Status of eigenvalues computation of a flavour non-degenerate Dirac operator

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The aim of this note is to report on the progresses achieved in the evaluation of the lowest eigenvalues of the non-degenerate Dirac operator by means of the Jacobi-Davidson (JD) routine, using a bispinor structure.

1 Basics

Since we will propose several tests, we need to recall the basic formulae for the 1-flavour (denoted by the subscript 1) and for the 2-flavours (denoted by the subscript ND = Non Degenerate) Dirac operators.
We will work within the twisted mass formalism where the fermionic terms in the action involve the following operators:

$$D_1 = \gamma\tilde{\nabla} - i\gamma_5 W_{cr} + \mu \quad , \quad D_{ND} = \gamma\tilde{\nabla} - i\gamma_5\tau_1 W_{cr} + \mu + \epsilon\tau_3 \ ,$$
$$W_{cr} = -\frac{a}{2}\nabla^*\nabla + M_{cr} \quad , \quad M_{cr} = \frac{1}{2\kappa_{cr}} - 4 \ .$$

In the above equations, the Pauli matrices operate in flavour space, μ is the twisted mass term while the real parameter ϵ denotes the mass splitting between the two flavours. (Note the different ϵ-sign convention compared to, among others, that used in our Lat'05 proceeding, hep-lat/0509154.)
Performing a chiral rotation and by rescaling the quark fields, the Dirac operators can be rewritten as

$$D_1 = \left[\gamma\tilde{\nabla} + W_{cr} \right] 2\kappa + i\mu\gamma_5\tau_3 \ , \tag{1}$$
$$D_{ND} = \left[\gamma\tilde{\nabla} + W_{cr} \right] 2\kappa + i\mu\gamma_5\tau_3 - \epsilon\tau_1 \ , \tag{2}$$

where we have also rescaled ϵ and μ by a factor 2κ, without changing their names. The situation of maximal twist is obtained by setting the hopping parameter κ to a sensible estimate of κ.

We will work with the γ_5 hermitian partners of the above Dirac operators

$$Q = \gamma_5 D = \begin{bmatrix} \tilde{Q} + i\mu & -\gamma_5\epsilon \\ -\gamma_5\epsilon & \tilde{Q} - i\mu \end{bmatrix} = \begin{bmatrix} Q_+ & -\epsilon\gamma_5 \\ -\epsilon\gamma_5 & Q_- \end{bmatrix} \ , \tag{3}$$
$$\tilde{Q} = \gamma_5 \left[\gamma\tilde{\nabla} - \frac{a}{2}\nabla^*\nabla + \frac{1}{2\kappa} - 4 \right] 2\kappa \ ,$$

and recall that the above illustrated flavour structure does not interfere with possible preconditionings, such as even-odd and mass shift. In fact, in eq. (3) we can still distinguish the terms coupling matter fields at the same site, such as the mass terms, from those acting on fields defined on different sites, such as $\tilde{Q}$.
The operator Q can be decomposed into four sub-matrices in the even-odd sites space:

$$\begin{aligned} Q = \begin{bmatrix} Q_{ee} & Q_{eo} \\ Q_{oe} & Q_{oo} \end{bmatrix} &= \begin{bmatrix} (\gamma_5 + i\mu\tau_3 - \epsilon\gamma_5\tau_1)_{ee} & Q_{eo} \\ Q_{oe} & (\gamma_5 + i\mu\tau_3 - \epsilon\gamma_5\tau_1)_{oo} \end{bmatrix} \\ &= \begin{bmatrix} Q_{ee} & 0 \\ Q_{oe} & 1 \end{bmatrix} \begin{bmatrix} 1 & Q_{ee}^{-1}Q_{eo} \\ 0 & \hat{Q}_{oo} \end{bmatrix} . \end{aligned}$$

