1 Notation

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. [**?**], but using Hermitian generators

$$T^{a\dagger} = T^a. \tag{1}$$

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

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

For a generic representation R, we define:

$$\begin{aligned} \mathrm{tr}_R\left(T^a T^b\right) &= T_R \delta^{ab}, & (3)\\ \sum_a \left(T^a T^a\right)_{AB} &= C_2(R)\delta_{AB}, & (4) \end{aligned}$$

which implies:

$$T_R = \frac{1}{N^2-1} C_2(R) d_R \tag{5}$$

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:

$$C_2(R) = \frac{1}{2}\left(nN + \sum_{i=1}^{m} n_i\left(n_i + 1 - 2i\right) - \frac{n^2}{N}\right) \tag{6}$$

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.

Table 1: Group invariants

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:

$$\begin{aligned} (X,Y) &= \mathrm{tr}\ \left(X^\dagger Y\right) = T_f X^a Y^a, & (7)\\ \|X\|^2 &= \mathrm{tr}\left(X^\dagger X\right) = \sum_{ij} |X_{ij}|^2 & (8) \end{aligned}$$

2 The Dirac operator

The massless Dirac operator is written as in Ref. [**?**]:

$$D = \frac{1}{2}\left\{\gamma_\mu\left(\nabla_\mu + \nabla^*_\mu\right) - \nabla^*_\mu\nabla_\mu\right\} \tag{9}$$

with

$$\begin{aligned}\nabla_\mu\phi(x) &= U^R(x,\mu)\phi(x+\mu) - \phi(x) &(10)\\ \nabla^*_\mu\phi(x) &= \phi(x) - U^R(x-\mu,\mu)^\dagger\phi(x-\mu) &(11)\end{aligned}$$

and therefore the action of the massive Dirac operator yields:

$$\begin{aligned}D_m\phi(x) &= (D+m)\phi(x)\\ &= -\frac{1}{2}\left\{(1-\gamma_\mu)\,U^R(x,\mu)\phi(x+\mu) + (1+\gamma_\mu)\,U^R(x-\mu,\mu)^\dagger\phi(x-\mu) - \right.\\ &\quad \left. -(8+2m)\phi(x)\right\}, \qquad (12)\end{aligned}$$

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:

$$S_f = \sum_{x,y}\phi^\dagger(x)D_m(x,y)\phi(y), \tag{13}$$

where

$$D_m(x,y) = \delta_{x,y} - \frac{\kappa}{2}\left[(1-\gamma_\mu)U^R(x,\mu)\delta_{y,x+\mu} + (1+\gamma_\mu)U^R(x-\mu,\mu)^\dagger\delta_{y,x-\mu}\right], \tag{14}$$

and the Hermitian Dirac operator is obtained as:

$$Q_m = \gamma_5 D_m. \tag{15}$$

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

$$\left(\det D_m\right)^{N_f} = \int \mathcal{D}\phi\mathcal{D}\phi^\dagger e^{-\phi^\dagger Q_m^{-N_f}\phi} \equiv \int \mathcal{D}\phi\mathcal{D}\phi^\dagger e^{-S_{\rm pf}}. \tag{16}$$

3 Force for the HMC molecular dynamics

The HMC Hamiltonian is given by:

$$\mathcal{H} = \mathcal{H}_\pi + \mathcal{H}_G + \mathcal{H}_F\,, \tag{17}$$

where

$$\begin{aligned}\mathcal{H}_\pi &= \frac{1}{2}\sum_{x,\mu}(\pi(x,\mu),\pi(x,\mu)) = \frac{1}{2}T_f\sum_{a,x,\mu}\pi^a(x,\mu)^2\,, &(18)\\ \mathcal{H}_G &= \beta\sum_{\mu<\nu}\left(1 - \frac{1}{N}\mathrm{Re\ tr}\ \mathcal{P}_{\mu\nu}\right), &(19)\\ \mathcal{H}_F &= \phi^\dagger(Q_m^2 - \beta)^{-l}\phi\,,\quad l = \frac{N_f}{2} > 0\,, &(20)\end{aligned}$$

