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Bloch Waves, Magnetization and Domain Walls: The Case of the Gluon Propagator **

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** In memory and recognition of Daniel Zwanziger.

Abstract

We expand our previous study of replicated gauge configurations in lattice SU(N_c) Yang–Mills theory—employing Bloch's theorem from condensed matter physics—to construct gauge-fixed field configurations on significantly larger lattices than the original, or primitive, one. We present a comprehensive discussion of the general gauge-fixing problem, identifying advantages of the replicated-lattice approach. In particular, the consideration of Bloch waves leads us to a visualization of the extended gauge-fixed configurations in terms of (color) magnetization domains. Moreover, we are able to explore features of the method to optimize the evaluation of gauge fields in momentum space, furthering our knowledge of the "allowed momenta", an issue that has hindered wider applications of this approach up to now. Interestingly, our analysis yields both a better conceptual understanding of the problem and a more efficient way to compute the desired large-volume observables.

Keywords: lattice QCD; algorithms and theoretical developments; correlation functions; vacuum structure and confinement

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1. Introduction

We study the problem of fixing the so-called minimal Landau gauge in Yang–Mills theory using a replicated gauge-field configuration on an extended lattice Λ_z, obtained by copying—m times along each direction—the link configuration defined on the original lattice Λ_x [1]. We employ periodic boundary conditions (PBCs), both for the original and for the extended lattice. This setup is then used for the evaluation of the gluon propagator in pure gauge theory, aiming at explaining and understanding the results obtained from numerical simulations of the propagator in the infrared regime for two, three, and four space-time dimensions [2–4]. We recall that this method was first proposed by D. Zwanziger in Ref. [5], as a way to take the infinite-volume limit in lattice gauge theory in two steps.

In a previous study [1], we worked out the numerical implementation of the method and conducted a feasibility test—in two and three dimensions—applying it to the gauge-fixing problem and evaluating the lattice gluon propagator in momentum space $D(\vec{k})$ for the SU(2) case. We thus obtained results for two- and three-dimensional lattices of sides up to 16 times larger than the original one, corresponding to lattice volumes respectively up to a few hundred and a thousand times larger than the starting one. We also verified good agreement when comparing $D(\vec{k})$ with numerical data obtained by working directly on a large lattice of the same size as the extended lattice Λ_z. These results are shown in the two plots of Figure 1 in Ref. [1]. This exercise proved very promising since the computational cost could be greatly reduced, but there were a few unresolved issues, which we now address. More specifically, we found that a nonzero gluon propagator could be obtained only for certain values of momenta. These "allowed" momenta included the ones given by the discretization on the original (small) lattice Λ_x, but it was not clear to us if (and which) other momenta could also produce a nonzero value for $D(\vec{k})$. We also obtained that the gluon propagator at zero momentum was strongly suppressed when evaluated on Λ_z, a result that we interpreted just qualitatively, as a peculiar effect due to the extended gauge transformations. At that time, we could not offer, for either of these two results, a robust analytic explanation, which would complete our conceptual description of the proposed approach. In point of fact, achieving such a comprehension is essential also for a more efficient application of the method. Indeed, in Ref. [1], while thermalization and gauge fixing were carried out—in the numerical code—using only the original lattice Λ_x, we still needed to use the (gauge-fixed) gauge field defined on the extended lattice Λ_z for the evaluation of the gluon propagator. Clearly, a better understanding of the setup and its properties must allow the entire numerical implementation of the method to be based on variables defined solely on Λ_x, in order for the computational cost to be independent of the replica factor m. This is the main goal of the present work.

