



Four-dimensional factorization of the fermion determinant in lattice QCD



Leonardo Giusti ^{a,b,*}, Matteo Saccardi ^{a,b}

^a Dipartimento di Fisica, Università di Milano-Bicocca, Piazza della Scienza 3, I-20126 Milano, Italy

^b INFN, Sezione di Milano-Bicocca, Piazza della Scienza 3, I-20126 Milano, Italy

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ABSTRACT

In the last few years it has been proposed a one-dimensional factorization of the fermion determinant in lattice QCD with Wilson-type fermions that leads to a block-local action of the auxiliary bosonic fields. Here we propose a four-dimensional generalization of this factorization. Possible applications are more efficient parallelizations of Monte Carlo algorithms and codes, master field simulations, and multi-level integration.

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1. Introduction

In path integrals of lattice gauge theories with fermions, once the Grassmann variables have been analytically integrated out, the manifest locality of the action and of the observables is lost. The fermion determinant is a non-local functional of the background gauge field, and the resulting effective gauge theory is simulated with variants of the Hybrid Monte Carlo (HMC) algorithm [1]. In the vast majority of cases, the algorithm implements global updates for an importance sampling with a non-local action.

A few years ago it has been proposed a factorization of the gauge-field dependence of the fermion determinant in lattice QCD based on a domain decomposition of the lattice [2–5]. The factorization has been derived in full details by decomposing the lattice in overlapping domains along one of the dimensions only [5]. Once combined with the multi-boson idea [6], it leads to a local action in the block gauge, pseudofermion and multi-boson auxiliary fields [5]. Extensive numerical tests have been performed since then [4,5,7,8], and a first computation of the hadronic vacuum polarization contribution to the anomalous magnetic moment of the muon based on these ideas has been presented [9].

The aim of this letter is to generalize the factorization of the fermion determinant in Ref. [5] to four dimensions. This is not straightforward because, in a multi-dimensional decomposition, the domains may not be naturally the union of discon-

nected regions. The problem is solved by choosing judiciously a four-dimensional overlapping domain decomposition of the lattice which leads to a simple block decomposition of the Dirac operator with highly-suppressed elements in the off-diagonal blocks. These contributions can then be taken into account by introducing multi-boson auxiliary fields.

A four-dimensional factorization of the gauge-field dependence of the fermion determinant boosts our ability of simulating gauge theories with fermions, possibly triggering new perspectives in this field. It allows for highly efficient parallelizations, also on heterogeneous architectures, of Monte Carlo algorithms and of the corresponding codes by reducing very significantly the rate of data exchange among different (blocks of) computer nodes where the various domains of the lattice are mapped to. In master field simulations [10–12], it allows for a block-local accept/reject step in the HMC, solving the problem of the increasing numerical precision needed for larger and larger volumes. Finally, a block-local action of the auxiliary bosonic fields indeed opens the way to multi-level simulations of QCD in all four dimensions.

The letter is organized as follows: in Section 2 we introduce the four-dimensional domain decomposition of the lattice that we adopt, and in the following two Sections we derive the factorization of the gauge-field dependence of the determinant. In Section 5 the residual interactions among the various domains is taken exactly into account by introducing multiboson fields on their boundaries, while in Section 6 a fully block-local Monte Carlo updating scheme is discussed. We end the letter with our conclusions and outlook. Notations, conventions, and technical details are reported in several appendices.

* Corresponding author at: Dipartimento di Fisica, Università di Milano-Bicocca, Piazza della Scienza 3, I-20126 Milano, Italy.

E-mail addresses: leonardo.giusti@mib.infn.it (L. Giusti), m.saccardi@campus.unimib.it (M. Saccardi).

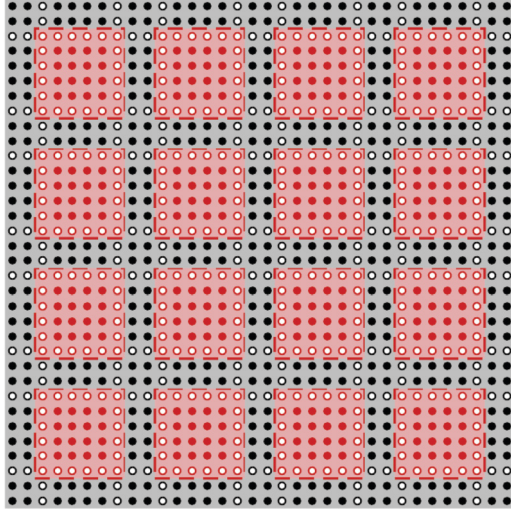


Fig. 1. Two-dimensional representation of the basic domain decomposition of the lattice in the disconnected domain Λ_0 (red square blocks) and the globally connected one Λ_1 (grey thick frame). The empty circles indicate the domain of hyperplanes $\partial\Pi$, see main text, with the red and black circles indicating $\partial\Lambda_0$ and $\partial\Pi_1$ respectively.

2. Four-dimensional domain decomposition of the lattice

We consider a four-dimensional hyperrectangular lattice of spacing a and lengths L_μ in the directions labeled by $\mu = 0, \dots, 3$. We are interested in decomposing this lattice in all the four dimensions by generalizing the one-dimensional domain decomposition introduced in Ref. [5], see also [7–9]. To this aim, we use some of the notation adopted in these papers by assuming familiarity of the reader with them.

We start by dividing the lattice in a domain Λ_0 made of hyperrectangular blocks embedded in a thick frame Λ_1 . In the two-dimensional representation shown in Fig. 1, the blocks are represented by red squares, while the grey region is the frame. By construction Λ_0 is a disconnected domain which can be decomposed as

$$\Lambda_0 = \bigcup_{\hat{a}} \Lambda_0^{\hat{a}} \quad (1)$$

where the label \hat{a} identifies the single hyperrectangle, see Appendix B for its definition. The domain Λ_1 spans the entire lattice and it is connected,¹ at variance of the one-dimensional decomposition [5]. Typically the linear extension B_μ of the blocks in each direction μ can be of a few fermi, while the thicknesses b_μ of the frame are typically of 0.5 fm or so. Following Refs. [2,5], for each block $\Lambda_0^{\hat{a}}$ we define

$$\partial\Lambda_0^{\hat{a}}, \quad \text{and} \quad \bar{\Lambda}_0^{\hat{a}} = \Lambda_0^{\hat{a}} \setminus \partial\Lambda_0^{\hat{a}}, \quad (2)$$

where $\partial\Lambda_0^{\hat{a}}$ is the inner boundary of the block (open red circles in Fig. 1) defined as the set of points in $\Lambda_0^{\hat{a}}$ at a distance a from the closest points of the lattice outside the block, the latter being the exterior boundary $\partial\Lambda_0^{\hat{a}*}$. The sub-block $\bar{\Lambda}_0^{\hat{a}}$ is therefore the set of the inner points of $\Lambda_0^{\hat{a}}$ (closed red circles in the same Figure). Analogously to Eq. (1), it is useful to define

¹ It is possible to introduce an even-odd decomposition of the domain Λ_0 , so that the union of the even and the odd blocks plays the same rôle as the domains Λ_0 and Λ_2 in the one-dimensional decomposition in Refs. [5,7,8]. The frame Λ_1 corresponds to the homologous one in these references.

