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Higher representations on the lattice: Numerical simulations.
SU(2) with adjoint fermions.

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We discuss the lattice formulation of gauge theories with fermions in arbitrary representations of the color group, and present in detail the implementation of the HMC/RHMC algorithm for simulating dynamical fermions. We discuss the validation of the implementation through an extensive set of tests, and the stability of simulations by monitoring the distribution of the lowest eigenvalue of the Wilson-Dirac operator. Working with two flavors of Wilson fermions in the adjoint representation, benchmark results for realistic lattice simulations are presented. Runs are performed on different lattice sizes ranging from $4^3 \times 8$ to $24^3 \times 64$ sites. For the two smallest lattices we also report the measured values of benchmark mesonic observables. These results can be used as a baseline for rapid cross-checks of simulations in higher representations. The results presented here are the first steps towards more extensive investigations with controlled systematic errors, aiming at a detailed understanding of the phase structure of these theories, and of their viability as candidates for strong dynamics beyond the Standard model.

I. INTRODUCTION

Recent algorithmic progress in simulations of QCD with dynamical fermions have shown that current computing facilities can reach beyond the quenched approximation without compromising the robustness of the formulation [1,6]. Besides their great relevance for lattice QCD, these improvements allow numerical simulations to be used as a quantitative, nonperturbative tool to study more generic strongly–interacting theories where the role of the fermion determinant is crucial: extensive Monte Carlo studies will enable to tame the systematic errors and therefore to obtain reliable information about the strong dynamics of theories beyond QCD. Examples that have a direct impact on physics beyond the Standard Model (BSM) include technicolor models [2,8] (see [9,10] for reviews), orientifold theories [11], and supersymmetry (see [12] for a recent review on the nonperturbative formulation of supersymmetry). Moreover the theoretical progresses in formulating QCD on the lattice provide the necessary tools for rigorous studies of BSM nonperturbative phenomena. This is of paramount importance in order to obtain reliable results as we move into the unknown territories of strongly–interacting BSM theories: the clean field–theoretical framework developed for QCD needs to be exported to the studies of BSM strong dynamics in order to obtain lattice results that are trustable and therefore can have an impact on the LHC phenomenology.

Simulations of the theories listed above share a common technical challenge: they all require fermion fields in representations larger than the fundamental, gauge groups SU($N$) with generic number of colors $N$, or a combination of both. Therefore a central ingredient of these simulations is a generalized Dirac operator, that can act on vectors of arbitrary dimension in color space. We developed such an operator and tested its inversion in a recent study of the quenched meson spectrum in the large-$N$ limit of pure Yang–Mills theories [13]. The same computational framework has also been used to assess the validity of the planar orientifold equivalence by numerical simulations in the quenched approximation [14].

Theories with two Dirac fermions in the two–index symmetric representation and small number of colors ($N = 2, 3$) are currently under scrutiny as viable candidates for strongly–interacting BSM candidates [15–17]. An important feature of these theories is that the number of fermions is close to the critical value where an IR conformal fixed point may appear [18]. The vicinity of the IR fixed point can induce a walking behaviour of the running coupling, which would make such theories phenomenologically viable. Whether or not this is really the case beyond perturbation theory can only be established by numerical simulations of such theories defined on the lattice. Recent studies of the running of the renormalized coupling in the Schrödinger functional (SF) scheme [19] with fundamental staggered fermions have provided first evidence of the existence of a conformal fixed point for $n_f = 12$ [20]. A similar study has also appeared for the SU(3) theory with fermions in the two–index symmetric representation [21], and for the SU(2) theory with fermions in the adjoint representation [22,23]. The results presented in those works confirm that the SF is indeed a valuable tool to study the RG structure of the theories under consideration. Further studies on the existence of an IR fixed point with fundamental fermions have appeared in the literature [24]. Several complementary approaches will be needed in order to fully under-
stand numerical simulations in the vicinity of an IR fixed point.

In this paper we discuss in detail the implementation of an algorithm for simulating gauge theories with dynamical Wilson fermions in an arbitrary representation, and arbitrary gauge group SU(N), and present the results of preliminary runs which are useful as a benchmark for future simulations. At this stage in our investigations, the emphasis is on the algorithm rather than the optimization or the phenomenological results. Sect. III summarizes the notation used for the Dirac operator, and introduces the conventions to deal with the higher representations. The HMC algorithm for two flavors is described in Sect. IIIA. In order to be able to simulate theories with an arbitrary number of flavors, the RHMC algorithm [6] has also been developed, as described in Sect. III B. Let us emphasize once again that, as numerical simulations move away from the well--known realms of QCD, we find it necessary to have a robust field--theoretical formulation and a tight control over the behaviour of the numerical simulations. These are necessary conditions if numerical simulations want to be in a position to test candidate theories for strong electroweak symmetry breaking with any degree of confidence.

We study the behaviour of the algorithm at different points in the space of bare lattice couplings by monitoring the time--history, the probability distribution and the correlation time of the plaquette and the lowest eigenvalue of the Dirac operator, in Sect. IV. In the same section we also study how the force is split in the terms of the rational approximation, in analogy with Ref. [6] where fundamental fermions were considered. We present results for $4^3 \times 8, 8^3 \times 16, 12^3 \times 24, 16^3 \times 32, 24^3 \times 64$ lattices, for the SU(2) theory with two flavours in the adjoint representation at two values of the coupling constant $\beta = 2$ and $\beta = 2.25$. The emphasis in this work is on the details of the implementation, and on the behaviour of the algorithm for the theory under consideration. These results are intended as benchmark for other softwares that simulate the same theory. When the exactness of numerical simulations cannot be judged by comparing with experimental data, a cross--check of all the available simulation softwares is essential before debating about the interpretation of the results. Up to date this preliminary cross--check is still missing, although several more complex and phenomenologically relevant results are currently available in the literature [22,23,25,30] (for studies with different number of colors or fermionic representation, see [20,21,24,31,49]). Therefore the authors encourage different groups to publish analogous studies, in order to fill this gap.

Some phenomenological results for the simulations presented in this work have been already published in a short paper [50] (see also [51,52]). A more detailed discussion of these results is currently in preparation.

II. WILSON FERMIONS IN A GENERIC REPRESENTATION

In four--dimensional Euclidean space the massless Wilson--Dirac operator is written following the notation in Ref. [53]:
is quadratic in the fermionic fields and therefore its contribution to the partition function can be computed exactly, yielding the fermionic determinant, \( \det D_m \). In numerical simulations, the latter determinant is conveniently replaced by the determinant of the Hermitian Dirac operator \( Q_m \), defined as usual as:

\[
Q_m = \gamma_5 D_m. 
\]  

(9)

The fermionic determinant for an even number \( n_f \) of degenerate flavours can be represented by introducing complex pseudofermionic (bosonic) fields \( \phi, \phi^\dagger \):

\[
(\det D_m)^{n_f} = (\det Q_m)^{n_f} = \int D\phi D\phi^\dagger e^{-S_f},
\]  

(10)

where the pseudofermionic action has the generic form:

\[
S_f = a^4 \sum_x \phi^\dagger(x) \left( Q_m^2 \right)^{-l} \phi(x), \quad l = n_f/2.
\]  

(11)

Note that we have used the same symbol \( S_f \) to denote the fermionic action written in term of the usual Grassmann variables and the pseudofermionic action written in terms of bosonic fields that is used in the numerical simulations; the meaning of the symbol will be specified by the context in which it is used. In the above expression the square of \( Q_m \) is used and not the matrix itself because \( Q_m \) may not be positive definite. The sum over spin and color indices in the above formulas has been omitted in order to simplify the notation.

For the gauge action we always use the Wilson action written in term of elementary \( 1 \times 1 \) plaquettes built of link variables in the fundamental representation:

\[
S_g = \beta \sum_{\mu<\nu} \left( 1 - \frac{1}{N} \text{Re} \text{tr} P_{\mu\nu} \right),
\]  

(12)

where \( \beta = 2N/g_0^2 \) is the lattice bare coupling. The algorithm can be generalized to other gauge actions without any major difficulty.

