

A local factorization of the fermion determinant in lattice QCD

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Abstract

We introduce a factorization of the fermion determinant in lattice QCD with Wilson-type fermions that leads to a bosonic action local in the block fields. The interaction among gauge fields on distant blocks is mediated by multiboson fields located on the boundaries of the blocks. The resultant multiboson domain-decomposed hybrid Monte Carlo passes extensive numerical tests carried out by measuring standard gluonic observables. The combination of the determinant factorization and of the one of the propagator, that we put forward recently, paves the way for multilevel Monte Carlo integration in presence of fermions. We test this possibility by computing the disconnected correlator of two flavor-diagonal pseudoscalar densities, and we observe a significant increase of the signal-to-noise ratio due to a two-level integration.

1 Introduction

State of the art algorithms for lattice QCD simulations require first to integrate out analytically the Grassmann quark fields, e.g. for two degenerate flavors, to work with the partition function

$$Z = \int [dU] \{\det D\}^2 e^{-S_G[U]} \quad (1.1)$$

with D the massive Dirac operator and S_G the gauge action, and then simulate this effective gauge theory by Monte Carlo techniques. As a result, the locality of the original action and of the observables is not manifest anymore, because the fermion determinant and the propagator are non-local functionals of the link variables U .

While necessary for making lattice QCD simulations feasible, the non-locality leads to severe limitations in practice. Local (link) update algorithms, the method of choice for pure gauge theory, are not competitive anymore. The effective gauge theory is instead simulated with variants of the *global* hybrid Monte Carlo (HMC) algorithm [1], with only its local variant performing comparably to other link update techniques¹ [5]. For the same reason, noise reduction techniques based on the locality of the theory, such as multihit or multilevel algorithms [6–11], have not yet been formulated successfully in theories with fermions. They are expected to lead to an impressive acceleration in those cases where the signal-to-noise ratio decreases exponentially with the distance between the sources [12, 13].

Over the last two decades, there have been many attempts to rewrite the fermion determinant via a local bosonic field theory. In the multiboson (MB) approach [14], the bosonic action is ultralocal. The back-reaction from the large number of bosonic fields which are typically required, however, results in stiff gauge links and thus in long autocorrelation times [15]. In the domain-decomposed hybrid Monte Carlo (DD-HMC), the determinants of the block Dirac operators are factorized. The remainder, however, is not small, depends on the gauge field values over all the lattice, and needs to be represented by boson fields with a nonlocal action [16].

The aim of this paper is to introduce a factorization of the fermion determinant in lattice QCD with Wilson-type fermions which can be represented by a bosonic theory with a local action in the block gauge and pseudofermion fields. The first step consists in factorizing out from the determinant the contribution depending from gauge fields in distant blocks, see Eq. (2.5). In the second step this factor, which deviates from the identity by terms suppressed as $\exp\{-M_\pi\Delta\}$ where M_π is the pion mass and Δ is the distance between the blocks, is taken exactly into account by introducing multiboson fields on the boundaries of the blocks involved. As a result the final bosonic action is local in the block fields.

Together with the factorization of the fermion observables presented in Ref. [17], this opens the way for multilevel simulations of QCD. We implement these ideas in

¹Attempts to make proposals including dynamical fermions based on link updates as in Refs. [2–4] have not been adopted in large scale projects.

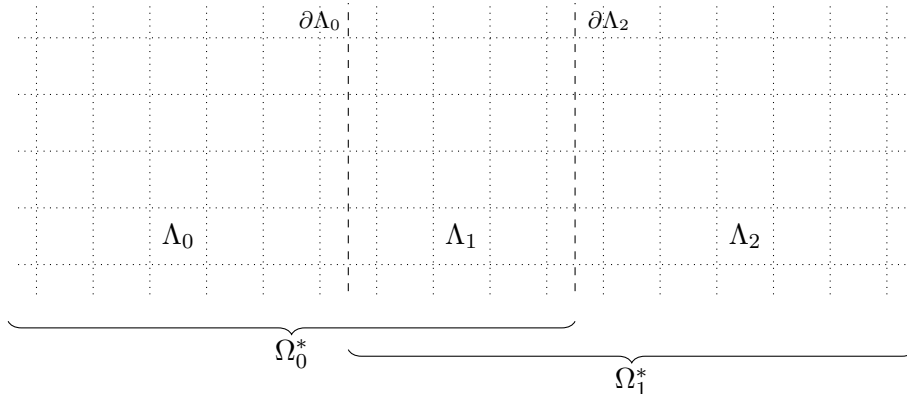


Figure 1: Decomposition of the lattice in tree thick time-slices.

a multiboson domain-decomposed hybrid Monte Carlo (MB-DD-HMC), which we test extensively by measuring the two-point correlators of the gluonic energy density, of the topological charge density, and of two flavor-diagonal pseudoscalar densities. In all cases we observe a significant increase of the signal-to-noise ratio due to a two-level integration.

2 Block decomposition of the determinant

The goal of the derivation in this and in the following section is a decomposition of the effective fermion action in terms which are local in the block gauge and scalar fields. The essential idea can already be presented by considering a lattice with open boundary conditions in the time direction and decompose it in three thick time-slices², see Fig. 1. The generic case is reported in appendix C. The blocks are labeled by Λ_i , $i = 0, 1, 2$, and the Hermitian $O(a)$ -improved massive Wilson–Dirac operator $Q = \gamma_5 D$, see appendix A, takes the block form

$$Q = \begin{pmatrix} Q_{\Lambda_{0,0}} & Q_{\Lambda_{0,1}} & 0 \\ Q_{\Lambda_{1,0}} & Q_{\Lambda_{1,1}} & Q_{\Lambda_{1,2}} \\ 0 & Q_{\Lambda_{2,1}} & Q_{\Lambda_{2,2}} \end{pmatrix}. \quad (2.1)$$

Following Ref. [17], we define the two-block operators

$$Q_{\Omega_i^*} = \begin{pmatrix} Q_{\Lambda_{i,i}} & Q_{\Lambda_{i,i+1}} \\ Q_{\Lambda_{i+1,i}} & Q_{\Lambda_{i+1,i+1}} \end{pmatrix}, \quad (2.2)$$

where $\Omega_i^* = \Lambda_i \cup \Lambda_{i+1}$ and $i = 0, 1$. The factorization of the determinant of Q is achieved as described in the following four steps.

²The block terminology and decompositions used here follow closely those in Ref. [17]. Throughout the paper dimensionful quantities are always expressed in units of the lattice spacing a , unless explicitly specified.

Step 1 Introduce the two-block partitioning of the lattice as defined in appendix B with $\Gamma = \Lambda_0 \cup \Lambda_2$ and $\Gamma^* = \Lambda_1$. Using Eq. (B.3) the determinant can be factorized as

$$\det Q = \det Q_{\Lambda_{1,1}} \det \begin{pmatrix} Q_{\Lambda_{0,0}} - Q_{\Lambda_{0,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,0}} & -Q_{\Lambda_{0,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,2}} \\ -Q_{\Lambda_{2,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,0}} & Q_{\Lambda_{2,2}} - Q_{\Lambda_{2,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,2}} \end{pmatrix}, \quad (2.3)$$

where the second matrix on the r.h.s. is the Schur complement associated to Γ .