The manuscript is organized as follows. In Section 2, we review—for general SU(N_c) gauge theory in the d-dimensional case—the numerical problem of imposing the minimal-Landau-gauge condition for a thermalized link configuration $\{U_\mu(\vec{x})\}$ on a lattice Λ_x, with PBCs, as well as the definition of the (lattice) gluon propagator in momentum space $D(\vec{k})$. Even though most of the topics discussed in this section are well known, the presentation is useful in order to set the notation and prepare the ground for our analysis of the replicated-lattice case. In particular, we explicitly address the invariance of the lattice formulation under translations and global gauge transformations, which will be important for our later discussion. Then, in Section 3, we extend the analysis to the case of a replicated field configuration, i.e., we discuss the minimal Landau gauge on the extended lattice Λ_z with PBCs, providing a more detailed description than the one presented in Ref. [1]. Specifically, after recalling the usual demonstration of Bloch's theorem for a crystalline solid and its more relevant consequences, we review the proof presented in Refs. [1,5], highlighting the properties of the translation operator $\mathcal{T}$ and the role played by global transformations. This analysis naturally suggests a new interpretation of the gauge-fixing condition for the extended lattice Λ_z, which is presented in Section 4. It also permits the visualization of the gauge-fixed configurations in terms of "domains", which will be later identified with different values of an effective (color) magnetization. Afterwards, we show, in Section 5, which gauge-fixed link variables are nonzero on the extended lattice when evaluated in momentum space. This is, of course, the essential ingredient to predict which momenta have a nonzero gluon propagator $D(\vec{k})$. From our presentation it will be clear that, for the majority of the momenta $\vec{k}$, the gluon propagator is indeed equal to zero. On the other hand, the allowed momenta, i.e., the momenta for which a nonzero $D(\vec{k})$ is obtained, include, but are not limited to, the momenta determined by the discretization on the original (small) lattice Λ_x. However, as we will see, the allowed momenta that are not defined on Λ_x depend on the outcome of the numerical gauge fixing, i.e., they are usually different for different gauge-fixed configurations. Hence, in a numerical simulation, they usually show very poor statistics. We also carefully analyze, in Section 5.4, the evaluation of the gluon propagator at zero momentum, as well as its limit for large values of the parameter m. Some of the analytic results presented in Section 5 are tested numerically in Section 6, where we also illustrate the color-magnetization domains for the different lattice replicas and we present our conclusions. Finally, details about the Cartan sub-algebra for the SU(N_c) group are reported in Appendix A.

2. Minimal Landau Gauge with PBCs

Let us first consider the usual minimal-Landau-gauge condition for Yang–Mills theory in the d-dimensional case and for the SU(N_c) gauge group, on a lattice Λ_x with volume $V = N^d$ and PBCs (see for example Ref. [6]). The gauge-fixing condition is imposed by minimizing—with respect to the gauge transformation $\{h(\vec{x})\}$—the functional [5]

$$\mathcal{E}_U[h] \equiv \frac{\mathrm{Tr}}{2\,N_c\,d\,V} \sum_{\mu=1}^{d} \sum_{\vec{x}\in\Lambda_x} \left[\,\mathbb{1} - U_\mu(h;\vec{x})\,\right] \left[\,\mathbb{1} - U_\mu(h;\vec{x})\,\right]^\dagger \tag{1}$$

$$= \frac{\Re\,\mathrm{Tr}}{N_c\,d\,V} \sum_{\mu=1}^{d} \sum_{\vec{x}\in\Lambda_x} \left[\,\mathbb{1} - U_\mu(h;\vec{x})\,\right]. \tag{2}$$

Here, Tr is the trace (in color space), † stands for the Hermitian conjugate, $\Re$ selects the real part, the vector $\vec{x}$ has integer components x_μ from 1 to N, and the transformed gauge link is given by

$$U_\mu(h;\vec{x}) \equiv h(\vec{x})\,U_\mu(\vec{x})\,h(\vec{x}+\hat{e}_\mu)^\dagger, \tag{3}$$

where the (thermalized) link configuration $\{U_\mu(\vec{x})\}$ is kept fixed, and $\hat{e}_\mu$ is the unit vector in the positive μ direction. Both $U_\mu(\vec{x})$ and the gauge-transformation variable $h(\vec{x})$ are SU(N_c) matrices in the fundamental $N_c \times N_c$ representation, and we denote by $\mathbb{1}$ the $N_c \times N_c$ identity matrix. As discussed below, this ensures a lattice implementation of the familiar Landau-gauge condition in the continuum, i.e., the condition of null divergence for the gauge field.

Let us impose periodicity by requiring that

$$U_\mu(\vec{x}+N\hat{e}_\nu) = U_\mu(\vec{x}) \tag{4}$$

and

$$h(\vec{x}+N\hat{e}_\nu) = h(\vec{x}) \tag{5}$$

for $\mu,\nu = 1,\ldots,d$. Combining these two conditions in (3), we obtain that

$$U_\mu(h;\vec{x}+N\hat{e}_\nu) = U_\mu(h;\vec{x}), \tag{6}$$

i.e., the gauge-transformed link variables $U_\mu(h;\vec{x})$ are also periodic[1] on Λ_x.