The partition function for the theory with \( n_f \) flavors of dynamical quarks can therefore be written as:

\[
Z = \int DU D\phi D\phi^\dagger e^{-S_g(U) - S_f(U,\phi,\phi^\dagger)}. 
\]  

(13)

It is also possible to work exclusively with link variables in the higher representation \( R \), by writing the gauge action as a function of the latter. We expect the two choices to yield the same physics in the continuum limit, while a different phase structure may appear at strong coupling. We will not investigate this option here.

### III. SIMULATION ALGORITHM

Simulations for this work are performed using the RHMC algorithm [54]. This is an exact algorithm which is flexible enough to cover all the cases of interest with good performances, while still maintaining a relatively simple form. The algorithm itself is a variation of the HMC algorithm [55] where rational approximations are used to compute fractional powers of the fermionic matrix \( Q_m^2 \) appearing for a generic number of flavors and pseudofermions. Both the HMC and RHMC set up a Markov chain of gauge field configurations yielding the desired limiting distribution using the same steps. The outline of the algorithms can be summarised as follows: i) generate new pseudofermion fields from a heat-bath; ii) evolve the gauge field configuration following the flow of a fictitious Hamiltonian with randomly chosen initial momenta for each link variable – this step is usually called molecular dynamic (MD) evolution; iii) perform a Metropolis test at the of the MD trajectory to correct for errors in the integration of the equation of motion at the previous step.

Our implementation of the HMC/RHMC is a straightforward adaptation of the standard technique to the case under consideration. As usual the bottleneck of the algorithm is the inversion of the Dirac operator \( Q_m^2 \) that is needed during the MD evolution. To reduce the number of steps in the integration of the equation of motion and thus the number of inversions, we use the second order Omelyan integrator [56] for the MD evolution with different time steps for the gauge and fermion action. Multiple pseudofermions and the even-odd preconditioning of the fermionic determinant are also used in this paper, but no other acceleration techniques are necessary for the purpose of this work. More extensive simulations will require a more careful study of these issues.

In the rest of this section we will describe the modifications required to handle fermions in a generic representation and the implementation details used in our code.

#### A. HMC molecular dynamics

In the following the expression for the force needed in the Molecular Dynamics is generalized to the case of fermions in a generic representation. Since simulations in arbitrary representations are still at their early stages, we decide to derive the forces in detail, in order to define the quantities that appear in the simulations as clearly as possible. Introducing for each link variable a conjugate momentum in the algebra of the gauge group:

\[
\pi(x, \mu) = i\pi^a(x, \mu) T_F^a, 
\]  

(14)

a fictitious Hamiltonian \( H \) is written on the group manifold as:

\[
H = H_\pi + H_g + H_f, 
\]  

(15)
where, assuming \( n_f = 2 \):

\[
H_\pi = \frac{1}{2} \sum_{x,\mu} \left( \pi(x,\mu) \right)  = \frac{1}{2} f F \sum_{a,x,\mu} \pi^a(x,\mu) \tag{16}
\]

\[
H_g = S_g = \beta \sum_{\mu<\nu} \left( 1 - \frac{1}{N} \text{Re tr} P_{\mu\nu} \right), \tag{17}
\]

\[
H_f = S_f = \sum_x \phi^\dagger(x) \left( Q^2_m - s \right)^{-1} \phi(x). \tag{18}
\]

Since the momenta are conjugate to the link variables, they are defined in the fundamental representation.

The cases where \( n_f \neq 2 \) are dealt using the RHMC algorithm described in the next section. Also note that an arbitrary shift \( s \) has been included in the fermionic action which will be useful for the discussion of the RHMC algorithm.

Denoting by \( \tau \) the fictitious time of this Hamiltonian system, the equation of motion are given by:

\[
\frac{d}{d\tau} U(x,\mu) = \pi(x,\mu) U(x,\mu), \quad (19)
\]

\[
\frac{d}{d\tau} \pi(x,\mu) = F(x,\mu), \quad (20)
\]

where the RHS of the second equation above defines the force \( F(x,\mu) \) that drives the time evolution of the momenta.

For a generic infinitesimal variation of a link variable:

\[
\delta U(x,\mu) = \delta \omega(x,\mu) U(x,\mu), \quad (21)
\]

where \( \delta \omega(x,\mu) = i \delta \omega^a(x,\mu) T^a_F \) is an element of the algebra, \( F(x,\mu) \) is obtained from the corresponding variation of the action through the equations:

\[
F(x,\mu) = F_g(x,\mu) + F_f(x,\mu),
\]

\[
\delta S_g = - (\delta \omega, F_g),
\]

\[
\delta S_f = - (\delta \omega, F_f).
\]

Since we use link variables in the fundamental representation for the gauge action \( S_g \), the variation of the latter is the usual one that appears in the HMC molecular dynamics evolution:

\[
\delta S_g = - \frac{\beta}{N} \sum_{x,\mu,a} \delta \omega^a(x,\mu) \text{Re tr} \left[ iT^a_F U(x,\mu) V^\dagger(x,\mu) \right], \quad (22)
\]

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

The fermionic force is obtained from the variation of the fermionic action as follows. Starting from:

\[
\delta S_f = - \phi^\dagger \left( Q^2_m - s \right)^{-1} \delta (Q^2_m) \left( Q^2_m - s \right)^{-1} \phi, \quad (23)
\]

let us define:

\[
\eta = \left( Q^2_m - s \right)^{-1} \phi, \quad (24)
\]

\[
\xi = Q_m \eta; \quad (25)
\]

using the fact that the matrix \( (Q^2_m - s) \) is hermitean, we can rewrite Eq. \( (23) \) as:

\[
\delta S_f = - 2 \text{Re} \left[ \xi \delta (Q_m) \eta \right]. \quad (26)
\]

Inserting the explicit form of \( Q_m \), Eq. \( (9) \), into Eq. \( (26) \) we obtain

\[
\delta S_f = \text{Re} \sum_{x,\mu} \left[ (\xi(x))^\dagger \delta U(x,\mu) \gamma_5 (1 - \gamma_\mu) \eta(x + \mu) + \eta(x) \delta U(x,\mu) \gamma_5 (1 - \gamma_\mu) \xi(x + \mu) \right], \quad (27)
\]

where we are implicitly summing over spin and color indices. We can now write the variation of \( U^R \) as:

\[
\delta U^R(x,\mu) = \delta \omega^R(x,\mu) U^R(x,\mu) = i \delta \omega^a(x,\mu) T^a_R U^R(x,\mu), \quad (28)
\]

where the \( \delta \omega^a(x,\mu) \) in the above equation are the same functions that define the variation of the gauge link in Eq. \( (21) \). Eq. \( (27) \) and \( (28) \) yield:

\[
\delta S_f = \sum_{x,\mu,a} \delta \omega^a(x,\mu) \text{Re tr}_{c,s} \left[ iT^a_R U^R(x,\mu) \gamma_5 \times \right. \left. \left( 1 - \gamma_\mu \right) \{ \eta(x + \mu) \otimes \xi(x) + \xi(x + \mu) \otimes \eta(x) \} \right]. \quad (29)
\]

Here the symbol \( \text{tr}_{c,s} \) indicates the trace over color and spin.

