the complex plane that were searched for eigenvalues, i.e. inside the curves all eigenvalues are captured.

One might suspect that the polynomial transformation $p_{\sigma,n}(D)$ goes along with a polynomial increase of the execution time due to additional matrix vector multiplications. That this is not so can be seen for the even-odd preconditioned matrix in Fig. (3) and for clover improvement in Fig. (4), where the dependence of the number of matrix vector multiplications and of the CPU time on the exponent $n$ are displayed.

For the even-odd preconditioned Wilson-Dirac matrix one can see that the run time increases strongly on the $4^4$ and is almost stable on the $8^4$ lattice, whereas a dramatic decrease is found on the realistic lattice sizes $12^3 \times 24$ and $16^3 \times 32$. For the last two lattices the CRAY T3E-1200 found an acceleration factor of 8, whereas the CRAY T3E-600 produced a gain factor of 9 and 14 respectively.

For the even-odd preconditioned Wilson-Dirac matrix this systematics seems to be delayed. On the $8^4$ lattice an increase in computing time is detected, whereas on the $12^3 \times 24$ an acceleration factor of 1.6 was found.

Furthermore the results indicate that the factor of acceleration grows with the size of the lattice.

Why does the polynomial transformation accelerate the algorithm?

At first one might expect that through the polynomial transformation the density of the eigenvalues is decreased. This would explain the

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2Surprisingly in some cases only for $n = 4$ no convergence was found.
acceleration, since the convergence is sensitive to this quantity. But if that is the right explanation, the number of matrix vector multiplications would be decreasing as well. Since this is not always the case (see Fig. (1) and Fig. (2)), a different mechanism must be at work. Taking a look at the time spent in the Arnoldi subroutines for different exponents $n$ immediately provides the answer: When employing the polynomial $p_{\sigma,n}$ one has to enter the Arnoldi subroutines less often, since in one Arnoldi step one performs $n$ multiplications instead of only one and thus saves the time normally spent in those routines. This means that for large $n$, the computing time is almost exclusively used for the matrix vector multiplications. Hence the optimal choice of polynomial is met, if just one Arnoldi factorization has to be performed.

4. Summary and comments

It could be shown that through the polynomial transformation $p_{\sigma,n}$ wedge-shaped spectral windows are accessible. In case of the even-odd preconditioned Wilson-Dirac matrix this led to an acceleration factor of an order of magnitude on typical lattices sizes, whereas for the clover improved Wilson-Dirac matrix a factor of the order of 2 was found. It could be shown that this factor grows with the size of the lattice. Comparing with a search for the eigenmodes of smallest modulus of $M$, which provides a similar part of the spectrum as $p_{\sigma,n}(D)$, the factor of acceleration is even larger.

The possible accuracy with which one can determine the eigenmodes is not affected by the polynomial transformation.

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