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 $\dot{\Box}$ indicates the derivative with respect to the molecular dynamics time):

$$\dot{U}(x\mu) = \pi(x,\mu)U(x,\mu)\,, \tag{21}$$

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:

$$0 = \dot{\mathcal{H}} = \dot{\mathcal{H}}_\pi + \dot{\mathcal{H}}_G + \dot{\mathcal{H}}_F\,. \tag{22}$$

For the first two derivatives we have:

$$\dot{\mathcal{H}}_\pi = \sum_{x,\mu}(\pi(x,\mu),\dot{\pi}(x,\mu)) = T_f\sum_{x,\mu}\sum_a \pi^a(x,\mu)\dot{\pi}^a(x,\mu) \tag{23}$$

$$\begin{aligned}\dot{\mathcal{H}}_G &= \sum_{x,\mu} -\frac{\beta}{N}\text{Re tr }\left[\dot{U}(x,\mu)V^\dagger(x,\mu)\right] = \\ &= \sum_{x,\mu} -\frac{\beta}{N}\text{Re tr }\left[\pi(x,\mu)U(x,\mu)V^\dagger(x,\mu)\right] = \\ &= \sum_{x,\mu}\sum_a -\frac{\beta}{N}\pi^a(x,\mu)\text{Re tr }\left[iT_f^aU(x,\mu)V^\dagger(x,\mu)\right]\,,\end{aligned} \tag{24}$$

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:

$$\dot{\mathcal{H}}_F = -\,\phi^\dagger(Q_m^2-\beta)^{-1}(\dot{Q_m^2})(Q_m^2-\beta)^{-1}\phi\,. \tag{25}$$

Defining:

$$\eta = (Q_m^2-\beta)^{-1}\phi\,, \tag{26}$$

$$\xi = Q_m\eta\,, \tag{27}$$

and using the fact that the matrix $(Q_m^2-\beta)$ is hermitean, we can rewrite Eq.(25) as

$$\dot{\mathcal{H}}_F = -2\;\xi^\dagger(\dot{Q_m})\eta\,. \tag{28}$$

Inserting the explicit form of Q_m, Eq.s (15) and (12), into Eq.(28) we obtain

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

$$= \mathrm{Re}\ \sum_{x,\mu} \xi(x)^\dagger \dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\eta(x+\mu) + \eta(x)^\dagger \dot{U}^R(x,\mu)\gamma_5(1-\gamma_\mu)\xi(x+\mu) \quad (29)$$

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

$$\dot{U}^R(x,\mu) = \pi^R(x,\mu)U^R(x,\mu) = i\pi^a(x,\mu)T_R^a U^R(x,\mu) \quad (30)$$

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.(30) in the expression for $\dot{\mathcal{H}}_F$ we find (capitalized Tr indicates the trace over color *and* spin indices as opposed to the lower case tr which is the trace over color only)

$$\dot{\mathcal{H}}_F = \sum_{x,\mu}\sum_a \pi^a(x,\mu)\mathrm{Re\ Tr}\ \left[iT_R^a U^R(x,\mu)\gamma_5(1-\gamma_\mu)\left\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\right\}\right] . \quad (31)$$

Inserting Eq.s (23),(24),(31) into Eq. (22) we obtain the equation of motion for the momenta $\pi^a(x,\mu)$

$$\dot{\pi}^a(x,\mu) = \dot{\pi}^a_G(x,\mu) + \dot{\pi}^a_F(x,\mu)\,, \quad (32)$$

$$\dot{\pi}^a_G(x,\mu) = \frac{\beta}{N}\frac{1}{T_f}\mathrm{Re\ tr}\ \left[iT_f^a U(x,\mu)V^\dagger(x,\mu)\right]\,, \quad (33)$$

$$\dot{\pi}^a_F(x,\mu) = -\frac{1}{T_f}\mathrm{Re\ Tr}\ \left[iT_R^a U^R(x,\mu)\gamma_5(1-\gamma_\mu)\left\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\right\}\right] . \quad (34)$$

