HiRep User Guide

Rudy Arthur, Vincent Drach, Martin Hansen, Sofie Martins, Claudio Pica, Antonio Rago, Fernando Romero-López

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1 How to cite

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Compare bibliography: [DDPP10]

2 Getting started

2.1 Dependencies

- GCC or different C-compiler
- MPI implementation, i.e. OpenMPI or MPICH for MPI support
- In order to make use of CUDA GPU acceleration compile with CUDA 11.x, for multi-GPU using a CUDA-aware MPI implementation

2.2 Compilation

2.2.1 Clone the directory

```
git clone https://github.com/claudiopica/HiRep
```

2.2.2 Adjust Make Flags

Adjust the file `Make/MkFlags` for the right compilation

- Gauge group SU(NG) or SO(NG)

```
NG=3

#CHOICES ARE GAUGE_SUN AND GAUGE_SON
GAUGE_GROUP = GAUGE_SUN
#GAUGE_GROUP = GAUGE_SON
```

- Representation

```
REPR = REPR_FUNDAMENTAL
#REPR = REPR_SYMMETRIC
#REPR = REPR_ANTISYMMETRIC
#REPR = REPR_ADJOINT
```

- Boundary Conditions

Uncomment the line here, when you want to establish certain boundary conditions into the respective direction.

```
#T => PERIODIC, ANTIPERIODIC, OPEN, THETA
#X => PERIODIC, ANTIPERIODIC, THETA
#Y => PERIODIC, ANTIPERIODIC, THETA
#Z => PERIODIC, ANTIPERIODIC, THETA
```

- Macro parameters

Then a number of macro parameters follow. Here you have to specify if you want to compile for certain boundary conditions by adding the identifier to the `MACRO` variable.

```
#MACRO += -DBC_T_THETA
#MACRO += -DBC_T_PERIODIC
MACRO += -DBC_T_ANTIPERIODIC
#MACRO += -DBC_T_OPEN
MACRO += -DBC_X_PERIODIC
MACRO += -DBC_Y_PERIODIC
MACRO += -DBC_Z_PERIODIC

#MACRO += -DBC_XYZ_TWISTED

#MACRO += -DHALFBG_SF
#MACRO += -DBASIC_SF
#MACRO += -DROTATED_SF
```

Specify, whether you want to compile with MPI either with or without GPU acceleration by using

```
#MACRO += -DWITH_MPI
```

For compilation with GPU acceleration for CUDA GPUs, add the identifier `-DWITH_GPU` to `MACRO`.

```
MACRO += -DWITH_GPU
```

- Compilers, wrappers, preprocessors

A number of example combinations are already given in `MkFlags`.

For compiling with `GCC` and `OpenMPI` one would compile with

```
CC = gcc
MPICC = mpicc
LDFLAGS =
INCLUDE =
```

Using Intel compilers and Intel's MPI implementation, one can use for example

```
CC = icc
MPICC = mpiicc
LDFLAGS = -L /opt/local/lib/mpich-devel-gcc7/ -L /opt/local/lib/
INCLUDE = -I /opt/local/include/mpich-devel-gcc7/
```

For CUDA acceleration, use `nvcc` and adjust the flag `-arch` according to the compute capability of the CUDA capable device.

```
CC = nvcc
CFLAGS = -O2 -Xcompiler '-std=c99 -fgcse-sm -fgcse-las -fgcse-after-reload'
GPUFLAGS = --x cu -arch=sm_70 -Xptxas -v -Xptxas -dlcm=ca -dc
LDFLAGS = -lcuda
```

For compilation with CUDA-aware MPI one needs to pass the MPI wrapper of the MPI implementation to the CUDA preprocessor using the flag `-ccbin`. For OpenMPI this is `mpicc`.

```
CC = nvcc
CFLAGS = -ccbin mpicc -Xcompiler '-std=c99 -fgcse-sm -fgcse-las -fgcse-after-reload'
GPUFLAGS = --x cu -arch=sm_70 -Xptxas -v -Xptxas -dlcm=ca -dc
LDFLAGS = -lcuda -lmpi
```

2.3 Run

2.3.1 Adjust input file

Compile the HiRep library for example in `LibHR` by typing `make`. An example of a C-file that generates a binary to run the HMC can be found in `HMC`, you can navigate into this directory and type `make` to create a binary. It is necessary to specify a number of parameters using an input file, see `HMC/input_file` for an example. For basic run variables, one can have a look at the section `Run control variables`.

```
run name = run1
save freq = 1
meas freq = 1
conf dir = cnfg
gauge start = random
last conf = +1
```

The "+" in front of `last conf` specifies the number of trajectories to be generated after the chosen startup configuration. I.e. if the startup configuration is trajectory number 5 and `last conf = 6` then one additional trajectory will be generated. If `last conf = +6` then six additional trajectories will be generated.

2.3.2 Execute Binary

Run the HMC using

```
$ ./hmc -i input_file
```

where `hmc` is the binary generated from `hmc.c`.

3 Input File Configuration

3.1 Integrator

The HiRep code uses a multilevel integrator and each integrator level has to be specified in the input file.

```
integrator {
    level = 0
    type = o2mn
    steps = 10
}
```

Variable	Description
`level`	unique integrator level (level 0 is the outermost level)
`type`	integrator type (see below)
`steps`	number of integration steps

The table below show the different integrators implemented in the HiRep code. The last column in the table show how many times the next integrator level will be called in each iteration of the given integrator.

Type	Description	Next level calls
`lf`	leap-frog integrator	1
`o2mn`	2nd order minimal norm (omelyan) integrator	2
`o4mn`	4th order minimal norm (omelyan) integrator	5

3.2 Plaquette gauge

This gauge monomial is the standard Wilson plaquette action.

$$S = -\frac{\beta}{N} \sum_{x,\mu>\nu} \mathrm{Re}\ \mathrm{tr}(U_\mu(x) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x))$$

The example below show how to specify a gauge monomial in the input file.

```
monomial {
    id = 0
    type = gauge
    beta = 2.0
    level = 0
}
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`beta`	bare coupling for the gauge field
`level`	integrator level where the monomial force is evaluated

3.3 Lüscher-Weisz gauge

This gauge monomial is the Lüscher-Weisz (tree-level Symanzik) gauge action, including the 1×1 plaquettes $P_{\mu\nu}$ and the 1×2 rectangular loops $R_{\mu\nu}$. The two coefficients below are related through $c_0 + 8c_1 = 1$ to ensure the correct continuum limit.

$$S = -\frac{\beta}{N}\sum_{x,\mu>\nu} c_0 \text{Re tr}[P_{\mu\nu}(x)] + c_1 \text{Re tr}[R_{\mu\nu}(x) + R_{\nu\mu}(x)]$$

The example below show how to specify a gauge monomial in the input file.

```
monomial {
    id = 0
    type = lw_gauge
    c0 = 1.666667
    beta = 2.0
    level = 0
}
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`beta`	bare coupling for the gauge field
`c0`	coefficient in front of the plaquette term
`level`	integrator level where the monomial force is evaluated

3.4 HMC Parameters

The HMC monomial is the standard term for simulating two mass degenerate fermions.

$$S = \phi^\dagger (D^\dagger D)^{-1} \phi$$

The example below show how to specify an HMC monomial in the input file.

```
monomial {
    id = 1
    type = hmc
    mass = -0.750
    mt_prec = 1e-14
    force_prec = 1e-14
    mre_past = 5
    level = 1
}
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`mass`	bare fermion mass
`mt_prec`	inverter precision used in the Metropolis test
`force_prec`	inverter precision used when calculating the force
`mre_past`	number of past solutions used in the chronological inverter
`level`	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm.

3.5 Twisted Mass

In this monomial the twisted mass is added before the Dirac operator has been even/odd preconditioned. The example below shows how to specify the monomial in the input file.

```
monomial {
    id = 1
    type = tm
    mass = -0.750
    mu = 0.1
    mt_prec = 1e-14
    force_prec = 1e-14
    mre_past = 5
```

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```
        level = 1
    }
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`mass`	bare fermion mass
`mu`	bare twisted mass
`mt_prec`	inverter precision used in the Metropolis test
`force_prec`	inverter precision used when calculating the force
`mre_past`	number of past solutions used in the chronological inverter
`level`	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm.

3.6 Twisted Mass Alternative

In this monomial the twisted mass is added after the Dirac operator has been even/odd preconditioned. The example below shows how to specify the monomial in the input file.

```
    monomial {
        id = 1
        type = tm_alt
        mass = -0.750
        mu = 0.1
        mt_prec = 1e-14
        force_prec = 1e-14
        mre_past = 5
        level = 1
    }
```

Variable	Description
id	unique monomial id
type	monomial type
mass	bare fermion mass
mu	bare twisted mass
mt_prec	inverter precision used in the Metropolis test
force_prec	inverter precision used when calculating the force
mre_past	number of past solutions used in the chronological inverter
level	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm.

3.7 Hasenbusch

The Hasenbusch term is a mass preconditioned term, used in connection with an HMC monomial.

$$S = \phi^\dagger \left(\frac{D^\dagger D}{(D+\Delta m)^\dagger (D+\Delta m)} \right) \phi$$

The example below show how to specify a Hasenbusch monomial in the input file.

```
monomial {
    id = 1
    type = hasenbusch
    mass = -0.750
    dm = 0.1
    mt_prec = 1e-14
    force_prec = 1e-14
    mre_past = 2
    level = 0
}
```

Variable	Description
id	unique monomial id
type	monomial type
mass	bare fermion mass
dm	shift in the bare mass
mt_prec	inverter precision used in the Metropolis test
force_prec	inverter precision used when calculating the force
mre_past	number of past solutions used in the chronological inverter
level	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm. In addition, the mass used in the associated HMC monomial should be the mass of this monomial plus the mass shift.

3.8 TM Hasenbusch

The example below show how to specify a Hasenbusch monomial with even odd preconditioned twisted mass

```
monomial {
    id = 1
    type = hasenbusch_tm
    mass = -0.750
    mu = 0
    dmu = 0.1
    mt_prec = 1e-14
    force_prec = 1e-14
    mre_past = 2
    level = 0
}
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`mass`	bare fermion mass
`mu`	twisted mass
`dmu`	shift in the twisted mass
`mt_prec`	inverter precision used in the Metropolis test
`force_prec`	inverter precision used when calculating the force
`mre_past`	number of past solutions used in the chronological inverter
`level`	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm. Further, the twisted mass μ used in the associated TM monomial should be the twisted mass of this monomial plus the twisted mass shift.

3.9 TM Hasenbusch Alternative

The example below show how to specify a Hasenbusch monomial with twisted even odd preconditioned operator.

```
monomial {
    id = 1
    type = hasenbusch_tm_alt
    mass = -0.750
    mu = 0
    dmu = 0.1
    mt_prec = 1e-14
    force_prec = 1e-14
    mre_past = 2
    level = 0
}
```

Variable	Description
id	unique monomial id
type	monomial type
mass	bare fermion mass
mu	bare twisted mass
dmu	shift in the twisted mass
mt_prec	inverter precision used in the Metropolis test
force_prec	inverter precision used when calculating the force
mre_past	number of past solutions used in the chronological inverter
level	integrator level where the monomial force is evaluated

When using the chronological inverter the force precision should be 10^{-14} or better to ensure reversibility in the algorithm. Further, the twisted mass μ used in the associated TM monomial should be the twisted mass of this monomial plus the twisted mass shift.

3.10 RHMC

The RHMC monomial uses a rational approximation to simulate an odd number of mass degenerate fermions.

$$S = \phi^\dagger (D^\dagger D)^{-n/d} \phi$$

The example below show how to specify an RHMC monomial in the input file.

```
monomial {
    id = 1
```