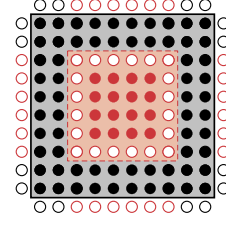


Fig. 2. A “framed domain” $\Omega_0^{\hat{a}}$ made by the union of a hyperrectangle $\Lambda_0^{\hat{a}}$ (red) and its frame $\Phi_1^{\hat{a}}$ (grey). The points of its exterior boundary $\partial\Omega_0^{\hat{a}*}$ are indicated with open circles outside the continuous black line. These circles are red, if they belong to $\partial\Lambda_0$, or black, if they belong to $\partial\Pi_1$ and in particular to $\partial\bar{\Omega}_0^{\hat{a}*}$.

$$\partial\Lambda_0 = \bigcup_{\hat{a}} \partial\Lambda_0^{\hat{a}}, \quad \bar{\Lambda}_0 = \bigcup_{\hat{a}} \bar{\Lambda}_0^{\hat{a}}. \quad (3)$$

The various boundary faces that form $\partial\Lambda_0$ belong to hyperplanes with normal directions parallel to the axes of the lattice (open circles in Fig. 1). The planes are spaced alternatively by B_μ and b_μ along each direction μ , and their ensemble is defined to be the domain $\partial\Pi$. The latter can be decomposed as

$$\partial\Pi = \partial\Lambda_0 \cup \partial\Pi_1, \quad (4)$$

where $\partial\Pi_1$ is represented by black open circles in Fig. 1. Notice that $\partial\Pi_1$ belongs to Λ_1 and that

$$\bar{\Lambda}_1 = \Lambda_1 \setminus \partial\Pi_1 \quad (5)$$

is a disconnected domain. Each block $\Lambda_0^{\hat{a}}$ has an associated “frame” $\Phi_1^{\hat{a}}$ defined as the grey region surrounding it, see Fig. 2 for a graphic representation and Appendix B for its precise definition. The set of blocks $\Phi_1^{\hat{a}}$ clearly forms an overlapping domain decomposition of Λ_1 . The “framed” counterpart of $\Lambda_0^{\hat{a}}$ is given by

$$\Omega_0^{\hat{a}} = \Lambda_0^{\hat{a}} \cup \Phi_1^{\hat{a}}, \quad (6)$$

a definition which requires obvious modifications for the blocks near the boundaries of the lattice, depending on the boundary conditions adopted. The blocks $\Omega_0^{\hat{a}}$ form an overlapping domain decomposition of the entire lattice L , see Fig. 1, similarly to what happens in the one-dimensional case [5,7]. Finally, we define

$$\partial\Omega_0^{\hat{a}*}, \quad \text{and} \quad \partial\bar{\Omega}_0^{\hat{a}*} = \partial\Omega_0^{\hat{a}*} \cap \partial\Pi_1 \quad (7)$$

where $\partial\Omega_0^{\hat{a}*}$ is the exterior boundary of $\Omega_0^{\hat{a}}$, see Fig. 2 for a graphic representation and Appendix B for the definition, while $\partial\bar{\Omega}_0^{\hat{a}*}$ is its subdomain belonging to $\partial\Pi_1$ (black open circles in the same Figure).

In the next Sections we will need the projection operators to the subspace of quark fields supported on the various sub-lattices, see Appendix C for their definitions. We will indicate them with the symbol \mathbb{P} associated to a subscript indicating the sub-lattice considered, e.g. $\mathbb{P}_{\Lambda_0^{\hat{a}}}$ for the block $\Lambda_0^{\hat{a}}$.

3. Block decomposition of the fermion determinant

We are interested in factorizing the gauge-field dependence of the determinant of the Wilson–Dirac operator D defined in Eq. (A.1) of Appendix A. To this aim, we start by decomposing the lattice L as

$$L = \partial\Lambda_0 \cup [\bar{\Lambda}_0 \cup \Lambda_1], \quad (8)$$

and, accordingly, we rewrite D as a 2×2 block matrix. By using Eq. (D.3) in Appendix D, the determinant can then be written as

$$\det D = \det D_{\bar{\Lambda}_0} \det D_{\Lambda_1} \det \tilde{D}_{\partial\Lambda_0}, \quad (9)$$

where²

$$\tilde{D}_{\partial\Lambda_0} = \bar{D}_{\partial\Lambda_0} - D_{\partial\Lambda_0, \Lambda_1} D_{\Lambda_1}^{-1} D_{\Lambda_1, \partial\Lambda_0} \quad (10)$$

and

$$\bar{D}_{\partial\Lambda_0} = D_{\partial\Lambda_0} - D_{\partial\Lambda_0, \bar{\Lambda}_0} D_{\bar{\Lambda}_0}^{-1} D_{\bar{\Lambda}_0, \partial\Lambda_0} = \sum_{\hat{a}} \bar{D}_{\partial\Lambda_0^{\hat{a}}}. \quad (11)$$

In the formulas above and throughout the paper, the subscript of an operator indicates the domain where the operator is restricted, e.g. $D_{\Lambda_0^{\hat{a}}}$ is the Wilson–Dirac operator restricted to the domain $\Lambda_0^{\hat{a}}$ with Dirichlet boundary conditions imposed on its external boundaries. When the subscript of the operator has two domains separated by a comma, this indicates a hopping term among these two domains, see for instance Appendix C. By noticing that

$$D_{\partial\Lambda_0, \Lambda_1} = \sum_{\hat{a}} D_{\partial\Lambda_0^{\hat{a}}, \Phi_1^{\hat{a}}}, \quad D_{\Lambda_1, \partial\Lambda_0} = \sum_{\hat{a}} D_{\Phi_1^{\hat{a}}, \partial\Lambda_0^{\hat{a}}}, \quad (12)$$

it is clear that

$$D_{\partial\Lambda_0, \Lambda_1} D_{\Lambda_1}^{-1} D_{\Lambda_1, \partial\Lambda_0} = \sum_{\hat{a}, \hat{a}'} D_{\partial\Lambda_0^{\hat{a}}, \Phi_1^{\hat{a}}} D_{\Lambda_1}^{-1} D_{\Phi_1^{\hat{a}'}, \partial\Lambda_0^{\hat{a}'}}. \quad (13)$$