Step 2 Use again Eq. (B.3) to obtain

$$\det Q = \frac{1}{\det Q_{\Lambda_{1,1}}^{-1} \det [P_{\Lambda_2} Q_{\Omega_1^*}^{-1} P_{\Lambda_2}] \det [P_{\Lambda_0} Q^{-1} P_{\Lambda_0}]}. \quad (2.4)$$

For the first two determinants in the denominator, the goal has been reached: they depend only on links from one or two time slices, respectively.

Step 3 Rewrite the last determinant as

$$\frac{1}{\det [P_{\Lambda_0} Q^{-1} P_{\Lambda_0}]} = \frac{1}{\det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}]} \det \begin{pmatrix} 1 & P_{\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} \\ P_{\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} & 1 \end{pmatrix}. \quad (2.5)$$

This step is suggested by the fact that for $x, y \in \Lambda_0$, the propagator elements $Q^{-1}(x, y)$ are expected to be well approximated by the inverse of $Q_{\Omega_0^*}$ up to corrections suppressed proportionally to $\exp\{-M_\pi \Delta\}$, where M_π is the pion mass and Δ is the thickness of the block Λ_1 [17], see also below.

Step 4 Reduce the last determinant in Eq. (2.5) to the one of a matrix acting on one of the boundaries only. To this end, Eq. (B.3) is employed once more

$$\det \begin{pmatrix} 1 & P_{\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} \\ P_{\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} & 1 \end{pmatrix} = \det \left(1 - P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} P_{\partial\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} P_{\partial\Lambda_0} \right), \quad (2.6)$$

where $P_{\partial\Lambda_0}$ and $P_{\partial\Lambda_2}$ are projectors on the inner boundary of the thick time-slices Λ_0 and Λ_2 respectively.

The factorized formula can finally be written as

$$\det Q = \frac{1}{\det Q_{\Lambda_{1,1}}^{-1} \det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}] \det [P_{\Lambda_2} Q_{\Omega_1^*}^{-1} P_{\Lambda_2}]} \det (1 - w), \quad (2.7)$$

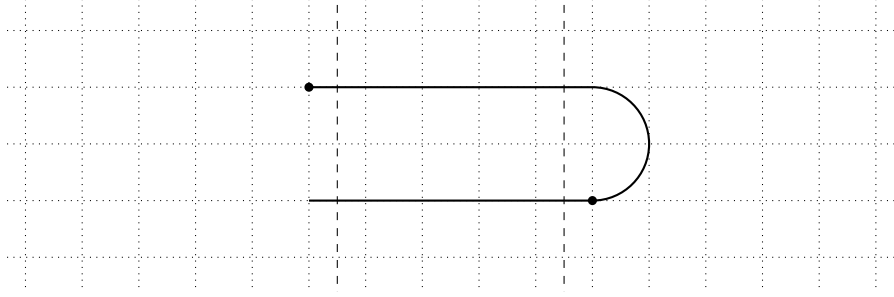


Figure 2: Representation of the operator w , black lines are full propagators while thick dots are insertions of the effective hops, see Eqs. (2.9).

where

$$w = P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} \quad (2.8)$$

acts on the inner boundary field $P_{\partial\Lambda_0} \psi$.

In Eq. (2.7) $\det Q_{11}^{-1}$ depends on the gauge field in the block Λ_1 , $\det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}]$ on the gauge fields in $\Lambda_0 \cup \Lambda_1$, and $\det [P_{\Lambda_2} Q_{\Omega_1^*}^{-1} P_{\Lambda_2}]$ on the gauge field in $\Lambda_1 \cup \Lambda_2$. Only the (small) correction $\det(1 - w)$ is a function of all links of the lattice. Note that $\det(1 - w)$ is real since all other determinants entering Eq. (2.7) are real.

2.1 Magnitude of w

To shed some light on the size of the contributions of the global determinant $\det(1 - w)$, one can rewrite the matrix in terms of the full propagator Q^{-1} . By considering two different partitions of the lattice in two blocks, first $\Lambda_0 \cup \Lambda_1$ and Λ_2 , and then Λ_0 and $\Lambda_1 \cup \Lambda_2$, it is easy to show that

$$\begin{aligned} P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} &= P_{\partial\Lambda_0} Q^{-1} \left\{ Q_{\Lambda_{1,2}} + Q_{\Lambda_{2,1}} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} \right\} , \\ P_{\partial\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} &= P_{\partial\Lambda_2} Q^{-1} \left\{ Q_{\Lambda_{1,0}} + Q_{\Lambda_{0,1}} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} \right\} . \end{aligned} \quad (2.9)$$

Therefore two propagators between the boundaries of the block Λ_0 and Λ_2 , each one multiplied by an effective boundary operator, appear in the definition of w (see Fig. 2). Numerical experience shows that, if the thickness Δ of the block Λ_1 is large enough, each of these propagators will be suppressed proportionally to $\exp\{-M_\pi \Delta/2\}$ [17]. Therefore the norm of w is expected to be suppressed as $\exp\{-M_\pi \Delta\}$.

2.2 Spectrum of w

Detailed knowledge of the spectrum of $1 - w$ is required for the next step. According to Eq. (2.8), the matrix w can be written as a product of two Hermitian matrices

$$w = [P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\partial\Lambda_0}] [Q_{\Lambda_{0,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,2}} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{2,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,0}}] \quad (2.10)$$

acting on the interior boundary of the block Λ_0 , which in turn implies that w is similar to w^\dagger [18]. The characteristic polynomial of w has therefore real coefficients, and the complex eigenvalues δ_i come in conjugate pairs. The spectrum of w is symmetric with respect to the real axis, and the determinant of $(1 - w)$ is real as anticipated. As a consequence of section 2.1, the modulus of the eigenvalues δ_i are expected to be suppressed proportionally to $\exp\{-M_\pi \cdot \Delta\}$.

3 Multiboson factorization

In the previous section, the goal of factorizing the determinant into contributions which depend on the gauge field in the neighboring thick time-slices has almost been reached. Only the determinant of $(1 - w)$ in Eq. (2.7) depends on the gauge field over the whole lattice. For a suitably chosen thickness of the central thick time-slice, however, all eigenvalues of w are expected to satisfy $|\delta_i| \ll 1$. This in turn implies a large spectral gap for the matrix $(1 - w)$, a fact which makes it possible to express its determinant through a polynomial approximation of $(1 - w)^{-1}$.