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```
        type = rhmc
        mass = -0.750
        n = 1
        d = 2
        mt_prec = 1e-14
        md_prec = 1e-14
        force_prec = 1e-14
        level = 0
    }
```

Variable	Description
`id`	unique monomial id
`type`	monomial type
`mass`	bare fermion mass
`n`	fraction numerator
`d`	fraction denominator
`mt_prec`	inverter precision used in the Metropolis test
`md_prec`	precision of the rational approximation
`force_prec`	inverter precision used when calculating the force
`level`	integrator level where the monomial force is evaluated

4 Supported Features

4.1 Introduction

4.1.1 Conventions

This section summarizes the main formulae that are used for implementing the HMC for dynamical Wilson fermions in higher representations. The Dirac operator is constructed following Ref. [@Luscher:1996sc], but using Hermitian generators

$$T^{a\dagger} = T^a.$$

For the fundamental representation, the normalization of the generators is such that:

$$\mathrm{tr}\,\left(T^a T^b\right) = \frac{1}{2}\delta^{ab}.$$

For a generic representation R, we define:

$$\mathrm{tr}_R\left(T^a T^b\right) = T_R \delta^{ab},$$

$$\sum_a \left(T^a T^a\right)_{AB} = C_2(R)\delta_{AB},$$

which implies:

$$T_R = \frac{1}{N^2-1} C_2(R) d_R$$

where d_R is the dimension of the representation R. The relevant group factors may be computed from the Young tableaux of the representation of $SU(N)$ by using the formula:

$$C_2(R) = \frac{1}{2}\left(nN + \sum_{i=1}^{m} n_i\left(n_i + 1 - 2i\right) - \frac{n^2}{N}\right)$$

where n is the number of boxes in the diagram, i ranges over the rows of the Young tableau, m is the number of rows, and n_i is the number of boxes in the i-th row.

R	d_R	T_R	$C_2(R)$
fund	N	$\frac{1}{2}$	$\frac{N^2-1}{2N}$
Adj	N^2-1	N	N
2S	$\frac{1}{2}N(N+1)$	$\frac{N+2}{2}$	$C_2(f)\frac{2(N+2)}{N+1}$
2AS	$\frac{1}{2}N(N-1)$	$\frac{N-2}{2}$	$C_2(f)\frac{2(N-2)}{N-1}$

A generic element of the algebra is written as: $X = iX^a T^a$, and the scalar product of two elements of the algebra is defined as:

$$(X, Y) = \mathrm{tr}\ \left(X^\dagger Y\right) = T_f X^a Y^a,$$

$$\|X\|^2 = \mathrm{tr}\left(X^\dagger X\right) = \sum_{ij} |X_{ij}|^2$$

γ matrices

We use the chiral representation for the Dirac γ matrices:

$$\gamma_\mu = \begin{pmatrix} 0 & e_\mu \\ e_\mu^\dagger & 0 \end{pmatrix},$$

where e_μ are 2×2 matrices given by $e_0 = -1$, $e_k = -i\sigma_k$,

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

We have:

$$\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

4.1.2 The Dirac operator

The massless Dirac operator is written as in Ref. [@Luscher:1996sc]:

$$D = \frac{1}{2}\left\{\gamma_\mu\left(\nabla_\mu + \nabla_\mu^*\right) - \nabla_\mu^*\nabla_\mu\right\}$$

with

$$\nabla_\mu \phi(x) = U^R(x,\mu)\phi(x+\mu) - \phi(x)$$

$$\nabla_\mu^* \phi(x) = \phi(x) - U^R(x-\mu,\mu)^\dagger \phi(x-\mu)$$

and therefore the action of the massive Dirac operator yields:

$$\begin{aligned} D_m\phi(x) =& (D+m)\phi(x) \\ =& -\frac{1}{2}\left\{(1-\gamma_\mu)\, U^R(x,\mu)\phi(x+\mu)\right. \\ &\left. +\,(1+\gamma_\mu)\, U^R(x-\mu,\mu)^\dagger\phi(x-\mu) - (8+2m)\phi(x)\right\}, \end{aligned} \tag{4.1}$$

where U^R are the link variables in the representation R.

Rescaling the fermion fields by $\sqrt{\kappa} = \left(\frac{2}{8+2m}\right)^{1/2}$, we can write the fermionic action as:

$$S_f = \sum_{x,y} \phi^\dagger(x) D_m(x,y)\phi(y),$$

where

$$D_m(x,y) = \delta_{x,y} - \frac{\kappa}{2}\left[(1-\gamma_\mu)U^R(x,\mu)\delta_{y,x+\mu} + (1+\gamma_\mu)U^R(x-\mu,\mu)^\dagger\delta_{y,x-\mu}\right],$$

and the Hermitian Dirac operator is obtained as:

$$Q_m = \gamma_5 D_m. \tag{4.2}$$

The fermionic determinant in the path integral can be represented by introducing complex pseudofermionic fields:

$$(\det D_m)^{N_f} = \int \mathcal{D}\phi\mathcal{D}\phi^\dagger e^{-\phi^\dagger Q_m^{-N_f}\phi} \equiv \int \mathcal{D}\phi\mathcal{D}\phi^\dagger e^{-S_{\rm pf}}.$$

4.1.3 Force for the HMC molecular dynamics

The HMC Hamiltonian is given by:

$$\mathcal{H} = \mathcal{H}_\pi + \mathcal{H}_G + \mathcal{H}_F\,,$$

where

$$\begin{aligned}
\mathcal{H}_\pi &= \frac{1}{2}\sum_{x,\mu}(\pi(x,\mu),\pi(x,\mu)) = \frac{1}{2}T_f\sum_{a,x,\mu}\pi^a(x,\mu)^2\,,\\
\mathcal{H}_G &= \beta\sum_{\mu<\nu}\left(1-\frac{1}{N}\mathrm{Re\,tr}\,\mathcal{P}_{\mu\nu}\right),\\
\mathcal{H}_F &= \phi^\dagger(Q_m^2-\beta)^{-l}\phi\,,\quad l=\frac{N_f}{2}>0\,,
\end{aligned} \tag{4.3}$$

and we have introduced for each link variable a conjugate momentum in the algebra of the gauge group: $\pi(x,\mu) = i\pi^a(x,\mu)T_f^a$. In the expression of $\mathcal{H}_F$ we omitted the sum over position, spin and color indices and we have also introduced an arbitrary shift β for the matrix Q_m^2, as this will be useful in the discussion for the RHMC algorithm.

The equation of motion for the link variables are given by (the $\dot{\square}$ indicates the derivative with respect to the molecular dynamics time):

$$\dot{U}(x\mu) = \pi(x,\mu)U(x,\mu)\,,$$

while the equation of motion for the momenta can be obtain as follows from the requirement that the hamiltonian $\mathcal{H}$ is a conserved quantity:

$$0 = \dot{\mathcal{H}} = \dot{\mathcal{H}}_\pi + \dot{\mathcal{H}}_G + \dot{\mathcal{H}}_F\,. \tag{4.4}$$

For the first two derivatives we have:

$$\dot{\mathcal{H}}_\pi = \sum_{x,\mu}(\pi(x,\mu),\dot{\pi}(x,\mu)) = T_f\sum_{x,\mu}\sum_a \pi^a(x,\mu)\dot{\pi}^a(x,\mu) \tag{4.5}$$

$$\begin{aligned}
\dot{\mathcal{H}}_G &= \sum_{x,\mu} -\frac{\beta}{N}\mathrm{Re\,tr}\left(\dot{U}(x,\mu)V^\dagger(x,\mu)\right)\\
&= \sum_{x,\mu} -\frac{\beta}{N}\mathrm{Re\,tr}\left(\pi(x,\mu)U(x,\mu)V^\dagger(x,\mu)\right)\\
&= \sum_{x,\mu}\sum_a -\frac{\beta}{N}\pi^a(x,\mu)\mathrm{Re\,tr}\left(iT_f^aU(x,\mu)V^\dagger(x,\mu)\right)\,,
\end{aligned} \tag{4.6}$$

where $V(x,\mu)$ is the sum of the staples around the link $U(x,\mu)$.

The computation of the fermionic force goes as follows. We only consider the case $l = 1$ since this is the only case relevant both for the HMC algorithm and the RHMC algorithm (see below). We have:

$$\dot{\mathcal{H}}_F = -\,\phi^\dagger (Q_m^2 - \beta)^{-1} (\dot{Q_m^2}) (Q_m^2 - \beta)^{-1} \phi\,. \tag{4.7}$$

Defining:

$$\eta = (Q_m^2 - \beta)^{-1}\phi\,, \tag{4.8}$$

$$\xi = Q_m \eta\,,$$

and using the fact that the matrix $(Q_m^2 - \beta)$ is hermitian, we can rewrite (4.7) as

$$\dot{\mathcal{H}}_F = -2\,\xi^\dagger (\dot{Q_m})\eta\,. \tag{4.9}$$

Inserting the explicit form of Q_m, eqs. (4.2) and (4.1) into eq. (4.9) we obtain

$$\begin{aligned}\dot{\mathcal{H}}_F &= \mathrm{Re}\sum_{x,\mu} \xi(x)^\dagger \dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\eta(x+\mu) + \xi(x+\mu)^\dagger \dot{U}^R(x,\mu)^\dagger \gamma_5(1+\gamma_\mu)\eta(x)\\ &= \mathrm{Re}\sum_{x,\mu} \xi(x)^\dagger \dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\eta(x+\mu) + \eta(x)^\dagger \dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\xi(x+\mu)\end{aligned}$$

where the sum over spin and color indices is intended and we made explicit the fact the the whole expression is real. We now use the fact that

$$\dot{U}^R(x,\mu) = \pi^R(x,\mu)U^R(x,\mu) = i\pi^a(x,\mu)T_R^a U^R(x,\mu) \tag{4.10}$$

Notice that, since we define $T_R^a(x,\mu) = R_* T^a(x,\mu)$, the $\pi^a(x,\mu)$ in the above equation are the same as those appearing in the expressions for $\dot{\mathcal{H}}_{\pi,G}$. Using eq. (4.10) in the expression for $\dot{\mathcal{H}}_F$ we find:

$$\begin{aligned}\dot{\mathcal{H}}_F = \sum_{x,\mu}\sum_a \pi^a(x,\mu)\mathrm{Re\ Tr}\ \big[&iT_R^a U^R(x,\mu)\gamma_5(1-\gamma_\mu)\\ &\big\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\big\}\big]\ .\end{aligned} \tag{4.11}$$

Note that capitalized Tr indicates the trace over both color and spin indices as opposed to the lower case tr, which is the trace over color only.

Inserting eq.s (4.5), (4.6) into eq. (4.4) we obtain the equations of motion for the momenta $\pi^a(x,\mu)$

$$\begin{aligned}\dot{\pi}^a(x,\mu) &= \dot{\pi}^a_G(x,\mu) + \dot{\pi}^a_F(x,\mu)\,,\\ \dot{\pi}^a_G(x,\mu) &= \frac{\beta}{N}\frac{1}{T_f}\mathrm{Re\ tr}\ \big[iT_f^a U(x,\mu)V^\dagger(x,\mu)\big]\ ,\\ \dot{\pi}^a_F(x,\mu) &= -\frac{1}{T_f}\mathrm{Re\ Tr}\ \big[iT_R^a U^R(x,\mu)\gamma_5(1-\gamma_\mu)\\ &\qquad \big\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\big\}\big]\ .\end{aligned}$$

For sake of convenience we introduce the following projectors P_R^a over the algebra in the representation R

$$P_R^a(F) = -\frac{1}{T_R}\mathrm{Re\ tr}\ [iT_R^a F]\ ,$$

which can be used to rewrite eq.s `eq:PIDOT2` and (4.12) in a more compact form:

$$\begin{aligned}\dot{\pi}^a_G(x,\mu) &= -\frac{\beta}{N}P_f^a\left(U(x,\mu)V^\dagger(x,\mu)\right)\ ,\\ \dot{\pi}^a_F(x,\mu) &= \frac{T_R}{T_f}P_R^a\big(U^R(x,\mu)\mathrm{tr}_{\mathrm{spin}}\,[\gamma_5(1-\gamma_\mu)\\ &\qquad \big\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\big\}\big)\ .\end{aligned}$$

4.1.4 Checks of the MD force

The formulae derived in the previous Section can be checked against two known examples. The first, and almost trivial, check is obtained by assuming that the representation R is again the fundamental representation. The well-known expression for the MD force for the usual HMC is then recovered.

The second case that has already been studied in the literature is the case of fermions in the adjoint representationof the gauge group SU(2) [@Donini:1996nr]. We agree with eq. (16) in Ref. [@Donini:1996nr], provided that we exchange the indices a and b in that formula.

4.1.5 HMC Algorithm

We briefly review the construction of the HMC algorithm [@{??}].

Given the action $S(\phi)$ of a system of bosonic fields ϕ, our goal is to generate a Markov process with fixed probability distribution $P_S(\phi) = 1/Z \exp[-S(\phi)]$. A sufficient condition to have such a Markov process is that it is ergodic and it satifies detailed balance:

$$P_S(\phi)P_M(\phi \to \phi') = P_S(\phi')P_M(\phi' \to \phi)\,.$$

We define $P_M(\phi \to \phi')$ with the following three-step process:

1. We expand the configuration space with additional fields, the "momenta" π randomly chosen with probability $P_k(\pi)$ such that $P_k(\pi) = P_k(-\pi)$ – usually one takes $P_k(\pi) \propto \exp[-\pi^2/2]$;
2. In the extended configuration space (ϕ, π), we generate a new configuration (ϕ', π') with probability $P_h((\phi, \pi) \to (\phi', \pi'))$ such that

   $$P_h((\phi, \pi) \to (\phi', \pi')) = P_h((\phi', -\pi') \to (\phi, -\pi))$$

   (reversibility condition)
3. We accept the new configuration ϕ' with probability

   $$P_A((\phi, \pi) \to (\phi', \pi')) = min\left\{1, \frac{P_S(\phi')P_k(\pi')}{P_S(\phi)P_k(\pi)}\right\}.$$

   It is easy to see that the resulting probability

   $$P_M(\phi \to \phi') = \int d\pi d\pi' P_k(\pi)P_h((\phi, \pi) \to (\phi', \pi'))P_A((\phi, \pi) \to (\phi', \pi'))\,,$$

   satisfies detailed balance. Care must be taken to ensure ergodicity.

As already stated, the distribution $P_k(\pi)$ is generally taken to be gaussian (this should also guarantee ergodicity). The process P_h is instead identified with the Hamiltonian flow of a yet unspecified Hamiltonian H in the phase space (ϕ, π) (giving to π the meaning of "momenta"). The time reversal symmetry of classical dynamics equation of motion guarantees the reversibility condition. The resulting probability P_h is then a delta function (the process is completely deterministic). Numerical integration to a given accuracy will result in a broader distribution and care must be taken to guarantee the reversibility condition in this case. Since we want a high acceptance rate (low correlation among the configurations), we must carefully choose the Hamiltonian H. One simple way is to take P_k to be gaussian and define $H(\pi, \phi) = -\ln[P_k(\pi)P_S(\phi)] = \pi^2/2 + S(\phi)$

(omitting irrelevant constants). If H is exactly conserved by the process P_h then the acceptance probability is 1.

When fermionic degrees of freedom are present in the action S, we can first integrate them out, resulting in a non local bosonic action and then apply the above scheme. In practice, to deal with a non-local action is not convienent from a numerical point a view and stochastic estimates are used.

Consider a quadratic fermionic term in the action: $S(\bar{\psi},\psi) = \bar{\psi}M\psi$ with a generic interaction matrix $M(\phi)$ function of the bosonic fields ϕ. The contribution of this term to the partition function is $\int d\bar{\psi}d\psi \exp[-S(\bar{\psi},\psi)] = \det[M(\phi)]$.

Assuming that the matrix $M(\phi)$ is positive definite, we can rewrite $\det[M] = \int d\bar{\eta}d\eta \exp[\bar{\eta}(M)^{-1}\eta]$, where $\bar{\eta}$,η are two new complex bosonic fields, called pseudofermions. This term can be taken into account generating random pseudofermions $\bar{\eta}$, η with the desidered probability distribution and keeping then fixed during the above HMC configuration generation for the remaining bosonic fields ϕ.

4.1.6 RHMC formulation

The fermionic part of the HMC hamiltonian, for N_f degenerate quarks and N_{pf} pseudofermions, can be written as:

$$\mathcal{H}_F = \sum_{k=1}^{N_{pf}} \phi_k^\dagger (Q_m^2)^{-l_k} \phi_k \; ; \; \sum_k l_k = \frac{N_f}{2} \,, \tag{4.12}$$

and $l_k > 0$. For the sake of simplicity we will set all the l_k to be equal:

$$\forall k, \; l_k = \frac{N_f}{2N_{pf}} \,.$$

In the RHMC algorithm [@Clark:2005sq] rational approximations are used whenever we need to take some fractional power of the positive definite fermion matrix Q_m^2.

In this implementation we use three different rational approximations.

The first one is used to approximate eq. (4.12) (we need only one approximation because all l_k are equal):

$$\mathcal{H}_F = \sum_{k=1}^{N_{pf}} \phi_k^\dagger r_a(Q_m^2) \phi_k \,, \tag{4.13}$$

$$(Q_m^2)^{-\frac{N_f}{2N_{pf}}} \simeq r_a(Q_m^2) = \alpha_0^a + \sum_{n=1}^{d_1} \alpha_n^a (Q_m^2 - \beta_n^a)^{-1} \,.$$

Using the formulas derived in the previous sections, it is easy to write the force corresponding to eq. (4.13). In fact, eq. (4.13) is nothing but a sum of terms of the form eq. (4.13) once we put $l = 1$, $\beta = \beta_n^a$. The RHMC force will be then given by a sum over $n = 1, \dots, d_1$ of terms given by eq. (4.12) multiplied by a factor α_n^a. Notice that since $l = 1$, to compute η as in eq. (4.8) a simple shifted inversion is required.

The second rational approximation is required in the heat bath update of pseudofermions. In order to generate pseudofermions distributed as in eq. (4.12), a simple two-step process is used. For each pseudofermion we first generate a gaussian distributed field $\tilde{\phi}_k$:

$$P(\tilde{\phi}_k) \propto \exp[-\tilde{\phi}_k^\dagger \tilde{\phi}_k] \,,$$

and then we set:

$$\phi_k = (Q_m^2)^{\frac{l_k}{2}} \tilde{\phi}_k \,,$$

making use of the fact that (Q_m^2) is hermitean (notice the plus sign in the exponent.) The RHMC algorithm uses a rational approximation to compute the above quantities (again we need only one approximation since all l_k are equal):

$$(Q_m^2)^{\frac{l_k}{2}} \simeq r_b(Q_m^2) = \quad \alpha_0^b + \sum_{n=1}^{d_2} \alpha_n^b (Q_m^2 - \beta_n^b)^{-1} \,.$$

The third rational approximation is used in the code for the Metropolis test. Starting from eq. (4.12) for each pseudofermion we can rewrite:

$$\phi_k^\dagger (Q_m^2)^{-l_k} \phi_k = \left\| (Q_m^2)^{-\frac{l_k}{2}} \phi_k \right\|^2 \,,$$

where we used the property that Q_m^2 is hermitean. The rational approximation needed in this case is:

$$(Q_m^2)^{-\frac{l_k}{2}} \simeq r_c(Q_m^2) = \quad \alpha_0^c + \sum_{n=1}^{d_3} \alpha_n^c (Q_m^2 - \beta_n^c)^{-1} \,.$$

Notice that if $d_2 = d_3$ the coefficients for the two approximations r_b and r_c can each be obtained from the other.

In order to compute the coefficients α_n, β_n appearing in the rational approximations the Remez algorithm is needed. In this implementation we do not compute those coefficients "on the fly", but rather we use a precomputation step to generate a table of coefficients form which we pick up the right values when needed. The generation of this table goes as follows.