If we decompose Λ_1 as the union of $\Phi_1^{\hat{a}}$ and its complement, the corresponding Schur decomposition of D_{Λ_1} , written in the 2×2 blocked form, allows us to rewrite its inverse as in Eq. (D.4). This in turn implies that

$$\mathbb{P}_{\Phi_1^{\hat{a}}} D_{\Lambda_1}^{-1} = D_{\Phi_1^{\hat{a}}}^{-1} - D_{\Phi_1^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\bar{\Omega}_0^{\hat{a}*}} D_{\Lambda_1}^{-1}, \quad (14)$$

$$D_{\Lambda_1}^{-1} \mathbb{P}_{\Phi_1^{\hat{a}}} = D_{\Phi_1^{\hat{a}}}^{-1} - D_{\Lambda_1}^{-1} D_{\partial\bar{\Omega}_0^{\hat{a}*}, \Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}}}^{-1}. \quad (15)$$

By inserting Eqs. (14) and (15) in Eq. (13), we obtain

$$\tilde{D}_{\partial\Lambda_0} = \hat{D}_{\partial\Lambda_0} - \hat{D}_{\partial\Lambda_0, \partial\Pi_1} D_{\Lambda_1}^{-1} \hat{D}_{\partial\Pi_1, \partial\Lambda_0} \quad (16)$$

where

$$\hat{D}_{\partial\Lambda_0, \partial\Pi_1} = - \sum_{\hat{a}} D_{\partial\Lambda_0^{\hat{a}}, \Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\bar{\Omega}_0^{\hat{a}*}}, \quad (17)$$

$$\hat{D}_{\partial\Pi_1, \partial\Lambda_0} = - \sum_{\hat{a}} D_{\partial\bar{\Omega}_0^{\hat{a}*}, \Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\Lambda_0^{\hat{a}}}, \quad (18)$$

and

$$\hat{D}_{\partial\Lambda_0} = \hat{D}_{\partial\Lambda_0}^d + \hat{D}_{\partial\Lambda_0}^h \quad (19)$$

with

$$\hat{D}_{\partial\Lambda_0}^d = \sum_{\hat{a}} \hat{D}_{\partial\Lambda_0^{\hat{a}}}, \quad \hat{D}_{\partial\Lambda_0}^h = \sum_{\hat{a} \neq \hat{a}'} \hat{D}_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}'}} \quad (20)$$

and

$$\hat{D}_{\partial\Lambda_0^{\hat{a}}} = \bar{D}_{\partial\Lambda_0^{\hat{a}}} - D_{\partial\Lambda_0^{\hat{a}}, \Phi_1^{\hat{a}}} D_{\Phi_1^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\Lambda_0^{\hat{a}}}, \quad (21)$$

$$\hat{D}_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}'}} = -\frac{1}{2} D_{\partial\Lambda_0^{\hat{a}}, \Phi_1^{\hat{a}}} \left[D_{\Phi_1^{\hat{a}}}^{-1} - D_{\Phi_1^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\bar{\Omega}_0^{\hat{a}*}} D_{\Phi_1^{\hat{a}'}}^{-1} + \right. \\ \left. D_{\Phi_1^{\hat{a}'}}^{-1} - D_{\Phi_1^{\hat{a}'}}^{-1} D_{\partial\bar{\Omega}_0^{\hat{a}'*}, \Phi_1^{\hat{a}'}} D_{\Phi_1^{\hat{a}'}}^{-1} \right] D_{\Phi_1^{\hat{a}'}, \partial\Lambda_0^{\hat{a}'}}. \quad (22)$$

² It is interesting to notice that $\tilde{D}_{\partial\Lambda_0}$ corresponds to the effective Wilson–Dirac operator, once the Grassmann field variables in $\bar{\Lambda}_0$ and Λ_1 have been integrated out in the path integral. Analogous considerations apply to other Schur complements throughout the paper.

Before proceeding further, it is already interesting to notice that $\hat{D}_{\partial\Lambda_0^{\hat{a}}}$ is the Schur complement of $D_{\Omega_0^{\hat{a}}}$ with respect to the decomposition $\Omega_0^{\hat{a}} = \partial\Lambda_0^{\hat{a}} \cup [\bar{\Lambda}_0^{\hat{a}} \cup \Phi_1^{\hat{a}}]$, and that the hopping terms among the blocks $D_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}'}}$ are suppressed with the thicknesses of the frame. To manipulate the last sum on the r.h.s. of Eq. (16), it is useful to define the Schur complement

$$\hat{D}_{\partial\Pi_1} = D_{\partial\Pi_1} - D_{\partial\Pi_1, \bar{\Lambda}_1} D_{\bar{\Lambda}_1}^{-1} D_{\bar{\Lambda}_1, \partial\Pi_1}. \quad (23)$$

Since $\partial\bar{\Omega}_0^{\hat{a}*} \in \partial\Pi_1$, in Eq. (16) we can replace $D_{\Lambda_1}^{-1}$ with its projection on $\partial\Pi_1$, which in turn is equal to $\hat{D}_{\partial\Pi_1}^{-1}$. Therefore, if we define the block matrix

$$\hat{W} = \begin{pmatrix} \hat{D}_{\partial\Lambda_0} & \hat{D}_{\partial\Lambda_0, \partial\Pi_1} \\ \hat{D}_{\partial\Pi_1, \partial\Lambda_0} & \hat{D}_{\partial\Pi_1} \end{pmatrix}, \quad (24)$$

it is immediate to see that

$$\det \hat{W} = \det \hat{D}_{\partial\Pi_1} \det \tilde{D}_{\partial\Lambda_0}. \quad (25)$$

By remembering that

$$\det D_{\Lambda_1} = \det D_{\bar{\Lambda}_1} \det \hat{D}_{\partial\Pi_1}, \quad (26)$$

Eq. (9) can thus be written as

$$\det D = \det D_{\bar{\Lambda}_0} \det D_{\bar{\Lambda}_1} \det \hat{W}. \quad (27)$$

Notice that the matrix \hat{W} acts on the fermion fields defined on the domain of the hyperplanes $\partial\Pi$ only. The off-diagonal blocks of \hat{W} are suppressed with the thicknesses of the frame of the blocks and depend on the gauge field in Λ_1 only. The one-dimensional decomposition in Ref. [5] is readily obtained as a particular case of Eq. (27) by noticing that in that case $\hat{D}_{\partial\Lambda_0}$ is identified with \hat{W} since the other blocks are absent, and that $\hat{D}_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}'}}$ takes contribution from the first and the third terms in the parenthesis in Eq. (22) only.