Note that the minimizing functional $\mathcal{E}_U[h]$ is non-negative[2] and, due to the cyclicity of the trace, it is invariant under *global* gauge transformations $h(\vec{x}) = v \in$ SU(N_c). At the same time, Equation (1) tells us that the minimal-Landau-gauge condition selects on each gauge orbit—defined by the original link configuration $\{U_\mu(\vec{x})\}$—the configuration whose distance from the trivial vacuum $U_\mu(\vec{x}) = \mathbb{1}$ is minimal [5]. Of course, there may be more than one minimum $\{U_\mu(h;\vec{x})\}$ of $\mathcal{E}_U[h]$ for a given $\{U_\mu(\vec{x})\}$, corresponding to different solutions of the minimization problem. Indeed, it is well-known that—both on the lattice and in the continuum formulation—there are multiple solutions to the general Landau-gauge-fixing problem along each gauge orbit, i.e., multiple configurations $\{U_\mu(h;\vec{x})\}$ corresponding to a null divergence of the gauge field [8–11]. These are called Gribov copies. Let us remark that not all such copies will be also (local, or relative) minima of $\mathcal{E}_U[h]$ since the minimal-Landau-gauge condition is more restrictive than the general one. The set of all local minima of the functional $\mathcal{E}_U[h]$ defines the first Gribov region Ω. It includes representative configurations of all gauge orbits, as well as some of their Gribov copies, while the remaining ones lie outside of Ω.

Clearly, if the configuration[3] $\{U_\mu(h;\vec{x})\}$ is a local minimum of the functional $\mathcal{E}_U[h]$, the stationarity condition implies that its first variation with respect to the matrices $\{h(\vec{x})\}$

be zero. This variation may be conveniently obtained [5,12] from a gauge transformation $h(\vec{x}) \to R(\tau;\vec{x})\,h(\vec{x})$, with $R(\tau;\vec{x})$ close to the identity and taken in a one-parameter subgroup of the gauge group SU(N_c). We thus write

$$R(\tau;\vec{x}) \equiv \exp\left[i\,\tau \sum_{b=1}^{N_c^2-1} \gamma^b(\vec{x})\,t^b \right] \approx \mathbb{1} + i\,\tau \sum_{b=1}^{N_c^2-1} \gamma^b(\vec{x})\,t^b, \tag{7}$$

where the parameter τ is real and small. Here, t^b are the $N_c^2 - 1$ traceless Hermitian generators of the SU(N_c) gauge group, and the factors $\gamma^b(\vec{x})$ are also real. About this, we recall that SU(N_c) is a real Lie group and that its Lie algebra $su(N_c)$ is also real [13]. Then, we can write any element $g \in$ SU(N_c) as $g = \exp\left(i \sum_b \gamma^b\, t^b \right)$, with $\gamma^b \in \mathbb{R}$, ensuring that $g^\dagger = g^{-1}$. At the same time, the condition $\text{Tr}\,(t^b) = 0$ implies that $\det(g) = 1$. We consider generators t^b to be normalized such that

$$\text{Tr}\,(t^b t^c) = 2\,\delta^{bc}, \tag{8}$$

which is the usual normalization condition satisfied by the Pauli matrices, in the SU(2) case, and by the Gell-Mann matrices, in the SU(3) case.

Using this one-parameter subgroup, we may regard $\mathcal{E}_U[h]$ as a function $\mathcal{E}_U[h](\tau)$ of τ. Its first derivative with respect to τ is then given, at $\tau = 0$, by

$$\begin{aligned} \mathcal{E}_U[h]'(0) &= \frac{\Re\,\text{Tr}}{N_c\,d\,V} \sum_{b,\,\mu,\,\vec{x}} -i \left[\gamma^b(\vec{x})\,t^b\,U_\mu(h;\vec{x}) - U_\mu(h;\vec{x})\,\gamma^b(\vec{x}+\hat{e}_\mu)\,t^b \right] \\ &= \frac{2\,\Re\,\text{Tr}}{N_c\,d\,V} \sum_{b,\,\mu,\,\vec{x}} \frac{\gamma^b(\vec{x})\,t^b}{2\,i} \left[U_\mu(h;\vec{x}) - U_\mu(h;\vec{x}-\hat{e}_\mu) \right], \end{aligned} \tag{9}$$

where $\vec{x} \in \Lambda_x$, the color index b takes values $1, \ldots, N_c^2 - 1$ and $\mu = 1, \ldots, d$. At the same time, we define the gauge-fixed (lattice) gauge field $A_\mu(h;\vec{x})$ using the relation

$$A_\mu(h;\vec{x}) \equiv \frac{1}{2\,i} \left[U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x}) \right]_{\text{traceless}} \tag{10}$$

$$= \frac{1}{2\,i} \left[U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x}) \right] - \mathbb{1}\,\frac{\text{Tr}}{2\,i\,N_c} \left[U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x}) \right] \tag{11}$$

$$= \frac{1}{2\,i} \left[U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x}) \right] - \mathbb{1}\,\frac{\Im\,\text{Tr}}{N_c} \left[U_\mu(h;\vec{x}) \right], \tag{12}$$

where $\Im$ selects the imaginary part of a complex number. Also, we write

$$A_\mu(h;\vec{x}) \equiv \sum_b A_\mu^b(h;\vec{x})\,t^b, \tag{13}$$

so that, recalling Equation (8), the color components $A_\mu^b(h;\vec{x})$ are given by

$$A_\mu^b(h;\vec{x}) = \frac{1}{2}\,\text{Tr}\left[A_\mu(h;\vec{x})\,t^b \right]. \tag{14}$$