First note that we need to compute rational approximations for a function $f(x)$ of the form $f(x) = x^l$ and the approximation must be accurate over the spectral range of the operator Q_m^2. To simplify the computation of the table we note that the following proposition holds: if $f(x)$ is a homogeneous function of degree l and $r(x)$ is an optimal (in the sense of relative error) rational approximation to $f(x)$ over the interval $[\epsilon, \mathrm{h}]$ to a given accuracy then $r(kx)/k^l$ is an optimal rational approximation for the same function and the same accuracy over the interval $[\epsilon/k, \mathrm{h}/k]$. Notice that the coefficients of the "rescaled" rational approximation are easily obtained from that of the original approximation. A simple corollary is that, given a homogeneuos function $f(x)$, we can divide the rational approximations with the same accuracy in classes distinguished by the ratio ϵ/h; within each class the coefficients of the rational approximations are easily related to each other, so that we only need to compute one rational approximation in each class. This is what is done in our implementation.

In detail: we generate a table containing the coefficients for the rational approximations belonging in different classes distinguished by the function $f(x)$ which we want to approximate and the accuracy which is required. We arbitrary set h to a fixed value equal to the absolute upper bound on the spectrum of the matrix Q_m^2. This choice fixes the representative of each class, because the lower bound of the approximation is now a function of h.

At run-time this table is used to generate optimal rational approximations rescaling the precomputed coefficients to the desired interval containing the spectrum of the matrix Q_m^2. This interval is obtained by computing the maximum and minimum eigenvalue of Q_m^2 on each configuration when needed. In our code we update this interval only before the metropolis test, while we keep it fixed during the molecular dynamics.

4.1.7 Even-Odd preconditioning

It is a very well know fact that the time spend for a simulation with dynamical fermions is dominated by the time required for the inversions of the Dirac operator. The convergence of such inversions can be improved using an appropriate precondining. The idea is to rewrite the fermionic determinant as a determinant (or product of determinants) of better conditioned matrix (matrices) than the original Dirac operator. For the non-improved Wilson action this can be easily done using the *even-odd* preconditioning. We start rewriting the Dirac operator D_m as a block matrix:

$$D_m = \begin{pmatrix} 4+m & D_{eo} \\ D_{oe} & 4+m \end{pmatrix} \ ,$$

where each block has a dimension half that of the original Dirac matrix. The diagonal blocks connecting sites with the same parity are proportional to the identity matrix, while off-diagonal blocks connect sites with opposite parity. We have (since D_m is γ_5-hermitean):

$$\gamma_5 D_{eo} \gamma_5 = D_{oe}^\dagger \ .$$

The determinant of the Dirac matrix D_m can be rewritten as:

$$\det D_m = \det \left((4+m)^2 - D_{oe} D_{eo} \right) = \det \left((4+m)^2 - D_{eo} D_{oe} \right) \equiv \det D_m^{eo} \ ,$$

using the well known formula for the determinant of a block matrix. Since the determinant of D_m and of D_m^{eo} are the same the latter can be used in numercal simulations. Note that the even-odd preconditioned matrix only connects sites with the same parity thus it have only half of the size of the original Dirac matrix and as D_m it is γ_5-hermitean. We define as before the hermitean matrix $Q_m^{eo} \equiv \gamma_5 D_m^{eo}$, which will be used in practice.

The formulation of the HMC algorithm does not change and the only difference is that pseudofermions fields are now only defined on half of the lattice sites, conventionally the even sites in what follows. We now give the explicit expression for the fermionic force for the preconditioned system described by the hamiltonian:

$$\mathcal{H}_F = \phi_e^\dagger ((Q_m^{eo})^2 - \beta)^{-1} \phi_e \ ,$$

where as before we are assuming $N_f = 2$ or a rational approximation of the actual fractional power function, and where we made explicit that ϕ_e is only defined on even sites. Eq. (4.9) is unchanged:

$$\dot{\mathcal{H}}_F = -2 \ \xi_e^\dagger (\dot{Q_m^{eo}}) \eta_e \, , \tag{4.14}$$

where as before we have defined:

$$\eta_e = ((Q_m^{eo})^2 - \beta)^{-1} \phi_e \, ,$$

$$\xi_e = Q_m^{eo} \eta_e \, .$$

The explicit form of Q_m^{eo} must be used at this point. We have:

$$(\dot{Q_m^{eo}}) = -\gamma_5 (\dot{D_{eo}} D_{oe} + D_{eo} \dot{D_{oe}}) \ . \tag{4.15}$$

Defining

$$\sigma_o = D_{oe} \eta_e \, ,$$

$$\rho_o = D_{oe}\xi_e \,,$$

and inserting eq. (4.15) into eq. (4.14) we find:

$$\begin{aligned}\dot{\mathcal{H}}_F = &- \sum_{\mu,x\in even} \mathrm{Tr}_{x,\mu}\left[\sigma_o(x+\mu)\otimes\xi_e(x)^\dagger + \rho_o(x+\mu)\otimes\eta_e(x)^\dagger\right] \\ &- \sum_{\mu,x\in odd} \mathrm{Tr}_{x,\mu}\left[\xi_e(x+\mu)\otimes\sigma_o(x)^\dagger + \eta_e(x+\mu)\otimes\rho_o(x)^\dagger\right]\end{aligned} \tag{4.16}$$

and for convenience we use the shorthand notation:

$$\mathrm{Tr}_{x,\mu}\left[\Phi\right] \equiv \mathrm{Re\ Tr}\ \left[\dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\Phi\right] \ .$$

From eq. (4.16) it is clear that the fermionic force has a different expression on sites of different parities. Proceeding as before we arrive at the final expressions. For $x \in even$:

$$\begin{aligned}\dot{\pi}^a_F(x,\mu) = -\frac{T_R}{T_f}P^a_R\big(U^R(x,\mu)\mathrm{tr}_{\mathrm{spin}}\left[\gamma_5(1-\gamma_\mu)\right. \\ \left.\left\{\sigma_o(x+\mu)\otimes\xi_e(x)^\dagger + \rho_o(x+\mu)\otimes\eta_e(x)^\dagger\right\}\right) \ ,\end{aligned}$$

while for $x \in odd$:

$$\begin{aligned}\dot{\pi}^a_F(x,\mu) = -\frac{T_R}{T_f}P^a_R\big(U^R(x,\mu)\mathrm{tr}_{\mathrm{spin}}\left[\gamma_5(1-\gamma_\mu)\right. \\ \left.\left\{\xi_e(x+\mu)\otimes\sigma_o(x)^\dagger + \eta_e(x+\mu)\otimes\rho_o(x)^\dagger\right\}\right) \ .\end{aligned}$$

4.2 Two-point functions

This is a summary of the formulae used for the mesonic two-pt functions.

Let Γ and Γ' be two generic matrices in the Clifford algebra, we define the two-pt function:

$$f_{\Gamma\Gamma'}(t) = \sum_{\mathbf{x}}\langle\bar{\psi}(\mathbf{x},t)\Gamma\psi(\mathbf{x},t)\bar{\psi}(0)\Gamma'\psi(0)\rangle$$

Performing the Wick contractions yields:

$$\begin{aligned}\langle\bar{\psi}(\mathbf{x},t)\Gamma\psi(\mathbf{x},t)\bar{\psi}(0)\Gamma'\psi(0)\rangle &= -\,\mathrm{tr}\left[\Gamma S(x-y)\Gamma' S(y-x)\right] \\ &= -\,\mathrm{tr}\left[\Gamma S(x-y)\Gamma'\gamma_5 S^\dagger(x-y)\gamma_5\right]\end{aligned}$$

In practice we invert the Hermitean Dirac operator $\gamma_5 D$ by solving the equation:

$$Q_{AB}(x-y)\eta^{\bar{A},x_0}_B(y) = \delta_{A,\bar{A}}\delta_{x,x_0}$$

where $A = \{a,\alpha\}$ is a collective index for colour and spin, and $\bar{A}$, x_0 are the position of the source for the inverter.

Using the field η that we obtain from the inverter, the correlator above becomes:

$$\langle\ldots\rangle = -\tilde{\Gamma}_{AB}\eta^{C,y}_B(x)\tilde{\Gamma}'_{CD}\eta^{D,y}_A(x)^*$$

where

$\tilde{\Gamma} = \gamma_5\Gamma$, and $\tilde{\Gamma}' = \gamma_5\Gamma'$.

4.3 Hasenbusch acceleration

Let us summarize the Hasenbusch trick (for two flavours)

$$\mathcal{H}_F = \phi^\dagger (Q_m^2)^{-1} \phi$$

where $Q_m = \gamma_5 D_m$ is the hermitian Dirac operator. After integration over the pseudofermions it gives the determinant:

$$\det Q_m^2 = \det D_m^\dagger D_m$$

The Hasenbusch trick can be rewritten in the following form :

$$\det Q_m^2 = \det W_- W_+ \det \frac{Q_m^2}{W_- W_+}$$

Where $W_\pm$ can be chosen arbitrarily as long as the determinant is well defined. We discuss in the next subsections various choices of $W_\pm$.

In any case the two term can be evaluated independently, and we have:

$$\mathcal{H}_{F_1} = \phi_1^\dagger (W_- W_+)^{-1} \phi_1, \quad , \mathcal{H}_{F_2} = \phi_2^\dagger Q_m^{-1} W_- W_+ Q_m^{-1} \phi_2$$

This can be combined with even-odd preconditioning.

4.3.1 Wilson Mass Shift

Assume

$$W_+ = (D_m + \delta_m), \quad W_- = W_+^\dagger = \left(D_m^\dagger + \delta_m\right)$$

Note that, as written in a comment in the code, $W_+ Q_m^{-1} = (aD + b) D^{-1} \gamma_5$.

Then

$$Q_m^{-1} \left(D_m^\dagger + \delta_m\right) (D_m + \delta_m) Q_m^{-1} = \left(\gamma_5 + \delta_m Q^{-1}\right) \left(\gamma_5 + \delta_m Q^{-1}\right)$$

The force can then be computed :

$$\begin{aligned} \dot{\mathcal{H}_{F_2}} =& - \delta_m \phi_2^\dagger \left[\left(\gamma_5 + \delta_m Q^{-1}\right) \dot{Q^{-1}} + \dot{Q^{-1}} \left(\gamma_5 + \delta_m Q^{-1}\right) \right] \phi_2 \\ =& - \delta_m \phi_2^\dagger \left[\left(\gamma_5 + \delta_m Q^{-1}\right) Q_m^{-1} \dot{Q} Q_m^{-1} \right] \phi_2 + \text{h.c} \end{aligned}$$

Note that the equation as now the standard form of the forces for the HMC algorithm provided that:

$$X \equiv Q^{-1} \phi_2, \quad \text{and} \quad Y^\dagger = \phi_2^\dagger (\gamma_5 + \delta_m Q^{-1}) Q_m^{-1}$$

From which we deduce

$$Y = Q_m^{-1} (\gamma_5 + \delta_m Q^{-1}) \phi_2 = D^{-1} (\phi_2 + \delta_m \gamma_5 X)$$

Which matches one comment in the the force_hmc.c file.

Even-Odd Preconditioning

Writing

$$D_m = \begin{pmatrix} 4+m & D_{eo} \\ D_{oe} & 4+m \end{pmatrix}$$

The determinant in the 2 flavour case can be written as follows:

$$\det D_m^2 = \det Q^2 \propto \det D_{eo}^\dagger D_{oe}$$

$$Q = \gamma_5 \begin{pmatrix} 1+4m & M_{\rm eo} \\ M_{\rm oe} & 1+4m \end{pmatrix} \equiv \gamma_5 \begin{pmatrix} M_{\rm ee} & M_{\rm eo} \\ M_{\rm oe} & M_{\rm oo} \end{pmatrix}$$

Note that $M_{\rm ee}^{-1}$ can be computed:

$$M_{\rm ee}^{-1} = \frac{1}{1+4m}$$

Now we can conveniently rewrite

$$Q_\pm = \begin{pmatrix} \gamma_5 M_{\rm ee} & 0 \\ \gamma_5 M_{\rm oe} & 1 \end{pmatrix} \begin{pmatrix} 1 & (M_{\rm ee})^{-1} M_{\rm eo} \\ 0 & \gamma_5 \left(M^{\rm oo} - \frac{1}{4+m} M_{\rm oe} M_{\rm eo} \right) \end{pmatrix}$$

From the last equation we deduce that:

$$\det Q = \det \gamma_5 M^{\rm ee} \det \gamma_5 \left(M_{\rm oo} - \frac{1}{4+m} M_{\rm oe} M_{\rm eo} \right) \propto \det \gamma_5 \left((4+m) M_{\rm oo} - M_{\rm oe} M_{\rm eo} \right)$$

Note that the first determinant is a constant that could be computed.

In the following we will denote

$$\hat{Q}_{m,eo} \equiv \gamma_5 \left((4+m)^2 - M_{\rm oe} M_{\rm eo} \right)$$

where $\hat{Q}_{m,eo}$ is defined on the odd sites of the lattice.

Now defining

$$W_+ = D_{m+\delta m}, \quad W_- = W_+^\dagger = D_{m+\delta m}^\dagger$$

$$\det Q_m (W_- W_+)^{-1} Q_m \propto \det Q_{m,eo} (\hat{D}_{m+\delta_m} \hat{D}_{m+\delta_m,eo})^{-1} Q_{m,eo}$$

We thus have

$$\mathcal{H}_{F_1} = \phi_1^\dagger \left(\hat{D}_{m+\delta m,eo} \hat{D}_{m+\delta_m,eo} \right)^{-1} \phi_1$$

and

$$\mathcal{H}_{F_2} = \phi_2^\dagger Q_{m,eo}^{-1} \hat{D}_{m+\delta_m,eo} \hat{D}_{m+\delta_m,eo} Q_{m,eo}^{-1} \phi_2$$

Note that as in the non-even-odd case this can be rewritten as:

$$\mathcal{H}_{F_2} = \phi_2^\dagger (\gamma_5 + \delta_m (1 + \delta_m (4+m)) Q_{m,eo}^{-1} (\gamma_5 + \delta_m (1 + \delta_m (4+m)) Q_{m,eo}^{-1} \phi_2$$

4.3.2 Twisted Mass Shift

Assume

$$W_+ = (Q_m + i\mu_2)\,, \quad W_- = W_+^\dagger = (Q_m - i\mu_2)$$

Note that $W_-W_+ = Q_m^2 + \mu_2^2$ and that $W_\pm^\dagger = W_\mp$.

Instead of dealing with $\det Q_m(W_-W_+)^{-1}Q_m$, we consider the slightly more general case where the determinant to evaluate is

$$\begin{aligned}\det{(Q_m + i\mu_1)(W_-W_+)^{-1}(Q_m - i\mu_1)} \propto &\int D\phi_2 D\phi_2^\dagger e^{-\phi_2^\dagger\left(Q_+(W_-W_+)^{-1}Q_-\right)^{-1}\phi_2]} \\ &= \int D\phi_2 D\phi_2^\dagger e^{-\phi_2 Q_-^{-1}W_-W_+Q_+^{-1}\phi_2}\end{aligned}$$

The following formulae can then be used for the case of several hasenbusch masses. The case of the determinant $\det Q_m(W_-W_+)^{-1}Q_m$ can be recovered by setting $\mu_1 = 0$ in the following equations.

We have:

$$\begin{aligned}&(Q_m - i\mu_1)^{-1}W_-W_+(Q_m + i\mu_1)^{-1} \\ &\quad =(1 - i(\mu_2 - \mu_1)(Q_m - i\mu_1)^{-1})(1 + i(\mu_2 - \mu_1)(Q_m - i\mu_1)^{-1}) \\ &\quad =1 + i(\mu_2 - \mu_1)(Q_m + i\mu_1)^{-1} - i(\mu_2 - \mu_1)(Q_m - i\mu_1)^{-1} + (\mu_2 - \mu_1)^2\big((Q_m + i\mu_1)(Q_m - i\mu_1)\big)^{-1} \\ &\quad =1 + (\mu_2 - \mu_1)^2\big(Q_m^2 + \mu_1^2\big)^{-1} + i(\mu_2 - \mu_1)(Q_m^2 + \mu_1^2)^{-1}(Q_m - i\mu_1)\end{aligned}$$

$$\begin{aligned}&-i(\mu_2 - \mu_1)(Q_m^2 + \mu_1^2)^{-1}(Q_m + i\mu_1) \\ &\quad =1 + (\mu_2 - \mu_1)\big(Q_m^2 + \mu_1^2\big)^{-1}\big((\mu_2 - \mu_1) + 2\mu_1\big) \\ &\quad =1 + (\mu_2^2 - \mu_1^2)\big(Q_m^2 + \mu_1^2\big)^{-1}\end{aligned}$$

The force can then be computed: (global sign and factor i have to be checked)

$$\begin{aligned}\dot{\mathcal{H}}_{F_2} =&i(\mu_2 - \mu_1)\phi_2^\dagger\Big[(1 - i(\mu_2 - \mu_1)(Q_m - i\mu_1)^{-1})(Q_m + \dot{i}\mu_1)^{-1} - (Q_m - \dot{i}\mu_1)^{-1}(1 + i(\mu_2 - \mu_1)(Q_m + i\mu_1)^{-1})\Big]\phi_2 \\ =&i(\mu_2 - \mu_1)\phi_2^\dagger\left[(1 - i(\mu_2 - \mu_1)(Q_m - i\mu_1)^{-1})(Q_m + i\mu_1)^{-1}\dot{Q_m}(Q_m + i\mu_1)^{-1}\right]\phi_2 + \text{h.c}\end{aligned}$$

$$X \equiv (Q_m + i\mu_1)^{-1}\phi_2, \quad \text{and} \quad Y^\dagger = i\phi_2^\dagger(1 - i(\mu_2 - \mu_1)(Q - i\mu_1)^{-1})(Q_m + i\mu_1)^{-1}$$

From which we deduce

$$\begin{aligned}Y =& -i(Q_m - i\mu_1)^{-1}(1 + i(\mu_2 - \mu_1)(Q + i\mu_1)^{-1})\phi_2 \\ =& -i(Q_m - i\mu_1)^{-1}(\phi_2 + i(\mu_2 - \mu_1)X)\end{aligned}$$

Note that in the particular case where $\mu_1 = 0$,

$$Q_m^{-1}W_-W_+Q_m^{-1} = (1 - i\mu_2Q_m^{-1})(1 + i\mu_2Q_m^{-1})) = 1 + \mu_2^2Q_m^{-2}$$

Which leads to

$$\dot{\mathcal{H}}_{F_2} = \quad \mu_2^2\phi_2^\dagger\dot{Q_m^{-2}}\phi_2$$

Note also that the forces are explicitly proportional to μ_2^2.

Even-Odd Preconditioning

Note that we have : $\widetilde{\mu} \equiv 2\kappa\mu$.

$$Q_{\pm} = \gamma_5 \begin{pmatrix} 1 \pm i\widetilde{\mu}\gamma_5 & M_{\mathrm{eo}} \\ M_{\mathrm{oe}} & 1 \pm i\widetilde{\mu}\gamma_5 \end{pmatrix} \equiv \gamma_5 \begin{pmatrix} M_{\mathrm{ee}}^{\pm} & M_{\mathrm{eo}} \\ M_{\mathrm{oe}} & M_{\mathrm{oo}}^{\pm} \end{pmatrix}$$

Note that M_{ee}^{-1} can be computed:

$$M_{\mathrm{ee}}^{-1} = (1 \pm i\widetilde{\mu}\gamma_5)^{-1} = \frac{1 \mp i\widetilde{\mu}\gamma_5}{1 + \widetilde{\mu}^2}$$

Now we can conveniently rewrite

$$Q_{\pm} = \begin{pmatrix} \gamma_5 M_{\mathrm{ee}}^{\pm} & 0 \\ \gamma_5 M_{\mathrm{oe}} & 1 \end{pmatrix} \begin{pmatrix} 1 & (M_{\mathrm{ee}}^{\pm})^{-1} M_{\mathrm{eo}} \\ 0 & \gamma_5 \left(M_{\mathrm{oo}}^{\pm} - M_{\mathrm{oe}} \left(M_{\mathrm{ee}}^{\pm}\right)^{-1} M_{\mathrm{eo}} \right) \end{pmatrix}$$

From the last equation we deduce that:

$$\det Q_{\pm} = \det \gamma_5 M_{\mathrm{ee}}^{\pm} \det \gamma_5 \left(M_{\mathrm{oo}}^{\pm} - M_{\mathrm{oe}} \left(M_{\mathrm{ee}}^{\pm}\right)^{-1} M_{\mathrm{eo}} \right)$$

Note that the first determinant is a constant that could be computed.

In the following we will denote

$$\hat{Q}_{\pm} \equiv \gamma_5 \left(M_{\mathrm{oo}}^{\pm} - M_{\mathrm{oe}} \left(M_{\mathrm{ee}}^{\pm}\right)^{-1} M_{\mathrm{eo}} \right)$$

where $\hat{Q}_{\pm}$ is defined on the odd sites of the lattice.

We thus have

$$\det Q_+ Q_- = \det Q_+ \det Q_- \propto \det \hat{Q}_+ \hat{Q}_-$$

and we thus get the following Hamiltonian:

$$\mathcal{H}_{F_1} = \phi_1^{\dagger} \left(\hat{Q}_+ \hat{Q}_- \right)^{-1} \phi_1$$

The corresponding force then reads :

$$\dot{\mathcal{H}_{F_1}} = -\phi_0^{\dagger} \left(\hat{Q}_-^{-1} \hat{Q}_+^{-1} \dot{\hat{Q}}_+ \hat{Q}_+^{-1} + \hat{Q}_-^{-1} \dot{\hat{Q}}_- \hat{Q}_-^{-1} \hat{Q}_+^{-1} \right) \phi_0$$

Now using that $Q_{\pm}^{\dagger} = Q_{\mp}$, the previous equation can be written:

$$\dot{\mathcal{H}_{F_1}} = -\left(Y_{\mathrm{o}}^{\dagger} \dot{\hat{Q}}_+ X_{\mathrm{o}} + \mathrm{h.c} \right)$$

with

$$X_{\mathrm{o}} = \hat{Q}_+^{-1} \phi_0, \quad .Y_{\mathrm{o}} = \left(\hat{Q}_+ \hat{Q}_- \right)^{-1} \phi_0,$$

where we have used that

$$\hat{Q}_{\pm}^{\dagger} = \hat{Q}_{\mp}.$$

Furthermore we have

$$\dot{\hat{Q}}_{\pm} = \gamma_5 \left(-\dot{M}_{\rm oe} \left(M_{\rm ee}^{\pm} \right)^{-1} M_{\rm eo} - M_{\rm oe} \left(M_{\rm ee}^{\pm} \right)^{-1} \dot{M}_{\rm eo} \right)$$

Now noting that

$$\dot{Q}_{\pm} = \gamma_5 \begin{pmatrix} 0 & \dot{M}_{\rm eo} \\ \dot{M}_{\rm oe} & 0 \end{pmatrix}$$

We have

$$\begin{aligned} Y^\dagger \dot{Q} X = & \begin{pmatrix} A^\dagger & B^\dagger \end{pmatrix} \gamma_5 \begin{pmatrix} 0 & \dot{M}_{\rm eo} \\ \dot{M}_{\rm oe} & 0 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\ = & A^\dagger \gamma_5 \dot{M}_{\rm oe} C + B^\dagger \gamma_5 \dot{M}_{\rm eo} D \end{aligned}$$

Now chosing $A^\dagger = Y_0^\dagger$, $C = \left(M_{\rm ee}^{+} \right)^{-1} M_{\rm eo} X_0$, $B^\dagger = Y_0^\dagger \gamma_5 M_{\rm oe} \left(M_{\rm ee}^{+} \right)^{-1} \gamma_5$, and $D = X_0$ allows to write:

$$\dot{\mathcal{H}}_{F_1} = Y^\dagger \dot{Q} X + \text{h.c}$$

with