4. Preconditioning of \hat{W}

By taking inspiration from the one-dimensional example, we would like to precondition \hat{W} so as to remain with a matrix which deviates from the identity by off-diagonal blocks which are suppressed with the thicknesses of the frame. To this aim we first notice that each block of the diagonal part $\hat{D}_{\partial\Lambda_0}^d$ in Eq. (20) depends on the gauge field in that (framed) block, while the elements of the off-diagonal component $\hat{D}_{\partial\Lambda_0}^h$ are suppressed with the thicknesses of the frame and depend on the gauge field in Λ_1 only. At variance of the one-dimensional case, here $\hat{D}_{\partial\Lambda_0}$ is not the only operator that appears in \hat{W} . We have to consider additional block matrices, e.g. $\hat{D}_{\partial\Pi_1}$, because the domain Λ_1 is not factorized. The operator $\hat{D}_{\partial\Pi_1}$ may also be decomposed in blocks similarly to $\hat{D}_{\partial\Lambda_0}$. For the factorization strategy of this letter, however, this decomposition is not necessary and we proceed by considering this operator as a unique global domain.

The structure of $\hat{D}_{\partial\Lambda_0}$ suggests that we can define a preconditioned operator \overline{W}_1 so that

$$\hat{W} = \begin{pmatrix} \hat{D}_{\partial\Lambda_0}^d & 0 \\ 0 & \hat{D}_{\partial\Pi_1} \end{pmatrix} \cdot \overline{W}_1, \quad (28)$$

where

$$\overline{W}_z = \left(\begin{array}{c|c} z\mathbb{P}_{\partial\Lambda_0} + [\hat{D}_{\partial\Lambda_0}^d]^{-1} \hat{D}_{\partial\Lambda_0}^h & \overline{W}_{\partial\Lambda_0, \partial\Pi_1} \\ \hline \overline{W}_{\partial\Pi_1, \partial\Lambda_0} & z\mathbb{P}_{\partial\Pi_1} \end{array} \right), \quad (29)$$

with $z \in \mathbb{C}$,

$$\overline{W}_{\partial\Lambda_0, \partial\Pi_1} = \sum_{\hat{a}} \mathbb{P}_{\partial\Lambda_0^{\hat{a}}} D_{\Omega_0^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\bar{\Omega}_0^{\hat{a}*}}, \quad (30)$$

and

$$\overline{W}_{\partial\Pi_1, \partial\Lambda_0} = \hat{D}_{\partial\Pi_1}^{-1} \hat{D}_{\partial\Pi_1, \partial\Lambda_0}. \quad (31)$$

Notice that the off-diagonal block operators of \overline{W}_z act on a subspace of $\partial\Pi$ identified by the projector $P_{\partial\Pi} = P_{\partial\Lambda_0} + P_{\partial\Pi_1}$ defined in Appendix C. Indeed at variance of $\mathbb{P}_{\partial\Lambda_0}$ and $\mathbb{P}_{\partial\Pi_1}$, the projectors $P_{\partial\Lambda_0}$ and $P_{\partial\Pi_1}$ include also the appropriate projectors on the spinor index for the inner and outer boundaries of the blocks $\Lambda_0^{\hat{a}}$ and $\Omega_0^{\hat{a}}$ respectively. As shown in Eq. (D.5) of Appendix D, it then holds

$$\det \overline{W}_1 = \det W_1, \quad \text{where} \quad W_z = P_{\partial\Pi} \overline{W}_z P_{\partial\Pi}, \quad (32)$$

with the dimensionality of the matrix W_z being smaller by essentially a factor 2 with respect to the one of \overline{W}_z . By combining Eqs. (27), (28) and (32) we obtain the final result

$$\det D = \frac{1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1} \right]} \det W_1. \quad (33)$$

The denominator in Eq. (33) has already a factorized dependence on the gauge field in the various blocks of Λ_0 . The next Section will be dedicated to the factorization of the remaining global contribution $\det W_1$.

5. Multi-boson factorization of $\det W_1$

For large enough thicknesses of the frame Λ_1 , we expect the matrix W_1 to have a large spectral gap, a fact which makes it effective to express its determinant through a polynomial approximation of W_1^{-1} . As reviewed in the Appendix D of Ref. [5], a generalization of Lüscher's original multiboson proposal [6] to complex matrices [13–15] starts by approximating the function $1/z$, with $z \in \mathbb{C}$, by the polynomial

$$P_N(z) \equiv \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^N (z - z_k), \quad (34)$$

where N is chosen to be even, the N roots of $P_N(z)$ are obtained by requiring that for the remainder polynomial R_{N+1} it holds $R_{N+1}(0) = 1$, and c_N is an irrelevant numerical constant. The roots z_k can be chosen to lie on an ellipse passing through the origin of the complex plane with center 1 and foci $1 \pm c$,

$$u_k = 1 - z_k = \cos\left(\frac{2\pi k}{N+1}\right) + i\sqrt{1-c^2} \sin\left(\frac{2\pi k}{N+1}\right), \quad (35)$$

where $k = 1, \dots, N$. This polynomial can be used to approximate the inverse determinant as

$$\det \overline{W}_1 = \frac{\det\{1 - R_{N+1}(\overline{W}_1)\}}{\det P_N(\overline{W}_1)}, \quad (36)$$

where, if the moduli of all eigenvalues of \overline{W}_1 are smaller than 1, the numerator of the r.h.s. converges exponentially to 1 as N is increased. Thanks to the γ_5 hermiticity of \hat{W} and of $\hat{D}_{\partial\Lambda_0}^d$, the matrix \overline{W}_1 can be written as a product of two Hermitian matrices which in turn implies that \overline{W}_1 is similar to \overline{W}_1^\dagger . Since the z_k come in complex conjugate pairs, the approximate determinant can then be written in a manifestly positive form,

$$\begin{aligned} \frac{1}{\det\{P_N(\overline{W}_1)\}} &= C \prod_{k=1}^{N/2} \det^{-1} \left[(z_k - \overline{W}_1)^\dagger (z_k - \overline{W}_1) \right] \\ &= C \prod_{k=1}^{N/2} \det^{-1} \left[W_{u_k}^\dagger \overline{W}_{u_k} \right] \end{aligned} \quad (37)$$

where C is again an irrelevant numerical constant and \overline{W}_z is defined in Eq. (29). As a result

$$\begin{aligned} \frac{\det D}{\det\{1 - R_{N+1}(W_1)\}} &\propto \frac{1}{\det D_{\Lambda_1}^{-1} \prod_{\hat{a}} \left[\det D_{\Phi_1^{\hat{a}}} \det D_{\Omega_0^{\hat{a}}}^{-1} \right]} \times \\ &\frac{1}{\prod_{k=1}^{N/2} \det \left[W_{u_k}^\dagger W_{u_k} \right]}, \end{aligned} \quad (38)$$

where we have replaced \overline{W}_{u_k} with W_{u_k} by using again the first relation in Eq. (32) which, for $z \neq 1$, is valid up to an irrelevant multiplicative constant. The first factor and the first product in the denominator on the r.h.s. can be included in the effective gluonic action via standard pseudofermions defined within the blocks labeled by the subscript of the operators.