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

$$P_R^a(F) = -\frac{1}{T_R}\mathrm{Re\ tr}\ \left[iT_R^a F\right]\,, \quad (35)$$

we can be used to rewrite Eq.s (33)-(34) in a more compact form:

$$\dot{\pi}^a_G(x,\mu) = -\frac{\beta}{N}P_f^a\left(U(x,\mu)V^\dagger(x,\mu)\right)\,, \quad (36)$$

$$\dot{\pi}^a_F(x,\mu) = \frac{T_R}{T_f}P_R^a\left(U^R(x,\mu)\mathrm{tr_{spin}}\left[\gamma_5(1-\gamma_\mu)\left\{\eta(x+\mu)\otimes\xi(x)^\dagger + \xi(x+\mu)\otimes\eta(x)^\dagger\right\}\right]\right) . \quad (37)$$

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) [**?**]. We agree with Eq. (16) in Ref. [**?**], provided that we exchange the indices a and b in that formula.

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:

$$P_S(\phi)P_M(\phi \to \phi') = P_S(\phi')P_M(\phi' \to \phi)\,. \tag{38}$$

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

$$P_M(\phi \to \phi') = \int d\pi d\pi' P_k(\pi)P_h((\phi, \pi) \to (\phi', \pi'))P_A((\phi, \pi) \to (\phi', \pi'))\,, \tag{39}$$

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 garantee 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 garantees the reversibility condition. The resulting probability P_h is then a delta function (the process is completly deterministic). Numerical integration to a given accuracy will result in a broader

distribution and care must be taken to garantee 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 to 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 stocastic extimates 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.

6 RHMC formulation

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

$$\mathcal{H}_F = \sum_{k=1}^{N_{pf}} \phi_k^\dagger (Q_m^2)^{-l_k} \phi_k \ ; \ \sum_k l_k = \frac{N_f}{2} \,, \tag{40}$$

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

$$\forall k, \ l_k = \frac{N_f}{2N_{pf}} \,. \tag{41}$$

In the RHMC algorithm [**?**] 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. (40) (we need only one approximation because all l_k are equal):

$$\mathcal{H}_F = \sum_{k=1}^{N_{pf}} \phi_k^\dagger r_a(Q_m^2) \phi_k \,, \tag{42}$$

$$(Q_m^2)^{-\frac{N_f}{2N_{pf}}} \simeq r_a(Q_m^2) = \alpha_0^a + \sum_{n=1}^{d_1} \alpha_n^a (Q_m^2 - \beta_n^a)^{-1} \,. \tag{43}$$

Using the formulas derived in Section 3, it is easy to write the force corresponding to Eq. (42). In fact, Eq. (42) is nothing but a sum of terms of the form Eq. (42) once we put $l = 1$, $\beta = \beta_n^a$. The RHMC force will be then given by a sum over $n = 1, \ldots, d_1$ of terms given by Eq.(37) multiplied by a factor α_n^a. Notice that since $l = 1$, to compute η as in Eq.(26) a simple shifted inversion is required.

The second rational approxmation is required in the heatbath update of pseudofermions. In order to generate pseudofermions distributed as in Eq. (40), a simple two-step process is used. For each pseudofermion we first generate a gaussian distributed field $\tilde{\phi}_k$:

$$P(\tilde{\phi}_k) \propto \exp[-\tilde{\phi}_k^\dagger \tilde{\phi}_k]\,, \tag{44}$$

and then we set:

$$\phi_k = (Q_m^2)^{\frac{l_k}{2}} \tilde{\phi}_k\,, \tag{45}$$

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):

$$(Q_m^2)^{\frac{l_k}{2}} \simeq r_b(Q_m^2) \quad = \quad \alpha_0^b + \sum_{n=1}^{d_2} \alpha_n^b (Q_m^2 - \beta_n^b)^{-1}\,. \tag{46}$$