$$X = \begin{pmatrix} \left(M_{\rm ee}^{+} \right)^{-1} M_{\rm eo} X_0 \\ X_0 \end{pmatrix}, \quad \text{and} \quad \text{Y} = \begin{pmatrix} \left(M_{\rm ee}^{-} \right)^{-1} M_{\rm eo} Y_0 \\ Y_0 \end{pmatrix}$$

We have used that $\dot{Q}_+ = \dot{Q}_-$ and

$$M_{\rm eo}^\dagger = \gamma_5 M_{\rm oe} \gamma_5$$

Determinant Ratio

We use that $\det Q_+ (W_- W_+)^{-1} Q_- = \det W_+^{-1} Q_+ Q_- W_-^{-1} \propto \det \hat{W}_+^{-1} \hat{Q}_+ \hat{Q}_- \hat{W}_-^{-1}$

We thus have to compute

$$\begin{aligned} \dot{\mathcal{H}}_{F_2} = & \phi_2^\dagger \big[\delta \hat{W}_- (\hat{Q}_+ \hat{Q}_-)^{-1} \hat{W}_+ + \hat{W}_- (\hat{Q}_+ \hat{Q}_-)^{-1} \delta \hat{W}_+ \\ & + \hat{W}_- \delta \hat{Q}_-^{-1} \hat{Q}_+^{-1} \hat{W}_+ + \hat{W}_- \hat{Q}_-^{-1} \delta \hat{Q}_+^{-1} \hat{W}_+ \big] \phi_2 \\ = & \phi_2^\dagger \big[\dot{\hat{W}}_- (\hat{Q}_+ \hat{Q}_-)^{-1} \hat{W}_+ + \hat{W}_- (\hat{Q}_+ \hat{Q}_-)^{-1} \delta \hat{W}_+ \\ & - \hat{W}_- \hat{Q}_-^{-1} \dot{\hat{Q}}_- \hat{Q}_-^{-1} \hat{Q}_+^{-1} \hat{W}_+ - \hat{W}_- \hat{Q}_-^{-1} \hat{Q}_+^{-1} \dot{\hat{Q}}_+ \hat{Q}_+^{-1} \hat{W}_+ \big] \phi_2 \end{aligned}$$

Now we introduce

$$X_W = (\hat{Q}_+ \hat{Q}_-)^{-1} \hat{W}_+ \phi_2, Y_W = \hat{Q}_+^{-1} \hat{W}_+ \phi_2 = \hat{Q}_- X_W$$

such that

$$\begin{aligned} \dot{\mathcal{H}}_{F_2} = & \quad \phi_2^\dagger \dot{\hat{W}}_- X_W + X_W^\dagger \delta \hat{W}_+ \phi_2 \\ & - \quad Y_W^\dagger \dot{\hat{Q}}_- X_W - X_W^\dagger \dot{\hat{Q}}_+ Y_W \end{aligned}$$

Now recalling that

$$\begin{aligned} \dot{\hat{Q}}_{\pm} = & - \gamma_5 \left(\dot{M}_{\rm oe} \left(1 \pm i \mu_1 \gamma_5 \right)^{-1} M_{\rm eo} + M_{\rm oe} \left(1 \pm i \mu_1 \gamma_5 \right)^{-1} \dot{M}_{\rm eo} \right) \\ \dot{\hat{W}}_{\pm} = & - \gamma_5 \left(\dot{M}_{\rm oe} \left(1 \pm i \mu_2 \gamma_5 \right)^{-1} M_{\rm eo} + M_{\rm oe} \left(1 \pm i \mu_2 \gamma_5 \right)^{-1} \dot{M}_{\rm eo} \right) \end{aligned}$$

Now can write the last expression in terms of $\dot{Q} \equiv \dot{Q}_{\pm}$.

$$\begin{aligned}\dot{\mathcal{H}_{F_2}} =& Y_1^\dagger \dot{Q} X_1 + X_1^\dagger \dot{Q} Y_1 - X_2^\dagger \dot{Q} Y_2 - Y_2^\dagger \dot{Q} X_2 \\ =& 2\,\mathrm{Re}\Big[\mathrm{Y}_1^\dagger \dot{\mathrm{Q}} \mathrm{X}_1 - \mathrm{Y}_2^\dagger \dot{\mathrm{Q}} \mathrm{X}_2\Big],\end{aligned}$$

with

$$Y_1 = \begin{pmatrix} (1+i\mu_1\gamma_5)^{-1} M_{\mathrm{eo}} Y_W \\ Y_W \end{pmatrix}, \quad Y_2 = \begin{pmatrix} (1+i\mu_2\gamma_5)^{-1} M_{\mathrm{eo}} \phi_2 \\ \phi_2 \end{pmatrix},$$
$$X_{1,2} = \begin{pmatrix} (1-i\mu_{1,2}\gamma_5)^{-1} M_{\mathrm{eo}} X_W \\ X_W \end{pmatrix}, \dot{Q} \equiv \dot{Q}_{\pm} = \gamma_5 \begin{pmatrix} 0 & \dot{M}_{\mathrm{eo}} \\ \dot{M}_{\mathrm{oe}} & 0 \end{pmatrix}$$

Twisted Wilson-Dirac Operator

Instead of applying the eo preconditionning to the twisted mass operator we can use the wilson dirac eo operator and do a different splitting.

We define:

$$Q_{\mathrm{eo}} \equiv \gamma_5 \big((4+m)^2 - D_{eo} D_{oe}\big)$$

Now we split the determinant as follows:

$$\det Q_{\mathrm{eo}}^2 = \det W_- W_+ \det \frac{Q_{\mathrm{eo}}^2}{W_- W_+}$$

And we choose

$$W_{\pm} = Q_{\mathrm{eo}} \pm i\mu$$

The corresponding Hamiltonian read:

$$\mathcal{H}_{F_1} = \phi_1^\dagger (W_- W_+)^{-1} \phi_1, \quad , \mathcal{H}_{F_2} = \phi_2^\dagger Q_{\mathrm{eo}}^{-1} W_- W_+ Q_{\mathrm{eo}}^{-1} \phi_2$$

Since the operator are now very similar to the non even-odd case, we can reuse some formulae. In particular, we can rewrite the Hamiltonian as follows:

$$\mathcal{H}_{F_1} = \phi_1^\dagger (Q_{\mathrm{eo}} + \mu^2)^{-1} \phi_1, \quad , \mathcal{H}_{F_2} = \phi_2^\dagger \big(1 + \mu^2 Q_{\mathrm{eo}}^{-1}\big) \phi_2$$

From which we have the following forces:

$$\begin{aligned}\dot{\mathcal{H}}_{F_1} =& \phi_1^\dagger W_+^{-1} \delta W_-^{-1} \phi_1 + \mathrm{h.c} \\ =& \phi_1^\dagger W_+^{-1} W_-^{-1} \dot{Q}_{\mathrm{eo}} W_-^{-1} \phi_1 + \mathrm{h.c}\end{aligned}$$

Now we want to rewrite the last equation as a function of

$$\dot{Q} = \gamma_5 \begin{pmatrix} 0 & \dot{D}_{\mathrm{eo}} \\ \dot{D}_{\mathrm{oe}} & 0 \end{pmatrix}$$

$$X_{\mathrm{o}} = W_+^{-1} \phi_1, \quad . Y_{\mathrm{o}} = (W_+ W_-)^{-1} \phi_1,$$

where we have used that

$$W_{\pm}^{\dagger} = W_{\mp}.$$

Furthermore we have

$$\dot{Q}_{\mathrm{eo}} = -\gamma_5 \left(\dot{M}_{\mathrm{oe}} M_{\mathrm{eo}} + M_{\mathrm{oe}} \dot{M}_{\mathrm{eo}} \right)$$

noting that

$$\begin{aligned} Y^{\dagger} \dot{Q} X = & \begin{pmatrix} A^{\dagger} & B^{\dagger} \end{pmatrix} \gamma_5 \begin{pmatrix} 0 & \dot{M}_{\mathrm{eo}} \\ \dot{M}_{\mathrm{oe}} & 0 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \\ = & A^{\dagger} \gamma_5 \dot{M}_{\mathrm{oe}} C + B^{\dagger} \gamma_5 \dot{M}_{\mathrm{eo}} D \end{aligned}$$

and chosing $A^{\dagger} = Y_0^{\dagger}$, $C = M_{\mathrm{eo}} X_0$, $B^{\dagger} = Y_0^{\dagger} \gamma_5 M_{\mathrm{oe}}$, and $D = X_0$ allows us to write:

$$\dot{\mathcal{H}_{F_1}} = -Y^{\dagger} \dot{Q} X + \mathrm{h.c}$$

with

$$X = \begin{pmatrix} M_{\mathrm{eo}} X_0 \\ X_0 \end{pmatrix}, \quad \text{and} \quad \mathrm{Y} = \begin{pmatrix} M_{\mathrm{eo}} Y_0 \\ Y_0 \end{pmatrix}$$

We have used that $M_{\mathrm{eo}}^{\dagger} = \gamma_5 M_{\mathrm{oe}} \gamma_5$.

Similarly for the second Hamiltonian we get:

$$\dot{\mathcal{H}}_{F_2} = \mu_2 \phi_2^{\dagger} \dot{Q_{\mathrm{eo}}^{-1}} \phi_2$$

which is exactly the force that appears in case of a pure Wilson-Dirac even-ddd preconditioned operator up to a multiplicative factor.

4.4 Clover Term

The clover term can be written as

$$D_{sw} = -\frac{c_{sw}}{4} \sum_x \sum_{\mu,\nu} \sigma_{\mu\nu} F_{\mu\nu}(x), \tag{4.17}$$

with the (unconventional) definition of $\sigma_{\mu\nu}$ given by

$$\sigma_{\mu\nu} = \frac{1}{2} [\gamma_\mu, \gamma_\nu].$$

With the Euclidean definition of the gamma matrices $\sigma_{\mu\nu}$ satisfies

$$\sigma_{\mu\nu}^{\dagger} = \sigma_{\nu\mu} = -\sigma_{\mu\nu} = \sigma_{\mu\nu}^{-1}.$$

For the Hermitian Dirac operator $\gamma^5 D$ we can make the following replacement without affecting any of the calculations presented here.

$$\sigma_{\mu\nu} \to \bar{\sigma}_{\mu\nu} = \gamma_5 \sigma_{\mu\nu}.$$

The field strength tensor is defined as

$$F_{\mu\nu}(x) = \frac{1}{8}\left\{Q_{\mu\nu}(x) - Q^{\dagger}_{\mu\nu}(x)\right\}$$

with

$$\begin{aligned} Q_{\mu\nu}(x) = & U_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x) \\ & + U_\nu(x)U^\dagger_\mu(x-\hat{\mu}+\hat{\nu})U^\dagger_\nu(x-\hat{\mu})U_\mu(x-\hat{\mu}) \\ & + U^\dagger_\mu(x-\hat{\mu})U^\dagger_\nu(x-\hat{\mu}-\hat{\nu})U_\mu(x-\hat{\mu}-\hat{\nu})U_\nu(x-\hat{\nu}) \\ & + U^\dagger_\nu(x-\hat{\nu})U_\mu(x-\hat{\nu})U_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x) \end{aligned}$$

Because $Q^{\dagger}_{\mu\nu} = Q_{\nu\mu}$ we have $F_{\mu\nu} = -F_{\nu\mu}$. For this reason we can change the sum over μ, ν in Eq. (4.17) to a sum over $\mu < \nu$ and a factor of two.

$$D_{sw} = -\frac{c_{sw}}{2}\sum_x \sum_{\mu<\nu} \sigma_{\mu\nu}F_{\mu\nu}(x)$$

The quantity $\sigma_{\mu\nu}F_{\mu\nu}$ is Hermitian and block diagonal. It can be written as

$$\sum_{\mu<\nu}\sigma_{\mu\nu}F_{\mu\nu} = \begin{pmatrix} A & B & 0 & 0 \\ B^\dagger & -A & 0 & 0 \\ 0 & 0 & C & D \\ 0 & 0 & D^\dagger & -C \end{pmatrix}$$

with the definitions

$$\begin{aligned} A &= -iF_{03} + iF_{12} \\ B &= -iF_{01} - F_{02} - F_{13} + iF_{23} \\ C &= iF_{03} + iF_{12} \\ D &= iF_{01} + F_{02} - F_{13} + iF_{23} \end{aligned}$$

4.4.1 Pseudofermion Forces

For the forces we use the following short-hand notation for the derivative with respect to the link variables.

$$\dot{S} = \partial^a_{x,\mu} S$$

To calculate the pseudofermion forces let us write down the action as

$$S = \phi^\dagger (H^{-2})\phi,$$

where $H = \gamma^5 D$ is the Hermitian Dirac operator. When differentiating the action we obtain

$$\dot{S} = -2\mathrm{Re}\ \xi^\dagger \dot{H}\eta, \tag{4.18}$$

with the definitions

$$\begin{aligned} \eta &= H^{-2}\phi, \\ \xi &= H\eta. \end{aligned}$$

Forces

Here we will only consider the forces from the clover term and not the hopping term. The clover part of the Dirac operator is given by

$$H_{sw} = -\frac{c_{sw}}{2}\sum_{\mu<\nu}\bar{\sigma}_{\mu\nu}F_{\mu\nu}(x) \tag{4.19}$$

When inserting Eq. (4.26) we obtain

$$\dot{S} = c_{sw}\sum_{\mu<\nu}\mathrm{Re}(\xi^\dagger\bar{\sigma}_{\mu\nu}\dot{F}_{\mu\nu}\eta).$$

From the definition of $F_{\mu\nu}$ it follows that

$$\begin{aligned}\dot{S} &= \frac{1}{8}c_{sw}\sum_{\mu<\nu}\mathrm{Re}(\xi^\dagger\bar{\sigma}_{\mu\nu}\dot{Q}_{\mu\nu}\eta + \xi^\dagger\bar{\sigma}^\dagger_{\mu\nu}\dot{Q}^\dagger_{\mu\nu}\eta),\\ &= \frac{1}{8}c_{sw}\sum_{\mu<\nu}\mathrm{Re}(\xi^\dagger\bar{\sigma}_{\mu\nu}\dot{Q}_{\mu\nu}\eta + \eta^\dagger\bar{\sigma}_{\mu\nu}\dot{Q}_{\mu\nu}\xi).\end{aligned}$$

This can in be written as

$$\dot{S} = \frac{1}{8}c_{sw}\sum_{\mu<\nu}\mathrm{Re\ tr}\left[\dot{Q}_{\mu\nu}\left\{\bar{\sigma}_{\mu\nu}\eta(x)\otimes\xi^\dagger(x) + \bar{\sigma}_{\mu\nu}\xi(x)\otimes\eta^\dagger(x)\right\}\right]$$

In a short hand notation we need to calculate

$$\dot{S} = \frac{1}{8}c_{sw}\mathrm{Re\ tr}[\dot{Q}_{\mu\nu}(x)X_{\mu\nu}(x)] \tag{4.20}$$

with

$$X_{\mu\nu}(x) = \bar{\sigma}_{\mu\nu}\eta(x)\otimes\xi^\dagger(x) + \bar{\sigma}_{\mu\nu}\xi(x)\otimes\eta^\dagger(x)$$

This matrix has the properties $X^\dagger_{\mu\nu} = X_{\nu\mu} = -X_{\mu\nu}$. The expression for $\dot{Q}_{\mu\nu}(x)$ contains eight different terms (two from each of the four leafs). The eight contributions to the force can be written as

$$\begin{aligned}F_1(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)X_{\mu\nu}(x)]\\ F_2(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})X^\dagger_{\mu\nu}(x-\hat{\nu})U_\nu(x-\hat{\nu})]\\ F_3(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})X^\dagger_{\mu\nu}(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})]\\ F_4(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)X_{\mu\nu}(x+\hat{\mu})U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)]\\ F_5(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)X^\dagger_{\mu\nu}(x+\hat{\mu})U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})]\\ F_6(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U_\nu(x+\hat{\mu})X_{\mu\nu}(x+\hat{\mu}+\hat{\nu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)]\\ F_7(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})X_{\mu\nu}(x+\hat{\nu})U^\dagger_\nu(x)]\\ F_8(x) &= \mathrm{Re\ tr}[\dot{U}_\mu(x)U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})X^\dagger_{\mu\nu}(x)]\end{aligned}$$

where each term should be multiplied by $c_{sw}/8$. The calculation can be done efficiently by noticing that several products and terms appear in multiple places. Introduce the intermediate variables

$$
\begin{aligned}
Z_0 &= X_{\mu\nu}(x) \\
Z_1 &= X_{\mu\nu}(x+\hat{\mu}) \\
Z_2 &= X_{\mu\nu}(x-\hat{\nu}) \\
Z_3 &= X_{\mu\nu}(x+\hat{\mu}-\hat{\nu}) \\
Z_4 &= X_{\mu\nu}(x+\hat{\mu}+\hat{\nu}) \\
Z_5 &= X_{\mu\nu}(x+\hat{\nu}) \\
W_0 &= U_{\mu}^{\dagger}(x-\hat{\nu}) \\
W_1 &= U_{\nu}(x-\hat{\nu}) \\
W_2 &= U_{\nu}(x+\hat{\mu}) \\
W_3 &= U_{\mu}^{\dagger}(x+\hat{\nu}) \\
W_4 &= U_{\nu}^{\dagger}(x) \\
W_5 &= U_{\nu}^{\dagger}(x+\hat{\mu}-\hat{\nu}) \\
W_6 &= W_0 W_1 \\
W_7 &= W_2 W_3 \\
W_8 &= W_7 W_4 - W_5 W_6
\end{aligned}
$$

The total force can now be written as

$$
F(x) = \frac{c_{sw}}{8}\dot{U}_{\mu}(x)\left\{W_8 Z_0 + Z_1 W_8 - W_5(W_0 Z_2 W_1 + Z_3 W_6) + (W_2 Z_4 W_3 + W_7 Z_5) W_4\right\}
$$

This brings us down to a total of 15 matrix multiplications and 6 additions.

Logarithmic Forces

In the case of even-odd preconditioning (see the next section) the action of the small determinant D_{oo} can be written as

$$
S_{sw} = -N_f \log\det D_{oo} = -N_f \ \mathrm{tr}\log D_{oo} = -N_f \sum_{x \ \mathrm{odd}} \mathrm{tr}\log D_{oo}(x)
$$

The derivative is given by

$$
\dot{S} = -N_f \sum_{x \ \mathrm{odd}} \mathrm{tr}\left[D_{oo}^{-1}(x)\dot{D}_{oo}(x)\right]
$$

with $D_{oo}(x)$ given by

$$
D_{oo}(x) = 4 + m_0 - \frac{c_{sw}}{2}\sum_{\mu<\nu}\sigma_{\mu\nu}F_{\mu\nu}(x)
$$

Both the determinant and the inverse of $D_{oo}(x)$ can be calculated from an LDL decomposition. If we insert the above definition we obtain

$$
\dot{S} = \frac{N_f c_{sw}}{2}\sum_{x \ \mathrm{odd}}\sum_{\mu<\nu}\mathrm{tr}(D_{oo}^{-1}(x)\sigma_{\mu\nu}\dot{F}_{\mu\nu}(x))
$$

$$\dot{S} = \frac{N_f c_{sw}}{2 \cdot 8} \sum_{x \text{ odd}} \sum_{\mu<\nu} \mathrm{tr}(D_{oo}^{-1}(x)\sigma_{\mu\nu}\dot{Q}_{\mu\nu}(x) + D_{oo}^{-1}(x)\sigma_{\mu\nu}^{\dagger}\dot{Q}_{\mu\nu}^{\dagger}(x))$$

Since D_{oo}^{-1} is Hermitian we can write the result as two times the real part. To simplify the result we define $X_{\mu\nu}(x) = D_{oo}^{-1}(x)\sigma_{\mu\nu}$ such that

$$\dot{S} = \frac{N_f c_{sw}}{8} \sum_{x \text{ odd}} \sum_{\mu<\nu} \mathrm{Re}\ \mathrm{tr}[X_{\mu\nu}(x)\dot{Q}_{\mu\nu}(x)]$$

This is equivalent to Eq. (4.29) except from the factor N_f and the definition of $X_{\mu\nu}(x)$. Notice that we still have the identity $X_{\mu\nu}^{\dagger} = -X_{\mu\nu}$. The sum over x can be extended to all sites by setting $X_{\mu\nu}$ to zero on the even sites. To calculate the inverse D_{oo}^{-1} we introduce the definitions:

$$D_{oo} = D_{oo}^{\dagger} = \begin{pmatrix} D_+ & 0 \\ 0 & D_- \end{pmatrix}$$

$$D_{oo}^{-1} = \begin{pmatrix} D_+^{-1} & 0 \\ 0 & D_-^{-1} \end{pmatrix}$$

$$D_+^{-1} = \begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix}$$

$$D_-^{-1} = \begin{pmatrix} D_{33} & D_{34} \\ D_{43} & D_{44} \end{pmatrix}$$

Because of hermiticity we know that $D_{12} = D_{21}^{\dagger}$ and $D_{34} = D_{43}^{\dagger}$. The six independent elements of $X_{\mu\nu}$ can now be written as

$$\begin{aligned}
X_{01} &= i(D_{34} + D_{43}) - i(D_{12} + D_{21}) \\
X_{02} &= \ (D_{12} - D_{21}) + \ (D_{43} - D_{34}) \\
X_{03} &= i(D_{22} - D_{11}) + i(D_{33} - D_{44}) \\
X_{12} &= i(D_{11} - D_{22}) + i(D_{33} - D_{44}) \\
X_{13} &= \ (D_{12} - D_{21}) + \ (D_{34} - D_{43}) \\
X_{23} &= i(D_{12} + D_{21}) + i(D_{34} + D_{43})
\end{aligned}$$

4.4.2 Even-odd Preconditioning

Method 1

We can write the determinant as

$$\det D = \det(D_{oo}) \det(D_{ee} - D_{eo}D_{oo}^{-1}D_{oe})$$

Use the notation

$$\begin{aligned}
Q_{oo} &= \gamma_5 D_{oo} \\
Q &= \gamma_5(D_{ee} - D_{eo}D_{oo}^{-1}D_{oe})
\end{aligned}$$

The action is

$$S = S_1 + S_2 = \phi_1^{\dagger} Q_{oo}^{-2} \phi_1 + \phi_2^{\dagger} Q^{-2} \phi_2$$

Forces for ϕ_1-term

The derivative is

$$\dot{S}_1 = -2\mathrm{Re}\left[\phi_1^\dagger (Q_{oo}^{-2} Q_{oo} \dot{Q}_{oo} Q_{oo}^{-2}) \phi_1\right]$$

and we can write it as

$$\dot{S}_1 = -2\mathrm{Re}\left[\xi^\dagger \dot{Q}_{oo} \eta\right]$$

with

$$\eta = Q_{oo}^{-2}\phi_1,$$
$$\xi = Q_{oo}\eta.$$

Forces for ϕ_2-term

The derivative is

$$\dot{S}_2 = -2\mathrm{Re}\left[\phi_2^\dagger (Q^{-2} Q \dot{Q} Q^{-2}) \phi_2\right]$$

and we can write it as

$$\dot{S}_2 = -2\mathrm{Re}\left[\xi^\dagger \dot{Q} \eta\right]$$

with

$$\eta = Q^{-2}\phi_2,$$
$$\xi = Q\eta.$$

The explicit expression for $\xi^\dagger \dot{Q} \eta$ is given by

$$\xi^\dagger \dot{Q}\eta = \xi^\dagger \gamma_5 \dot{D}_{ee}\eta - \xi^\dagger \gamma_5 \dot{D}_{eo} D_{oo}^{-1} D_{oe}\eta + \xi^\dagger \gamma_5 D_{eo} D_{oo}^{-1} \dot{D}_{oo} D_{oo}^{-1} D_{oe}\eta - \xi^\dagger \gamma_5 D_{eo} D_{oo}^{-1} \dot{D}_{oe}\eta$$

and it can be written as

$$\xi^\dagger \dot{Q}\eta = \xi^\dagger \gamma_5 \dot{D}_{ee}\eta - \xi^\dagger \gamma_5 \dot{D}_{eo}\eta_1 + \xi_1^\dagger \gamma_5 \dot{D}_{oo}\eta_1 - \xi_1^\dagger \gamma_5 \dot{D}_{oe}\eta$$

with

$$\eta_1 = D_{oo}^{-1} D_{oe}\eta$$
$$\xi_1 = D_{oo}^{-1} D_{oe}\xi$$

Method 2

The action of D_{oo} can also be expressed directly as the logarithm of the determinant.

$$S = -2\log\det D_{oo} + \phi^\dagger Q^{-2}\phi$$

This is the approach implemented in the code.

4.4.3 LDL factorization

With even-odd preconditioning we need to calculate the inverse D_{oo}^{-1} when applying the dirac operator and when calculating the forces. Because this matrix is Hermitian and block diagonal it can be inverted locally with an exact solver. The most practical solver is via an LDL decomposition.

$$A = LDL^\dagger$$

Sum over j

$$D_j = A_{jj} - \sum_{k=1}^{j-1} L_{jk} L_{jk}^* D_k$$

Sum over $i > j$.

$$L_{ij} = \frac{1}{D_j} \left(A_{ij} - \sum_{k=1}^{j-1} L_{ik} L_{jk}^* D_k \right)$$

The determinant is given by

$$\det(A) = \prod_k D_k$$

LDL Decomposition

Calculates the LDL decomposition $A = LDL^\dagger$ in-place. After the decomposition, the lower triangular part of A is L and the diagonal is D.