Then, since the generators t^b are traceless, it is evident that the term proportional to the identity matrix $\mathbb{1}$ in Equations (11) and (12) does not contribute to $A_\mu^b(h;\vec{x})$, see Equation (14), i.e.,

$$A_\mu^b(h;\vec{x}) = \text{Tr}\left\{ t^b \left[\frac{U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x})}{4\,i} \right] \right\} = \Re\,\text{Tr}\left[t^b\,\frac{U_\mu(h;\vec{x})}{2\,i} \right]. \tag{15}$$

We may thus rewrite the first derivative of the minimizing functional from Equation (9) as

$$\mathcal{E}_U[h]'(0) \;=\; \frac{2}{N_c\, d\, V} \sum_{b,\,\mu,\,\vec{x}} \gamma^b(\vec{x}) \left[A_\mu^b(h;\vec{x}) \;-\; A_\mu^b(h;\vec{x}-\hat{e}_\mu) \right], \tag{16}$$

which provides a nice analogy with the continuum case as shown next.[4]

Of course, if $\{U_\mu(h;\vec{x})\}$ is a stationary point of $\mathcal{E}_U[h](\tau)$ at $\tau = 0$, we must have

$$\mathcal{E}_U[h]'(0) \;=\; 0 \tag{19}$$

"along" any direction $\sum_b \gamma^b(\vec{x}) t^b$, i.e., for every set of $\gamma^b(\vec{x})$ factors. This implies that the lattice divergence

$$\left(\nabla\cdot A^b\right)(h;\vec{x}) \;\equiv\; \sum_{\mu=1}^{d} \left[A_\mu^b(h;\vec{x}) - A_\mu^b(h;\vec{x}-\hat{e}_\mu) \right] \tag{20}$$

of the gauge-fixed gauge field $A_\mu(h;\vec{x})$ is zero, i.e.,

$$\left(\nabla\cdot A^b\right)(h;\vec{x}) \;=\; 0 \qquad\qquad \forall\ \vec{x}, b, \tag{21}$$

and the gauge field $A_\mu(h;\vec{x})$ is transverse. The above Equations (20) and (21) give the lattice formulation of the usual Landau gauge-fixing condition in the continuum and, due to Equation (8), are clearly equivalent to

$$(\nabla\cdot A)(h;\vec{x}) \;=\; 0 \qquad \forall\ \vec{x} \tag{22}$$

with, see Equations (13) and (20),

$$(\nabla\cdot A)(h;\vec{x}) \;\equiv\; \sum_{\mu=1}^{d} \left[A_\mu(h;\vec{x}) - A_\mu(h;\vec{x}-\hat{e}_\mu) \right] \;=\; \sum_{b=1}^{N_c^2-1} t^b \left(\nabla\cdot A^b\right)(h;\vec{x}). \tag{23}$$

Let us stress that the gauge transformation $\{h(\vec{x})\}$ depends on $\mathcal{N}_p \equiv V\,(N_c^2-1)$ free parameters $\gamma^b(\vec{x})$ and the minimization process enforces the corresponding $\mathcal{N}_p$ constraints (21).

Clearly, since the link variables $U_\mu(h;\vec{x})$ satisfy PBCs, the same is true for the gauge fields $A_\mu(h;\vec{x})$, defined in Equations (10)–(12). Thus, it is convenient to consider the Fourier transform (see [14])

$$\widetilde{A}_\mu^b(h;\vec{k}) \;\equiv\; \sum_{\vec{x}\in\Lambda_x} A_\mu^b(h;\vec{x}) \, \exp\left[-\frac{2\pi i}{N} \left(\vec{k}\cdot\vec{x} + \frac{k_\mu}{2} \right) \right], \tag{24}$$

where the wave-number vectors $\vec{k}$ have integer components k_μ, which are usually restricted to the so-called first Brillouin zone[5] $k_\mu = 0, 1, \ldots, N-1$. Let us notice that, according to this definition, the contribution to the Fourier transform coming from the link between $\vec{x}$ and $\vec{x} + \hat{e}_\mu$ is calculated at its midpoint $\vec{x} + \hat{e}_\mu/2$. For later convenience, let us also define the Fourier transform of the gauge link

$$\widetilde{U}_\mu(h;\vec{k}) \;\equiv\; \sum_{\vec{x}\in\Lambda_x} U_\mu(h;\vec{x}) \, \exp\left[-\frac{2\pi i}{N} \left(\vec{k}\cdot\vec{x} \right) \right]. \tag{25}$$