For the sake of convenience we introduce the following projectors \( P^a_R \) over the algebra in the representation \( R \):

\[
P^a_R(F) = - \frac{1}{T_F} \text{Re} \text{tr}_{c} \left[ iT^a_R F \right], \quad (30)
\]

and the following trace operator:

\[
\text{Tr}_{x,\mu}(\eta, \xi) = \text{tr}_{s} \left[ \gamma_5 (1 - \gamma_\mu) \{ \eta(x + \mu) \otimes \xi(x) + \xi(x + \mu) \otimes \eta(x) \} \right]. \quad (31)
\]

The forces are then given by:

\[
F^a_G(x,\mu) = - \frac{\beta}{N} P^a_R \left( U(x,\mu) V^\dagger(x,\mu) \right), \quad (32)
\]

\[
F^a_{\bar{F}}(x,\mu) = P^a_R \left( U^R(x,\mu) \text{Tr}_{x,\mu}(\eta, \xi) \right). \quad (33)
\]

Note that when \( R \) is chosen to be the fundamental representation, the usual expressions for the fermionic force are recovered. Explicit expressions for the forces had already been computed for the case of fermions in the adjoint representation of the gauge group SU(2) in Ref. \[57\]. As an analytic check, we have verified that our result above agrees with Eq. \( (16) \) in Ref. \[57\].

**B. RHMC implementation**

The fermionic part of the HMC hamiltonian, for \( n_f \) degenerate fermions and \( N_{pf} \) pseudofermions, can be written as:

\[
H_f = \sum_{k=1}^{N_{pf}} \delta_k \phi^\dagger_k Q^2_m - i \phi_k + \sum_{k=1}^{N_{pf}} \phi_k ; \quad \sum_{k=1}^{N_{pf}} \delta_k = \frac{n_f}{2}. \quad (34)
\]
For the sake of simplicity we will set all the $l_k$ to be equal:

$$
\forall k, \quad l_k = \frac{n_f}{2N_{pf}}. \tag{35}
$$

The above decomposition is used in the RHMC algorithm [54], where rational approximations are used to compute the fractional powers of the positive definite fermion matrix $Q^2_m$. Even though we will work at fixed $n_f = 2$ in this paper, the RHMC is particularly useful if one wants an algorithm that can be easily generalized to an arbitrary number of fermions. Three different rational approximations are used for this implementation.

The first rational approximation is required in the heat–bath update of pseudofermions. In order to generate pseudofermions distributed as in Eq. (34), a simple two-step process is used. For each pseudofermion we first generate a gaussian distributed field $\tilde{\phi}_k$ with probability:

$$
P(\tilde{\phi}_k) \propto \exp[-\tilde{\phi}_k^2], \tag{36}
$$

and then we set:

$$
\phi_k = (Q^2_m)^{\frac{1}{2}} \tilde{\phi}_k, \tag{37}
$$

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

$$
r_a(Q^2_m) = \alpha_0^a + \sum_{n=1}^{d_1} \alpha_n^a (Q^2_m - s_n^a)^{-1} \simeq (Q^2_m)^{\frac{1}{2}}. \tag{38}
$$

The second rational approximation is used to approximate Eq. (34) during the molecular dynamics evolution (as before only one approximation is needed because all $l_k$ are equal):

$$
H_F = \sum_{k=1}^{N_{pf}} \phi_k^\dagger r_b(Q^2_m) \phi_k, \tag{39}
$$

$$
r_b(Q^2_m) = \alpha_0^b + \sum_{n=1}^{d_2} \alpha_n^b (Q^2_m - s_n^b)^{-1} \simeq (Q^2_m)^{-l_k}. \tag{40}
$$

Using the formulas derived in Section IIIA it is easy to write the force corresponding to Eq. (39). In fact, Eq. (39) is nothing but a sum of terms of the form Eq. (40) once we put $l = 1$, $s = s_n$. The RHMC force will be then given by a sum over $n = 1, \ldots, d_2$ of terms given by Eq. (39) multiplied by a factor $\alpha_n^b$. It is possible to compute all the $\eta$’s defined in Eq. (21) corresponding to different $s_n$ simultaneously with a multi-shift inverter.

The third rational approximation is used for the Metropolis test. Starting from Eq. (34), for each pseudofermion we can rewrite:

$$
\phi^\dagger_k (Q^2_m)^{-l_k} \phi_k = \| (Q^2_m)^{-\frac{1}{2}} \phi_k \|^2, \tag{41}
$$

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

$$
r_c(Q^2_m) = \alpha_0^c + \sum_{n=1}^{d_3} \alpha_n^c (Q^2_m - s_n^c)^{-1} \simeq (Q^2_m)^{-\frac{1}{2}}. \tag{42}
$$

Notice that if $d_1 = d_3$ the coefficients for the two approximations $r_a$ and $r_c$ can each be obtained from the other.

The coefficients $\alpha_n$, $s_n$ appearing in the rational approximations are computed using the Remez algorithm. In this implementation we do not compute the coefficients “on the fly” but instead the required values are taken from a look-up table that has been precomputed, according to the following prescription.

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 $Q^2_m$. 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 $[\epsilon, l]$ 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 $[\epsilon/k, l/k]$. Moreover the coefficients of this “rescaled” rational approximation are easily obtained from that of the original approximation. A simple corollary is that we can divide the optimal rational approximations of a given homogeneous function $f(x)$ with the same relative precision, in classes labeled by the ratio $\epsilon/h$. Within each of these classes 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. Thus all that is needed in practice is a table containing the coefficients of rational approximations for each of these classes, for each function $f(x)$ which we want to approximate and for each relative precision which is required. At run-time this table is used to generate optimal rational approximations rescaling the pre-computed coefficients to the desired interval containing the spectrum of the matrix $Q^2_m$. This interval is obtained by computing the maximum and minimum eigenvalue of $Q^2_m$ on each configuration when needed.

C. Even-Odd preconditioning

As already pointed out above, the time required for the inversions of the Dirac operator is one of the dominant contributions to the total cost of the simulation. The convergence of such inversions can be improved using an appropriate preconditioning. The idea behind preconditioning is to rewrite the fermionic determinant as a determinant (or product of determinants) of one (or more) better conditioned matrix (matrices) than the original Dirac operator. Very effective preconditionings are at the heart of the recent progress in simulations of QCD with
dynamical fermions. For the scope of this work, we use a simple even-odd preconditioning \[58\]. We review the main features of even–odd preconditioning here in order to explain the modifications that are required when considering higher-dimensional representations. We divide the lattice in a sublattice of even points \(\Lambda_0\) and another sublattice of odd points \(\Lambda_o\), and we rewrite 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 thus it has only relations. Note that the even-odd preconditioned matrix are the same the latter can be used in numerical simulations. We have:

The explicit form of \(Q\)

where as before we have defined:

\[
\eta_o = D_{oe}\eta_e, \quad \xi_o = D_{oe}\xi_e,
\]

and inserting Eq. \((50)\) into Eq. \((47)\), we arrive at the same expression as before for the variation of the action, but with a minus sign:

\[
\delta S_F = -\sum_{\mu,x} \Re \text{tr}_e \left[ \delta U^R(x,\mu) \text{Tr}_{x,\mu}(\eta,\xi) \right]
\]

From Eq. \(\delta S_F\) and proceeding as before we arrive at the final expression for the force. This again coincides with Eq. \(\delta S_F\) but with the opposite sign:

\[
F^a_F(x,\mu) = -P^a_R(U^R(x,\mu)\text{Tr}_{x,\mu}(\eta,\xi))
\]

### D. Some details on the implementation

As the algorithm is implemented for the first time, we describe in this section some general features of our code and the technical solutions adopted to manage fermions fields defined in an arbitrary representation.

At this early stage in our physics studies we prioritize the flexibility of the code over the optimization aspects. The code is written in ANSI C for maximum portability to different architectures. This choice is justified, in our opinion, by the fact that, on this relatively small scale, C codes maintain a much higher overall simplicity and clarity compared to e.g. C++ codes with a comparable low overhead.