5.1. Multiboson action

Each of the $N/2$ factors in the last product in the denominator of the r.h.s. of Eq. (38) can be represented, up to an irrelevant multiplicative constant, as

$$\frac{1}{\det \left[W_{u_k}^\dagger W_{u_k} \right]} \propto \int d\chi_k d\chi_k^\dagger e^{-|W_{u_k} \chi_k|^2}. \quad (39)$$

The $N/2$ multiboson fields χ_k are defined on the subspace of $\partial\Pi$ identified by the projector $P_{\partial\Pi}$. Each of them can be decomposed as $\chi = \chi_{\partial\Lambda_0} + \chi_{\partial\Pi_1}$, with $\chi_{\partial\Lambda_0} = P_{\partial\Lambda_0} \chi$ and $\chi_{\partial\Pi_1} = P_{\partial\Pi_1} \chi$. As a result

$$\begin{aligned} |W_z \chi|^2 &= \sum_{\hat{a}} \left| P_{\partial\Lambda_0^{\hat{a}}} \left[z \chi_{\partial\Lambda_0} + [\hat{D}_{\partial\Lambda_0^{\hat{a}}}^d]^{-1} \hat{D}_{\partial\Lambda_0^{\hat{a}}}^h \chi_{\partial\Lambda_0} \right. \right. \\ &\left. \left. + D_{\Omega_0^{\hat{a}}}^{-1} D_{\Phi_1^{\hat{a}}, \partial\bar{\Omega}_0^{\hat{a}*}} \chi_{\partial\Pi_1} \right] \right|^2 + \left| z \chi_{\partial\Pi_1} + W_{\partial\Pi_1, \partial\Lambda_0} \chi_{\partial\Lambda_0} \right|^2. \end{aligned} \quad (40)$$

The term on the second line of the r.h.s. of Eq. (40) depends on the gauge field in Λ_1 only. The gauge field within the domain Λ_0 appears only on the first line. As a result the dependence of the multi-boson action from the gauge field in the blocks $\Lambda_0^{\hat{a}}$ is factorized. Moreover, all contributions in Eq. (40) are highly suppressed with the thicknesses of the frame. This implies that the order N of the multi-boson polynomial can be rather low, i.e. of the order of ten or so [5].

5.2. Reweighting factor

A given correlation function of a string of fields O can finally be written as

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N}, \quad (41)$$

where $\langle \cdot \rangle_N$ indicates the expectation value for an importance sampling with N multi-bosons in the action, and

$$\mathcal{W}_N = \det\{1 - R_{N+1}(W_1)\}. \quad (42)$$

By using Eq. (34), up to an irrelevant numerical multiplicative constant, the reweighting factor can be written as

$$\mathcal{W}_N \propto \frac{1}{\det \left\{ W_1^{-1} \prod_{k=1}^{N/2} [W_{u_k}^\dagger]^{-1} W_{u_k}^{-1} \right\}}, \quad (43)$$

a representation which suggests the random noise estimator

$$\mathcal{W}_N = \frac{\int [d\eta][d\eta^\dagger] e^{-\xi^\dagger W_1^{-1} \xi}}{\int [d\eta][d\eta^\dagger] e^{-\eta^\dagger \eta}}, \quad \xi = \prod_{k=1}^{N/2} W_{u_k}^{-1} \eta. \quad (44)$$

The expectation value can then be computed as

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N} = \langle O_{\text{fact}} \rangle_N + \langle O \frac{\mathcal{W}_N}{\langle \mathcal{W}_N \rangle_N} - O_{\text{fact}} \rangle_N, \quad (45)$$

where $O_{\text{fact}} = O$ if the observable is already factorized, otherwise it has to be a rather precise factorized approximation of O (see Ref. [4] for instance). As a result, $\langle O_{\text{fact}} \rangle_N$ can be computed with a fully factorized integration algorithm, while the last (small) contribution on the r.h.s. of Eq. (45) can be estimated in the standard way.

6. Block-local updates

The factorization of the fermionic contribution to the effective gluonic action in Eqs. (38)–(40) allows for a decoupling of the link variables in different blocks $\Lambda_0^{\hat{a}}$. This can be achieved by generalizing the Domain Decomposed Hybrid Monte Carlo (DD-HMC) proposed many years ago [3] to a MultiBoson Domain Decomposed Hybrid Monte Carlo (MB-DD-HMC) [5]. To this aim, the molecular dynamics evolution is restricted to the subset of all link variables, referred to as the *active link variables*, which have both endpoints in the same block $\Lambda_0^{\hat{a}}$ and at most one endpoint on the inner boundary of the block (white open circles in Fig. 1). From Eqs. (38)–(40), it is clear that the active link variables in different blocks are decoupled from each other during the molecular dynamics evolution because the multiboson fields and the inactive gauge links are kept constant in this phase of the simulation. The accept/reject step can thus be carried out independently on each block $\Lambda_0^{\hat{a}}$, i.e. there will be blocks where the proposed new configuration is accepted and blocks where it is not. In between every update cycle, the gauge field is then translated by a random vector v , i.e.

$$U_\mu(x) \rightarrow U_\mu(x+v), \quad (46)$$

to ensure that all link variables are treated equally on average. Before restarting the molecular dynamics evolution, new pseudofermion and multiboson fields need to be generated. The pseudofermions can be generated locally in each block $\Lambda_0^{\hat{a}}$. The multibosons, instead, require a global inversion of the Dirac operator but on a vector belonging to the domain $\partial\Pi$ which is much smaller than the entire lattice.³

In such an updating scheme, one needs to be sure that a good fraction of the link variables can be updated in each step. This is the case if the linear extensions of the blocks are at least of a few fermi. If, for instance, we consider blocks with an extension of 2.5 fm and a frame of 0.5 fm in all directions, the fraction of the active links is readily computed to be approximately 50%, a value which increases very rapidly with the size of the blocks.

7. Conclusions and outlook

The factorization of the gauge-field dependence of the fermion determinant clearly boosts our ability of simulating gauge theories in the presence of fermions. In particular the complete four-dimensional factorization of the molecular dynamics evolution and of the accept/reject steps may change the way we simulate lattice gauge theories in several ways:

Parallelization – During the molecular dynamics evolution and in the accept-reject step the link variables in different blocks are decoupled from each other, and the HMC runs independently in each block. On heterogeneous architectures, one can envisage to simulate each block on a sub-set of nodes which have faster connections (or, for instance, on a single GPU) without the need to communicate during long periods of simulation time. A communication overhead is required only when the gauge field is shifted and the multiboson fields are generated. This is typically a very small fraction of the computer time of the simulation.