Recalling that we are interested in the evaluation of the determinant, we can restrict on the operator $\hat{Q}$ defined only on half of the lattice, say the odd-to-odd sites. Inserting also the flavour structure, we can rewrite the EO-preconditioned operator as

$$\hat{Q} \equiv \hat{Q}_{oo} = \gamma_5 \begin{bmatrix} 1 + i\mu\gamma_5 - \frac{M_{oe}(1-i\mu\gamma_5)M_{eo}}{1+\mu^2-\epsilon^2} & -\epsilon\left(1 + \frac{M_{oe}M_{eo}}{1+\mu^2-\epsilon^2}\right) \\ -\epsilon\left(1 + \frac{M_{oe}M_{eo}}{1+\mu^2-\epsilon^2}\right) & 1 - i\mu\gamma_5 - \frac{M_{oe}(1+i\mu\gamma_5)M_{eo}}{1+\mu^2-\epsilon^2} \end{bmatrix} , \tag{4}$$

where the nearest neighbours sites are coupled by

$$(M_{eo(oe)})_{x,y} = \kappa \sum_{\mu} \left[\ (1+\gamma_\mu) \ U_\mu^\dagger(y) \ \delta_{y,x-\hat{\mu}} + (1-\gamma_\mu) \ U_\mu(x) \ \delta_{y,x+\hat{\mu}} \ \right] . \tag{5}$$

In the following we will often refer to the hermitian operator

$$\hat{S} = \hat{Q}\hat{Q}^\dagger \tag{6}$$

2 Structure for JD

Since we are aiming at the (Chebyshev) polynomial approximation of the hermitian $\hat{S}$ operator in eq. (6), we need to evaluate its lowest and largest eigenvalues [1].

The chosen algorithm is the Jacobi-Davidson (JD), which was already implemented for the 1-flavour operator in eq. (1). The corresponding routine makes largely use of ATLAS and LAPACK routines, and was adapted to handle structures called spinor, which are defined over the 'volume plus boundary' lattice points.

The implementation of the JD-routine to the 2-flavour case, involving the application of the Dirac operator in eq. (6) to two spinors, is not straightforward since this operation mixes the contribution of the two spinors, as evident from the (flavour space) off-diagonal parts of eq. (4).
However, noting that the boundary are filled (and used) only when the Dirac operator is applied (more rigorously, only when the nearest neghborough interaction in eq. (5) is called), we create a copy of the existing JD-routine handling now a so called 'bispinor'

[1] Both eigenvalues $\lambda_{min,max}$ are needed for instance, for the determination of the approximation interval $[\lambda_{min}/\lambda_{max}, 1]$.

structure Φ, a new object made out of two spinors (an upper part ϕ_{up} and a lower part ϕ_{dn}), defined over the 'volume' lattice points alone

$$\Phi = \begin{pmatrix} \phi_{up} \\ \phi_{dn} \end{pmatrix} .$$

Whenever the EO-preconditioned Dirac operator in eq. (4) is called

1. the volume site values of the bispinor are copied into two spinor arrays (ψ_1, ψ_2)

$$\phi_{up}(x) \to \psi_1(x) \quad , \quad \phi_{dn}(x) \to \psi_2(x)$$

2. the Dirac operator in eq. (4) is applied

$$\begin{pmatrix} \psi'_1 \\ \psi'_2 \end{pmatrix} \; = \; \hat{Q} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} ,$$

   filling and using the boundary whenever the interaction in eq. (5) is called,

3. the volume site values of the resulting two spinors are used to create the outcoming bispinor

$$\psi'_1(x) \to \phi'_{up}(x) \quad , \quad \psi'_2(x) \to \phi'_{dn}(x) \qquad \Rightarrow \qquad \Phi' = \begin{pmatrix} \phi'_{up} \\ \phi'_{dn} \end{pmatrix} .$$

Even if this (double copying) procedure involves a little waste of CPU-time (see below), it appears to us as the safest and fastest way to implement the JD-routine. In fact, besides adapting the JD for the new bispinor structure, it involves only the implementation of few linear algebra routines and (at least) one solver for the determination of $\Phi = \hat{S}^{-1}\eta$, given the source η.

3 Properties under mass sign transformation

Before discussing all the tests we performed, we should sketch for definitiveness many important properties which will be use thought the next sections.