Now, in order to write down the inverse Fourier transform, we recall that, in one dimension (and with k taking values $0, 1, \ldots, N-1$), we find [15,16]

$$\sum_{x=1}^{N} e^{-\frac{2\pi i}{N} k\, x} \;=\; \sum_{x=0}^{N-1} \left(e^{-\frac{2\pi i}{N} k} \right)^{x} \;=\; \frac{1 - \left[\exp\left(-2\pi i\, k/N\right) \right]^{N}}{1 - \exp\left(-2\pi i\, k/N\right)} \;=\; 0 \tag{26}$$

for $k \neq 0$. Thus, the above expression is equal to $N\,\delta(k,0)$, where $\delta(\,,\,)$ stands for the Kronecker delta function. Analogously, in the d-dimensional case, we have

$$\sum_{\vec{x} \in \Lambda_x} e^{-\frac{2\pi i}{N} \vec{k}\cdot\vec{x}} \;=\; \prod_{\nu=1}^{d} \left[\sum_{x_\nu = 1}^{N} e^{-\frac{2\pi i}{N} k_\nu x_\nu} \right] \;=\; N^d\, \delta(\vec{k},\vec{0}) \;=\; V\, \delta(\vec{k},\vec{0}), \tag{27}$$

where $\delta(\vec{k},\vec{0})$ is a shorthand for $\prod_{\nu=1}^{d} \delta(k_\nu, 0)$. Conversely, we have

$$\sum_{\vec{k} \in \widetilde{\Lambda}_x} e^{\frac{2\pi i}{N} \vec{k}\cdot\vec{x}} \;=\; V\, \delta(\vec{x},\vec{0}), \tag{28}$$

where $\widetilde{\Lambda}_x$ stands for the first Brillouin zone (for the Λ_x lattice). Hence, it is straightforward to verify that the inverse Fourier transform, corresponding to Equation (24), is given by

$$A^b_\mu(h;\vec{x}) \;\equiv\; \frac{1}{V} \sum_{\vec{k} \in \widetilde{\Lambda}_x} \widetilde{A}^b_\mu(h;\vec{k})\, \exp\left[\frac{2\pi i}{N} \left(\vec{k}\cdot\vec{x} + \frac{k_\mu}{2} \right) \right]. \tag{29}$$

As mentioned above, the term $i\pi k_\mu / N$ in the exponent of Equation (24) is obtained by considering the gauge field at the midpoint $\vec{x} + \hat{e}_\mu/2$ of a lattice link.[6] This term is essential in order to show that, in momentum space, Equation (21) becomes

$$0 \;=\; \frac{1}{V} \sum_{\vec{k} \in \widetilde{\Lambda}_x} \sum_{\mu=1}^{d} \widetilde{A}^b_\mu(h;\vec{k})\, \exp\left(\frac{2\pi i}{N} \vec{k}\cdot\vec{x} \right) 2\, i\, \sin\left(\frac{\pi\, k_\mu}{N} \right), \tag{30}$$

yielding (for each $\vec{k}$) the lattice transversality condition

$$\sum_{\mu=1}^{d} \widetilde{A}^b_\mu(h;\vec{k})\, p_\mu(\vec{k}) \;=\; 0, \tag{31}$$

where

$$p_\mu(\vec{k}) \;\equiv\; 2\, \sin\left(\frac{\pi\, k_\mu}{N} \right) \tag{32}$$

are the components of the lattice momentum $\vec{p}(\vec{k})$ [15,16]. Indeed, without the factor $\exp\left(i\pi k_\mu/N\right)$, we would obtain the condition

$$\sum_{\mu=1}^{d} \widetilde{A}^b_\mu(h;\vec{k}) \left[1 \,-\, \cos\left(\frac{2\,\pi\, k_\mu}{N} \right) \,+\, i\, \sin\left(\frac{2\pi\, k_\mu}{N} \right) \right] \;=\; 0, \tag{33}$$

which looks very different from the Landau gauge condition in the continuum.