Master field simulations – During the molecular dynamics evolution and for the accept-reject step, an inversion of the global lattice Dirac operator is never required. In master field simulations in the presence of fermions [10–12], this solves the problem of the increasing numerical precision needed for inverting the Dirac operator on larger and larger volumes.

Multi-level integration – The update procedure sketched in Section 6 calls for a two-level Monte Carlo integration scheme [5] where first n_0 level-0 independent configurations of the gauge field are generated over the entire lattice, and then for each of them n_1 level-1 configurations of the active links are generated by keeping fixed the inactive links and the multiboson fields. The two-level estimate of an observable is then computed by averaging over the $n_0 \cdot n_1^{n_b}$ configurations obtained at a cost proportional to $n_0 \cdot n_1$, where n_b is the number of blocks in Λ_0 . This two-level integration can in principle be generalized to a multi-level scheme by iterating the domain decomposition and the integration procedure. Extensive numerical tests which have been performed in the one-dimensional case [4,5,7–9] have already shown the benefit of the multi-level integration in solving the signal to noise ratio problem in the computation of correlation functions in lattice QCD.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. $O(a)$ -improved Wilson-Dirac operator

The massive $O(a)$ -improved Wilson-Dirac operator is defined as⁴ [16,17]

$$D = D_w + D_{sw} + m_0, \quad (A.1)$$

where m_0 is the bare quark mass, D_w is the massless Wilson-Dirac operator

$$D_w = \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - \nabla_\mu^* \nabla_\mu \}, \quad (A.2)$$

³ The localization of the generation of the multiboson fields is beyond the scope of this paper.

⁴ Throughout this appendix the lattice spacing is set to unity for notational simplicity.

with γ_μ being the Dirac matrices and the summation over repeated indices is understood. The covariant forward and backward derivatives ∇_μ and ∇_μ^* are defined to be

$$\begin{aligned}\nabla_\mu \psi(x) &= U_\mu(x) \psi(x + \hat{\mu}) - \psi(x), \\ \nabla_\mu^* \psi(x) &= \psi(x) - U_\mu^\dagger(x - \hat{\mu}) \psi(x - \hat{\mu}),\end{aligned}\quad (\text{A.3})$$

where $U_\mu(x)$ are the link fields and $\hat{\mu}$ is the unit versor along the direction μ . By inserting Eq. (A.3) in Eq. (A.2), the Wilson operator reads

$$\begin{aligned}D_W \psi(x) &= 4\psi(x) - \frac{1}{2} \sum_{\mu=0}^3 \left\{ U_\mu(x) (1 - \gamma_\mu) \psi(x + \hat{\mu}) \right. \\ &\quad \left. + U_\mu^\dagger(x - \hat{\mu}) (1 + \gamma_\mu) \psi(x - \hat{\mu}) \right\}.\end{aligned}\quad (\text{A.4})$$

The second term on the r.h.s. of Eq. (A.1) is the Sheikholeslami-Wohlert operator defined as

$$D_{sw} \psi(x) = c_{sw} \frac{i}{4} \sigma_{\mu\nu} \widehat{F}_{\mu\nu}(x) \psi(x), \quad (\text{A.5})$$

where $\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$, and $\widehat{F}_{\mu\nu}(x)$ is the clover discretization of the field strength tensor which is given by

$$\widehat{F}_{\mu\nu}(x) = \frac{1}{8} \{ Q_{\mu\nu}(x) - Q_{\nu\mu}(x) \}, \quad (\text{A.6})$$

with

$$\begin{aligned}Q_{\mu\nu}(x) &= U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x) \\ &\quad + U_\nu(x) U_\mu^\dagger(x - \hat{\mu} + \hat{\nu}) U_\nu^\dagger(x - \hat{\mu}) U_\mu(x - \hat{\mu}) \\ &\quad + U_\mu^\dagger(x - \hat{\mu}) U_\nu^\dagger(x - \hat{\mu} - \hat{\nu}) U_\mu(x - \hat{\mu} - \hat{\nu}) U_\nu(x - \hat{\nu}) \\ &\quad + U_\nu^\dagger(x - \hat{\nu}) U_\mu(x - \hat{\nu}) U_\nu(x + \hat{\mu} - \hat{\nu}) U_\mu^\dagger(x).\end{aligned}\quad (\text{A.7})$$

It is also possible to use the alternative expression for D_{sw} given by

$$D_{sw} + (4 + m_0) \rightarrow (4 + m_0) \exp \left\{ \frac{c_{sw}}{4 + m_0} \frac{i}{4} \sigma_{\mu\nu} \widehat{F}_{\mu\nu} \right\}, \quad (\text{A.8})$$

which has been proposed in the context of master field simulations [12].

Appendix B. Definitions of basic domains

To easily label the various subdomains considered in this letter, it is useful to introduce a non-overlapping domain decomposition of the lattice so that the entire lattice L is decomposed as

$$L = \bigcup_{\hat{a}} \Gamma^{\hat{a}}, \quad (\text{B.1})$$

where $\Gamma^{\hat{a}}$ is a basic hyperrectangular cell, see Fig. B.3 for a 2-dimensional representation. Each cell has dimension $G_\mu = B_\mu + b_\mu$

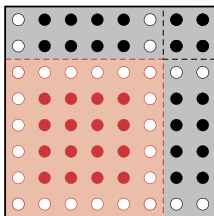


Fig. B.3. Two-dimensional representation of a basic cell $\Gamma^{\hat{a}}$.

in the direction μ and it is uniquely identified by the position of its lower-left corner, given in four-dimensional Cartesian coordinates (in units of G_μ) by $\hat{a} = \{a_0, a_1, a_2, a_3\}$, where

$$a_\mu = 0, \dots, \frac{L_\mu}{G_\mu} - 1, \quad \mu = 0, \dots, 3, \quad (\text{B.2})$$

where L_μ is the length of the lattice along direction μ . As a result, the global lattice coordinates of the lower-left point of the basic cell are given by $x_\mu = G_\mu \cdot a_\mu$ (no summation over repeated indices is meant here).