3.1 Polynomial approximation

As reviewed in appendix D, a generalization of Lüscher's original multiboson proposal [14] to complex matrices [19–21] starts by approximating the function $1/z$, with $z \in \mathbb{C}$, by the polynomial

$$P_N(z) \equiv \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^N (z - z_k), \quad (3.1)$$

where N is chosen to be even, and the N roots of $P_N(z)$ are obtained by requiring that for the remainder polynomial R_{N+1} holds $R_{N+1}(0) = 1$. 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 $1 \pm c$, see appendix D,

$$u_k = 1 - z_k = \cos\left(\frac{2\pi k}{N+1}\right) + \beta\sqrt{1-c^2} \sin\left(\frac{2\pi k}{N+1}\right), \quad k = 1, \dots, N. \quad (3.2)$$

3.2 Approximation of the determinant

This polynomial can be used to approximate the inverse determinant

$$\det(1 - w) \det\{P_N(1 - w)\} = \det\{1 - R_{N+1}(1 - w)\}, \quad (3.3)$$

where, if for all eigenvalues of w holds $|\delta_i| < 1$, the right hand side converges exponentially to 1 as N is increased. Since the determinant of w is real and the u_k come in complex conjugate pairs, the approximate determinant can be written in a manifestly positive form

$$\det\{P_N(1 - w)\}^{-1} = C \prod_{k=1}^{N/2} \det^{-1}\{(u_k - w)^\dagger (u_k - w)\} = C \prod_{k=1}^{N/2} \det^{-1}(W_{\sqrt{u_k}}^\dagger W_{\sqrt{u_k}}) \quad (3.4)$$

with a irrelevant constant C and

$$W_z = \begin{pmatrix} z P_{\partial\Lambda_0} & P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} P_{\partial\Lambda_2} \\ P_{\partial\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} P_{\partial\Lambda_0} & z P_{\partial\Lambda_2} \end{pmatrix}. \quad (3.5)$$

In the last equality of Eq. (3.4), the reverse substitution of the one in Eq. (2.6) has been performed. For the determination of the approximation, it is advantageous to work with the operator w (acting on $\partial\Lambda_0$ only) since the order of the polynomial is reduced by about a factor 2 for a given accuracy. The expression (3.4) with W_z acting on $\partial\Lambda_0$ and $\partial\Lambda_2$, however, allows in the next step for a fully factorized domain-decomposition of the fermion action.

3.3 Multiboson action

For two flavors of quarks we can finally represent the determinants by scalar fields [22]³

$$\begin{aligned} \frac{\det Q^2}{\det\{1 - R_{N+1}(1 - w)\}^2} &= \frac{1}{\det [Q_{\Lambda_{1,1}}^{-1}]^2 \cdot \det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}]^2 \cdot \det [P_{\Lambda_2} Q_{\Omega_1^*}^{-1} P_{\Lambda_2}]^2} \times \\ &\times \det \{P_N(1 - w)\}^{-2} = C' \int [d\phi_0 d\phi_0^\dagger] e^{-|P_{\Lambda_0} Q_{\Omega_0^*}^{-1} \phi_0|^2} \int [d\phi_1 d\phi_1^\dagger] e^{-|Q_{\Lambda_{1,1}}^{-1} \phi_1|^2} \\ &\int [d\phi_2 d\phi_2^\dagger] e^{-|P_{\Lambda_2} Q_{\Omega_1^*}^{-1} \phi_2|^2} \cdot \prod_{k=1}^N \left\{ \int [d\chi_k d\chi_k^\dagger] e^{-|W_{\sqrt{w_k} \chi_k}|^2} \right\}, \end{aligned} \quad (3.6)$$

where C' is another irrelevant numerical constant. Each scalar field ϕ_i is confined to the corresponding region Λ_i , $i = 0, 1, 2$. The N fields χ_k live on the outer boundaries of region Λ_1 . We can decompose them as $\chi_k = \eta_k + \xi_k$, with $\eta_k = P_{\partial\Lambda_0} \chi_k$ and $\xi_k = P_{\partial\Lambda_2} \chi_k$, and split explicitly the contributions from the inner boundaries of region Λ_0 and Λ_2 as

$$\begin{aligned} |W_z \phi_k|^2 &= |z|^2 |\eta_k|^2 + |z|^2 |\xi_k|^2 + |P_{\partial\Lambda_2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} \eta_k|^2 + |P_{\partial\Lambda_0} Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} \xi_k|^2 \\ &+ [z(\xi_k, Q_{\Lambda_{2,1}} Q_{\Omega_0^*}^{-1} \eta_k) + z^*(\xi_k, Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} \eta_k) + \text{c.c.}], \end{aligned} \quad (3.7)$$

The dependence of the bosonic action from the gauge field in block Λ_0 and Λ_2 is thus factorized. Interestingly, the terms in Eq. (3.7) which will contribute to the forces in region Λ_0 always start (or end) on the inner boundary of Λ_2 and vice versa. The matrices in Eq. (3.7) contain one boundary to boundary quark propagator which is suppressed exponentially in Δ , see Eq. (2.9), and so do the corresponding forces.

3.4 Order of the polynomial

The order of the polynomial can be fixed, for the required precision, by employing Eq. (D.2) in appendix D. This guarantees that

$$\max_{\|v\|=1} \|[1 - (1 - w)P_N(1 - w)]v\| \leq \max_i |\delta_i|^{N+1} = |\delta|_{\max}^{N+1} \quad (3.8)$$

³The identity $\det Q_{\Lambda_{1,1}}^{-1} \cdot \det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}] = \det Q_{\Omega_0^*}^{-1}$ can be used to speed up the simulation when the region 1 is active.

where v is a generic vector on which w act. Then Eq. (3.3), when $|\delta|_{\max}^{N+1} \ll 1$ and $\text{Tr } R_{N+1}(1-w) \ll 1$, implies

$$\det(1-w) \det\{P_N(1-w)\} = 1 - \text{Tr } R_{N+1}(1-w) + \dots \quad (3.9)$$

At the first order in the expansion, the relative error which one makes on the determinant is therefore

$$|\text{Tr } R_{N+1}(1-w)| \leq \sum_i |\delta_i|^{N+1} \leq \sum_{i=1}^{N_{\text{ev}}} |\delta_i|^{N+1} + (6L^3 - N_{\text{ev}}) |\delta_{N_{\text{ev}}+1}|^{N+1}, \quad (3.10)$$

where in the last inequality the contribution from the N_{ev} eigenvalues with the highest modules, i.e. $|\delta_i|$ sorted decreasingly, has been treated separately and L is the spatial length in lattice units. If the bulk of the modes have modulus significantly smaller than $|\delta|_{\max}$ and if N is large, the sum on the r.h.s. of Eq. (3.10) will not generate a large factor, see below. Given the distribution of the eigenvalues of w , the circle centered in 1 with radius 1 is a natural choice for the polynomial approximating $(1-w)^{-1}$ that we adopt in the following. However one could optimize further the approximation by working with an ellipse, and tuning the value of c .