3.1 Parity of the operator

Denoting with $\hat{Q}(\mu, \epsilon)$ the Dirac operator in eq. (4) with given values of the mass parameter, we note that

$$\begin{aligned} \tau_1 \hat{Q}(\mu,\epsilon)\tau_1 &= \hat{Q}(-\mu,\epsilon) & (7)\\ \tau_3 \hat{Q}(\mu,\epsilon)\tau_3 &= \hat{Q}(\mu,-\epsilon) & (8)\\ \tau_2 \hat{Q}(\mu,\epsilon)\tau_2 &= \hat{Q}(-\mu,-\epsilon) \end{aligned}$$

$$\hat{Q}(\mu,\epsilon) - \hat{Q}(\mu,-\epsilon) = -2\epsilon\gamma_5 \begin{pmatrix} 0 & A \\ A & 0 \end{pmatrix} \quad , \quad A = \left[1 + \frac{M_{oe}M_{eo}}{1+\mu^2\,\epsilon^2}\right] \tag{9}$$

$$\hat{Q}^\dagger(\mu,\epsilon) = \hat{Q}(-\mu,\epsilon) \tag{10}$$

which, together with eq. (7) yields

$$\tau_1 \hat{Q}(\mu,\epsilon)\tau_1 = \hat{Q}^\dagger(\mu,\epsilon) \tag{11}$$

3.2 Parity of the eigenvectors

As we aim at the eigenvalues computation of the hermitian operator $\hat{S}$ in eq. (6) by means of the Jacobi-Davidson method, we will assume that a real eigenvalue λ and an eigenvector $|\lambda\rangle$ exist:

$$\langle\lambda|\ \hat{S}(\mu,\epsilon)\ |\lambda\rangle = \langle\lambda|\ \hat{Q}(\mu,\epsilon)\hat{Q}^\dagger(\mu,\epsilon)\ |\lambda\rangle = \lambda$$

We are going to demonstrate that the many operators $\hat{S}(\pm\mu,\pm\epsilon)$ have the same spectrum of eigenvalues λ's, with corresponding eigenvectors $|\lambda\rangle$'s related by τ_i-multiplications.

for instance, note that

$$\text{defining} \quad |\tilde{\lambda}_1\rangle \equiv \tau_1\ |\lambda\rangle \quad \Rightarrow \quad \hat{S}(-\mu,\epsilon)\ |\tilde{\lambda}_1\rangle = \lambda\ |\tilde{\lambda}_1\rangle \tag{12}$$

since

$$\langle\tilde{\lambda}|\ \hat{S}(-\mu,\epsilon)\ |\tilde{\lambda}\rangle = \langle\lambda|\ \tau_1\hat{Q}(-\mu,\epsilon)\hat{Q}^\dagger(-\mu,\epsilon)\tau_1\ |\lambda\rangle = \langle\lambda|\ \hat{Q}(\mu,\epsilon)\hat{Q}^\dagger(\mu,\epsilon)\ |\lambda\rangle = \lambda$$

Analogous conclusions can be drawn for

$$|\tilde{\lambda}_3\rangle \equiv \tau_3\ |\lambda\rangle \quad \Rightarrow \quad \hat{S}(\mu,-\epsilon)\ |\tilde{\lambda}_3\rangle = \lambda\ |\tilde{\lambda}_3\rangle \tag{13}$$

$$|\tilde{\lambda}_2\rangle \equiv i\tau_2\ |\lambda\rangle \quad \Rightarrow \quad \hat{S}(-\mu,-\epsilon)\ |\tilde{\lambda}_2\rangle = \lambda\ |\tilde{\lambda}_2\rangle \tag{14}$$

4 Tests

In this section we will report the successful checks we have done in order to convince first of all ourselves that the proposed method is correct. The tests concern the construction of the non-degenerate operator and the computation of the eigenvalues, separately. We will therefore divide the discussion into two subsections.

4.1 Operator

The following tests refers to the application of the non-degenerate 2-flavour EO-precond. Dirac operator in eq. (4) on random fields (spinor or bispinor structure will be explicitly declared), on either a thermalised or a random gauge configuration. The tests have been performed on a hypercubic 4^4 lattice, using both a workstation (serial code) and few processors of a PC cluster (parallel code).

1. Test against 1-flavour case: $\epsilon = 0$
   Setting $\epsilon = 0$, applying the non-degenerate operator $\hat{Q}$ in eq. (4) on two random spinors X_{up}, X_{dn}, produces the same two outputs (Y_{up} and Y_{dn}) as the application of the 1-flavour Dirac operators $\hat{Q}_+$ on X_{up} and $\hat{Q}_-$ on X_{dn}. We call $\hat{Q}_{+,-}$ the diagonal entries of the matrix in eq. (4), evaluated at $\epsilon = 0$.