```
do i=0, N-1
    do k=0, i-1
        A_ii = A_ii - L_ik * conj(L_ik) * A_kk
    enddo
    do j=i+1, N-1
        do k=0, i-1
            A_ji = A_ji - A_jk * conj(L_ik) * A_kk
        enddo
        A_ji = A_ji/A_ii
    enddo
enddo
```

Forward substitution

Calculates $x = L^{-1}b$.

```
do i=0, N-1
    x_i = b_i
    do k=0, i-1
        x_i = x_i - A_ik * x_k
    enddo
enddo
```

Backward substitution with diagonal

Calculates $x = (L^\dagger)^{-1} D^{-1} x$.

```
do i=N-1, 0
    x_i = x_i/A_ii
    do k=i+1, N-1
        x_i = x_i - conj(A_ki) * x_k
    enddo
enddo
```

Full inversion

This algorithm calculates the inverse $B = A^{-1}$ from the LDL decomposition. Because the inverse is Hermitian we only calculate the lower triangular part.

```
do i=0, N-1
    B_ii = 1
    do j=i, N-1
        do k=i, j-1
            B_ji = L_jk * B_ki
        enddo
    enddo
    do j=N-1, i
        B_ji = B_ji/L_ii
        do k=j+1, N-1
            B_ji = conj(L_kj) * B_ki
        enddo
    enddo
enddo
```

4.5 Exponential Clover Term

The exponential version of the clover term (including mass term) can be written as

$$D_{sw} = \sum_x (4 + m_0) \exp(A(x)), \text{ with } A(x) = -\frac{c_{sw}}{4(4+m_0)} \sum_{\mu,\nu} \sigma_{\mu\nu} F_{\mu\nu}(x) \tag{4.21}$$

where $\sigma_{\mu\nu}$ is again defined by

$$\sigma_{\mu\nu} = \frac{1}{2}[\gamma_\mu, \gamma_\nu].$$

As for the clover term above, we can simplify the sum over $\mu\nu$ to a sum over $\mu < \nu$ and introduce a factor of two. We define

$$A(x) = -\frac{c_{sw}}{2(4+m_0)} \sum_{\mu<\nu} \sigma_{\mu\nu} F_{\mu\nu}(x) \tag{4.22}$$

The quantity $\sigma_{\mu\nu}F_{\mu\nu}$ is Hermitian and block diagonal. It can be written as

$$A(x) = -\frac{c_{sw}}{2(4+m_0)}\sum_{\mu<\nu}\sigma_{\mu\nu}F_{\mu\nu} = \begin{pmatrix} a & b & 0 & 0 \\ b^\dagger & -a & 0 & 0 \\ 0 & 0 & c & d \\ 0 & 0 & d^\dagger & -c \end{pmatrix} \equiv \begin{pmatrix} A^+ & 0 \\ 0 & A^- \end{pmatrix}, \tag{4.23}$$

where $A^\pm$ are 2×2 matrices in spin space and a, b, c, d are $N_F \times N_F$.

This formulation of $A(x)$ as a block matrix will be useful for the exponentiation.

4.5.1 Evaluation of the operator

The evaluation of the exponential of $A(x)$ can be split as:

$$\exp A(x) = \begin{pmatrix} \exp A^+ & 0 \\ 0 & \exp A^- \end{pmatrix}$$

and so, the problem is reduced to the exponential of two $(2N_F)\times(2N_F)$ matrices. The evaluation can be performed in two ways.

1. Using the Taylor expansion:

$$\exp(A^\pm) = \sum_{k=0}^{N}\frac{1}{k!}(A^\pm)^k.$$

2. Using the Horner scheme:

$$\exp(A^\pm) = \sum_{k=0}^{\dim A^\pm - 1} b_k (A^\pm)(A^\pm)^k, \tag{4.24}$$

where b_k are computed recursively as follows. We start with

$$q_{N,0} = 1/N!, q_{N,1\cdots(\dim A^\pm)-1} = 0.$$

Then, the recursion proceeds:

$$\begin{aligned} q_{n,0} &= -p_0 q_{n+1,\dim A^\pm - 1} + 1/n!, \\ q_{n,i} &= -p_i q_{n+1,\dim A^\pm - 1} + q_{n+1,i-1}, \\ &\text{with } i = 1\cdots(\dim A^\pm) - 1, \end{aligned} \tag{4.25}$$

where p_i represent the coefficients of the characteristic polynomial of the matrix $A^\pm$:

$$P(A^\pm) = \sum_{n=0}^{\dim A\pm} p_n (A^\pm)^n.$$

For instance, the characteristic polynomial of a 4×4 traceless matrix has the following coefficients:

$$p_0 = \frac{1}{8}\left(\mathrm{tr}A^2\right)^2 - \frac{1}{4}\mathrm{tr}A^4,\ p_1 = -\frac{1}{3}\mathrm{tr}A^3,\ p_2 = -\frac{1}{2}\mathrm{tr}A^2,\ p_3 = 0,\ p_3 = 1.$$

Finally, the coefficients of eq. (4.24) are $b_k = q_{0,k}$.

The Horner scheme method is currently implemented only for $SU(2)$ and $SU(3)$ with fundamental fermions.

4.5.2 Pseudofermion Forces

For the forces we use the following short-hand notation for the derivative with respect to the link variables.

$$\dot{S} = \partial^a_{x,\mu} S.$$

To calculate the pseudofermion forces let us write down the action as

$$S = \phi^\dagger (H^{-2}) \phi,$$

where $H = \gamma^5 D$ is the Hermitian Dirac operator. When differentiating the action we obtain

$$\dot{S} = -2\mathrm{Re}\ \xi^\dagger \dot{H} \eta, \tag{4.26}$$

with the definitions

$$\eta = H^{-2}\phi,$$
$$\xi = H\eta.$$

Forces

Here we will only consider the forces from the clover term. For the exponential version of the clover term, the implementation is very similar to the traditional clover term.

The clover part of the Dirac operator is given by

$$H_{sw} = (4+m_0)\gamma_5 \exp\left(-\frac{c_{sw}}{2(4+m_0)} \sum_{\mu<\nu} \sigma_{\mu\nu} F_{\mu\nu}(x)\right) = (4+m)\gamma_5 \exp A(x). \tag{4.27}$$

An optimized way of calculating the derivative is provided by the double Horner scheme. The basic idea is that the derivative of a matrix can be expressed as:

$$de^A = \sum_{k=0}^{\dim A - 1} \sum_{l=0}^{\dim A - 1} C_{kl}(A) A^l dA A^k, \tag{4.28}$$

where the C_{kl} coefficients depend on the matrix A, similarly to the ones eq. (4.24). They are calculated performing first the iteration in eq. `horner`, and then repeating the iteration process on the result of the first iteration. For compactness, we shall omit the limits of the sum henceforth. When inserting eq. (4.27) in eq. (4.26), and using eq. (4.28) we obtain

$$\dot{S} = c_{sw} \sum_k \sum_{\mu<\nu} \mathrm{Re}(\xi^\dagger_k \bar{\sigma}_{\mu\nu} \dot{F}_{\mu\nu} \eta_k),$$

with $\$\xi_k = \sum_l \begin{pmatrix} C^+_{kl} (A^+)^l \xi^+ \\ C^-_{kl} (A^-)^l \xi^- \end{pmatrix}$, and $\eta_k = \begin{pmatrix} (A^+)^k \eta^+ \\ (A^-)^k \eta^- \end{pmatrix}$.$

From the definition of $F_{\mu\nu}$ it follows that

$$\begin{aligned}\dot{S} &= \frac{1}{8} c_{sw} \sum_k \sum_{\mu<\nu} \mathrm{Re}(\xi^\dagger_k \bar{\sigma}_{\mu\nu} \dot{Q}_{\mu\nu} \eta_k + \xi^\dagger_k \bar{\sigma}^\dagger_{\mu\nu} \dot{Q}^\dagger_{\mu\nu} \eta_k), \\ &= \frac{1}{8} c_{sw} \sum_k \sum_{\mu<\nu} \mathrm{Re}(\xi^\dagger_k \bar{\sigma}_{\mu\nu} \dot{Q}_{\mu\nu} \eta_k + \eta^\dagger_k \bar{\sigma}_{\mu\nu} \dot{Q}_{\mu\nu} \xi_k).\end{aligned}$$

This can in be written as

$$\dot{S} = \frac{1}{8} c_{sw} \sum_{\mu<\nu} \mathrm{Re\ tr} \left[\dot{Q}_{\mu\nu} \sum_k \left\{ \bar{\sigma}_{\mu\nu} \eta_k(x) \otimes \xi_k^\dagger(x) + \bar{\sigma}_{\mu\nu} \xi_k(x) \otimes \eta_k^\dagger(x) \right\} \right]$$

As for the clover term above we need to calculate now

$$\dot{S} = \frac{1}{8} c_{sw} \mathrm{Re\ tr} [\dot{Q}_{\mu\nu}(x) X_{\mu\nu}(x)] \tag{4.29}$$

now with

$$X_{\mu\nu}(x) = \sum_k \bar{\sigma}_{\mu\nu} \eta_k(x) \otimes \xi_k^\dagger(x) + \bar{\sigma}_{\mu\nu} \xi_k(x) \otimes \eta_k^\dagger(x).$$

The total force can now be expressed as in the clover term above.

4.5.3 Even-odd preconditioning

Even-odd preconditioning is particularly simple for the exponential case, since the force coming from the little determinant vanished. This can be seen because of the fact that:

$$\det D_{oo} = \exp(\log \det D_{oo}) = \exp(\mathrm{tr} \log D_{oo}) = 1,$$

and so it is a constant term in the action that does not contribute to the force.

4.5.4 Implementation of $X_{\mu\nu}$ using Taylor series

In the current version of the code, the horner scheme is only implemeted for $SU(2)$ and $SU(3)$ with fundamental fermions. For other theories, a less efficient, but more flexible, alternative is used. For this, we use the Taylor series:

$$dA = \sum_{k=0}^{N} \sum_{l=0}^{N-k} \frac{1}{(k+l+1)!} A^k dA A^l,$$

with N sufficiently large. The implementation changes only in the definition of $X_{\mu\nu}$:

$$X_{\mu\nu}(x) = \sum_{k=0}^{N} \bar{\sigma}_{\mu\nu} \eta_k(x) \otimes \xi_k^\dagger(x) + \bar{\sigma}_{\mu\nu} \xi_k(x) \otimes \eta_k^\dagger(x),$$

where now:

$$\xi_k = \sum_l \frac{1}{(k+l+1)!} \begin{pmatrix} (A^+)^l \xi^+ \\ (A^-)^l \xi^- \end{pmatrix}, \text{ and } \eta_k = \begin{pmatrix} (A^+)^k \eta^+ \\ (A^-)^k \eta^- \end{pmatrix}.$$

4.6 Stout smearing

The implementation follows [hep-lat/0311018] closely. We define the smeared links as

$$U'_\mu(x) = e^{Q_\mu(x)} U_\mu(x)$$

where $\Sigma_\mu(x)$ is an element of the Lie algebra, defined via the projection

$$Q_\mu(x) = \mathcal{P}\{\Omega_\mu(x)\}.$$

The projection operator is not unique, but the most common choice is

$$\mathcal{P}(\Omega) = \frac{1}{2}(\Omega - \Omega^\dagger) - \frac{1}{2N}\mathrm{tr}(\Omega - \Omega^\dagger).$$

However, in a setup with mixed representations, it is convenient to use the following two-step procedure for the projection. This allows us to project matrices from different representations onto the generators of the fundamental representation.

$$A^a_\mu(x) = -\frac{1}{T_f}\mathrm{tr}[iT^a_R\Omega_\mu(x)]$$
$$Q_\mu(x) = iT^a_F A^a_\mu(x)$$

The matrix $\Omega_\mu(x)$ is defined as

$$\Omega_\mu(x) = U_\mu(x)V_\mu(x)$$

$$V_\mu(x) = \sum_{\nu\neq\mu}\rho_{\mu\nu}\left(U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x) + U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})\right)$$

For the force calculation we use the chain rule.

$$\frac{dS}{dU} = \frac{dS}{dU'}\frac{dU'}{dU}$$

The first derivative on the right-hand side is the usual force $\Sigma'_\mu(x)$ evaluated using the smeared links. The second term is the derivative of the smeared links with respect to the fundamental links. This can be written in the following way, because the derivative of the action is surrounded by a trace.

$$\frac{dS}{dU} = e^Q\Sigma' + \frac{d\Omega}{dU}\mathcal{P}(X)$$

When using a Taylor expansion to define the exponential function, we can use the following definition of X.

$$X = \sum_{n=0}^{\infty}\sum_{k=0}^{n}Q^kU\Sigma'Q^{n-k}$$

The derivative of the Ω matrix is the last missing piece. Define $\Lambda = \mathcal{P}(X)$ and consider

$$\frac{d}{dU_\mu(x)}U_\mu(x)V_\mu(x)\Lambda_\mu(x)$$

Here we have a sum over $\nu \neq \mu$. There are eight contributions to the above derivative.

$$\rho_{\mu\nu}U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)\Lambda_\mu(x)$$

$$\rho_{\nu\mu}U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})\Lambda_\nu(x-\hat{\nu})U_\nu(x-\hat{\nu})$$

$$\rho_{\mu\nu}U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})\Lambda^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})$$

$$\rho_{\nu\mu}U_\nu(x+\hat{\mu})U^\dagger_\mu(x+\hat{\nu})U^\dagger_\nu(x)\Lambda^\dagger_\nu(x)$$

$$\rho_{\mu\nu}U^\dagger_\nu(x+\hat{\mu}-\hat{\nu})U^\dagger_\mu(x-\hat{\nu})U_\nu(x-\hat{\nu})\Lambda_\mu(x)$$

$$\rho_{\nu\mu} U_\nu^\dagger(x-\hat{\nu}+\hat{\mu}) \Lambda_\nu^\dagger(x-\hat{\nu}+\hat{\mu}) U_\mu^\dagger(x-\hat{\nu}) U_\nu(x-\hat{\nu})$$

$$\rho_{\mu\nu} U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) \Lambda_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$$

$$\rho_{\nu\mu} \Lambda_\nu(x+\hat{\mu}) U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu}) U_\nu^\dagger(x)$$

This can be simplified because several products appear more than once and we can use $\Lambda^\dagger = -\Lambda$ to remove some of the Hermitian conjugates. In the following we also assume that $\rho_{\mu\nu} = \rho_{\nu\mu}$.

$$\rho_{\mu\nu} W_2 U_\nu^\dagger(x) \{\Lambda_\mu(x) - \Lambda_\nu(x)\}$$

$$\rho_{\mu\nu} U_\nu^\dagger(x+\hat{\mu}-\hat{\nu}) U_\mu^\dagger(x-\hat{\nu}) \{\Lambda_\nu(x-\hat{\nu}) - \Lambda_\mu(x-\hat{\nu})\} U_\nu(x-\hat{\nu})$$

$$\rho_{\mu\nu} U_\nu^\dagger(x+\hat{\mu}-\hat{\nu}) \{W_1 \Lambda_\mu(x) - \Lambda_\nu(x+\hat{\mu}-\hat{\nu}) W_1\}$$

$$\rho_{\mu\nu} \{\Lambda_\nu(x+\hat{\mu}) W_2 - W_2 \Lambda_\mu(x+\hat{\nu})\} U_\nu^\dagger(x)$$

Here

$$W_1 = U_\mu^\dagger(x-\hat{\nu}) U_\nu(x-\hat{\nu})$$
$$W_2 = U_\nu(x+\hat{\mu}) U_\mu^\dagger(x+\hat{\nu})$$

This brings us down to 13 multiplications.

5 Analysis

5.1 Contractions

5.1.1 Connected two point correlation functions

First we choose interpolating operators with the quantum numbers of the meson we would like to study:

$$O_M = \bar{\psi}^{(1)}(x)\Gamma\psi^{(2)}(x)$$

$$\bar{O}_M = \bar{\psi}^{(2)}(x)\bar{\Gamma}\psi^{(1)}(x)$$

where $\bar{\Gamma} = \gamma_0\Gamma^\dagger\gamma_0$. The gamma matrix is chosen to have the same J^{PC} quantum numbers as the meson we want to create. We then calculate the expectation value to create a meson at y and destroy it again at x:

$$\begin{aligned}\langle O_M(x)\bar{O}'_M(y)\rangle =&\langle\bar{\psi}^{(1)}(x)\Gamma\psi^{(2)}(x)\bar{\psi}^{(2)}(y)\bar{\Gamma}'\psi^{(1)}(y)\rangle\\ =&\Gamma_{\alpha\beta}\bar{\Gamma}'_{\gamma\delta}\langle\bar{\psi}^{(1)}_\alpha(x)\psi^{(2)}_\beta(y)\bar{\psi}^{(2)}_\gamma(y)\psi^{(1)}_\delta(x)\rangle\\ =&-\Gamma_{\alpha\beta}\bar{\Gamma}'_{\gamma\delta}\langle\psi^{(2)}_\beta(x)\bar{\psi}^{(2)}_\gamma(y)\psi^{(1)}_\delta(y)\bar{\psi}^{(1)}_\alpha(x)\rangle\end{aligned}$$

where the sign in the last line comes from exchanging the anticommuting $\bar{\psi}_\alpha$ three times. Wick contracting where $\langle\psi_\alpha(x)\bar{\psi}_\beta(y)\rangle = S_{\alpha\beta}(x,y)$ gives

$$\begin{aligned}\langle O_M(x)\bar{O}'_M(y)\rangle =&-\Gamma_{\alpha\beta}S^{(2)}_{\beta\gamma}(x,y)\bar{\Gamma}'_{\gamma\delta}S^{(1)}_{\delta\alpha}(y,x)\\ =&-\mathrm{Tr}\left[\Gamma S^{(2)}(x,y)\bar{\Gamma}'S^{(1)}(y,x)\right]\end{aligned}$$

To get correlation functions we Fourier transform, ie. sum over all source and sink seperations while projecting onto the momentum we want to give to the particle:

$$\begin{aligned}C(t-\tau,\vec{p}) =&\sum_{\vec{x}\vec{y}} e^{-i\vec{p}(\vec{x}-\vec{y})}\langle O_M(\vec{x},t)O'_M(\vec{y},\tau)\rangle\\ =&-\sum_{\vec{x}\vec{y}} e^{-i\vec{p}(\vec{x}-\vec{y})}\mathrm{Tr}\left[\Gamma S^{(2)}(x,y)\bar{\Gamma}'S^{(1)}(y,x)\right]\end{aligned}$$

here $x = (\vec{x},t)$ and $y = (\vec{y},\tau)$ and the zero momentum correlator is:

$$C(t-\tau,0) = -\sum_{\vec{x}\vec{y}}\mathrm{Tr}\left[\Gamma S^{(2)}(x,y)\bar{\Gamma}'S^{(1)}(y,x)\right]$$

We now use γ_5 Hermiticity: $\gamma_5 S^\dagger(x,y)\gamma_5 = S(y,x)$,

$$C(t-\tau,0) = -\sum_{\vec{x}\vec{y}}\mathrm{Tr}\left[\gamma_5\Gamma S^{(2)}(x,y)\bar{\Gamma}'\gamma_5 S^{\dagger(1)}(x,y)\right] \tag{5.1}$$

5.1.2 Point Sources

Using a delta function source and solving the Dirac equation gives a point propagator,

$$D_{\alpha a,\beta b}(x,y)S_{\beta b,\gamma c}(y,z)=\delta(x,z)\delta_{ac}\delta_{\alpha\gamma}$$

usually $z=(\vec{0},0)$ so we get $S(y,0)=\gamma_5 S^\dagger(0,y)\gamma_5$. Then we use these to calculate correlation functions,

$$C(t,0)=-\sum_{\vec{x}}\mathrm{Tr}e^{-i\vec{p}\vec{x}}\left[\gamma_5\Gamma S(x,0)\bar{\Gamma}'\gamma_5 S(x,0)\right] \tag{5.2}$$

Translational invariance in the limit of infinitely many gauge configurations implies $S(x,y)=S(|x-y|)$, so the sum over $\vec{y}$ in equation `eq:corr` just gives V times equation `eq:pointcorr`. We place the source at the time origin so $\tau=0$.

5.1.3 One-end Trick

For this method it helps to write all the indices out,

$$C(t-\tau,0)=-\sum_{\vec{x}\vec{y}}(\gamma_5\Gamma)_{\alpha\beta}S^{(2)}_{\beta\gamma,bc}(x,y)(\bar{\Gamma}'\gamma_5)_{\gamma\delta}S^{\dagger(1)}_{\delta\alpha,cb}(x,y)$$

Greek indices $\alpha,\beta,\gamma,\delta,...$ are spinor indices and Latin indices $a,b,c,d...$ are colour indices. The one-end trick involves inserting a delta function in colour, spin and space.

$$C(t-\tau,0)=-\sum_{\vec{x}\vec{y}\vec{z}}(\gamma_5\Gamma)_{\alpha\beta}S^{(2)}_{\beta\gamma,bc}(\vec{x},t;\vec{y},\tau)\delta_{\gamma\lambda}\delta_{cd}\delta(\vec{y},\vec{z})(\bar{\Gamma}'\gamma_5)_{\lambda\delta}S^{\dagger(1)}_{\delta\alpha,db}(\vec{x},t;\vec{z},\tau)$$

The delta function is aproximated with a $Z(2)\times Z(2)$ noise source on timeslice τ

$$\delta_{\gamma\lambda}\delta_{cd}\delta(\vec{y},\vec{z})\approx\frac{1}{K}\sum_{k=0}^{K}|\eta^{(k)}_{\gamma c}(\vec{y})\rangle\langle\eta^{(k)}_{\lambda d}(\vec{z})|$$

which is exact in the limit $K\to\infty$.

$$C(t-\tau,0)=-\frac{1}{K}\sum_{k=0}^{K}\sum_{\vec{x}\vec{y}\vec{z}}(\gamma_5\Gamma)_{\alpha\beta}S^{(2)}_{\beta\gamma,bc}(\vec{x},t;\vec{y},\tau)|\eta^{(k)}_{\gamma c}(\vec{y})\rangle\langle\eta^{(k)}_{\lambda d}(\vec{z})|(\bar{\Gamma}'\gamma_5)_{\lambda\delta}S^{\dagger(1)}_{\delta\alpha,db}(\vec{x},t;\vec{z},\tau) \tag{5.3}$$

Defining

$$\phi^{(k)}_{\beta,b}(\vec{x},t;\tau)=\sum_{\vec{y}}S^{(2)}_{\beta\gamma,bc}(\vec{x},t;\vec{y},\tau)|\eta^{(k)}_{\gamma c}(\vec{y})\rangle$$

and

$$\phi^{\Gamma(k)}_{\alpha,b}(\vec{x},t;\tau)=\sum_{\vec{z}}S^{(1)}_{\alpha\delta,bd}(\vec{x},t;\vec{z},\tau)(\bar{\Gamma}'\gamma_5)^\dagger_{\delta\lambda}|\eta^{(k)}_{\lambda d}(\vec{z})\rangle$$

the correlator can be evaluated as,

$$C(t-\tau,0)=-\frac{1}{K}\sum_{k=0}^{K}\sum_{\vec{x}}(\gamma_5\Gamma)_{\alpha\beta}\phi^{(k)}_{\beta,b}(\vec{x},t;\tau)\phi^{\Gamma\dagger(k)}_{\alpha,b}(\vec{x},t;\tau)$$

Implementation in HiRep

In HiRep the code `Spectrum/mk_mesons_with_z2semwall.c` does two solves to calculate $S^{(1)}|\eta\rangle$ and $S^{(2)}(\bar{\Gamma}'\gamma_5)^\dagger|\eta\rangle$. HiRep has

$$\rho = \rho_c(\vec{y})$$

a $Z(2) \times Z(2)$ colour vector at all (even) spatial sites $\vec{y}$ and non-zero only on timeslice τ.

$$\rho^\alpha_\beta = \delta_{\alpha\beta}\rho^\alpha$$

eg.

$$\rho^1_\beta = \begin{pmatrix} 0 \\ \rho^1 \\ 0 \\ 0 \end{pmatrix}$$

It then solves for the four objects

$$\chi^\alpha_\beta = S_{\beta\gamma}\rho^\alpha_\gamma$$

eg.

$$\chi^0_\beta = \begin{pmatrix} S_{00}\rho^0 \\ S_{10}\rho^0 \\ S_{20}\rho^0 \\ S_{30}\rho^0 \end{pmatrix}$$

For every different Γ that is required it does four more inversions,

$$\chi^{\Gamma\alpha}_\beta = S_{\beta\gamma}(\Gamma\gamma_5)^\dagger_{\gamma\delta}\rho^\alpha_\delta$$

before calculating the correlator as,

$$C(t-\tau,0) = -\frac{1}{K}\sum_{k=0}^{K}\sum_{\lambda=0}^{3}\sum_{\vec{x}}(\gamma_5\Gamma)_{\alpha\beta}\chi^\lambda_{\beta,b}(\vec{x},t;\tau)\chi^{\Gamma\lambda\dagger}_{\alpha,b}(\vec{x},t;\tau)$$

where the λ sum is over the 4 spinor components.

We should be able to improve the signal and reduce the number of inversions with two modifications. First, instead of having a different noise vector for every spin component we reuse the same noise, i.e.

$$\rho^\alpha_\beta = \delta_{\alpha\beta}\rho$$

for fixed ρ. Using less noise seems to be generally preferred.

Secondly there is no need to invert for every different Γ. Let,

$$\chi^{\Gamma\alpha}_\beta = (\Gamma\gamma_5)^\dagger_{\gamma\alpha}\chi^\gamma_\beta$$

This is true because,

$$(\Gamma\gamma_5)^\dagger_{\gamma\alpha}\chi^\gamma_\beta = (\Gamma\gamma_5)^\dagger_{\gamma\alpha}S_{\beta\delta}\rho^\gamma_\delta = (\Gamma\gamma_5)^\dagger_{\gamma\alpha}S_{\beta\delta}\delta_{\gamma\delta}\rho = (\Gamma\gamma_5)^\dagger_{\gamma\alpha}S_{\beta\gamma}\rho = S_{\beta\gamma}(\Gamma\gamma_5)^\dagger_{\gamma\alpha}\rho$$

then the correlation function is