The third rational approximation is used in the code for the Metropolis test. Starting from Eq. (40), for each pseudofermion we can rewrite:

$$\phi_k^\dagger (Q_m^2)^{-l_k} \phi_k = \left\| (Q_m^2)^{-\frac{l_k}{2}} \phi_k \right\|^2\,, \tag{47}$$

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

$$(Q_m^2)^{-\frac{l_k}{2}} \simeq r_c(Q_m^2) \quad = \quad \alpha_0^c + \sum_{n=1}^{d_3} \alpha_n^c (Q_m^2 - \beta_n^c)^{-1}\,. \tag{48}$$

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 dinamics.

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:

$$D_m = \begin{pmatrix} 4+m & D_{eo} \\ D_{oe} & 4+m \end{pmatrix} \ , \tag{49}$$

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):

$$\gamma_5 D_{eo} \gamma_5 = D_{oe}^\dagger \ . \tag{50}$$

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

$$\det\, D_m = \det\, ((4+m)^2 - D_{oe} D_{eo}) = \det\, ((4+m)^2 - D_{eo} D_{oe}) \equiv \det\, D_m^{eo} \ , \tag{51}$$

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:

$$\mathcal{H}_F = \phi_e^\dagger ((Q_m^{eo})^2 - \beta)^{-1} \phi_e \ , \tag{52}$$

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.(28) is unchanged :

$$\dot{\mathcal{H}}_F = -2 \ \xi_e^\dagger (\dot{Q_m^{eo}}) \eta_e \, , \tag{53}$$

where as before we have defined:

$$\eta_e = ((Q_m^{eo})^2 - \beta)^{-1} \phi_e \, , \tag{54}$$

$$\xi_e = Q_m^{eo} \eta_e \, . \tag{55}$$

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

$$(\dot{Q_m^{eo}}) = -\gamma_5 (\dot{D_{eo}} D_{oe} + D_{eo} \dot{D_{oe}}) \ . \tag{56}$$

Defining

$$\sigma_o = D_{oe} \eta_e \, , \tag{57}$$

$$\rho_o = D_{oe} \xi_e \, , \tag{58}$$

and inserting Eq.(56) into Eq.(53), we find:

$$\dot{\mathcal{H}}_F = - \sum_{\mu, x \in even} \mathrm{Tr}_{x,\mu} \left[\sigma_o(x+\mu) \otimes \xi_e(x)^\dagger + \rho_o(x+\mu) \otimes \eta_e(x)^\dagger \right] - \\ - \sum_{\mu, x \in odd} \mathrm{Tr}_{x,\mu} \left[\xi_e(x+\mu) \otimes \sigma_o(x)^\dagger + \eta_e(x+\mu) \otimes \rho_o(x)^\dagger \right] \tag{59}$$

and for convenience we use the shorthand notation:

$$\mathrm{Tr}_{x,\mu} \left[\Phi \right] \equiv \mathrm{Re \ Tr} \ \left[\dot{U}^R(x,\mu) \gamma_5 (1 - \gamma_\mu) \Phi \right] \ . \tag{60}$$

From Eq.(59) 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 $x \in even$:

$$\dot{\pi}_F^a(x,\mu) = -\frac{T_R}{T_f} P_R^a \left(U^R(x,\mu) \mathrm{tr}_{\mathrm{spin}} \left[\gamma_5 (1-\gamma_\mu) \right. \right. \\ \left. \left. \left\{ \sigma_o(x+\mu) \otimes \xi_e(x)^\dagger + \rho_o(x+\mu) \otimes \eta_e(x)^\dagger \right\} \right] \right) , \qquad (61)$$

while for $x \in odd$:

$$\dot{\pi}_F^a(x,\mu) = -\frac{T_R}{T_f} P_R^a \left(U^R(x,\mu) \mathrm{tr}_{\mathrm{spin}} \left[\gamma_5 (1-\gamma_\mu) \right. \right. \\ \left. \left. \left\{ \xi_e(x+\mu) \otimes \sigma_o(x)^\dagger + \eta_e(x+\mu) \otimes \rho_o(x)^\dagger \right\} \right] \right) . \qquad (62)$$