2. Test at $\mu = 0$
   Setting $\mu = 0$ the application of $\hat{Q}$ on two random spinors X_{up}, X_{dn} gives the same results as the application of $\hat{Q}^\dagger$ on the same random spinor, independently of the value of ϵ, see eq. (10).

3. Testing the parity properties of the operator

   - We have tested eq. (7) applying separately $\hat{Q}$ on two random spinors X_{up}, X_{dn} and $\hat{Q}$ with opposite μ-mass term on X_{dn}, X_{up} (note the inverted dn, up order). The spinors from the two applications, Y_{up}, Y_{dn}, have been shown to be related by a tau_1 multiplication.
   - Moreover, we have also applied the operators $\hat{Q}$ and $\hat{Q}^\dagger$ keeping the same μ-mass value, showing that the resulting outcomes are related by a τ_1 multiplication, as predicted by eq. (11) (the upper spinor of the first application is identical to the lower spinor of the second application, and vice versa).
   - Similarly as before, we tested eq. (8) applying separately $\hat{Q}$ on two random spinors X_{up}, X_{dn} and $\hat{Q}$ with opposite ϵ-mass value on the two spinors $X_{up}, -X_{dn}$. The resulting spinors Y_{up}, Y_{dn} of the two applications have been show to be related by a τ_3 multiplication.
   - Finally, we tested the correct implementation of the non-degenerate Dirac operator in eq. (4), verifying eq. (9). We have applied in fact separately the operator $\hat{Q}$ with positive and negative ϵ-mass value on two random spinors X_{up}, X_{dn} and compared the results with the outcomes obtained applying the operator in the r.h.s. of that equation.

4. Test for the hermitian $\hat{Q}\hat{Q}^\dagger$ operator
   Since our aim is the eigenvalue computation of $\hat{S}$, we construct the routine which applies in one shot the hermitian operator $\hat{Q}\hat{Q}^\dagger$ to two random spinors X_{up}, X_{dn}. We check the new routine comparing the two resulting spinors Y_{up}, Y_{dn}, with those obtained applying $\hat{Q}^\dagger$ and $\hat{Q}$ sequently.

5. Test for the bispinor structure
   Finally, we focus on the possibility that the non-degenerate Dirac operator handles only bispinors. However, since the application of eq. (4) mixes the single-flavour contributions, due to a non-vanishing ϵ-mass value, our routine should first split the values stored in one bispinor array into two spinor arrays. After the application of $\hat{S}$, the two outcoming spinor arrays are then composed into a single bispinor array. Whenever possible, we performed the same tests as before.

For all the discussed cases, in addition to few single components (fixed site, spin and colour indices), we compared also the norm and the norm difference.

4.2 Eigenvalue and Time Lost

Once we are confident that the (hermitian, EO-precond., 2-flavoured, non-degenerate) operator $\hat{S}$ acting on one bispinor field is correctly implemented, we can use it as the operator of which we wish to compute the eigenvalues and eigenvectors by mean of the Jacobi-Davidson method.

In the following we summarise all the tests done by using both the serial code as well as the parallelised code, for the eigenvalues, λ's, and eigenvectors, $|\lambda\rangle$'s, computation of $\hat{S}$.

1. Test for degeneracy at $\epsilon = 0$
   The first check aimed at a comparison between the λ's computed for the 2-flavour operator $\hat{S}$ in with respect to the those for its 1-flavour counterpart. Obviously, the comparison is possible only if we set $\epsilon = 0$. Running the two codes separately, we found indeed the same lowest eigenvalues, as expected double degenerate for the operator in eq. (6). This case is illustrated in the 2nd., 3rd. and 4th. column of Tab. 1.