3.5 Reweighting factor

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

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N} = \frac{\langle O_{\text{fact}} \rangle_N}{\langle \mathcal{W}_N \rangle_N} + \frac{\langle O \mathcal{W}_N - O_{\text{fact}} \rangle_N}{\langle \mathcal{W}_N \rangle_N}, \quad (3.11)$$

where O_{fact} is a rather precise factorized approximation of O , see Ref. [17] for instance, and $\langle \cdot \rangle_N$ indicates the expectation value in the theory defined by the multiboson action at finite N . Since both the action and the observable are factorized, the expectation value $\langle O_{\text{fact}} \rangle_N$ can be computed with a multilevel algorithm by generating gauge field configurations with the multiboson action at finite N . All other quantities in Eq. (3.11) can be computed with a one-level Monte Carlo procedure. For two flavors, the reweighting factor \mathcal{W}_N is

$$\mathcal{W}_N = \det\{1 - R_{N+1}(1-w)\}^2. \quad (3.12)$$

This expression is easily evaluated as

$$\mathcal{W}_N = \frac{\int [d\eta] [d\eta^\dagger] e^{-|(1-R_{N+1})^{-1}\eta|^2}}{\int [d\eta] [d\eta^\dagger] e^{-\eta^\dagger \eta}}, \quad (3.13)$$

where the exponent can be computed by a Taylor expansion, and as usual the integral over η can be replaced by random samples. For the special case of a circle, the simplification $R_{N+1}(1-w) = w^{N+1}$ applies.

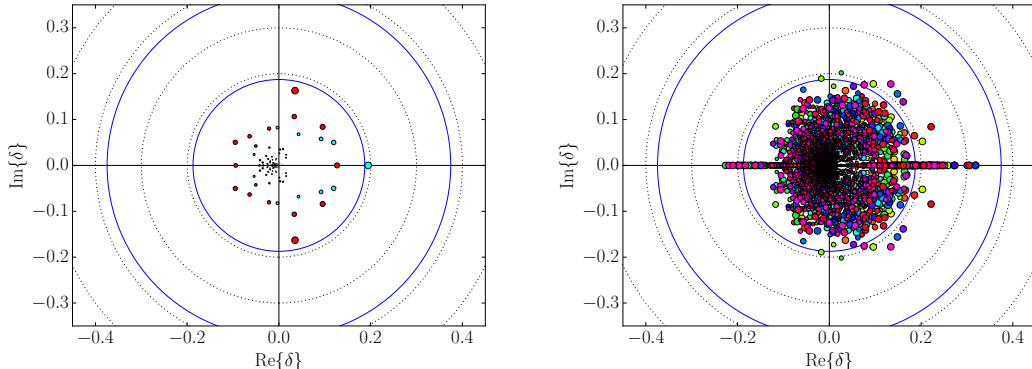


Figure 3: Left: eigenvalues δ_i of w ($\Delta = 12$) with the largest norm for two typical configurations. Right: as on the left but for all the 200 configurations. In both panels the blue circles have radius $\bar{\delta} = \exp\{-M_\pi\Delta\}$ and $2\bar{\delta}$.

4 Numerical tests on the spectrum of w

The feasibility of the whole proposal hinges crucially on the assumption that the spectrum of the operator w is confined into a disk around 1 in the complex plane, with a radius significantly below unity. Only in this case, a small number of bosonic fields N in Eq. (3.7) leads to a good enough approximation at reasonable computational cost.

To test this assumption, we have generated a set of 200 configurations with the Wilson gluonic action and with two flavors of non-perturbatively $O(a)$ -improved Wilson quarks as defined in appendix A, with $\beta = 5.3$, $c_{\text{SW}} = 1.90952$, $c_{\text{F}} = c'_{\text{F}} = 1$, $k = 0.13625$, $T \times L^3 = 64 \times 32^3$ and open boundary conditions. The lattice spacing is 0.0652(6) fm, while the pion mass in lattice units is $M_\pi = 0.1454(5)$ corresponding to 440(5) MeV [23].

For $\Delta = 8, 12$ and 16, we have computed with the Arnoldi algorithm the 60 approximate eigenvalues δ_i of w with the largest absolute value. On the left plot of Fig. 3, they are shown for $\Delta = 12$ and on two typical configurations. As expected, the eigenvalues are either real or appear in complex conjugate pairs. For one configuration (green points) the eigenvalue with the largest absolute value is real, while for the other one (red points) two eigenvalues with opposite imaginary parts have the largest absolute value. We find that both possibilities are common, see last column of Table 1. In the right plot of Figure 3 we show the eigenvalues δ_i again for $\Delta = 12$ but for all configurations. The blue circles in these plots have radius $\bar{\delta}$ and $2\bar{\delta}$, where

$$\bar{\delta} = \exp\{-M_\pi\Delta\}. \quad (4.1)$$

The distribution of the eigenvalue with the largest magnitude is shown in the left plot of Figure 4. It is peaked at a value slightly smaller than $\bar{\delta}$, denoted by a vertical blue line, and extends up to $\sim 2\bar{\delta}$. The results for the largest eigenvalue norm computed over the 200 configurations, its average value and the estimate of its standard deviation are

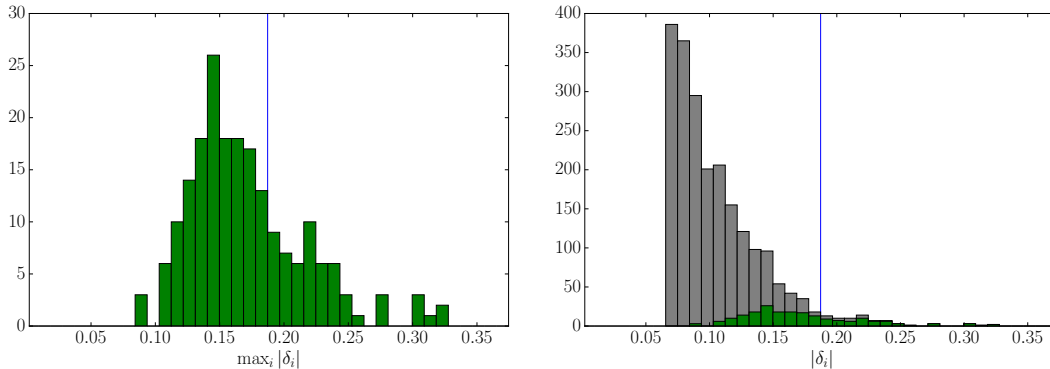


Figure 4: Left: distribution of the eigenvalue of w ($\Delta = 12$) with the largest absolute value. The vertical blue line is at $|\delta_i| = \bar{\delta}$. Right: as in left but for the eigenvalues with $|\delta_i| > 0.35 \bar{\delta}$.

Table 1: Properties of the spectrum of w for different values of Δ . f_{Re} is the fraction of configurations for which δ_i with the largest absolute value is real.