Actually, one can verify that Equations (31) and (33) have the same (formal) continuum limit [14] but with different discretization errors. To this end, we write

$$\frac{2\,\pi\, k_\mu}{N} \;=\; a\, \frac{2\,\pi\, k_\mu}{a\, N} \;\equiv\; a\; \hat{p}_\mu, \tag{34}$$

where a is the lattice spacing and $\hat{p}_\mu$ is now a continuum momentum in physical units, and take the limit $a \to 0$ with $\hat{p}_\mu$ kept fixed. We find, in both cases, that the term multiplying

$\widetilde{A}_\mu^b(h;\vec{k})$ is proportional to $\hat{p}_\mu$, yielding the desired transversality condition. However, in the first case the discretization error is of order a^2, while in the second it is of order a. Moreover, Equation (32) provides a more natural definition of the lattice-momentum components than the expression in square brackets in Equation (33) since

$$p^2(\vec{k}) \;=\; \sum_{\mu=1}^{d} p_\mu^2(\vec{k}) \;\equiv\; \sum_{\mu=1}^{d} 4\,\sin^2\left(\frac{\pi\,k_\mu}{N}\right) \tag{35}$$

are the eigenvalues of (minus) the usual lattice Laplacian

$$-\Delta(\vec{x},\vec{y}) \;\equiv\; \sum_{\mu=1}^{d}\left[\,2\,\delta(\vec{x},\vec{y}) \;-\; \delta(\vec{x}+\hat{e}_\mu,\vec{y}) \;-\; \delta(\vec{x}-\hat{e}_\mu,\vec{y})\,\right], \tag{36}$$

corresponding to the plane-wave eigenvectors $\exp\left(-2\pi i\vec{k}\cdot\vec{y}/N\right)$.

2.1. Numerical Gauge Fixing

In order to minimize $\mathcal{E}_U[h]$ numerically, it is sufficient to implement an iterative algorithm that monotonically decreases the value of the minimizing functional. Indeed, since $\mathcal{E}_U[h]$ is bounded from below, an algorithm of this kind is expected to converge. As the simplest approach, one can sweep through the lattice Λ_x and apply—for each lattice site $\vec{x}$—a convenient update

$$h(\vec{x}) \;\to\; h'(\vec{x}) = r(\vec{x})\,h(\vec{x}), \tag{37}$$

where $r(\vec{x}) \in \mathrm{SU}(N_c)$, while keeping all the other matrices $h(\vec{x})$ fixed. In other words, a single-site update at $\vec{x}$ corresponds to $\{h(\vec{x})\} \;\to\; \{h'(\vec{x})\}$, where the new set of gauge transformations is unaltered except for applying $r(\vec{x})$ to $h(\vec{x})$ as above. From Equations (2) and (3), we see that the corresponding change $\mathcal{E}_U[h'] \,-\, \mathcal{E}_U[h]$ in the minimizing functional due to this update is given by

$$\begin{aligned} &\frac{\Re\,\mathrm{Tr}}{N_c\,d\,V}\sum_{\mu=1}^{d}\left[\,U_\mu(h;\vec{x}) \,+\, U_\mu(h;\vec{x}-\hat{e}_\mu)^\dagger \,-\, r(\vec{x})\,U_\mu(h;\vec{x}) \,-\, U_\mu(h;\vec{x}-\hat{e}_\mu)\,r(\vec{x})^\dagger\,\right] \\ =\;\; &\frac{\Re\,\mathrm{Tr}\,[\,w(\vec{x})\,]}{N_c\,d\,V} \,-\, \frac{\Re\,\mathrm{Tr}\,[\,r(\vec{x})\,w(\vec{x})\,]}{N_c\,d\,V}, \end{aligned} \tag{38}$$

with

$$w(\vec{x}) \;\equiv\; \sum_{\mu=1}^{d}\left[\,U_\mu(h;\vec{x}) \,+\, U_\mu(h;\vec{x}-\hat{e}_\mu)^\dagger\,\right]. \tag{39}$$

Then, for the change to be negative, the single-site update must satisfy the inequality

$$-\Re\,\mathrm{Tr}\,[\,r(\vec{x})\,w(\vec{x})\,] \;\leq\; -\Re\,\mathrm{Tr}\,[\,w(\vec{x})\,]\,. \tag{40}$$