The major difference with respect to conventional codes – i.e. codes for simulations of the SU(3) gauge group with fundamental fermions – is obviously that all operations involving gauge links or pseudofermions fields must be able to handle matrices and vectors of arbitrary dimension. In the generic case of four–dimensional SU(\(N\)) with fermions in a representation \(R\), link matrices for the gauge action have dimension \(N \times N\), the represented gauge links have dimension \(d_R \times d_R\) and fermion fields have dimension \(4d_R\). These numbers indicate how the cost of the simulation scales both in memory and in the number of floating point operations per application of the Dirac operator as \(N\) and \(R\) are varied. One simple way to handle this objects would be to have functions that implement operations on them taking as an additional parameter the dimensions of the objects themselves. However we found it more flexible to use the following approach. We use preprocessor macros instead of functions\(^1\). We fix the gauge group and the representation \(R\) at compile time as this gives the opportunity

---

\(^1\) Inline functions could work just as well, however the handling of inlining is a feature which depends on the compiler.
to more optimizations (e.g. partial unrolling of loops)\textsuperscript{2}. All of the required macros are automatically generated in a pre-compiling step. We use a simple Perl program for this purpose whose input parameters are the number of colors \(N\) and the representation \(R\) and whose output is a C header file containing the macro functions. The whole process of header generation and compilation is managed through a custom Makefile system and it is thus completely transparent to the end user.

A second difference with respect to conventional codes, is that it is convenient, although not strictly necessary, to have a second copy of the gauge field in the representation \(R\). This is only used in the computation of the fermionic force, see Eq. (63), and it is also useful to impose boundary conditions on the fermion fields. Every time the gauge field is updated during the molecular dynamics evolution, the represented gauge field needs to be recomputed.

At this early stage of simulations, we chose to use double precision everywhere in the code to reduce the risk of problems arising from numerical accuracy. This is done at the expense of optimal performance, which we feel is justified in this study of the algorithm implementation and behavior. As the source of random numbers, we use the RANLUX generator\textsuperscript{58}.

IV. BEHAVIOR OF THE ALGORITHM

In this section we shall discuss some simple tests of the RHMC algorithm with the aim to show the correctness of our implementation. The majority of the tests performed for this purpose were run on the lattice T2-B11 (see Tab. IV C below) which corresponds to our biggest volume and the lightest mass at \(\beta = 2\). For all the tests in this section we have used even-odd preconditioning and two pseudofermion fields.

A. Preliminary Tests

A simple test of the algorithm is to look at the expectation value \(\langle \exp(-\Delta H) \rangle\), where \(\Delta H\) is the difference of the values of the Hamiltonian \(H\) at the beginning and at the end of a trajectory in the Molecular Dynamics evolution. This expectation value should always be 1 (a result known as Creutz equality \textsuperscript{60}). Moreover since the RHMC is an exact algorithm, i.e. there are no corrections due to the errors occurring in the Molecular Dynamics integration, a good test of the algorithm is to check whether or not there is any dependence of any quantity on the integration step size \(\Delta \tau\). The average plaquette \(\langle P \rangle\) is a good candidate to this purpose because it can be measured with high accuracy.

We show in Fig. 1 the quantities \(\langle \exp(-\Delta H) \rangle\) (upper panel) and the average plaquette (lower panel) for four different step sizes of the MD integration. No statistically significant deviations from the expected behavior are seen. The value of \(\langle P \rangle\) is consistently independent on \(\Delta \tau\) and the Creutz’s equality \(\exp(-\Delta H) = 1\) is satisfied. Notice also that for the latter quantity the error bars become smaller as \(\Delta \tau\) goes to zero, as expected from the fact that \(\langle \Delta H \rangle\) is also vanishing in the same limit. This is explicitly shown in the upper panel of Fig. 2. As expected for a second order integrator (see \textsuperscript{61}), the quantity \(\langle \Delta H \rangle\) is proportional to \(\Delta \tau^4\) with very good accu-

\textsuperscript{2}This also means that recompiling is needed whenever the number of colors or the fermions representation is changed. However since the total compilation time, including the automatic generations of required header, is less than one minute and independent on \(N\), this can hardly be a problem.
racy (the red curve in the plot is the best fit to that functional form with one free parameter). The acceptance probability $P_{\text{acc}}$ can also be used as a test of the correctness of the algorithm. In fact in the large volume limit this probability is given by $P_{\text{acc}} = \text{erfc}(\sqrt{\langle \Delta H \rangle}/2)$ [62]. We show the measured value of the acceptance rate as a function of the average Hamiltonian variation in the lower panel of Fig. 2. The same figure shows also the predicted behavior (solid curve). We found a convincing agreement with the expectations.

As a last test in this section we measured reversibility violations in the MD. We remind the reader that this is a necessary condition for the correctness of the algorithm. The discussion will follow that of Ref. [63]. At the “microscopic” level, reversibility violations can occur when updating the gauge variables and in the momenta update during the MD evolution. We deal with the first source of non-reversibility using the trick suggested in Ref. [3]: the link update Eq. (19) is implemented by left multiplication of non-reversibility using the trick suggested in Ref. [3]: the link update Eq. (19) is implemented by left multiplication of an exactly unitary matrix

$$|\delta H| = \frac{6.0 \times 10^{-7}}{10^{-7}}$$

FIG. 3: Reversibility test for several values of the time–step used for the MD integration.

FIG. 4: Time–history for the thermalization of the plaquette in the SU(3) theory with two flavours in the fundamental representation on a 16$^3$ lattice at $\beta = 5.6$ and $\kappa = 0.15750$. The black line shows the evolution of the plaquette value using our HMC algorithm, while the red line represents the same quantity using the DD-HMC algorithm. Trajectory number has been scaled by a factor of 7 for the DD-HMC data.

automatically by a Perl program. As a first non–trivial test of our implementation, our code should correctly reproduce the results for simulations in the fundamental representation of SU(3). The code has been benchmarked for SU(3) with $n_f = 2$ against simulations obtained using the DD–HMC algorithm [3] on small lattices. Fig. IV.B shows the thermalization of the plaquette at $\beta = 6.0$. On small lattices, the DD–HMC only updates a small fraction of the links in the system, and therefore the thermalization is much slower in units of MC trajectories. To compare the two time–histories we have therefore rescaled the trajectory number for the DD–HMC data. The figure shows a very good agreement between the two simulations, in particular for the equilibrium value of the plaquette.

Another test of the algorithm is obtained by simulating the SU(3) theory with two flavors in the fundamental representation and in the two–index antisymmetric one. For the theory with three colors the two representations are equivalent and related by charge conjugation. We have compared the outcomes of two simulations on 4$^3 \times 8$ lattice at $\beta = 5.6$ and $\kappa = 0.15600$. The time–history of the plaquette and its probability distribution for the two simulations are summarized in Fig. 5. Once again we find a very convincing agreement between the two simulations.

C. SU(2) $n_f = 2$ two–index symmetric

The theory with two colors and two Dirac fermions in the two–index symmetric (2S) representation has been proposed as a phenomenologically relevant candidate for a minimal walking technicolor theory. For the specific case of the SU(2) color group, the 2S representation is equivalent to the adjoint representation and is therefore

B. Checks for SU(3) with $n_f = 2$ in the fundamental representation

The routines that perform linear algebra operations in color space for arbitrary representations are generated
TABLE I: List of runs for the T2 theory at inverse coupling \( \beta = 2.0 \). The standard runs are performed using link variables in the real adjoint representation. The primed run is constructed in an algorithmic way as complex matrices. In order to simplify the comparison with the runs in Ref. [25], we list both the values of \( \kappa \) and \( m \) real, which makes it less intensive from the computational point of view. Analytical results for the \( A \) parameter, the renormalization constant, and the possibility of an Aoki phase at finite lattice spacing have been presented in Ref. [64], where the theory was denoted T2. We will adopt the same conventions here. Preliminary results from lattice simulations of this theory were presented in Ref. [25]. In this subsection we build upon this previous experience and provide some more extensive description of the behaviour of numerical simulations in the space of bare parameters. The list of runs is summarized in Tab. IV C for inverse coupling \( \beta = 2.0 \) and in Tab. IV C for inverse coupling \( \beta = 2.25 \).