2. Test for $\kappa = 0$
   The simplicity of this test consists in the fact that by setting $\kappa = 0$ the hopping term in eq. (5) vanishes and the matrix in eq. (4) reduces to a diagonal one in space and time indices. Moreover, imposing $\epsilon = 0$, it also becomes diagonal in flavour space, $\hat{S} = \begin{pmatrix} 1+\mu^2 & 0 \\ 0 & 1+\mu^2 \end{pmatrix}$. The resulting degenerate eigenvalue will $\lambda = 1 + \mu^2$. The results are consistent with the explained predictions, as illustrated in the 2nd. column of Tab. 1.

	$\kappa = 0$	$\kappa \neq 0$		
λ	$\epsilon = 0, \mu = 0.5$	$\epsilon = 0, \mu = 0.05$	$\epsilon = 0, \mu = 0.5$	$\epsilon = \mu = 0.5$
1	1.250	7.445708096e-02	7.923313798e-01	2.917788497e-02
2	1.250	7.445708096e-02	7.923313798e-01	3.160717696e-02
3	1.250	7.910082938e-02	8.011715990e-01	4.298394254e-02
4	1.250	7.910082938e-02	8.011715990e-01	4.443633930e-02

Table 1: *The columns illustrate the 4 lowest eigenvalues λ's evaluated on a random configuration using a lattice of 4^4 sites. The same test with similar results have been performed on a thermalised configuration and on a larger lattice of 8^4 sites. The degenerate eigenvalue λ are not identical, since the illustrated numbers have been truncated, but the difference lies on the 16th. digit.*

3. Test for small ϵ
   As was already mentioned, the ϵ-term plays the rôle of the mass-splitting. If the value of ϵ is set to be small in comparison to μ, eq. (4) suggests that lowest eigenvalues should be linear in ϵ for sufficiently small ϵ-mass values. We verify this expectation numerically as it is evident from Tab. 2.

4. Test for λ-parity
   The next test concern the behaviour of the λ once we reverse the sign of the mass parameters. Following to Subsect. (3.2), we check that the operations $\mu \to -\mu$ and $\epsilon \to -\epsilon$ do not change the eigenvalues, λ's.

5. Test for $|\lambda\rangle$-parity
   As one of the most important check of the implemented JD-routine, we carefully look at the behaviour of the eigenvectors $|\lambda\rangle$'s under sign reversal of the mass parameters. Referring to eqs. (12-14), we checked that by applying the Dirac operator $\hat{S}(-\mu, \epsilon)$ [$\hat{S}(\mu, -\epsilon)$] to the eigenvectors $|\tilde{\lambda}_1\rangle$ [$|\tilde{\lambda}_3\rangle$], we obtained the

	$\kappa \neq 0$; $\mu = 0.05$			
λ	$\epsilon = 0$	$\epsilon = 0.001$	$\epsilon = 0.002$	$\epsilon = 0.003$
1	7.445708096e-02	7.391683060e-02	7.337144289e-02	7.282447271e-02
2	7.445708096e-02	7.498464266e-02	7.548073272e-02	7.589007216e-02
3	7.910082938e-02	7.859472224e-02	7.812636981e-02	7.775103000e-02
4	7.910082938e-02	7.962588307e-02	8.016225747e-02	8.070626799e-02

Table 2: *The columns illustrate the 4 lowest eigenvalues λ's evaluated on a random configuration, with parameters κ and μ fixed. While at $\epsilon = 0$ the double degeneracy is evident (2.nd column), the increase of the ϵ-mass value is reflected into an almost linear splitting of the two nearly degenerate λ's from the original degenerate eigenvalue (3rd. $\rightarrow$ 5th. columns).*

same eigenvalue, λ. In addition, we checked that at the end of the eigenvalues computation, the following relations were fulfilled

$$|\lambda\rangle = \left\{ \begin{array}{c} \tau_1 \, |\tilde{\lambda}_1\rangle \\ \tau_3 \, |\tilde{\lambda}_3\rangle \end{array} \right\} \quad \text{or} \quad \left(\begin{array}{c} |\tilde{\lambda}_1\rangle_{up} \\ |\tilde{\lambda}_1\rangle_{dn} \end{array} \right) = \left(\begin{array}{c} |\lambda\rangle_{dn} \\ |\lambda\rangle_{up} \end{array} \right) \quad ; \quad \left(\begin{array}{c} |\tilde{\lambda}_3\rangle_{up} \\ |\tilde{\lambda}_3\rangle_{dn} \end{array} \right) = \left(\begin{array}{c} |\lambda\rangle_{up} \\ -|\lambda\rangle_{dn} \end{array} \right)$$

These properties have been checked both on fixed (sites, spin, colour) components as well as on the norm of the eigenvectors $|\lambda\rangle$'s.