To map the blocks of the decomposition in Fig. 1 to the basic cells, the latter are further decomposed in 2^4 blocks as depicted in Fig. B.3. Within each cell, the 16 blocks can be identified by their local Cartesian coordinates in each direction μ , i.e. by $\hat{d} = \{d_0, d_1, d_2, d_3\}$ with $d_\mu = 0, 1$. In particular, the lower-left block ($\hat{d} = \hat{0}$) of $\Gamma^{\hat{a}}$ identifies the block $\Lambda_0^{\hat{a}}$ of Λ_0 , with their lower-left corners coinciding. The other blocks of the basic cell belong to Λ_1 , and the coordinates of their lower-left point are given by $x_\mu = G_\mu \cdot a_\mu + B_\mu \cdot d_\mu$ with $\hat{d} \neq \hat{0}$. With those definitions we can finally write

$$\Gamma^{\hat{a}} = \Lambda_0^{\hat{a}} \bigcup_{\substack{\hat{d} \neq \hat{0} \\ d_\mu = 0, 1}} \Lambda_1^{(\hat{a}, \hat{d})}. \quad (\text{B.3})$$

For each block $\Lambda_1^{\hat{a}}$, it is useful to define its ‘‘frame’’ $\Phi_1^{\hat{a}}$, which is shown in Fig. 2, as

$$\Phi_1^{\hat{a}} = \bigcup_{\substack{(\hat{c}, \hat{d}) \neq (\hat{0}, \hat{0}) \\ c_\mu, d_\mu = 0, 1 | (d-c)_\mu = 0, 1}} \Lambda_1^{(\hat{a} - \hat{c}, \hat{d})}. \quad (\text{B.4})$$

Therefore, the ‘‘framed’’ domain

$$\Omega_0^{\hat{a}} = \Lambda_0^{\hat{a}} \cup \Phi_1^{\hat{a}} \quad (\text{B.5})$$

is made of 3^4 blocks with the obvious modifications for the blocks near the boundaries of the lattice depending on the boundary conditions adopted. The blocks $\Phi_1^{\hat{a}}$ clearly form an overlapping domain decomposition of the entire domain Λ_1 . Analogously, the blocks $\Omega_0^{\hat{a}}$ form an overlapping domain decomposition of the entire lattice L , similarly to what happens in the one-dimensional case [5,7].

Appendix C. Projectors

In this Appendix we define projectors on the various domains introduced in Section 2. For $\Lambda_0^{\hat{a}}$ the projector is defined as

$$\mathbb{P}_{\Lambda_0^{\hat{a}}} \psi(x) = \begin{cases} \psi(x) & \text{if } x \in \Lambda_0^{\hat{a}}, \\ 0 & \text{otherwise,} \end{cases} \quad (\text{C.1})$$

i.e. it localizes the quark field $\psi(x)$ inside the domain indicated in the subscript. It follows that

$$\mathbb{P}_{\Lambda_0} = \sum_{\hat{a}} \mathbb{P}_{\Lambda_0^{\hat{a}}}. \quad (\text{C.2})$$

Projectors on other domains, e.g. $\mathbb{P}_{\Omega_0^{\hat{a}}}$, \mathbb{P}_{Ω_0} , $\mathbb{P}_{\partial\Lambda_0^{\hat{a}}}$, $\mathbb{P}_{\partial\Lambda_0}$, etc., are defined analogously.

Projectors on the inner and outer boundaries of $\Lambda_0^{\hat{a}}$ are indicated with $P_{\partial\Lambda_0^{\hat{a}}}$ and $P_{\partial\Lambda_0^{\hat{a}*}}$ respectively, and they are defined so that

$$\begin{aligned}P_{\partial\Lambda_0^{\hat{a}}} D_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}*}} &= D_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}*}} P_{\partial\Lambda_0^{\hat{a}*}}, \\ P_{\partial\Lambda_0^{\hat{a}*}} D_{\partial\Lambda_0^{\hat{a}*}, \partial\Lambda_0^{\hat{a}}} &= D_{\partial\Lambda_0^{\hat{a}*}, \partial\Lambda_0^{\hat{a}}} P_{\partial\Lambda_0^{\hat{a}}}.\end{aligned}\quad (\text{C.3})$$

From Eq. (A.4) it holds

$$\begin{aligned} [D_{\partial\Lambda_0^{\hat{a}*}, \partial\Lambda_0^{\hat{a}}} \psi](x) = & -\mathbb{P}_{\partial\Lambda_0^{\hat{a}*}} \sum_{\mu=0}^3 \left[U_{\mu}(x) \frac{1-\gamma_{\mu}}{2} \mathbb{P}_{\partial\Lambda_0^{\hat{a}}} \psi(x+\hat{\mu}) \right. \\ & \left. + U_{\mu}^{\dagger}(x-\hat{\mu}) \frac{1+\gamma_{\mu}}{2} \mathbb{P}_{\partial\Lambda_0^{\hat{a}}} \psi(x-\hat{\mu}) \right], \end{aligned} \quad (\text{C.4})$$

and analogously for $D_{\partial\Lambda_0^{\hat{a}}, \partial\Lambda_0^{\hat{a}*}}$ with $\mathbb{P}_{\partial\Lambda_0^{\hat{a}}} \longleftrightarrow \mathbb{P}_{\partial\Lambda_0^{\hat{a}*}}$. This implies that

$$P_{\partial\Lambda_0^{\hat{a}}} \psi(x) = \begin{cases} 0 & \text{if } x \notin \partial\Lambda_0^{\hat{a}}, \\ \frac{1-\gamma_{\mu}}{2} \psi(x) & \text{if } x \in \partial\Lambda_0^{\hat{a}} \text{ and } \exists! \mu \mid (x-\hat{\mu}) \in \partial\Lambda_0^{\hat{a}*}, \\ \frac{1+\gamma_{\mu}}{2} \psi(x) & \text{if } x \in \partial\Lambda_0^{\hat{a}} \text{ and } \exists! \mu \mid (x+\hat{\mu}) \in \partial\Lambda_0^{\hat{a}*}, \\ \psi(x) & \text{otherwise,} \end{cases} \quad (\text{C.5})$$

and analogously for $P_{\partial\Lambda_0^{\hat{a}*}}$, i.e. with respect to $\mathbb{P}_{\partial\Lambda_0^{\hat{a}}}$ and $\mathbb{P}_{\partial\Lambda_0^{\hat{a}*}}$ they include also the appropriate projectors on the spinor index on each face of the boundaries. It follows that

$$P_{\partial\Lambda_0} = \sum_{\hat{a}} P_{\partial\Lambda_0^{\hat{a}}}, \quad (\text{C.6})$$

and analogously for $P_{\partial\Lambda_0^*}$, $P_{\partial\Omega_0^{\hat{a}}}$, $P_{\partial\Omega_0^{\hat{a}*}}$, etc. The projector $P_{\partial\Pi}$ is defined as $P_{\partial\Lambda_0}$ but extended to all points of each hyperplane, while $P_{\partial\Pi_1}$ is defined from

$$P_{\partial\Pi} = P_{\partial\Lambda_0} + P_{\partial\Pi_1}. \quad (\text{C.7})$$