This theory allows us to perform a non-trivial check of our code generation. The link variables in the higher representation can be built in two different manners: in one case we construct real matrices according to Eq. [7], while in the other case we use our generic algorithm for constructing the 2S complex representation of SU(\( N \)), as described in App. [13]. As expected, for a given configuration in the fundamental representation the two representations yield exactly the same matrices; the generic algorithm produces complex matrices with vanishing imaginary parts. Evolving the configuration using the HMC with the two different representations yields compatible results as one can see by the comparison of the runs T2-A1 and T2-A1′ shown in Fig. IV C for the case of the plaquette.

The critical value of the hopping parameter has been computed in perturbation theory in Ref. [64], to which we refer the reader for the notation and results used in what follows. Using the cactus resummed formula for the theory under consideration, we find:

\[
m_c = g_0^2 2C_2(R) \times (−0.162857)/\tilde{c}_0
\]

where \( \tilde{c}_0 \) is a function of \( g_0 \) defined by solving the following equation:

\[
\tilde{c}_0 = e^{-g_0^2/(16\tilde{c}_0)} \left( 1 - \frac{g_0^2}{24\tilde{c}_0} \right).
\]

For \( \beta = 2.0 \) and \( \beta = 2.25 \) the above formula yields respectively \( m_c = -1.73 \) (\( \kappa_c = 0.220 \)) and \( m_c = -1.47 \) (\( \kappa_c = 0.198 \)). A non–perturbative determination of the chiral limit in the space of bare parameters (\( \beta, \kappa \)) can be obtained by linear extrapolation of the PCAC mass, or of the mass squared of the pseudoscalar Goldstone boson. Due to the power divergencies in the renormalization of the bare quark mass, any perturbative computation of \( m_c \) is expected to receive non–perturbative corrections \( \mathcal{O}(e^{-1/\tilde{c}_0^2}/a) \). Therefore the perturbative computation can at best yield an indication of the location of the critical point. The detailed study of these quantities is presented in the next section.

In order to check that the range of \( \kappa \) values does not lead to exceptionally small values of the eigenvalues of the Dirac operator, we have monitored the distribution...
of the smallest eigenvalue of $Q^{ac}$ following the study in Ref. [4]. The histograms that describe the distribution of the lowest eigenvalue of $|Q^{ac_i}|$ are displayed in Fig. [IV C] for the simulations at $\beta = 2.25$. At the values of $\kappa$ that we have considered, the spectrum of the Dirac operator has a clear gap. This is reflected in a smooth behaviour of the simulations even at the lightest masses, as can be seen in the time–histories for the plaquette and the solver number reported in Fig. [IV C]. The results obtained with fundamental fermions in Ref. [4] suggest that the width of the distribution scales like $a/\sqrt{V}$ as the continuum and thermodynamic limits are approached. A comparison of the standard deviations of the eigenvalue distributions for the simulations at $\beta = 2.25$ shows that this scaling is well verified for the theory under consideration (Fig. [IV C]).

As a final test of the algorithm we monitored the MC integration forces for the RHMC algorithm. Compatibility with the absence of exceptionally small eigenvalues, these forces appear to behave smoothly as a function of the bare mass and we observe a very mild (consistent with zero) dependence on the size of the lattice at constant $am_0$. In the upper panel of Fig. [IV D] we show the modulus of the force $|F_\mu^\nu(x,\mu)|$ averaged over all the lattice points $x$ and all directions $\mu$ for each term of the rational approximation indexed by $n$. Data for two different volumes at the same value of the bare quark mass are shown corresponding to the lattices T2-E2 and T2-F0. The average fermionic force appears to change very little once the equilibrium is reached which is reflected in the plot by the fact that errors on this quantity is really small and not visible on the scale of the graph. The relative error for the average force ranges from a few permille for $n = 1$ to less than one percent for $n = 11$. The variation with volume is also very small: the two average values appear to be always consistent with each other within errors. In the bottom panel of Fig. [IV D] we report for completeness the size of the rational approximation coefficients used in the simulation. Their variation is also quite small, given that the distribution of the smallest and largest eigenvalues is very well reflected in the smooth behaviour of the simulations.