Common possible choices[7] for $r(\vec{x})$—usually written as a linear combination of the identity matrix $\mathbb{1}$ and of the matrix $w(\vec{x})$—can be found in Refs. [18–22]. In particular, in the SU(2) case, the matrix $w(\vec{x})$ is proportional to an SU(2) matrix. On the contrary, in the general $\mathrm{SU}(N_c)$ case, it is simply an $N_c \times N_c$ complex matrix, and one needs to project this matrix onto the gauge group (see Refs. [18,22]). Let us note that, from the point of view of the organization of the numerical algorithm, one does not need to store both the gauge transformation $\{h(\vec{x})\}$ and the link configuration $\{U_\mu(\vec{x})\}$. Indeed, every time a single-site update (37) is performed, one can modify the gauge configuration directly, by evaluating the products[8]

$$U_\mu(h;\vec{x}) \;\to\; r(\vec{x})\, U_\mu(h;\vec{x}) \qquad \text{and} \qquad U_\mu(h;\vec{x}-\hat{e}_\mu) \;\to\; U_\mu(h;\vec{x}-\hat{e}_\mu)\, r(\vec{x})^\dagger, \tag{41}$$

for each direction $\mu = 1,\ldots,d$. An iteration of the method corresponds to a full sweep of the lattice, applying the above single-site updates at each point $\vec{x}$.

As a check of convergence of the (iterative) minimization algorithm after t sweeps over the lattice, one can "monitor" the behavior of several different quantities[9] [19–21], e.g.,

$$\Delta\mathcal{E} \;\equiv\; \mathcal{E}_U[h;t] \,-\, \mathcal{E}_U[h;t-1], \tag{42}$$

$$(\nabla A)^2 \;\equiv\; \frac{1}{(N_c^2-1)\,V} \sum_b \sum_{\vec{x}\in\Lambda_x} \left[\left(\nabla\cdot A^b\right)(h;\vec{x}) \right]^2, \tag{43}$$

$$\Sigma_Q \;\equiv\; \frac{1}{N} \sum_{b,\,\mu,\,x_\mu} \left[Q_\mu^b(h;x_\mu) - \widehat{Q}_\mu^b(h) \right]^2 \Big/ \;\sum_{b,\,\mu} \left[\widehat{Q}_\mu^b(h) \right]^2, \tag{44}$$

where all quantities are evaluated using the gauge-transformed configuration $\{U_\mu(h;\vec{x})\}$, the color index b takes values $1,\ldots,N_c^2-1$ and, as always throughout this work, $\mu = 1,\ldots,d$ and $x_\mu = 1,\ldots,N$. In Equation (44) above, we define

$$Q_\mu^b(h;x_\mu) \;\equiv\; \sum_{\substack{x_\nu \\ \nu\neq\mu}} A_\mu^b(h;\vec{x}) \tag{45}$$

and

$$\widehat{Q}_\mu^b(h) \;\equiv\; \frac{1}{N} \sum_{x_\mu} Q_\mu^b(h;x_\mu) \;=\; \frac{1}{N} \sum_{\vec{x}} A_\mu^b(h;\vec{x})\,. \tag{46}$$

One can check that, if the Landau-gauge-fixing condition (21) is satisfied, then $Q_\mu^b(h;x_\mu)$ must be independent of x_μ. Indeed, from Equations (20) and (21), we obtain[10]

$$\begin{aligned} 0 \;&=\; \sum_{\substack{x_\nu \\ \nu\neq\mu}} \left(\nabla\cdot A^b\right)(h;\vec{x}) \;=\; \sum_{\substack{x_\nu \\ \nu\neq\mu}} \sum_{\sigma=1}^{d} \left[A_\sigma^b(h;\vec{x}) - A_\sigma^b(h;\vec{x}-\hat{e}_\sigma) \right] \\ &=\; \sum_{\substack{x_\nu \\ \nu\neq\mu}} \left[A_\mu^b(h;\vec{x}) - A_\mu^b(h;\vec{x}-\hat{e}_\mu) \right] + \sum_{\substack{x_\nu \\ \nu\neq\mu}} \sum_{\sigma\neq\mu} \left[A_\sigma^b(h;\vec{x}) - A_\sigma^b(h;\vec{x}-\hat{e}_\sigma) \right], \end{aligned} \tag{47}$$

for any $\mu = 1,\ldots,d$ and $x_\mu = 1,\ldots,N$. Here, the first term on the r.h.s. is simply given by $Q_\mu^b(h;x_\mu) - Q_\mu^b(h;x_\mu-1)$, while the second one may be written as

$$\sum_{\sigma\neq\mu} \left\{ \sum_{\substack{x_\nu \\ \nu\neq\mu,\sigma}} \sum_{x_\sigma} \left[A_\sigma^b(h;\vec{x}) - A_\sigma^b(h;\vec{x}-\hat{e}_\sigma) \right] \right\}. \tag{48}$$

Let us stress that, in the above formulae, the coordinate x_μ is fixed and all other coordinates are summed over. In particular, in Equation (48), we single out the sum over the coordinate x_σ. This makes it evident that, with respect to this coordinate, one has a telescopic sum, yielding (for each direction $\sigma \neq \mu$)

$$\sum_{\substack{x_\nu \\ \nu\neq\mu,\sigma}} \left[A_\sigma^b(h;\vec{x}) \Big|_{x_\sigma=N} - A_\sigma^b(h;\vec{x}) \Big|_{x_\sigma=0} \right]. \tag{49}$$

Then, when PBCs are imposed along the direction σ, the last expression cancels out and we get

$$Q^b_\mu(h; x_\mu) \;=\; Q^b_\mu(h; x_\mu - 1), \tag{50}$$

i.e., the "charges" $Q^b_\mu(h; x_\mu)$ are constant, they do not depend on x_μ, for any direction μ.