Appendix D. LU decomposition of a 2×2 block matrix

A 2×2 block matrix can be decomposed as

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & BD^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} S_A & 0 \\ C & D \end{pmatrix}, \quad (\text{D.1})$$

where the Schur complement is defined as

$$S_A = A - BD^{-1}C. \quad (\text{D.2})$$

Its determinant can then be factorized

$$\det M = \det D \det (A - BD^{-1}C), \quad (\text{D.3})$$

while the inverse is given by

$$M^{-1} = \begin{pmatrix} S_A^{-1} & -S_A^{-1}BD^{-1} \\ -D^{-1}CS_A^{-1} & D^{-1} + D^{-1}CS_A^{-1}BD^{-1} \end{pmatrix}. \quad (\text{D.4})$$

It is worth noting that S_A^{-1} is the exact inverse of M in the domain where A is defined. If B and C act only on subspaces identified by the projectors \mathcal{P}_1 and \mathcal{P}_2 in the first and the second block respec-

tively a simplification occurs, e.g. the inverse D^{-1} in the second determinant on the r.h.s. of Eq. (D.3) can be restricted to the subspace identified by \mathcal{P}_2 . This in turn implies that

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det A \det D \det \begin{pmatrix} \mathbb{1} & \mathcal{A}^{-1}B \\ \mathcal{D}^{-1}C & \mathbb{1} \end{pmatrix} \quad (\text{D.5})$$

where $\mathcal{A}^{-1} = \mathcal{P}_1 A^{-1} \mathcal{P}_1$, $\mathcal{B} = \mathcal{P}_1 B \mathcal{P}_2$, $\mathcal{C} = \mathcal{P}_2 C \mathcal{P}_1$, and $\mathcal{D}^{-1} = \mathcal{P}_2 D^{-1} \mathcal{P}_2$. Notice that the dimensionality of the last matrix on the r.h.s. of Eq. (D.5) is smaller with respect to the one of the original matrix on the l.h.s.

References

- [1] S. Duane, A.D. Kennedy, B.J. Pendleton, D. Roweth, Hybrid Monte Carlo, Phys. Lett. B 195 (1987) 216–222, [https://doi.org/10.1016/0370-2693\(87\)91197-X](https://doi.org/10.1016/0370-2693(87)91197-X).
- [2] M. Lüscher, Solution of the Dirac equation in lattice QCD using a domain decomposition method, Comput. Phys. Commun. 156 (2004) 209–220, [https://doi.org/10.1016/S0010-4655\(03\)00486-7](https://doi.org/10.1016/S0010-4655(03)00486-7), arXiv:hep-lat/0310048.
- [3] M. Lüscher, Schwarz-preconditioned HMC algorithm for two-flavour lattice QCD, Comput. Phys. Commun. 165 (2005) 199–220, <https://doi.org/10.1016/j.cpc.2004.10.004>, arXiv:hep-lat/0409106.
- [4] M. Cè, L. Giusti, S. Schaefer, Domain decomposition, multi-level integration and exponential noise reduction in lattice QCD, Phys. Rev. D 93 (9) (2016) 094507, <https://doi.org/10.1103/PhysRevD.93.094507>, arXiv:1601.04587.
- [5] M. Cè, L. Giusti, S. Schaefer, A local factorization of the fermion determinant in lattice QCD, Phys. Rev. D 95 (3) (2017) 034503, <https://doi.org/10.1103/PhysRevD.95.034503>, arXiv:1609.02419.
- [6] M. Lüscher, A new approach to the problem of dynamical quarks in numerical simulations of lattice QCD, Nucl. Phys. B 418 (1994) 637–648, [https://doi.org/10.1016/0550-3213\(94\)90533-9](https://doi.org/10.1016/0550-3213(94)90533-9), arXiv:hep-lat/9311007.
- [7] L. Giusti, M. Cè, S. Schaefer, Multi-boson block factorization of fermions, EPJ Web Conf. 175 (2018) 01003, <https://doi.org/10.1051/epjconf/201817501003>, arXiv:1710.09212.
- [8] M. Cè, L. Giusti, S. Schaefer, Local multiboson factorization of the quark determinant, EPJ Web Conf. 175 (2018) 11005, <https://doi.org/10.1051/epjconf/201817511005>, arXiv:1711.01592.
- [9] M. Dalla Brida, L. Giusti, T. Harris, M. Pepe, Multi-level Monte Carlo computation of the hadronic vacuum polarization contribution to $(g_{\mu} - 2)$, Phys. Lett. B 816 (2021) 136191, <https://doi.org/10.1016/j.physletb.2021.136191>, arXiv:2007.02973.
- [10] M. Lüscher, Stochastic locality and master-field simulations of very large lattices, EPJ Web Conf. 175 (2018) 01002, <https://doi.org/10.1051/epjconf/201817501002>, arXiv:1707.09758.
- [11] L. Giusti, M. Lüscher, Topological susceptibility at $T > T_c$ from master-field simulations of the SU(3) gauge theory, Eur. Phys. J. C 79 (3) (2019) 207, <https://doi.org/10.1140/epjc/s10052-019-6706-7>, arXiv:1812.02062.
- [12] A. Francis, P. Fritsch, M. Lüscher, A. Rago, Master-field simulations of O(a)-improved lattice QCD: algorithms, stability and exactness, Comput. Phys. Commun. 255 (2020) 107355, <https://doi.org/10.1016/j.cpc.2020.107355>, arXiv:1911.04533.
- [13] A. Borici, P. de Forcrand, Systematic errors of Lüscher's fermion method and its extensions, Nucl. Phys. B 454 (1995) 645–662, [https://doi.org/10.1016/0550-3213\(95\)00429-V](https://doi.org/10.1016/0550-3213(95)00429-V), arXiv:hep-lat/9505021.
- [14] A. Borici, P. de Forcrand, Variants of Lüscher's fermion algorithm, Nucl. Phys. B, Proc. Suppl. 47 (1996) 800–803, [https://doi.org/10.1016/0920-5632\(96\)00178-8](https://doi.org/10.1016/0920-5632(96)00178-8), arXiv:hep-lat/9509080.
- [15] B. Jegerlehner, Improvements of Lüscher's local bosonic fermion algorithm, Nucl. Phys. B 465 (1996) 487–506, [https://doi.org/10.1016/0550-3213\(96\)00055-7](https://doi.org/10.1016/0550-3213(96)00055-7), arXiv:hep-lat/9512001.
- [16] B. Sheikholeslami, R. Wohlert, Improved continuum limit lattice action for QCD with Wilson fermions, Nucl. Phys. B 259 (1985) 572, [https://doi.org/10.1016/0550-3213\(85\)90002-1](https://doi.org/10.1016/0550-3213(85)90002-1).
- [17] M. Lüscher, S. Sint, R. Sommer, P. Weisz, Chiral symmetry and O(a) improvement in lattice QCD, Nucl. Phys. B 478 (1996) 365–400, [https://doi.org/10.1016/0550-3213\(96\)00378-1](https://doi.org/10.1016/0550-3213(96)00378-1), arXiv:hep-lat/9605038.