<table>
<thead>
<tr>
<th>lattice</th>
<th>$V$</th>
<th>$-am_0$</th>
<th>$N_{tra}$</th>
<th>$\langle P \rangle$</th>
<th>$\tau$</th>
<th>$\lambda$</th>
<th>$\tau_\lambda$</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2-C0</td>
<td>$16 \times 8^3$</td>
<td>0.95</td>
<td>7601</td>
<td>0.63577(16)</td>
<td>5.45(72)</td>
<td>3.582(13)</td>
<td>8.6(1.4)</td>
</tr>
<tr>
<td>T2-C1</td>
<td>$16 \times 8^3$</td>
<td>0.975</td>
<td>7701</td>
<td>0.63843(15)</td>
<td>5.43(71)</td>
<td>2.982(12)</td>
<td>6.65(96)</td>
</tr>
<tr>
<td>T2-C2</td>
<td>$16 \times 8^3$</td>
<td>1</td>
<td>7801</td>
<td>0.64136(15)</td>
<td>5.10(64)</td>
<td>2.427(11)</td>
<td>6.28(88)</td>
</tr>
<tr>
<td>T2-C3</td>
<td>$16 \times 8^3$</td>
<td>1.025</td>
<td>7801</td>
<td>0.64463(15)</td>
<td>4.29(50)</td>
<td>1.894(10)</td>
<td>6.07(84)</td>
</tr>
<tr>
<td>T2-C4</td>
<td>$16 \times 8^3$</td>
<td>1.05</td>
<td>7801</td>
<td>0.64793(15)</td>
<td>3.48(36)</td>
<td>1.459(79)</td>
<td>4.39(52)</td>
</tr>
<tr>
<td>T2-C5</td>
<td>$16 \times 8^3$</td>
<td>1.075</td>
<td>6400</td>
<td>0.65179(16)</td>
<td>2.99(32)</td>
<td>1.0692(74)</td>
<td>4.27(55)</td>
</tr>
<tr>
<td>T2-C6</td>
<td>$16 \times 8^3$</td>
<td>1.1</td>
<td>6400</td>
<td>0.65566(16)</td>
<td>3.28(37)</td>
<td>0.7564(60)</td>
<td>3.77(45)</td>
</tr>
<tr>
<td>T2-C7</td>
<td>$16 \times 8^3$</td>
<td>1.125</td>
<td>7073</td>
<td>0.66037(15)</td>
<td>2.99(30)</td>
<td>0.4854(43)</td>
<td>3.03(31)</td>
</tr>
<tr>
<td>T2-C8</td>
<td>$16 \times 8^3$</td>
<td>1.15</td>
<td>6400</td>
<td>0.66550(16)</td>
<td>3.31(37)</td>
<td>0.2779(31)</td>
<td>2.80(29)</td>
</tr>
<tr>
<td>T2-C9</td>
<td>$16 \times 8^3$</td>
<td>1.175</td>
<td>6400</td>
<td>0.67177(17)</td>
<td>3.24(36)</td>
<td>0.1351(18)</td>
<td>2.80(29)</td>
</tr>
<tr>
<td>T2-D0</td>
<td>$24 \times 12^3$</td>
<td>0.95</td>
<td>10201</td>
<td>0.63531(0)</td>
<td>6.16(74)</td>
<td>3.5058(50)</td>
<td>3.08(26)</td>
</tr>
<tr>
<td>T2-D1</td>
<td>$24 \times 12^3$</td>
<td>1</td>
<td>8652</td>
<td>0.64099(64)</td>
<td>4.92(58)</td>
<td>2.4218(44)</td>
<td>3.10(29)</td>
</tr>
<tr>
<td>T2-D2</td>
<td>$24 \times 12^3$</td>
<td>1.05</td>
<td>7819</td>
<td>0.64763(70)</td>
<td>6.79(99)</td>
<td>1.4936(51)</td>
<td>5.80(78)</td>
</tr>
<tr>
<td>T2-D3</td>
<td>$24 \times 12^3$</td>
<td>1.075</td>
<td>7186</td>
<td>0.65163(68)</td>
<td>4.61(58)</td>
<td>1.0553(40)</td>
<td>4.95(64)</td>
</tr>
<tr>
<td>T2-D4</td>
<td>$24 \times 12^3$</td>
<td>1.1</td>
<td>6393</td>
<td>0.65582(76)</td>
<td>4.09(51)</td>
<td>0.7202(30)</td>
<td>7.8(1.3)</td>
</tr>
<tr>
<td>T2-D5</td>
<td>$24 \times 12^3$</td>
<td>1.125</td>
<td>6200</td>
<td>0.66058(78)</td>
<td>3.97(50)</td>
<td>0.4419(22)</td>
<td>5.98(91)</td>
</tr>
<tr>
<td>T2-D6</td>
<td>$24 \times 12^3$</td>
<td>1.15</td>
<td>1599</td>
<td>0.66588(15)</td>
<td>3.71(90)</td>
<td>0.2271(31)</td>
<td>6.6(2.1)</td>
</tr>
<tr>
<td>T2-D7</td>
<td>$24 \times 12^3$</td>
<td>1.175</td>
<td>5582</td>
<td>0.67207(79)</td>
<td>4.22(58)</td>
<td>0.08641(90)</td>
<td>3.78(49)</td>
</tr>
<tr>
<td>T2-D8</td>
<td>$24 \times 12^3$</td>
<td>1.18</td>
<td>4081</td>
<td>0.67347(92)</td>
<td>4.01(63)</td>
<td>0.06561(92)</td>
<td>10.2(5)</td>
</tr>
<tr>
<td>T2-D9</td>
<td>$24 \times 12^3$</td>
<td>1.185</td>
<td>4201</td>
<td>0.67509(93)</td>
<td>3.42(49)</td>
<td>0.05196(71)</td>
<td>3.53(51)</td>
</tr>
<tr>
<td>T2-D10</td>
<td>$24 \times 12^3$</td>
<td>1.19</td>
<td>3501</td>
<td>0.67663(10)</td>
<td>4.15(70)</td>
<td>0.03985(61)</td>
<td>5.2(1.0)</td>
</tr>
<tr>
<td>T2-E0</td>
<td>$32 \times 16^4$</td>
<td>1.15</td>
<td>5446</td>
<td>0.665894(14)</td>
<td>3.22(40)</td>
<td>0.2227(10)</td>
<td>3.05(36)</td>
</tr>
<tr>
<td>T2-E1</td>
<td>$32 \times 16^3$</td>
<td>1.175</td>
<td>2192</td>
<td>0.672235(73)</td>
<td>2.80(50)</td>
<td>0.07036(90)</td>
<td>5.9(1.5)</td>
</tr>
<tr>
<td>T2-E2</td>
<td>$32 \times 16^3$</td>
<td>1.18</td>
<td>4606</td>
<td>0.673657(49)</td>
<td>3.46(47)</td>
<td>0.05167(50)</td>
<td>6.1(1.1)</td>
</tr>
<tr>
<td>T2-E3</td>
<td>$32 \times 16^3$</td>
<td>1.185</td>
<td>4313</td>
<td>0.675170(50)</td>
<td>2.99(39)</td>
<td>0.03751(38)</td>
<td>4.66(75)</td>
</tr>
<tr>
<td>T2-E4</td>
<td>$32 \times 16^3$</td>
<td>1.19</td>
<td>5404</td>
<td>0.676637(44)</td>
<td>3.29(40)</td>
<td>0.02474(28)</td>
<td>7.9(1.5)</td>
</tr>
<tr>
<td>T2-F0</td>
<td>$64 \times 24^4$</td>
<td>1.18</td>
<td>458</td>
<td>0.673737(46)</td>
<td>4.0(1.9)</td>
<td>0.04436(51)</td>
<td>3.5(1.5)</td>
</tr>
<tr>
<td>T2-F1</td>
<td>$64 \times 24^4$</td>
<td>1.185</td>
<td>291</td>
<td>0.675184(59)</td>
<td>2.3(1.1)</td>
<td>0.02836(59)</td>
<td>4.2(2.5)</td>
</tr>
<tr>
<td>T2-F2</td>
<td>$64 \times 24^4$</td>
<td>1.19</td>
<td>349</td>
<td>0.676649(52)</td>
<td>1.63(59)</td>
<td>0.01520(39)</td>
<td>5.7(3.6)</td>
</tr>
</tbody>
</table>

TABLE II: List of runs for the T2 theory at inverse coupling $\beta = 2.25$. In the last two columns we give the average of the smallest eigenvalue of $|Q^{ac_i}|$ and its integrated autocorrelation time.
The dependence of the average fermionic forces on the bare quark mass is shown in Fig. IV D for the T2-F lattice. The change with the quark mass is quite small but visible in this case, and more pronounced for higher values of $n$, corresponding to smaller shifts.

D. Autocorrelation times

The integrated autocorrelation time for the plaquette during our runs is computed in units of molecular dynamics time following Ref. [65]. The results are reported in Tab. IV C, where an increase of the autocorrelation time is clearly visible as we move to lighter fermion masses. In all cases the autocorrelation time is short compared to the total length of the simulations, which guarantees that the binned configurations used for our analyses can be considered as independent and therefore the statistical error is correctly estimated from the variance of the ensembles. It is worthwhile to emphasize that extensive simulations of QCD have shown that the autocorrelation time depends on the trajectory length [66], and on the lattice spacing. Our runs are all performed with trajectories of unit length. Moreover a critical slowing down of the topological modes has been highlighted in the time–histories of the topological charge [67]. Therefore we expect that the observables that are more strongly correlated with topology, show a greater correlation length as we approach the continuum limit. These issues need to be kept in mind as the simulations evolve and more precise estimates of the phenomenological quantities will be sought. Finally, one should keep in mind that autocorrelations depend on the observables, and should be monitored for all the relevant quantities in order to fully control the systematics in the simulations. For our runs at $\beta = 2.25$ we changed the MC integrator parameters to keep the plaquette autocorrelation time roughly constant, which is why the data in Tab. IV C do not show the same increase in autocorrelation times.

V. BENCHMARK MESONIC OBSERVABLES

Phenomenological results on the spectrum of the T2 theory are extracted from the study of lattice two–point functions. In this study we do not attempt to perform an investigation of the phenomenology of this theory, which will be presented in a forthcoming paper. Our aim is to provide lattice results useful as a benchmark for future investigations, and to define the observables and the analysis procedure that we use here and in subsequent papers. In this section we describe in detail the procedure used to extract mesonic observables, such as the mass of the pseudoscalar or vector mesons, and the corresponding

FIG. 7: Probability distribution of the lowest eigenvalue of the Dirac operator for $\beta = 2.25$.

FIG. 8: Time-histories for the plaquette and the solver number for the T2-B11 lattice at $\beta = 2$.