$$C(t-\tau,0) = -\frac{1}{K}\sum_{k=0}^{K}\sum_{\lambda=0}^{3}\sum_{\vec{x}}(\gamma_5\Gamma)_{\alpha\beta}\chi^\lambda_{\beta,b}(\vec{x},t;\tau)\chi^{\Gamma\lambda\dagger}_{\alpha,b}(\vec{x},t;\tau)$$

as before. By using the spin_matrix object in HiRep to construct the objects $\chi^\lambda_{\beta,b}$ the correlators can be calculated with only $4N_F$ inversions.

5.1.4 Disconnected

The Disconnected contributions occur when we have fermion species of the same type in the hadron interpolator O_M:

$$O_M(x) = \bar{\psi}(x)\Gamma\psi(x)$$

The same manipulations that lead to equation (5) give,

$$\begin{aligned}\langle O_M(x)\bar{O}'_M(y)\rangle = & \langle\bar{\psi}(x)\Gamma\psi(x)\bar{\psi}(y)\bar{\Gamma}'\psi(y)\rangle \\ =&\Gamma_{\alpha\beta}\bar{\Gamma}'_{\gamma\delta}\langle\bar{\psi}_\alpha(x)\psi_\beta(y)\bar{\psi}_\gamma(y)\psi_\delta(x)\rangle\end{aligned}$$

There are two allowed Wick contractions,

$$\langle O_M(x)\bar{O}'_M(y)\rangle = -\mathsf{Tr}\left[\Gamma S(x,y)\bar{\Gamma}'S(y,x)\right] + \mathsf{Tr}\left[\Gamma S(x,x)\right]\mathsf{Tr}\left[\bar{\Gamma}'S(y,y)\right]$$

the connected and disconnected contributions. Fourier transforming the first term gives us the same result as before. For the disconnected part,

$$D(t-\tau,\vec{p}) = \sum_{\vec{x}\vec{y}} e^{-i\vec{p}(\vec{x}-\vec{y})}\mathsf{Tr}\left[\Gamma S(x,x)\right]\mathsf{Tr}\left[\bar{\Gamma}'S(y,y)\right]$$

again $x=(\vec{x},t)$ and $y=(\vec{y},\tau)$, the zero momentum correlator is

$$\begin{aligned}D(t-\tau,0) = & \sum_{\vec{x}\vec{y}}\mathsf{Tr}\left[\Gamma S(x,x)\right]\mathsf{Tr}\left[\bar{\Gamma}'S(y,y)\right] \\ =&\sum_{\vec{x}}\mathsf{Tr}\left[\Gamma S(x,x)\right]\sum_{\vec{y}}\mathsf{Tr}\left[\bar{\Gamma}'S(y,y)\right]\end{aligned}$$

This means we have to evaluate objects like,

$$d(t) = \sum_{\vec{x}}\mathsf{Tr}\left[\Gamma S(x,x)\right] = \sum_{\vec{x}}\Gamma_{\alpha\beta}S_{\beta\alpha}(x,x)$$

Using

$$\phi^{(k)}_{\beta,b}(\vec{x},t;\tau) = \sum_{\vec{y}}S_{\beta\gamma,bc}(\vec{x},t;\vec{y},\tau)|\eta^{(k)}_{\gamma c}(\vec{y})\rangle$$

which implies

$$\begin{aligned}\frac{1}{K}\sum_k^K\sum_{\vec{x}}\mathsf{Tr}\left[\langle\eta^{(k)}(\vec{x})|\Gamma|\phi^{(k)}(\vec{x},t;\tau)\rangle\right] =&\frac{1}{K}\sum_k^K\sum_{\vec{x}}\Gamma_{\beta\gamma}|\phi^{(k)}_{\gamma,b}(\vec{x},t;\tau)\rangle\langle\eta^{(k)}_{\beta b}(\vec{x})|\\ =&\frac{1}{K}\sum_k^K\sum_{\vec{x}}\Gamma_{\beta\gamma}\sum_{\vec{y}}S_{\gamma\alpha,bc}(\vec{x},t;\vec{y},\tau)|\eta^{(k)}_{\alpha c}(\vec{y})\rangle\langle\eta^{(k)}_{\beta b}(\vec{x})|\end{aligned}$$

Using the limit $K\to\infty$ this becomes,

$$\begin{aligned}\sum_{\vec{x}}\Gamma_{\beta\gamma}\sum_{\vec{y}}S_{\gamma\alpha,bc}(\vec{x},t;\vec{y},\tau)\delta_{bc}\delta_{\alpha\beta}\delta(\vec{y},\vec{x}) =&\sum_{\vec{x}}\Gamma_{\beta\gamma}S_{\gamma\beta,bb}(\vec{x},t;\vec{x},\tau)\\ d(t,\tau) =&\mathsf{Tr}\left[\Gamma S(\vec{x},t;\vec{x},\tau)\right]\end{aligned}$$

We want only cases where $t=\tau$ so we need either (a) four noise vectors on every timeslice or (b) noise vectors that are nonzero on all timeslices. In case (b) we would evaluate,

$$\frac{1}{K}\sum_k^K\sum_{\vec{x}}\mathsf{Tr}\left[\langle\eta^{(k)}(\vec{x},t)|\Gamma|\phi^{(k)}(\vec{x},t)\rangle\right]$$

with

$$\phi^{(k)}_{\beta,b}(\vec{x},t)=\sum_{\vec{y}}S_{\beta\gamma,bc}(\vec{x},t;\vec{y},\tau)|\eta^{(k)}_{\gamma c}(\vec{y},\tau)\rangle$$

5.1.5 Cancelling Backwards Propagation

The two point function evaluated in the centre of the lattice is (including the backward propagating part to give the extra factor of 2),

$$C(T/2,\vec{p})=\frac{|Z_\pi|^2}{2E_\pi(\vec{p})}2e^{-E_\pi(\vec{p})(T/2)}$$

therefore

$$\frac{1}{2}C(T/2,\vec{p})e^{-E_\pi(\vec{p})(T/2-t)}=\frac{|Z_\pi|^2}{2E_\pi(\vec{p})}e^{-E_\pi(\vec{p})(T-t)}$$

then

$$C_\rightarrow(t,\vec{p})=C(t,\vec{p})-\frac{1}{2}C(T/2,\vec{p})e^{-E_\pi(\vec{p})(T/2-t)}$$

is the forward propagating part only. $E_\pi(\vec{p})$ is obtained by fitting the zero momentum correlator and using $E(\vec{p})=\sqrt{m_\pi^2+\vec{p}^2}$. The factor $C(T/2,\vec{p})$ can be obtained also from the zero momentum correlator, by fitting to obtain $|Z_\pi|^2$ and using the fact that this is momentum independent. Since 0 momentum results are used this might not be too noisy.

Alternatively the Wilson action is invariant under

$$\begin{aligned}\psi(x)\to\mathcal{P}_\mu[\psi(x)]=\gamma_\mu\psi(P_\mu[x])\\ \bar{\psi}(x)\to\mathcal{P}_\mu[\bar{\psi}(x)]=\bar{\psi}(P_\mu[x])\gamma_\mu\end{aligned}$$

where $P_\mu[x]$ reverses the sign of all the components of x except the μ one. Time reversal corresponds to $\mathcal{T} = \mathcal{P}_1\mathcal{P}_2\mathcal{P}_3$.

$$\psi(x) \to \mathcal{T}[\psi(x)] = \gamma_0\gamma_5\psi(T[x])$$
$$\bar{\psi}(x) \to \mathcal{T}[\bar{\psi}(x)] = \bar{\psi}(T[x])\gamma_5\gamma_0$$

Using this the T symmetry of operators used to construct the correlators can be calculated to calculate the sign on the backwards propagating part.

$$\langle O_1(t)O_2(0)\rangle = C(t) = A\left(e^{-Et} + \tau_1\tau_2 e^{-E(T-t)}\right)$$

where $\tau_i = \pm 1$ is the $\mathcal{T}$ eigenvalue of O_i.

We mostly use correlators where $O_1 = O_2$ so $\tau_1\tau_2 = 1$ then the correlator is

$$C_{pp}(t,\vec{p}) = \frac{|Z_\pi|^2}{2E_\pi(\vec{p})}\left(e^{-E_\pi(\vec{p})t} + e^{-E_\pi(\vec{p})(T-t)} + e^{-E_\pi(\vec{p})(2T-t)} + \dots\right)$$

The subscript on C_{pp} refers to the fact that both propagators used periodic boundary conditions. We want to cancel the backwards propagating part which can be done by solving the forward propagator $S(0,x)$ using antiperiodic time bc's and the backward $S(x,0)$ with periodic time bc's to give an extra minus sign,

$$C_{ap}(t,\vec{p}) = \frac{|Z_\pi|^2}{2E_\pi(\vec{p})}\left(e^{-E_\pi(\vec{p})t} - e^{-E_\pi(\vec{p})(T-t)} + e^{-E_\pi(\vec{p})(2T-t)} - \dots\right)$$

so,

$$C_{ap}(t,\vec{p}) + C_p(t,\vec{p}) = \frac{2|Z_\pi|^2}{2E_\pi(\vec{p})}\left(e^{-E_\pi(\vec{p})t} + e^{-E_\pi(\vec{p})(2T-t)} + \dots\right)$$

cancelling the subleading exponential. This method requires two inversions and the calculation of

$$S_{A\pm P}(x,y) = S_A(x,y) \pm S_P(x,y)$$

Where the subscript refers to (A)ntiperiodic/(P)eriodic boundary conditions. Then,

$$C_\pm(t-\tau,0) = -\sum_{\vec{x}\vec{y}} \mathrm{Tr}\left[\gamma_5\Gamma S_{A\pm P}(x,y)\bar{\Gamma}'\gamma_5 S_{A\pm P}(x,y)\right]$$

where $C_+(t-\tau,0)$ gives the forward propagating part from 0 to T and $C_-(t-\tau,0)$ gives the backwards propagating part from $2T$ to T.

5.1.6 Form Factors and Sequential Sources

The electromagnetic form factor of a 'pion' requires the evaluation of the matrix element

$$\langle\pi(p_f)|V_\mu|\pi(p_i)\rangle = (p_i + p_f)_\mu f(q^2)$$

where $q^2 = (p_i - p_f)^2$ and

$$V_\mu = q_u\bar{u}\gamma_\mu u + q_d\bar{d}\gamma_\mu d$$

is the electromagnetic current and q_i is the charge of the fermion i. This is the local (not conserved) current, so there will be a factor Z_V for renormalization. The matrix elements required look like:

$$C_3(t_f,t,t_i,\vec{p_i},\vec{p_f}) = Z_V\sum_{\vec{x}\vec{y}\vec{z}} e^{-i\vec{p_f}(\vec{x}-\vec{y})}e^{i\vec{p_i}(\vec{y}-\vec{z})}\langle 0|\bar{u}\gamma_5 d(\vec{x},t_f)V_0(\vec{y},t)\bar{d}\gamma_5 u(\vec{z},t_i)|0\rangle$$

We take the $\mu = 0$ component since this is statistically cleaner and also nonzero independant of the momentum direction. The contractions give three propagators eg. taking the $\bar{d}\gamma_\mu d$ part of V_μ,

$$Z_V \sum_{\vec{x}\vec{y}\vec{z}} e^{-i\vec{p_f}(\vec{x}-\vec{y})} e^{-i\vec{p_i}(\vec{y}-\vec{z})} Tr\left[S_u(\vec{z},t_i;\vec{x},t_f)\gamma_5 S_d(\vec{x},t_f;\vec{y},t)\gamma_0 S_d(\vec{y},t;\vec{z},t_i)\gamma_5\right]$$

There are also disconnected contributions from contracting the two fermions in the current together but we ignore those. The usual sequential source trick consists of solving

$$S_u(\vec{x},t;\vec{z},t_i) = \sum_{\vec{y},\tau} D_u(\vec{x},t;\vec{y},\tau)\delta(\vec{y},\tau;\vec{z},t_i)$$

to get the point-to-all propagator (for a specific $\vec{z}$ and t_i as well as dropping the sum over $\vec{z}$ and using translational invarience). Then taking a single timeslice of the propagator $S_u(\vec{x},t_f;\vec{z},t_i)$ and solving,

$$\begin{aligned} D_d(\vec{x},t_f;\vec{y},t) G_{du}(\vec{y},t;\vec{p_f};t_f;\vec{z},t_i) =& e^{i\vec{p_f}\vec{x}}\gamma_5 S_u(\vec{x},t_f;\vec{z},t_i) \\ G_{du}(\vec{y},t;\vec{p_f};t_f;\vec{z},t_i) =& \sum_{\vec{x}} e^{i\vec{p_f}\vec{x}} S_d(\vec{y},t;\vec{x},t_f)\gamma_5 S_u(\vec{x},t_f;\vec{z},t_i) \end{aligned}$$

to get the all-to-all-to-point contribution. Then

$$\begin{aligned} \gamma_5\left[G_{du}(\vec{y},t;\vec{p_f};t_f;\vec{z},t_i)\right]^\dagger\gamma_5 =& \sum_{\vec{x}} e^{-i\vec{p_f}\vec{x}}\gamma_5 S_u^\dagger(\vec{x},t_f;\vec{y},t)\gamma_5\gamma_5\gamma_5\gamma_5\gamma_5 S_d^\dagger(\vec{z},t_i;\vec{x},t_f)\gamma_5 \\ =& \sum_{\vec{x}} e^{-i\vec{p_f}\vec{x}} S_u(\vec{z},t_i;\vec{x},t_f)\gamma_5 S_d(\vec{x},t_f;\vec{y},t) \\ =& G_{ud}(\vec{z},t_i;t_f;\vec{p_f};\vec{y},t) \end{aligned}$$

$$C_3(t_f,t,t_i,\vec{p_i},\vec{p_f}) = Z_V \sum_{\vec{y}} e^{-i(\vec{p_i}-\vec{p_f})\vec{y}} Tr\left[G_{ud}(\vec{z},t_i;t_f;\vec{p_f};\vec{y},t)\gamma_0 S_d(\vec{y},t;\vec{z},t_i)\gamma_5\right] \tag{5.4}$$

This Z_V factor is unknown. We show how to calculate it later, or cancel it, but an alternative is to use the conserved vector current in place of the local current:

$$V_\mu = \frac{1}{2}\left[\bar{\psi}(x+\mu)(1+\gamma_\mu)U_\mu^\dagger(x)\psi(x) - \bar{\psi}(x)(1-\gamma_\mu)U_\mu^\dagger(x)\psi(x+\mu)\right]$$

The trace in (5.4) becomes

$$\begin{aligned} Tr[&S_d(\vec{y},t+1;\vec{z},t_i)\gamma_5(1+\gamma_0)U_0^\dagger(\vec{y},t)G_{ud}(\vec{z},t_i;t_f;\vec{p_f};\vec{y},t) - \\ &S_d(\vec{y},t;\vec{z},t_i)\gamma_5(1-\gamma_0)U_0(\vec{y},t)G_{ud}(\vec{z},t_i;t_f;\vec{p_f};\vec{y},t+1)] \end{aligned}$$

If we use this then all the following formulas are the same except $Z_V \to 1$.

There is an alternative that doesn't require the sequential source trick. Using the properties of our noise sources,

$$S_d(\vec{x},t_f;\vec{y},t) \approx \frac{1}{K}\sum_{i=0}^{K} |\psi^{(i)}(\vec{x},t_f)\rangle\langle\eta^{(i)}(\vec{y},t)|$$

the three point correlation function becomes,

$$\begin{aligned} Z_V \frac{1}{K}\sum_{i=0}^{K}\sum_{\vec{x}\vec{y}} e^{-i\vec{p_f}(\vec{x}-\vec{y})} e^{i\vec{p_i}\vec{y}} Tr\left[\langle\eta^{(i)}(\vec{y},t)|\gamma_0 S_d(\vec{y},t;\vec{0},0)\gamma_5 S_u(\vec{0},0;\vec{x},t_f)\gamma_5|\psi^{(i)}(\vec{x},t_f)\rangle\right] \\ Z_V \frac{1}{K}\sum_{i=0}^{K}\sum_{\vec{x}\vec{y}} e^{-i\vec{p_f}(\vec{x}-\vec{y})} e^{i\vec{p_i}\vec{y}} Tr\left[\langle\eta^{(i)}(\vec{y},t)|\gamma_0 S_d(\vec{y},t;\vec{0},0) S_u^\dagger(\vec{x},t_f;\vec{0},0)|\psi^{(i)}(\vec{x},t_f)\rangle\right] \end{aligned}$$

Using this method we can inject arbitrary momentum at the source without the need for extra inversions.

Two Point Function

A complete set of hadrons is given by,

$$\sum_n \frac{|n\rangle\langle n|}{2E_n V}$$

the first term is the pion. The two point function (from point sources) is,

$$\begin{aligned} C(t,\vec{p}) = & \sum_{\vec{x}} e^{-i\vec{p}\vec{x}}\langle O_\pi(\vec{x},t)O_\pi^\dagger(\vec{0},0)\rangle \\ = & \sum_{\vec{x}}\sum_n e^{i\vec{p}\vec{x}}\frac{\langle 0|O_\pi(\vec{x},t)|n\rangle\langle n|O_\pi^\dagger(\vec{0},0)|0\rangle}{2E_n} \end{aligned}$$

Use $\sum_{\vec{y}} e^{-i\vec{p}\vec{y}}O_n^\dagger(\vec{y},0)|0\rangle = |n(\vec{p})\rangle$, the time evolution operator e^{-Ht} and also the fact that the lightest meson dominates the sum to get,

$$C(t,\vec{p}) = \sum_{\vec{x}\vec{y}\vec{z}}\sum_{\vec{p'}} e^{-i\vec{p}\vec{x}}\frac{\langle 0|O_\pi(\vec{x},0)O_\pi^\dagger(\vec{y},0)e^{i\vec{p'}\vec{y}}|0\rangle\langle 0|e^{i\vec{p'}\vec{z}}O_\pi(\vec{z},0)O_\pi^\dagger(\vec{0},0)|0\rangle}{2E_\pi(\vec{p'})}e^{-E_\pi(\vec{p'})t}$$

The sum over $\vec{p'}$ gives a delta function leaving,

$$C(t,\vec{p}) = \sum_{\vec{x}\vec{y}} e^{-i\vec{p}\vec{x}}\frac{\langle 0|O_\pi(\vec{x},0)O_\pi^\dagger(\vec{y},0)|0\rangle\langle 0|O_\pi(\vec{y},0)O_\pi^\dagger(\vec{0},0)|0\rangle}{2E_\pi(\vec{p})}e^{-E_\pi(\vec{p})t}$$

Translational invarience lets us write,

$$C(t,\vec{p}) = \sum_{\vec{x}\vec{y}} e^{-i\vec{p}(\vec{x}-\vec{y})}e^{-i\vec{p}\vec{y}}\frac{\langle 0|O_\pi(\vec{0},0)O_\pi^\dagger(\vec{x}-\vec{y},0)|0\rangle\langle 0|O_\pi(\vec{y},0)O_\pi^\dagger(\vec{0},0)|0\rangle}{2E_\pi(\vec{p})}e^{-E_\pi(\vec{p})t}$$

Now changing variables gives us two Fourier transforms,

$$C(t,\vec{p}) = \frac{\langle 0|O_\pi(\vec{0},0)|\pi(p)\rangle\langle\pi(p)|O_\pi^\dagger(\vec{0},0)|0\rangle}{2E_\pi(\vec{p})}e^{-E_\pi(\vec{p})t}$$

and finally using the time evolution operator we get,

$$C(t,\vec{p}) = \frac{|Z_\pi|^2}{2E_\pi(\vec{p})}e^{-E_\pi(\vec{p})t}$$

where

$$Z_\pi = \langle\pi(p)|O_\pi^\dagger(\vec{0},0)|0\rangle$$

Three Point Function

In less detail we insert two complete sets of states into the correlator (point sources so $(\vec{x_i},t_i) = (\vec{0},0)$)

$$\begin{aligned} \langle\pi(p_f)|V_\mu|\pi(p_i)\rangle = & \langle 0|O(\vec{p_f},t_f)V_\mu(\vec{x},t)O^\dagger(\vec{p_i},t_i)|0\rangle \\ = & \langle 0|O(\vec{0},0)|\pi(\vec{p_f})\rangle\frac{e^{-(t_f-t)E_\pi(\vec{p_f})}}{2E_\pi(\vec{p_f})}\langle\pi(\vec{p_f})|V_\mu(\vec{0},0)|\pi(\vec{p_i})\rangle \\ & \times\frac{e^{-(t-t_i)E_\pi(\vec{p_i})}}{2E_\pi(\vec{p_i})}\langle\pi(\vec{p_i})|O^\dagger(\vec{0},0)|0\rangle \\ = & \frac{Z_{\pi,f}^\dagger Z_{\pi,i}}{4E(\vec{p_f})E(\vec{p_i})}\langle\pi(\vec{p_f})|V_\mu(\vec{0},0)|\pi(\vec{p_i})\rangle e^{-(t_f-t)E_\pi(\vec{p_f})-(t-t_i)E_\pi(\vec{p_i})} \end{aligned}$$

if $t < t_f$ we have the backwards contribution and the exponential changes to

$$-e^{-(t-t_f)E_\pi(\vec{p_f})-(T-t+t_i)E_\pi(\vec{p_i})}$$

Correlator Ratios: Z_V

Z_V can be obtained as follows: The ratio,

$$\begin{aligned}\frac{C_\rightarrow(t_f,\vec{0})}{C_3(t_f,t,\vec{p_i},\vec{p_f})} &= \frac{\frac{|Z_\pi(\vec{0})|^2}{2m_\pi}e^{-m_\pi t_f}}{\frac{|Z_\pi(\vec{0})|^2}{4m_\pi^2}\langle\pi(\vec{0})|V_\mu|\pi(\vec{0})\rangle e^{-(t_f-t)m_\pi - t m_\pi}} \\ &= \frac{1}{\frac{1}{2m_\pi}\langle\pi(\vec{0})|V_\mu|\pi(\vec{0})\rangle} \\ &= \frac{1}{\frac{1}{2m_\pi}2m_p i f(0)/Z_V} = Z_V.\end{aligned}$$

Where we used that the renormalized form factor $f(0) = 1$

Correlator Ratios: $f(q)$

There are various ways to cancel the unwanted terms and get $f(q)$,

RBC-UKQCD Ratio

We examine the ratio,

$$2m_\pi \frac{C_3(t,t_f,\vec{p},\vec{0})C_\rightarrow(t,\vec{0})}{C_3(t,t_f,\vec{0},\vec{0})C_\rightarrow(t,\vec{p})}$$

Assuming Z_π is momentum independant (this also works (probably) if $Z_\pi = E(\vec{p})f_\pi$, which is the case for $O = \bar{u}\gamma_0\gamma_5 d$ type interpolators) the numerator is,

$$\frac{Z_V|Z_\pi|^2}{4E(\vec{p})E(\vec{0})}f(q^2)(E(\vec{p})+m_\pi)\frac{|Z_\pi|^2}{2E(\vec{0})}e^{-E(\vec{p})t-E(\vec{0})(t_f-t)-E(\vec{0})t}$$

and the denominator is,

$$\frac{Z_V|Z_\pi|^2}{4E(\vec{0})E(\vec{0})}f(0)(m_\pi+m_\pi)\frac{|Z_\pi|^2}{2E(\vec{p})}e^{-E(\vec{0})t-E(\vec{0})(t_f-t)-E(\vec{p})t}$$

Cancelling leaves,

$$2m_\pi \frac{C_3(t,t_f,\vec{p},\vec{0})C_\rightarrow(t,\vec{0})}{C_3(t,t_f,\vec{0},\vec{0})C_\rightarrow(t,\vec{p})} = f(q^2)(E(\vec{p})+m_\pi)$$

note there is no Z_V here.

Bonnet et. al. Ratio

$$\frac{2Z_V m_\pi}{E(\vec{p})+m_\pi}\frac{C_3(t,t_f,\vec{p},\vec{0})C_{\rightarrow}(t,\vec{0})}{C_{\rightarrow}(t,\vec{p})C_{\rightarrow}(t_f,\vec{0})}$$

the numerator of the right term is,

$$\frac{|Z_\pi|^2}{4E(\vec{p})m_\pi}f_B(q^2)(E(\vec{p})+m_\pi)\frac{|Z_\pi|^2}{2m_\pi}e^{-E(\vec{p})t-m_\pi(t_f-t)-m_\pi t}$$

the denominator of the right term is,

$$\frac{|Z_\pi|^2}{2m_\pi}\frac{|Z_\pi|^2}{2E(\vec{p})}e^{-m_\pi t-m_\pi(t_f-t)-E(\vec{p})t}$$

Cancelling leaves,

$$\frac{f_B(q^2)(E(\vec{p})+m_\pi)}{2E(\vec{p})}$$

the kinematic factors are cancelled

$$\frac{2Z_V m_\pi}{E(\vec{p})+m_\pi}\frac{f_B(q^2)(E(\vec{p})+m_\pi)}{2E(\vec{p})}=Z_V f_B(q^2)=f(q^2)$$

you need to actually know Z_V or use the conserved current.

5.2 Estimation of Disconnected Contributions

5.2.1 Conventions

We choose the hermitian basis of gamma matrices given in Tab. 1. Each element of the basis is referred by an index in [0,15] shown in the following table

No	Matrix
0	γ_5
1	γ_1
2	γ_2
3	γ_3
4	$-\mathrm{i}\gamma_0\gamma_5$
5	$-\mathrm{i}\gamma_0\gamma_1$
6	$-\mathrm{i}\gamma_0\gamma_2$
7	$-\mathrm{i}\gamma_0\gamma_3$
8	1
9	$-\mathrm{i}\gamma_5\gamma_1$
10	$-\mathrm{i}\gamma_5\gamma_2$
11	$-\mathrm{i}\gamma_5\gamma_3$
12	γ_0
13	$-\mathrm{i}\gamma_5\gamma_0\gamma_1$
14	$-\mathrm{i}\gamma_5\gamma_0\gamma_2$
15	$-\mathrm{i}\gamma_5\gamma_0\gamma_3$

5.2.2 Singlet Two-Point Functions

Consider a gauge theory on a group G coupled to N_f fermions in an arbitrary representation R. Let us denote:

$$C(t,x_0)=\frac{1}{N_f}\sum_{\vec{x}}\langle\bar{q}\Gamma q(x)\bar{q}\Gamma q(x_0)\rangle$$

where q,$\bar{q}$ are the N_f quark fields and Γ denotes as arbitrary Dirac structure. The $1/N_f$ factor is only there for convenience. The Wick contractions read:

$$C(t,x_0)=\sum_{\vec{x}}\langle-\mathrm{tr}\left(\Gamma S(x,x_0)\Gamma S(x_0,x)\right)+N_f\,\mathrm{tr}\left(\Gamma S(x,x)\right)\mathrm{tr}\left(\Gamma S(x_0,x_0)\right)\rangle$$

5.2.3 Stochastic Evaluation of Disconnected Loops

The simple one consist to evaluate stochastically the disconnected contribution without any variance reduction techniques. Considering a general volume source ξ, we define ϕ using the Dirac operator D:

$$\phi=D^{-1}\xi$$

For a given element X of the basis defined in the previous section, we then have

$$\sum\left(\xi^* X\phi\right)_R=\sum XM^{-1}+\text{noise}$$

where the symbol $(\ldots)_R$ refers to the average over R samples of the stochastic source.

It should be observed that in evaluating the disconnected contributions to the neutral meson correlators each one of the two quark loops arising from Wick contractions must be averaged over completely *independent* smaples of stochastic sources for the purpose of avoiding unwanted biases.

Implemented Source Types

We use XX noise sources. The user can switch between the following different source types

- type 0: Pure volume source
- type 1: Gauge fixed wall source
- type 2: Volume sources with time and spin dilution
- type 3: Volume sources with time, spin and color dilution
- type 4: Volume source with time, spin, color and even-odd dilution
- type 6: Volume source with spin, color and even-odd dilution

5.2.4 Output

The code does not perform any average on the stochastic noise or on the dilution indices. This allows to keep as much information as possible and to vary the number of stochastic sources at the analysis level.

The indices are always