Δ	ncfg	$\bar{\delta}$	$\langle \max_i \delta_i \rangle$	$\sigma(\max_i \delta_i)$	$\max \max_i \delta_i $	$f_{\text{Re}}[\%]$
8	200	0.3273	0.2886	0.0616	0.5130	48.5
12	200	0.1710	0.1692	0.0453	0.3193	46.5
16	200	0.1072	0.0951	0.0284	0.1977	45.5

also reported in Table 1. On the right plot of Figure 4 we also report the distribution of the absolute value of the eigenvalues limited to those with $|\delta_i| > 0.35 \bar{\delta}$.

A clear message emerges from this data. The largest eigenvalue of the relevant operator w decreases proportionally to $\exp\{-M_\pi \Delta\}$, with a prefactor of order 1. This in turn implies that $(1 - w)$ has a large gap if Δ is properly tuned. The relative error on the determinant computed as in Eq. (3.10) at various values of N compares well with $|\delta|_{\text{max}}^{N+1}$ configuration by configuration. No big prefactors appear because the eigenvalues do not accumulate near the maximum one, and the approximation gets exponentially more precise toward the center of the circle. We have also computed the reweighting factor as defined in Eq. (3.13). Its value, again for $N = 12$ and estimated with 4 random sources per configuration, deviates from 1 by at most $4.5 \cdot 10^{-6}$ again in line with the expectation. At the level of precision of most contemporary simulations the impact of the reweighting factor is therefore negligible.

5 Numerical implementation of MB-DD-HMC

The effective action in Eq. (3.6) can be simulated using variants of the hybrid Monte-Carlo algorithm [1]. The implementation does not pose particular problems. To define the setup for the tests discussed below, we mention a few essential points only. In the

following we distinguish two basic contributions: the determinants of the block operators such as $\det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}]$, and the multiboson contributions responsible for the coupling between the blocks Λ_0 and Λ_2 .

5.1 Block action

In the denominator of Eq. (3.6), there are three determinants deriving from the block decomposition of the fermion determinant. For the sake of the presentation we focus on $\det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}]$, the other two being treated analogously. Since in general the thick time-slices are not particularly thin, further decomposition of this determinant is necessary in order to have a cost-efficient simulation. One possibility is to apply mass-preconditioning [24, 25], that is to write

$$\det [P_{\Lambda_0} Q_{\Omega_0^*}^{-1} P_{\Lambda_0}] = \prod_{i=1}^{N_\mu-1} \frac{\det [P_{\Lambda_0} \{Q_{\Omega_0^*}(\mu_i)\}^{-1} P_{\Lambda_0}]}{\det [P_{\Lambda_0} \{Q_{\Omega_0^*}(\mu_{i+1})\}^{-1} P_{\Lambda_0}]} \cdot \det [P_{\Lambda_0} \{Q_{\Omega_0^*}(\mu_{N_\mu})\}^{-1} P_{\Lambda_0}] \quad (5.1)$$

with $0 = \mu_1 < \mu_2 < \dots < \mu_{N_\mu}$ and $Q_{\Omega_0^*}(\mu) = Q_{\Omega_0^*} + i\mu P_{\Lambda_0}$. The pseudofermion heatbath is then performed using

$$[P_{\Lambda_0} \{Q_{\Omega_0^*}(\mu)\}^{-1} P_{\Lambda_0}]^{-1} = Q_{\Lambda_{0,0}} - Q_{\Lambda_{0,1}} Q_{\Lambda_{1,1}}^{-1} Q_{\Lambda_{1,0}} + i\mu P_{\Lambda_0}. \quad (5.2)$$

In the numerical tests described in the following we have used $N_\mu = 5$, with twisted-mass values $\mu_i = 0.0, 0.001, 0.005, 0.1, 0.5$ for $i = 1, \dots, 5$.

5.2 Multiboson action

The contribution of the multiboson fields is by construction small and therefore preconditioning does not seem to be necessary in a first implementation. The computation of the forces themselves is straightforward, while the heatbath for the bosonic fields requires further attention.

For the fields χ_k , distributed according to the action $S_{b,k} = |W_{\sqrt{u_k}} \chi_k|^2$, the heatbath can be performed in the usual fashion, by acting with the inverse of $W_{\sqrt{u_k}}$ on Gaussian random fields located on the inner boundaries of region Λ_0 and Λ_2 . One way to solve the corresponding linear system is discussed in appendix E. The cost of these inversions is a negligible compared to the one of the molecular dynamics evolution. In the numerical tests presented in the following we have used $N = 12$ multiboson fields χ_k , with the roots z_k chosen to lie on the circle of radius 1 centered in 1.

6 Numerical tests of MB-DD-HMC

In order to test the potentiality of the two-level MB-DD-HMC algorithm described in the previous section, we have taken a subset of $n_0 = 32$ configurations spaced by at least 80 molecular dynamics units (MDUs) among the 200 described in Section 4, which we

can safely assume to be independent.⁴ Starting from each of them, we have generated $n_1 = 45$ level-1 configurations spaced by 4 MDUs by keeping fixed the links in region Λ_1 . The latter extends between time slices 24 and 35, corresponding to a thickness of $\Delta \approx 0.8$ fm and $M_\pi \Delta \approx 1.7$.

For the gauge variables in each of the two active regions Λ_0 and Λ_2 , the molecular dynamics in the HMC can be integrated with the following nested three level scheme. The forces deriving from the multiboson fields are integrated on the outermost level with a second order OMF [26] integrator, with 12 steps per trajectory of length 2. On the second level, all forces deriving from the block determinants in Eq. (5.1) are integrated, with one step of the fourth order OMF integrator per outer step. The third level, which consists again of one fourth order OMF step, takes care of the gauge forces. This scheme, which is very similar to the ones used in Ref. [27], leads to an acceptance rate of 94%.

6.1 Correlation functions of gluonic operators

The primary local gluonic observables that we measure to test the algorithm are the energy and the topological charge densities summed over the time-slices, i.e.

$$\bar{e}(x_0) = \frac{1}{4} \sum_{\vec{x}} F_{\mu\nu}^a(x) F_{\mu\nu}^a(x), \quad \bar{q}(x_0) = \frac{1}{64\pi^2} \sum_{\vec{x}} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x), \quad (6.1)$$

where the gluon field strength tensor is the one in Eq. (A.6) but with the trace removed. In particular we focus on the expectation value

$$C_e(x_0) = \frac{1}{L^3} \langle \bar{e}(x_0) \rangle, \quad (6.2)$$

and on the correlators

$$C_{ee}(x_0, y_0) = \frac{1}{L^3} \langle \bar{e}(x_0) \bar{e}(y_0) \rangle_c, \quad (6.3)$$

$$C_{qq}(x_0, y_0) = \frac{1}{L^3} \langle \bar{q}(x_0) \bar{q}(y_0) \rangle. \quad (6.4)$$

In an analysis of 200 level-0 configurations each spaced by 8 MDUs, autocorrelations of $\bar{e}(x_0)$ and $\bar{q}(x_0)$ are not detectable.