FIG. 9: The distribution width $\Delta \lambda_0$ of the lowest eigenvalue of the Dirac operator scales like $V^{-1/2}$. Results for $\beta = 2.25$. 

is clearly visible as we move to lighter fermion masses.
generate fermion fields, so that we only consider flavor where

\[ \psi \]

momentum as follows:

\[ \bar{\psi}_1(x)\Gamma\psi_2(x)\bar{\psi}_2(0)\psi_1(0) = -\text{tr} [\Gamma S(x)\Gamma' S(-x)] = -\text{tr} [\Gamma S(x)\Gamma' \gamma_5 S^l(x)\gamma_5] \]

In practice we invert the Hermitian Dirac operator \( Q = \gamma_5 D \) by solving the equation:

\[ Q(x, y)_{AB} \eta_{B}^{A, 0}(y) = \delta_{A, A'} \delta_{x, 0} \]

where capital Latin letters like \( A = \{a, \alpha\} \) are collective indices for color and spin, and \( A, x = 0 \) is the position of the source for the inverter. The inversion is performed using a QMR recursive algorithm with even–odd preconditioning of the Dirac operator, which is stopped when the residue is less than \( 10^{-8} \). Using the solution \( \eta \) obtained from the inversion, the above correlator is re-expressed as:

\[ \langle \ldots \rangle = -\tilde{\Gamma}_{AB} C^{B, y}(x) \tilde{\Gamma}_{CD} D^{C, y}(x)^* \]

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

Following Ref. [68], masses and decay constants for the pseudoscalar meson are extracted from the asymptotic behaviour of the correlators \( f_{PP} \) and \( f_{AP} \) at large Euclidean time. The pseudoscalar mass and the vacuum–to–meson matrix element are obtained from the correlator of two pseudoscalar densities:

\[ f_{PP}(t) = -\frac{G_{PS}^2}{\eta_{PS}} \exp \left\{ -M_{PS} t \right\} + \ldots . \]

The meson mass is obtained by fitting the effective mass to a constant, while the coupling \( G_{PS} \) is extracted from the amplitude of the two–point function \( f_{PP} \). For the precise definition of the effective mass and coupling, we refer the reader to Ref. [68]. On the other hand the ratio

\[ m_{\text{eff}}(t) = \frac{1}{2} \left[ (\partial_0 + \partial_0^2) f_{AP}(t) \right] / f_{PP}(t) \]

yields the PCAC mass \( m \) with corrections of \( O(\alpha) \) for the unimproved theory. On the relatively small lattices that we have used in this study, it is difficult to isolate clearly the contribution from the lowest state, that dominates the large–time behaviour of two–point correlators. Fig. [12] illustrates the typical quality of the plateau that is fitted to extract the pion mass. The data on the plot correspond to the effective mass obtained from two \( f_{PP} \) two–point function, whose asymptotic behaviour is governed by the mass of the lightest pseudoscalar meson. Lattices with a smaller time extent do not show such a clear plateau; for these smaller lattices the determination of the masses is affected by larger systematics due to the contamination from heavier states.

Note that the decay constant is not computed directly; it is obtained from the values computed above as:

\[ F_{PS} = \frac{m}{M_{PS}} G_{PS} \].
The decay constant extracted from bare lattice correlators is related to its continuum counterpart by the renormalization constant \( Z_A \) which has been recently computed in perturbation theory in Ref. \[54\].

Finally the mass of the vector state is extracted from the \( f_{VV} \) correlator, again following the procedure outlined in Ref. \[68\].

**A. Results**

A first set of results were obtained from runs on the T2-A lattices. Our results are summarized in Tab. \[III\]. The results obtained on such small lattices are affected by large systematic errors, and hence are not suitable for reliable phenomenology. On one hand the limited extension of the T2-A lattices in the time direction means that it is virtually impossible to identify a proper plateau. As a consequence we estimate the mass of the relevant states from the value of the effective mass at the centre of the lattice. For the heavier masses we find that our results are in agreement with the data presented in Ref. \[25\].

However, for these larger values of the bare mass, we see that all masses are \( O(1) \) in units of the inverse lattice spacing, and therefore we expect these results to be affected by large lattice artefacts. Smaller masses are needed in order to identify the chiral dynamics that is relevant for phenomenological studies. The lattices T2-A6, T2-A7, and T2-A8 yield smaller masses, but the lightest pseudoscalar meson has a mass \( \sqrt{am} \) which is still large in units of the UV cutoff. The study of the eigenvalue distributions presented in the previous section suggests that it is not possible to go to lighter masses on the T2-A lattices without entering the regime where the algorithm becomes unstable, or the system gets close to a phase transition.

The results obtained on the T2-B lattices for the pseudoscalar mass, the PCAC mass, the vector meson mass, the axial vector meson mass, and the vacuum–to–meson matrix element are reported in Tab. \[IV\]. As a result of the reduced width in the eigenvalue distribution, we can afford to simulate closer to the chiral limit, with a PCAC mass smaller than 0.1.

Several combinations of interest are also summarized in Tab. \[V\] the ratio of the pseudoscalar mass squared to the PCAC mass, the bare pseudoscalar decay constant, and the mass of the vector meson in units of the pseudoscalar decay constant. They are computed from the primary observables discussed above, and the error propagation is done by the usual jackknife method. The main

![FIG. 12: Effective mass plot for the pion mass. The points correspond to the effective mass extracted from \( f_{PP}(t) \). The data refer to the T2-F0 lattice.](image)

**TABLE III:** Results for the PCAC mass, for the pseudoscalar mass and coupling, for the vector meson mass, and the pseudoscalar decay constant, from simulations on the T2-A lattices.

<table>
<thead>
<tr>
<th>lattice</th>
<th>( am )</th>
<th>( \sqrt{am} )</th>
<th>( \sqrt{am}^2 )</th>
<th>( aM_V )</th>
<th>( aF_{PS} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2-A1</td>
<td>1.0199(14)</td>
<td>2.5711(12)</td>
<td>1.134(8)</td>
<td>2.5814(13)</td>
<td>0.3499(11)</td>
</tr>
<tr>
<td>T2-A2</td>
<td>0.7997(14)</td>
<td>2.2313(16)</td>
<td>1.277(10)</td>
<td>2.2516(17)</td>
<td>0.4102(16)</td>
</tr>
<tr>
<td>T2-A3</td>
<td>0.6718(14)</td>
<td>2.0212(19)</td>
<td>1.351(12)</td>
<td>2.0517(21)</td>
<td>0.4442(20)</td>
</tr>
<tr>
<td>T2-A4</td>
<td>0.5188(13)</td>
<td>1.7708(24)</td>
<td>1.435(14)</td>
<td>1.8222(26)</td>
<td>0.4748(26)</td>
</tr>
<tr>
<td>T2-A5</td>
<td>0.3129(23)</td>
<td>1.362(7)</td>
<td>1.356(34)</td>
<td>1.457(8)</td>
<td>0.4578(68)</td>
</tr>
<tr>
<td>T2-A6</td>
<td>0.2599(39)</td>
<td>1.196(18)</td>
<td>1.157(63)</td>
<td>1.280(20)</td>
<td>0.421(12)</td>
</tr>
<tr>
<td>T2-A7</td>
<td>0.1601(30)</td>
<td>0.868(27)</td>
<td>0.776(47)</td>
<td>0.901(31)</td>
<td>0.3301(97)</td>
</tr>
<tr>
<td>T2-A8</td>
<td>0.0921(16)</td>
<td>0.677(24)</td>
<td>0.607(27)</td>
<td>0.684(28)</td>
<td>0.2433(61)</td>
</tr>
</tbody>
</table>

**TABLE IV:** Fitted values for the masses and vacuum–to–meson matrix element in lattice units for the T2-B lattices.

<table>
<thead>
<tr>
<th>lattice</th>
<th>( am )</th>
<th>( \sqrt{am} )</th>
<th>( aF_{PS} )</th>
<th>( M_V )</th>
<th>( M_{V/F} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>T2-B7</td>
<td>0.2209(30)</td>
<td>5.98(14)</td>
<td>3.99(14)</td>
<td>3.19(12)</td>
<td></td>
</tr>
<tr>
<td>T2-B8</td>
<td>0.1874(40)</td>
<td>5.82(24)</td>
<td>3.54(20)</td>
<td>3.29(19)</td>
<td></td>
</tr>
<tr>
<td>T2-B9</td>
<td>0.1624(37)</td>
<td>5.58(26)</td>
<td>0.31(18)</td>
<td>3.40(20)</td>
<td></td>
</tr>
<tr>
<td>T2-B10</td>
<td>0.1307(42)</td>
<td>5.30(41)</td>
<td>0.266(21)</td>
<td>3.58(30)</td>
<td></td>
</tr>
<tr>
<td>T2-B11</td>
<td>0.0455(14)</td>
<td>2.79(39)</td>
<td>0.154(8)</td>
<td>2.38(31)</td>
<td></td>
</tr>
</tbody>
</table>

**TABLE V:** Fitted values for the relevant combinations of \( m, M_{PS}, G_{PS}, \) and \( M_V \) for the T2-B lattices. The value of the PCAC mass is reported again for clarity.