```
#T #iGamma #iSrc #\[color and/or e/o \] #Re #Im
```

where iGamma refers to the index of the Gamma matrix defined in Table 1.

5.2.5 Debugging Options

If the code is executed with the following additional arguments

the code will read the two files and perform the contraction accordingly computing $\chi^\dagger \Gamma \psi$

5.3 Mesonic Correlators of the Isotriplet

The two fermionic flavors are denoted by u and d. We are interested in the mesonic correlators

$$C_{\Gamma_1,\Gamma_2}(x-y) = \left\langle (\bar{u}\Gamma_1 d)^\dagger (x) (\bar{u}\Gamma_2 d)(y) \right\rangle = \\ = \left\langle \left(\bar{d}\gamma_0\Gamma_1^\dagger\gamma_0 u\right)(x) (\bar{u}\Gamma_2 d)(y) \right\rangle$$

where Γ_i are the generic producs of the γ-matrices.

We can integrate out the fermionic fields explicitly. Here we use the definition $H(x,y) = G(x,y)\gamma_5$ for the hermitian Dirac operator, with $G(x,y)$ defined as its inverse.

$$\begin{aligned} C_{\Gamma_1,\Gamma_2}(x-y) &= -\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 G(x,y)\Gamma_2 G(y,x)\right]\right\rangle = \\ &= -\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 G(x,y)\Gamma_2\gamma_5 G(x,y)^\dagger\gamma_5\right]\right\rangle = \\ &= -\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 H(x,y)\gamma_5\Gamma_2 H(x,y)^\dagger\gamma_5\right]\right\rangle \ . \end{aligned}$$

Since the γ-matrices commute, we can conclude that the matrix $\gamma_0\Gamma^\dagger\gamma_0$ is equal to Γ up to a sign

$$\gamma_0\Gamma^\dagger\gamma_0 = s(\Gamma)\Gamma \qquad \text{with } s(\Gamma) = \pm 1 \ .$$

In addition, a generic matrix Γ has the following properties:

1. Its matrix elements can be 0, ± 1, $\pm i$
2. Its entries are either all real or all imaginary
3. In each row and correspondingly each column, there is only one non-zero element

Consequently, we can write

$$\Gamma_{\alpha\beta} = t_\alpha(\Gamma)\delta_{\sigma_\alpha(\Gamma),\beta}$$

where $\sigma(\Gamma)$ constitutes a permutation of four elements. Putting this together we find

$$\begin{aligned} C_{\Gamma_1,\Gamma_2}(x-y) &= -s(\Gamma_1)\left\langle \mathrm{tr}\left[\gamma_5\Gamma_1 H(x,y)\gamma_5\Gamma_2 H(x,y)^\dagger\right]\right\rangle = \\ &= -s(\Gamma_1)\sum_{\alpha\beta} t_\alpha(\gamma_5\Gamma_1)t_\beta(\gamma_5\Gamma_2)\times\left\langle \mathrm{tr}\left[H_{\sigma_\alpha(\gamma_5\Gamma_1),\beta}(x,y)H_{\alpha,\sigma_\beta(\gamma_5\Gamma_2)}(x,y)^\dagger\right]\right\rangle \ . \end{aligned}$$

5.3.1 Implementation of the Point-To-All Propagator

In order to calculate mesonic masses we are interested in correlators satisfying $\Gamma_1 = \Gamma_2$. Using translational invariance, we can set $y = 0$. In this case the formula simplifies to

$$C_\Gamma(x) = -s(\Gamma)\sum_{\alpha\beta} t_\alpha(\gamma_5\Gamma)t_\beta(\gamma_5\Gamma)\times\left\langle \mathrm{tr}\left[H_{\sigma_\alpha(\gamma_5\Gamma),\beta}(x,0)H_{\alpha,\sigma_\beta(\gamma_5\Gamma)}(x,0)^\dagger\right]\right\rangle \ . \tag{5.5}$$

This is implemented into HiRep in the following way

- The data of the point-like source $\xi^{(\alpha,a)}$ defined by

  $$\xi^{(\alpha,a)}_{\beta b}(x) = \delta_{\alpha,\beta}\delta_{a,b}\delta_{x,0} \ ,$$

  The function `quark_propagator` applies the inverse of the hermitian Dirac operator to the source

  $$\eta^{(\alpha,a)} = H\xi^{(\alpha,a)} \qquad \eta^{(\alpha,a)}_{\beta b}(x) = H^{ba}_{\beta\alpha}(x,0) \ .$$

- The functions `void *_correlator(float *out, suNf_spinor **qp)`in `Observables/mesons.c` implement the formulae (5.5), where `out` stands for the correlator and `qp` for the spinor array. The functions $s(\Gamma)$, $t_\alpha(\gamma_5\Gamma)$ and $\sigma_\alpha(\gamma_5\Gamma)$ where calculated using `Mathematica`, see file `mesons.nd` and implemented in the code using macros, defined as follows\

_C1_ =$\sigma_1(\gamma_5\Gamma)$
_C2_ =$\sigma_2(\gamma_5\Gamma)$
_C3_ =$\sigma_3(\gamma_5\Gamma)$
_C4_ =$\sigma_4(\gamma_5\Gamma)$

If $t_\alpha(\gamma_5\Gamma)$ are read:

_S0_ =$-s(\Gamma)$
_S1_ =$t_1(\gamma_5\Gamma)$
_S2_ =$t_2(\gamma_5\Gamma)$
_S3_ =$t_3(\gamma_5\Gamma)$
_S4_ =$t_4(\gamma_5\Gamma)$

whereas if $t_\alpha(\gamma_5\Gamma)$ are imaginary:

_S0_ =$s(\Gamma)$
_S1_ =$-it_1(\gamma_5\Gamma)$
_S2_ =$-it_2(\gamma_5\Gamma)$
_S3_ =$-it_3(\gamma_5\Gamma)$
_S4_ =$-it_4(\gamma_5\Gamma)$

5.4 Mesonic Correlators of the Isosinglet

We are now concerned with the genertic mesonic correlator given by

$$C_{\Gamma_1,\Gamma_2}(x-y) = \left\langle \left(\bar{u}\gamma_0\Gamma_1^\dagger\gamma_0 u\right)(x)\,(\bar{u}\Gamma_2 u)\,(y)\right\rangle$$

considering only a single flavor u.

Integration of the fermionic fields now yiels one additional term, the hairpin diagram

$$\begin{aligned} C_{\Gamma_1,\Gamma_2}(x-y) &= -\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 G(x,y)\Gamma_2 G(y,x)\right]\right\rangle + \left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 G(x,x)\right]\mathrm{tr}\left[\Gamma_2 G(y,y)\right]\right\rangle \\ &= -\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 H(x,y)\gamma_5\Gamma_2 H(x,y)^\dagger\gamma_5\right]\right\rangle + \left\langle \mathrm{tr}\left[\gamma_5\gamma_0\Gamma_1^\dagger\gamma_0 H(x,x)\right]\mathrm{tr}\left[\gamma_5\Gamma_2 H(y,y)\right]\right\rangle \ . \end{aligned}$$

All other contributions are identical to the contributions to the isotriplet correlator. We can, therefore, focus on the contribution through the hairpin diagram. Using the formulae `eq:gamma0_adj` we can write

$$\left\langle \mathrm{tr}\left[\gamma_0\Gamma_1^\dagger\gamma_0 G(x,x)\right]\mathrm{tr}\left[\Gamma_2 G(y,y)\right]\right\rangle = \quad = s(\Gamma_1)\sum_{\alpha\beta} t_\alpha(\Gamma_1)t_\beta(\Gamma_2)\times\left\langle \mathrm{tr}G_{\sigma_\alpha(\gamma_5\Gamma_1),\alpha}(x,x)\ \mathrm{tr}G_{\sigma_\beta(\gamma_5\Gamma_2),\beta}(y,y)\right\rangle \ . \tag{5.6}$$

5.4.1 All-to-all Propagator

It is clear from (5.6), from the fact that we are employing point source, that one must compute the entire inverse matrix of the Dirac operator. The alternative is to use a statistic estimate for H followed by variance reduction procedures.

Suppose there are N_s available random fermion sources $\xi^{(i)}$ such that the only non-zero correlators are

$$\left\langle \xi^{(i)}_{\alpha a}(x)^\dagger \xi^{(j)}_{\beta b}(y) \right\rangle = \delta_{\alpha,\beta}\delta_{a,b}\delta_{x,y}\delta_{i,j} \ .$$

Current literature proposes mainly either Gaussian noise or Z_2 noise. In the following, we will choose Z_2 noise, following [FM99]. Each component of the spinor is randomly chosen from the values $\pm 1/\sqrt{2}$.

Then the matrix H can be estimated as follows:

$$H^{ab}_{\alpha\beta}(x,y) \simeq \sum_{i=1}^{N_s} \eta^{(i)}_{\alpha a}(x)\xi^{(i)}_{\beta b}(y)^\dagger \eta^{(i)} \equiv H\xi^{(i)} \tag{5.7}$$

Stochastic estimation can then be used to calculate the relevant tracks for correlators

$$\mathrm{tr}\left[\Gamma_1 G(x,y)\Gamma_2 G(y,x)\right] = \sum_{ij} \xi^{(i)}(x)^\dagger \gamma_5\Gamma_1\eta^{(j)}(x) \times \xi^{(j)}(y)^\dagger\gamma_5\Gamma_2\eta^{(i)}(y)$$

$$\mathrm{tr}\left[\Gamma G(x,x)\right] = \sum_{i} \xi^{(i)}(x)^\dagger \gamma_5\Gamma\eta^{(i)}(x) \, .$$

5.4.2 Variance reduction

The noise obtained from stochastic estimation of the matrix G in the formula `naive_noisy_estimate` can be reduced using the trick from [MM01] for Wilson fermions. Here, the Dirac operator has the form $D = 1 - K$. As a result, for the matrix G the following formula applies

$$\begin{aligned} G = D^{-1} = (1-K)^{-1} = \\ = 1 + K + \cdots + K^m + K^{n_1} G K^{n_2} \end{aligned}$$

with $n_1 + n_2 = n = m + 1$. In particular, for the evaluation of the hairpin diagram

$$\begin{aligned} \mathrm{tr}\left[\Gamma G(x,x)\right] = \quad & \mathrm{tr}\Gamma + \mathrm{tr}\left[\Gamma K^4\right](x,x) + \mathrm{tr}\left[\Gamma K^6\right](x,x) + \cdots + \\ & + \mathrm{tr}\left[\Gamma K^{2k}\right](x,x) + \mathrm{tr}\left[\Gamma K^{n_1} G K^{n_2}\right](x,x) \end{aligned}$$

with $m = 2k$. (TODO: fix this sentence) Here, we can use the fact that the matrix K connects first neighboring sites as thus $K^p(x,x) \neq 0$ only when p is even. Further, $r_0 = 1$ and consequently $K^2(x,x) = 0$ The first $k+1$ terms can be calculated explicitly and we can estimate the last term stochastically.

$$\begin{aligned} \mathrm{tr}\left[\Gamma G(x,x)\right] = & \mathrm{tr}\Gamma + \mathrm{tr}\left[\Gamma K^4\right](x,x) + \mathrm{tr}\left[\Gamma K^6\right](x,x) + \cdots + \\ & + \mathrm{tr}\left[\Gamma K^{2k}\right](x,x) + \sum_{iy} \xi^{(i)}(y)^\dagger \gamma_5 K^{n_2}(y,x)\Gamma K^{n_1}(x,y)\eta^{(i)}(y) \end{aligned}$$

[MM01] use this trick only for the calculation of the hairpin diagram. It might be possible to generalize it to the the isotriplet part as well, as an alternative to the point-to-all propagator.

5.4.3 Time dilution

This is a trick introduced in [FJC+05] for noise reduction in the computation of null-moment propagators. Whenever stochastic estimation of the H matrix is required, such as in (5.7), it is possible to replace each stochastic source $\xi^{(i)}$ with a set of sources each with support on a different time slice.

$$\xi^{(i)} \to \xi^{(i,\tau)}(\mathbf{x},t) = \xi^{(i)}(\mathbf{x},t)\delta_{t,\tau}$$

Stochastic estimation is now obtained similarly to the naive case:

$$H^{ab}_{\alpha\beta}(x,y) \simeq \sum_{i=1}^{N_s}\sum_{\tau=1}^{N_t} \eta^{(i,\tau)}_{\alpha a}(x)\xi^{(i,\tau)}_{\beta b}(y)^\dagger \eta^{(i,\tau)} \equiv H\xi^{(i,\tau)} \tag{5.8}$$

5.4.4 Implementation Scheme

TODO: Add this to function reference instead if this is still implemented this way

The following functions will be implemented

- Calculation of the exact terms of the formula `hairpin_with_variance_reduction`
- `void GAMMA_variance_reduction_exact_terms(float *out, int k)`

  Here, `out` is a real vector with its components equal to the volume and k corresponds to the index in the γ-matrix.

  This function evaluates

  $$h_k(x) = \mathrm{tr}\left[\Gamma K^{2k}\right](x,x) = \left(\frac{\kappa}{2}\right)^{2k}\sum_{\mathcal{C}_x}\mathrm{tr}\left(\Gamma\tilde{\gamma}(\mathcal{C}_x)\right)\mathcal{W}(\mathcal{C}_x)$$

  where $\mathcal{C}_x = (x,\hat{\mu}_1,\hat{\mu}_2,\dots,\hat{\mu}_{2k})$ is the generic closed path of x of length $2k$ obtained by moving from x in the directions $\hat{\mu}_i$. $\mathcal{W}(\mathcal{C}_x)$ is the trace of the parallel transport through $\mathcal{C}_x$ in the corresponding fermionic representation. $\tilde{\gamma}(\mathcal{C}_x)$. is the matrix defined as

  $$\tilde{\gamma}(\mathcal{C}_x) = (1-\gamma_{\hat{\mu}_1})(1-\gamma_{\hat{\mu}_2})\cdots(1-\gamma_{\hat{\mu}_{2k}})$$

  having defined $\gamma_{-\hat{\mu}_i} = -\gamma_{\hat{\mu}_i}$.

  It should be noted that since $(1-\gamma_{\hat{\mu}_i})(1-\gamma_{-\hat{\mu}_i}) = 0$, one can exclude the paths in which a pair of subsequences $(\dots,\hat{\mu}_i,-\hat{\mu}_i,\dots)$ appears from the sum. In addition, the matrix $\tilde{\gamma}(\mathcal{C}_x)$ does not depend on x. There is is convenient to compute the list of paths and the matrix $\tilde{\gamma}(\mathcal{C}_x)$ only once.

- It is convenient to have a function that calculates the traces of the parallel transports:
- `void tr_r_pexp(complex *out, int *path, int length)`

  Here again `out` is the complex vector with number of components according to the volume and $\phi(x)\backslash$ is the number of directions (`length`) of which the path is composed.

  This returns

  $$\phi(x) = \mathrm{tr}_{\mathbf{R}}\left[U_{x,\hat{\mu}_1}U_{x+\hat{\mu}_1,\hat{\mu}_2}\cdots\right]$$

- Calculation of the time-diluted estimators