6. The case of large μ

   The behaviour of the lowest EW with increasing values of μ turns out to be not simple as for the previous case. A possible explanation can be argued looking at eq. (4), where among other places, the μ term enters non-trivially also as a coefficient of the nearest neighbours interaction terms. Referring again to Tab. 1, the 4th and the 5th. columns show the case of large μ and two possible extreme values of the mass-splitting term: $\epsilon = 0$ and $\epsilon = \mu$, respectively.

7. Test for time lost

   This test should give us an estimate of the time 'lost' by the code, while computing the lowest λ, in the conversion from bispinor to two spinors and vice versa. The percentage of time spent for this operation with respect to the total amount of time needed for the $S = QQ^\dagger$ application is illustrated in the first line of Tab. 3. We should stress that this most interesting value remains acceptable small, even if it varies with the lattice size and the kind of parallelisation from 1% to 7%. However, we found that the larger the volume the stable, around 6%, the results. Our conclusion inspecting the first line of Tab. 3 is that, with respect to the full eigenvalues computation, the percentage of time lost by the code in the bispinor $\leftrightarrow$ two spinors is definitively less than 10%.

   In addition, in the second line of Tab. 3 we also provide the percentage of time spent by the code in the subroutine that applies the $\hat{S} = \hat{Q}\hat{Q}^\dagger$ matrix to a bispinor, with respect to the total time required for eigenvalues and eigenvectors computation. The time spent in lineal algebra operations is reported in the third line. Finally we also give the number of S applications needed to compute the 10 lowest eigenvalues.

In all the cases illustrated in Tab. 3, we divided the lattice over 4 Processors, considering hence different sub-lattices.
We do not report another table referring to the computed 4 highest λ's, since the program used still required high accuracy, while for our purpose of evaluating the interval of the polynomial approximation, also a rough estimate of the maximal eigenvalue will be sufficient (we guess that a 1% relative accuracy should be sufficient).

$\mu = 0.5$	1-Dim. parallelisation				2-Dim. parallelisation		
$\epsilon = 0.0025$	$L = 4$	$L = 8$	$L = 12$	$L = 16$	$L = 8$	$L = 12$	$L = 16$
bispinor $\leftrightarrow$ spinors	0.3%	4.0%	2.5%	3.8%	2.5%	3.9%	3.1%
$S\ \Phi$	47.9%	56%	53.5%	55.2%	69.5%	68.1%	67.9%
Lin. Alg.	51.8%	40%	44%	41%	28%	28%	29%
Nr. ($S\Phi$) application	2340	3932	6001	7991	4279	5999	7671

Table 3: *The illustrated outcomes refer to the computation of the 10 lowest eigenvalues, keeping the mass parameters μ and ϵ fixed. The most interesting values in the first line teaches us that the time overhead due to the bispinors $\leftrightarrow$ two spinors remains acceptable small. The values in the second line show the time consumption of the matrix-vector computation, while time requested by linear algebra operations is illustrated in the third line. Finally, the fourth line shows the number of $S = QQ^\dagger$ applications.*

5 New Files

As already anticipated, the bunch of tests has been performed both on one P4 workstation as well as on 4 processors of the CILEA Xeon cluster. In the latter case, we also checked the correct running choosing 1- and 2- dimensional parallelisation.
The implementation of the JD-routine for the bispinor structure can be called 'maximal', in the sense that so far we have 'maximally' implemented all the necessary routines to work directly with bispinors. For our purposes, we implemented therefore many linear algebra routines and two new solvers (bicgstab_complex_bi and cg_her_bi). The conversion bispinors $\leftrightarrow$ two spinors has been used uniquely (and unavoidably) in the evaluation of the matrix-vector multiplication, by mean of a decompose-compose process, and thus is the only place where the above discussed time loss occurs.

The whole bunch of new files carry names derived from the original ('spinor' case) ones, ending with the suffix '_bi', in order to signal that they refer to the code using the bispinor structure.