\( aF_{PS} \) has been used in Ref. \[25\]. The two choices differ by a factor \( \sqrt{8} \). Our choice for the normalization of \( aF_{PS} \) yields \( F_a = 93 \) MeV in QCD.

\( \gamma \) yields 8. Our choice for the normalization of \( aF_{PS} \)
phenomenological conclusions of this paper are obtained from these values.

The computation of the pseudoscalar decay constant in the chiral limit is the method of choice to set the lattice scale. In a technicolor theory the decay constant is related to the vacuum expectation value of the Higgs field, and therefore \( F_{PS} = 250 \) GeV. A realistic determination of the physical value of \( F_{PS} \) would be beyond the scope of this work. Here we simply report the values of \( F_{PS} \) in Tab. III and IV.

The ratio \( M_V / F_{PS} \) is also an interesting quantity of a Technicolor theory. Our result for this quantity are summarized in Tab. V.

We stress again that the results in this section are only benchmarks: they are useful for checking future numerical simulations but not to draw any solid phenomenological conclusion about this theory.

VI. CONCLUSIONS

In this paper we have described the generalization of the HMC and RHMC algorithms to the case of generic representations of the color group \( SU(N) \). We have developed a general framework that can deal with Wilson fermions in arbitrary representations and generic number of colors \( N \). We have put the emphasis in describing in detail the algorithmic issues that need to be faced in generalizing existing code to arbitrary representations. Since simulations for these new theories are still in their infancy, and even the simplest results are not known a priori, numerous independent studies will be welcome. We have provided an extensive number of tests of the algorithm and a detailed study of its behavior for the SU(2) gauge theory with fermions in the adjoint representation. Our benchmark result are ideally suited for validating lattice simulations of theories with fermions in higher representations.

We have presented benchmark results on small \( 8^3 \times 16 \) lattices, giving full the details of the procedure we used, so as to make all the results presented in this work reproducible beyond any ambiguity. On these small lattice, our results should be easily reproducible without any major investment of computational resources. We provided a large number of benchmark quantities, ranging from the average value of the plaquette to mesonic observables.

The results in this paper are the first step in a more comprehensive program that aims to study nonperturbative phenomena beyond QCD. Robust results for the spectrum and decay constants in technicolor theories are an important ingredient to search for strongly-interacting BSM physics at the LHC. The techniques that have been developed for QCD offer all the theoretical and algorithmic tools needed to develop a comprehensive study of technicolor on the lattice. Lattice results will be important in order to test these theories as potential candidates for BSM physics. We stress again that an uncompromising theoretical formulation is mandatory for such studies that are investigating unknown theories in order to have some real predictive power. First numerical results should be benchmarked carefully against each other in order to verify that systematics are under control.

It is worthwhile to emphasize once again that the algorithmic framework that we have developed here can be readily used to study the planar orientifold equivalence and lattice supersymmetry. Preliminary results in this direction have already appeared [13].

Acknowledgements

During the long gestation of this work, we have enjoyed discussing its progress with many people. We want to thank Adi Armoni, Francis Bursa, Simon Catterall, Bigio Lucini, Martin Lüscher, Francesco Sannino, Misha Shifman and Gabriele Veneziano for discussions about various aspects of this work. LDD acknowledges the kind hospitality of the Isaac Newton Institute, CERN, and Odense University while this work was progressing. Workshops at the INI, the Niels Bohr Institute, and Edinburgh provided a lively atmosphere for discussions. We thank SUPA for funding the workshop in Edinburgh. LDD is funded by an STFC Advanced Fellowship. The work of C.P. has been supported by contract No. DE-AC02-98CH10886 with the U.S. Department of Energy during the initial stages of this work. A.P. is supported by an STFC special project grant and by the “Fondazione Angelo Della Riccia”.

Appendix A: Group–theoretical factors

The normalization of the generators in a generic representation \( R \) of \( SU(N) \) is fixed by requiring that:

\[
[T_R^a, T_R^b] = i f^{abc} T_R^c,
\]

where the structure constants \( f^{abc} \) are the same in all representations. We define:

\[
\text{tr}_R (T_R^a T_R^b) = \text{tr} (T_R^a T_R^b) = T_R \delta^{ab},
\]

\[
\sum_a (T_R^a T_R^a)_{AB} = C_2(R) \delta_{AB},
\]

and hence:

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

where \( d_R \) is the dimension of the representation \( R \). The quadratic Casimir operators may be computed from the Young tableaux of the representation of \( SU(N) \) by using the formula:

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

The quantities \( d_R \), \( T_R \), \( C_2(R) \) are listed in Tab. VI for the fundamental, adjoint, 2–index symmetric, and 2–index antisymmetric representations.

### Appendix B: Two–index representations

The hermitian generators \( T_R^a \) for the fundamental representation used are of the following form. For each pair of integers \( 1 \leq k < l \leq N \), we define two generators as:

\[
(T_F^{i,j+})_{mn} = \frac{1}{2} (\delta_{mk} \delta_{nl} + \delta_{ml} \delta_{nk}) ,
\]

\[
(T_F^{i,j-})_{mn} = \frac{1}{2} (\delta_{mk} \delta_{nl} - \delta_{ml} \delta_{nk}) ,
\]

and for each \( 1 \leq k < N \) one more generator is defined as:

\[
(T_F^k) = \frac{1}{\sqrt{2k(k+1)}} \text{diag}(1,1,\ldots,-k,0,\ldots,0) .
\]

The generators \( T_F^a \) are normalized so that \( T_F = 1/2 \). The generators for the other representations are obtained as follows.

We first give the explicit form for the representation functions \( R \) which map \( U \rightarrow U^R \). 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 hermitian matrices to be \( e_{Adj}^a = T_R^a / \sqrt{T_F} \), \( a = 1, \ldots, N^2 - 1 \) (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 \( i \leq j \), for the \( N \times N \) symmetric matrices is given by:

\[
i \neq j , \quad (e_S^{(ij)})_{kl} = \frac{1}{\sqrt{2}} (\delta_{ik} \delta_{jl} + \delta_{jk} \delta_{il}) , \quad (B4)
\]

\[
i = j , \quad (e_S^{(ii)})_{kl} = \delta_{kl} \delta_{il} . \quad (B5)
\]

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

\[
(e_S^{(ij)})_{kl} = \frac{1}{\sqrt{2}} (\delta_{ik} \delta_{jl} - \delta_{jk} \delta_{il}) . \quad (B6)
\]

The maps \( R \) are explicitly given by:

\[
(R^{Adj} U)_{ab} = U^{Adj}_{ab} = \text{tr} \left[ e_{Adj}^a U e_{Adj}^b U^\dagger \right] , \quad a,b = 1, \ldots, N^2 - 1 , \quad (B7)
\]

\[
(R^S U)_{(ij)(lk)} = U^S_{(ij)(lk)} = \text{tr} \left[ (e_S^{(ij)})^\dagger U (e_S^{(lk)})^T U^\dagger \right] , \quad i \leq j,l \leq k , \quad (B8)
\]

\[
(R^A U)_{(ij)(lk)} = U^A_{(ij)(lk)} = \text{tr} \left[ (e_A^{(ij)})^\dagger U (e_A^{(lk)})^T U^\dagger \right] , \quad i < j,l < k . \quad (B9)
\]

The generators \( T_R^a \) used are defined as the image of the generators in the fundamental under the differential of the maps \( R \) defined above: \( T_R^a = R_* T_F^a \). 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 Tab. VI.

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[38] B. Lucini (2009), 0911.0020.
[50] E. Bilgici et al. (2009), 0910.0792.