  ```
  void time_diluted_stochastic_estimate
  (suNf_spinor *csi, suNf_spinor **eta,
  int nm, float *mass, double ac)\
  ```

  With the parameters: `csi` is the spinor ξ
  `path` is the list of $N_t \times \mathrm{nm}$ spinors along the $\eta^{(\tau,m)}$ \

  This function generates the spinor ξ with Z_2 noise. Here the spinors are defined as

$$\xi^{(\tau)}(\mathbf{x},t) = \xi(\mathbf{x},t)\delta_{t,\tau}$$

and then returned as

```
$$\eta^{(\tau,m)} \equiv H_m \xi^{(\tau)}$$

using the inverter of the Dirac operator with parameters `nm`, `mass` and `acc`.

The calculation of the hairpin term

` `\
` void GAMMA_hairpin_VR_TD(float **out,`\
`      int n1, int n2, int nrs,`\
`      int nm, float *mass, double acc)`\

Takes the parameters
                `out` = list of real `nm` vectors with the number of components␣
↪corresponding to the volume
                ` n1, n2 ` = parameters of the variance reduction algorithm
                ` nrs ` = number of random sources for the statistical estimation
                ` nm, mass ` = number and list of masses
                `acc` = inverter parameter
    ` `\
```

The functions above implement the formula (5.8), summing exact terms and the statistical term, generated with `nrs` to dilute, for a total of $\times N_t$ matrix invertions for each mass value and returns the result as `out`.

6 Writing A Program in HiRep

6.1 Global Objects

Structures and variables that are stored in `global.h`.

6.2 Blablabla

Bibliography

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