The two-level estimates of the same quantities have been carried out by first averaging, for each of the n_0 configurations, the densities over the n_1 level-1 background fields. This gives n_0 measurements of the improved observables. The figure of merit is the variance of this estimator. In the situation where autocorrelations among the n_0 level-0 configurations can be neglected, the square root of the variance divided by $\sqrt{n_0}$ gives the error of the measurement. Since the cost of the simulation scales linearly in n_1 , the variance itself should decrease with n_1 to break even.

⁴Since with $N = 12$ the reweighting factor is negligible within the statistical precision of our observables, for testing purposes it is appropriate to use the level-0 configurations already generated with the exact action.

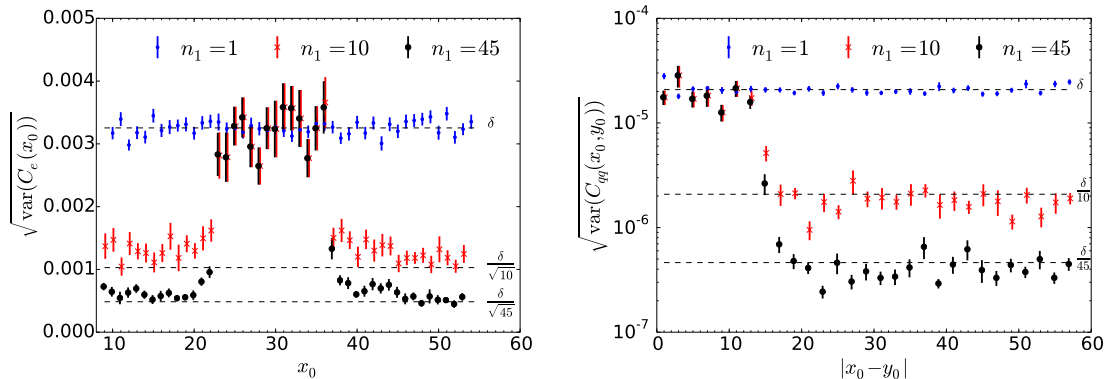


Figure 5: In the left panel, the square root of the variance of the energy density averaged over the time slice x_0 is shown. In the frozen central region this does not profit from the level-1 updates, while in the active regions, it decreases with the square root of their inverse number. The right plot demonstrates the effectiveness of the multilevel algorithm for the topological charge density correlation function. The time slices x_0 and $y_0 = 30 - x_0$ are chosen such that they are symmetric with respect to the frozen region Λ_1 . Once $|x_0 - y_0| > 12$ they enter the active regions where the square root variance decreases with $1/n_1$. In both plots, the horizontal lines indicate the ideal scaling behavior as expected from the variance measured at level-0.

The square root of the variance of $C_e(x_0)$ as a function of x_0 is shown in the left panel of Fig. 5. In the central region, the links are frozen during the level-1 updates. We therefore do expect the same variance as in the level-0 estimator, just the error of the variance is larger due to the smaller value of n_0 in this case. Once we move into the active regions Λ_0 and Λ_2 , however, the variance of the estimator is clearly improved, in agreement with what is expected from ideal scaling, i.e. $\sqrt{\text{var}(C_e)} \propto 1/\sqrt{n_1}$.

In the right panel the same analysis is shown for the two-point function C_{qq} , and analogous results are obtained for C_{ee} . Here the full benefit of the method can be realized, because an improved estimator can be constructed by averaging for each of the n_0 fields the densities in region Λ_0 and Λ_2 independently before constructing the two-point function. As optimal scaling in this case we expect a reduction of the square root of the variance, and therefore the error, with $1/n_1$. The numerical data is in agreement with such a reduction once x_0 and y_0 are in two different active regions.

The picture emerging from this analysis is just in line with expectations. In the region where the links are frozen during the level-1 updates no benefit from the multilevel is observed. As soon as the densities are in the active regions Λ_0 and Λ_2 , the square root of the variances of the one- and two-point functions are reduced by $1/\sqrt{n_1}$ and $1/n_1$ respectively. The two-level Monte Carlo works at full potentiality in these regions, with a net gain in the computational cost of the two-point functions of n_1 . This in turn implies that links in the active regions Λ_0 and Λ_2 are regularly updated during the level-1 MB-DD-HMC. In particular no freezing induced by multiboson fields is observed.

6.2 Disconnected pseudoscalar propagator

Quark-line disconnected correlation functions serve as a second test of the method, following our quenched results presented in Ref. [17]. We restrict ourselves to the correlation between two flavor-diagonal pseudoscalar densities,

$$C_{P_d}(y_0, x_0) = \frac{1}{L^3} \left\langle \sum_{\vec{x}} \text{tr} \left\{ Q^{-1}(x, x) \right\} \times \sum_{\vec{y}} \text{tr} \left\{ Q^{-1}(y, y) \right\} \right\rangle \quad (6.5)$$

which are decomposed as in Eq. (6.1) of Ref. [17]

$$C_{P_d}(y_0, x_0) = C_{P_d}^{(f)}(y_0, x_0) + C_{P_d}^{(r_1)}(y_0, x_0) + C_{P_d}^{(r_2)}(y_0, x_0). \quad (6.6)$$

In the first contribution, the two propagators in Eq. (6.5) are replaced by approximate propagators with Dirichlet boundary conditions imposed at $x_0^{\text{cut}} = 30$, making this term amenable to multilevel integration. The other two contributions are correction terms which make the equation exact, containing once or twice, respectively, the difference between the full and approximate propagator. Note that in this case there are several options for imposing Dirichlet boundary conditions. They may, for instance, be imposed on the (opposite) respective ends of the frozen region Λ_1 .

All the traces appearing on the r.h.s. of Eq. (6.6) are estimated stochastically by inverting the various Dirac operators on the very same $n_{\text{src}} = 500$ Gaussian random sources η_i , defined on the whole space-time volume, and by contracting the solution with a time-slice of η_i , see Ref. [17] for more details⁵. A rough measure of the autocorrelation function of $\sum_{\vec{x}} \text{tr} \left\{ Q^{-1}(x, x) \right\}$ from level-0 configurations shows that the autocorrelation time is approximately $\tau_{\text{int}} = 10$ MDUs. The 32 configurations can thus be safely considered as independent when used for level-0 measurements.

As for the gluonic two-point function above, the $C_{P_d}^{(f)}(y_0, x_0)$ contribution, for $x_0 < 24$ and $y_0 > 35$, is estimated by first averaging, for each of the level-0 configurations, the two traces independently over the n_1 level-1 background fields. The product of the two means constitutes the improved estimator which is then averaged over the n_0 measurements. For the other two contributions such an improved estimator is not available. The correlation functions $C_{P_d}^{(r_1)}$ and $C_{P_d}^{(r_2)}$ as a whole are first averaged over level-1, giving again n_0 measurements which are then processed in the usual manner.