8 Conventions used in the code

8.1 Representations

The hermitean generators T_f^a for the fundamental representation used are of the form:

$$\begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} , \begin{pmatrix} 0 & i & 0 & \dots \\ -i & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} , \begin{pmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & -2 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} , \qquad (63)$$

normalized so that $T_f = 1/2$. The generators for the other representations will be obtained in the following.

We first give the explicit form for the representation functions R which map $U \to U^R$. We define for each representation an orthonormal base e_R for the appropriate vector space of matrices.

For the Adjoint representation we define the base e_{Adj} for the $N \times N$ traceless hemitean matrices to be $e_{Adj}^a = T_f^a / \sqrt{T_f}$, $a = 1, \dots, N^2 - 1$ (i.e. proportional to the generators of the fundamental representation and normalized to 1.)

For the two-index Symmetric representation the base $e_S^{(ij)}$, with $i \le j$, for the $N \times N$ symmetric matrices is given by:

$$i \neq j , \quad e_S^{(ij)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} , \qquad (64)$$

$$i = j , \quad e_S^{(ii)} = \begin{pmatrix} 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} , \qquad (65)$$

where the non zero entries are at position (i,j), etc.

For the two-index Antisymmetric representation the base $e^{(ij)}_{AS}$, with $i < j$, for the $N \times N$ symmetric matrices is given by:

$$e^{(ij)}_{AS} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 & \dots \\ -1 & 0 & 0 & \dots \\ 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix}, \tag{66}$$

where, as above, the non zero entries are at position (i, j).

The maps R are explicitly given by:

$$(R^{Adj}U)_{ab} = U^{Adj}_{ab} = \text{tr}\, \left[e^a_{Adj} U e^b_{Adj} U^\dagger \right] , a, b = 1, \dots, N^2 - 1 , \tag{67}$$

$$(R^S U)_{(ij)(lk)} = U^S_{(ij)(lk)} = \text{tr}\, \left[(e^{(ij)}_S)^\dagger U e^{(lk)}_S U^T \right] , i \le j, l \le k , \tag{68}$$

$$(R^A U)_{(ij)(lk)} = U^A_{(ij)(lk)} = \text{tr}\, \left[(e^{(ij)}_A)^\dagger U e^{(lk)}_A U^T \right] , i < j, l < k . \tag{69}$$

The generators T^a_R used are defined as the image of the generators in the fundamental under the differential of the maps R defined above: $T^a_R = R_* T^a_f$. Explicit expression can easily be worked out form the definition above. The invariants T_R and $C_2(R)$ for the generators defined in this way are given in Table (1).

8.2 γ matrices

We use the chiral representation for the Dirac γ matrices:

$$\gamma_\mu = \begin{pmatrix} 0 & e_\mu \\ e^\dagger_\mu & 0 \end{pmatrix} , \tag{70}$$

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

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} , \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} , \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{71}$$

We have:

$$\gamma_5 = \gamma_0\gamma_1\gamma_2\gamma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} . \tag{72}$$

9 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:

$$f_{\Gamma\Gamma'}(t) = \sum_{\mathbf{x}} \langle \bar\psi(\mathbf{x}, t)\Gamma\psi(\mathbf{x}, t)\bar\psi(0)\Gamma'\psi(0)\rangle \tag{73}$$

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:

$$Q_{AB}(x-y)\eta_B^{\bar{A},x_0}(y) = \delta_{A,\bar{A}}\delta_{x,x_0} \tag{74}$$

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:

$$\langle\ldots\rangle = -\tilde{\Gamma}_{AB}\eta_B^{C,y}(x)\tilde{\Gamma}'_{CD}\eta_A^{D,y}(x)^* \tag{75}$$

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