While for the first contribution the scaling of the square root variance is expected to be proportional to n_1^{-1} , for the second and the third it goes at most with $n_1^{-1/2}$. Since n_1 has to be counted in number of independent measurements and the level-1 updates are spaced by 4 MDUs only, in the plots we opt for normalizing the number of level-1 updates as $\bar{n}_1 = n_1 / (2 \tau_{\text{int}}) = n_1 / 5$. This rescaling has no impact on the correctness of the procedure itself, but relates only to the level of improvement which one can expect from a given number of level-1 updates.

⁵At variance with Ref. [17], here we did not use the hopping parameter variance reduction in the singlet evaluation.

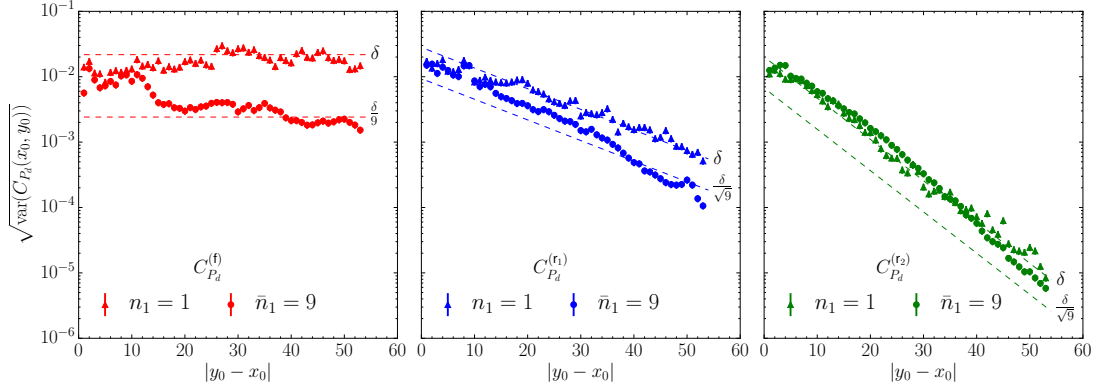


Figure 6: The square root of the variance of the three contributions of the disconnected correlator of two flavor-diagonal pseudoscalar densities, see Eq. (6.6), are shown as a function of the time separation $|y_0 - x_0|$. The dashed lines indicate the expected asymptotic form, which is constant for the first contributions and falls exponentially $\exp\{-M_\pi|y_0 - x_0|/2\}$ and $\exp\{-M_\pi|y_0 - x_0|\}$ for the second and third contribution, respectively. In all panels, the lower line indicates the expected reduction from the level-1 updates.

The numerical results for the square root of the variance of $C_{P_d}^{(f)}$, $C_{P_d}^{(r_1)}$, and $C_{P_d}^{(r_2)}$ are plotted in Fig. 6 as a function of the time separation of the pseudoscalar densities. In all cases x_0 and y_0 belong to different domains, $y_0 > x_0$, and they are chosen to be as much as possible equidistant from x_0^{cut} . These plots can be directly compared with those on the right column of Fig. 4 in Ref. [17].

Our findings are very similar to the quenched case [17], once one takes into account that in the present computation 12 slices are frozen instead of 1. The square root of the variance of $C_{P_d}^{(f)}$, left plot of Fig. 6, is a flat function of $|y_0 - x_0|$ with sizeable deviations near the boundaries of the domains. Up to the largest value that we have, $\bar{n}_1 = 9$, the square root variance decreases approximately as \bar{n}_1^{-1} for large $|y_0 - x_0|$, i.e. the two-level Monte Carlo works as expected. For $C_{P_d}^{(r_1)}$ and $C_{P_d}^{(r_2)}$, center and right plots in Fig. 6, a strong dependence on $|y_0 - x_0|$ is observed. They are compatible with an exponential behavior of the form $\exp\{-M_\pi|y_0 - x_0|/2\}$ and $\exp\{-M_\pi|y_0 - x_0|\}$ respectively as suggested by theory.

The picture which emerges is analogous to the one in the quenched case [17]. At large time distances, the statistical error of the standard estimate of the disconnected pseudoscalar propagator is dominated by the one on $C_{P_d}^{(f)}$. This is the contribution for which the multilevel is efficient. The second largest contribution is the statistical error on $C_{P_d}^{(r_1)}$ which, however, is exponentially suppressed as $\exp\{-M_\pi|y_0 - x_0|/2\}$. Therefore, once the two-level integration is switched on and a large enough number of n_1 level-1 configurations is generated, the signal-to-noise ratio increases exponentially in $|y_0 - x_0|$ with respect to the standard Monte Carlo.

7 Conclusions

The gauge field dependence of the fermion determinant is factorizable by combining a domain decomposition with a multiboson representation of the (small) interaction among gauge fields on distant blocks.

The resulting action is local in the block scalar and gauge fields and can be simulated by variants of the standard hybrid Monte Carlo algorithm. The measurements of local gluonic observables, such as the energy and the topological charge densities, reveal a good efficiency of the algorithm in updating the gauge field. No particular freezing of the links is observed. The locality of the action can be beneficial for simulations using parallel computers due to reduced communication.

When combined with the recently proposed factorization of the fermion propagator [17], this setup naturally allows for multilevel Monte Carlo integration also in the presence of fermions, opening new perspectives in lattice gauge theories. The numerical test of the disconnected correlator of two flavor-diagonal pseudoscalar densities that we have reported indeed shows that the signal-to-noise ratio increases exponentially with the time distance of the sources when a two-level integration is at work.

Many interesting computations in lattice QCD and other theories are expected to profit from these improvements, especially those which suffer from signal-to-noise ratios which decrease exponentially with the time distance of the sources. Prime examples here are disconnected correlators and/or baryonic two- and three-point functions.

The proposed method relies on two key ingredients: the locality of the Wilson Dirac operator and the (configuration by configuration) exponential decrease of its inverse with the distance between the sink and the source. The ideas and the computational strategy presented here may, therefore, be applicable to very different theories with fermions if they enjoy these very basic properties.

8 Acknowledgments

Simulations have been performed on the PC-clusters Galileo and Marconi at CINECA (CINECA-INFN and CINECA-Bicocca agreements), PAX at DESY, and Wilson at Milano-Bicocca. We thank these institutions for the computer resources and the technical support. Numerical simulations have been carried out with a modified version of the open-QCD code version 1.4 [28].

A $O(a)$ -improved Wilson–Dirac operator

The massive $O(a)$ -improved Wilson–Dirac operator is defined as [27, 29, 30]

$$D = D_w + \delta D_v + \delta D_b + m_0 , \tag{A.1}$$

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

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

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

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

where $U_\mu(x)$ are the link fields. The boundary corrections terms are defined to be

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

$$\delta D_b \psi(x) = \{(c_F - 1) \delta_{x_0,1} + (c'_F - 1) \delta_{x_0,T-1}\} \psi(x), \quad (\text{A.5})$$

where with open boundary conditions in the time direction $c'_F = c_F$, $\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu]$, and the field strength of the gauge field is

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

with

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

We are also interested in the operator $Q = \gamma_5 D$, which is Hermitian since D satisfies the γ_5 -hermiticity relation $D = \gamma_5 D^\dagger \gamma_5$.

B LU decomposition of a 2×2 block matrix

A 2×2 block matrix can be decomposed as

$$Q = \begin{pmatrix} Q_\Gamma & Q_{\partial\Gamma} \\ Q_{\partial\Gamma^*} & Q_{\Gamma^*} \end{pmatrix} = \begin{pmatrix} I & Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} \\ 0 & I \end{pmatrix} \begin{pmatrix} S_\Gamma & 0 \\ Q_{\partial\Gamma^*} & Q_{\Gamma^*} \end{pmatrix}, \quad (\text{B.1})$$

where the Schur complement is defined as

$$S_\Gamma = Q_\Gamma - Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*}. \quad (\text{B.2})$$

Its determinant can then be factorized

$$\det Q = \det (Q_\Gamma - Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*}) \det Q_{\Gamma^*}, \quad (\text{B.3})$$

while the inverse is given by

$$Q^{-1} = \begin{pmatrix} S_\Gamma^{-1} & -S_\Gamma^{-1} Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} \\ -Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*} S_\Gamma^{-1} & Q_{\Gamma^*}^{-1} + Q_{\Gamma^*}^{-1} Q_{\partial\Gamma^*} S_\Gamma^{-1} Q_{\partial\Gamma} Q_{\Gamma^*}^{-1} \end{pmatrix}. \quad (\text{B.4})$$

It is worth noting that S_Γ^{-1} is the exact inverse of Q if the source and the sink positions are both in Γ .

When z is contained in an ellipse centered at a distance d from the origin on the positive real axis, with major and minor radii a and b respectively and with focus distance $c = \sqrt{a^2 - b^2}$, the polynomial approximation of $1/z$ of order n is

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

where

$$R_{N+1}(z) \equiv \frac{T_{N+1}\left(\frac{d-z}{c}\right)}{T_{N+1}\left(\frac{d}{c}\right)}, \quad (\text{D.2})$$

with $T_k(z)$ being the Chebyshev polynomial of the first kind of degree k . The N roots of $P_N(z)$ are obtained by requiring that $R_{N+1}(0) = 1$, and they are given by

$$z_k = d \left(1 - \cos \frac{2\pi k}{N+1} \right) - \beta \sqrt{d^2 - c^2} \sin \frac{2\pi k}{N+1}, \quad k = 1, \dots, N. \quad (\text{D.3})$$

They lie on the ellipse in the complex plane with center d , foci $d \pm c$, and which passes through zero. By using the definition of the Chebyshev polynomials, a uniform error bound on the approximation is given by

$$|1 - zP_N(z)| = |R_{N+1}(z)| \leq \left(\frac{a + \sqrt{a^2 - c^2}}{d + \sqrt{d^2 - c^2}} \right)^{N+1} \left\{ 1 + \left[\frac{a}{c} + \left(\frac{a^2}{c^2} - 1 \right)^{1/2} \right]^{-2N-2} \right\}. \quad (\text{D.4})$$

D.1 The circle

In the limit $c \rightarrow 0$, when the ellipse becomes a circle centered in d with radius $a = b$, it holds

$$|R_{N+1}(z)| \equiv \left| \frac{d-z}{d} \right|^{N+1}. \quad (\text{D.5})$$

The bound becomes

$$|1 - zP_N(z)| = |R_{N+1}(z)| \leq \left(\frac{a}{d} \right)^{N+1}, \quad (\text{D.6})$$

which corresponds to the limit of Eq. (D.4) when $c \rightarrow 0$. The Zangwill lemma guarantees that the polynomial is optimal in this case. The roots of $P_N(z)$ are again given by Eq. (D.3) with $c = 0$. They lie on a circle centered in d of radius d . If we choose $d + a = 1$ and define the spectral gap as $d - a = \epsilon$ we get

$$|R_{N+1}(z)| \leq \left(\frac{a}{d} \right)^{N+1} = \left(\frac{1 - \epsilon}{1 + \epsilon} \right)^{N+1}. \quad (\text{D.7})$$

In the limit in which $\epsilon \ll 1$

$$\left(\frac{1 - \epsilon}{1 + \epsilon} \right)^{N+1} \sim e^{-2\epsilon(N+1)}, \quad (\text{D.8})$$

which shows that the polynomial approximation converges exponentially in N with a rate twice the (small) gap.

E Inverse of W_z

The operator W_z , defined in Eq. (3.5), acts on the union of the inner boundaries of region Λ_0 and Λ_2 . For the heatbath of the bosonic fields, the solution to the equation $W_z\chi = \eta$ needs to be found. This is not trivial, because the definition of W_z itself contains matrix inverses. Following the general idea of Eq. (3.12) of Ref. [16], we recast this problem into the solution of an extended system, from which a suitable projection gives the desired result. In particular we define complex vectors on an extended lattice, the latter being the ordinary lattice augmented by a copy of region Λ_1 . On this space acts the matrix \bar{Q} , defined by

$$\bar{Q} \equiv \begin{pmatrix} Q_{\Lambda_0,0} & Q_{\Lambda_0,1} & 0 & 0 \\ Q_{\Lambda_1,0} & Q_{\Lambda_1,1} & 0 & z^{-1}Q_{\Lambda_1,2} \\ z^{-1}Q_{\Lambda_1,0} & 0 & Q_{\Lambda_1,1} & Q_{\Lambda_1,2} \\ 0 & 0 & Q_{\Lambda_2,1} & Q_{\Lambda_2,2} \end{pmatrix}. \quad (\text{E.1})$$

This is an ordinary sparse matrix, which is amenable to the standard iterative algorithms for the solution of linear systems. Since it is in general not well conditioned, it turns out to be profitable to use the deflation techniques introduced in Ref. [33] to accelerate the computation.

By using the matrix \bar{Q} , it is easy to show that the following identity holds

$$zW_z^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \bar{Q}^{-1} \begin{pmatrix} Q_{\Lambda_0,1} Q_{\Lambda_1,1}^{-1} Q_{\Lambda_1,0} & 0 \\ Q_{\Lambda_1,0} & z^{-1}Q_{\Lambda_1,2} \\ z^{-1}Q_{\Lambda_1,0} & Q_{\Lambda_1,2} \\ 0 & Q_{\Lambda_2,1} Q_{\Lambda_1,1}^{-1} Q_{\Lambda_1,2} \end{pmatrix}, \quad (\text{E.2})$$

where the two components on which the matrix acts are the two inner boundaries of region Λ_0 and Λ_2 , respectively. The computation of the inverse of W_z is thus reduced to a sequence of solutions of sparse linear systems.

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