Also, note that the quantity $(\nabla A)^2$ is invariant under global gauge transformations $v \in \mathrm{SU}(N_c)$. Indeed, from Equations (3) and (11) we have that, for $h(\vec{x}) \to v\, h(\vec{x})$, the gauge field $A_\mu(h; \vec{x})$ changes as

$$A_\mu(h; \vec{x}) \;\to\; v\, A_\mu(h; \vec{x})\, v^\dagger \tag{51}$$

and the same form holds for the transformation of $(\nabla \cdot A)(h; \vec{x})$, see Equation (23). The above statement then follows if we write, see Equation (8),

$$(\nabla A)^2 \;\equiv\; \frac{\mathrm{Tr}}{2\,(N_c^2 - 1)\, V} \sum_{\vec{x} \in \Lambda_x} \Big[(\nabla \cdot A)(h; \vec{x}) \Big]^2 \tag{52}$$

and use the cyclicity of the trace. This result is expected if we interpret Equation (16) as a directional derivative of the minimizing functional $\mathcal{E}_U[h]$ along the "direction" specified by the vector with components $\gamma^b(\vec{x})$ so that $\left(\nabla \cdot A^b\right)(h; \vec{x})$ are the (color) components of its gradient. Then, since $\mathcal{E}_U[h]$ is invariant under global gauge transformations,[11] one should have that the magnitude of its gradient—which quantifies the steepness of the minimizing function at a given point in the link-configuration space—is also invariant under such global transformations, even though its components $\left(\nabla \cdot A^b\right)(h; \vec{x})$ are not.

Similarly, we can write Σ_Q as

$$\Sigma_Q \;=\; \frac{1}{N} \sum_{\mu=1}^{d} \sum_{x_\mu=1}^{N} \mathrm{Tr} \left[Q_\mu(h; x_\mu) - \widehat{Q}_\mu(h) \right]^2 \Big/ \sum_{\mu=1}^{d} \mathrm{Tr} \left[\widehat{Q}_\mu(h) \right]^2, \tag{53}$$

with

$$Q_\mu(h; x_\mu) \;\equiv\; \sum_{b=1}^{N_c^2-1} t^b\, Q^b_\mu(h; x_\mu) \qquad \text{and} \qquad \widehat{Q}_\mu(h) \;\equiv\; \sum_{b=1}^{N_c^2-1} t^b\, \widehat{Q}^b_\mu(h). \tag{54}$$

Then, clearly we have invariance under a global gauge transformation v, see Equations (45) and (46), since $Q_\mu(h; x_\mu) \to v\, Q_\mu(h; x_\mu)\, v^\dagger$ and $\widehat{Q}_\mu(h) \;\to\; v\, \widehat{Q}_\mu(h)\, v^\dagger$.

We see, therefore, that all the three quantities proposed to monitor the convergence of the algorithm, given in Equations (42)–(44), are invariant under a global gauge transformation, just as the minimizing functional in Equation (1).

2.2. Gluon Propagator

The lattice space-time gluon propagator is defined as[12]

$$D^{bc}_{\mu\nu}(\vec{x}_1, \vec{x}_2) \;\equiv\; \left\langle A^b_\mu(h; \vec{x}_1)\, A^c_\nu(h; \vec{x}_2) \right\rangle, \tag{55}$$

where $\langle \cdot \rangle$ stands for the path-integral (Monte Carlo) average. If we impose translational invariance, i.e., if we consider the quantity $D^{bc}_{\mu\nu}(\vec{x}_1 - \vec{x}_2) \equiv D^{bc}_{\mu\nu}(\vec{x}_1, \vec{x}_2)$, corresponding to total momentum conservation, we can also write

$$D^{bc}_{\mu\nu}(\vec{x}) \;=\; \left\langle A^b_\mu(h; \vec{x})\, A^c_\nu(h; \vec{0}) \right\rangle \;=\; \frac{1}{V} \sum_{\vec{x}_2 \in \Lambda_x} \left\langle A^b_\mu(h; \vec{x} + \vec{x}_2)\, A^c_\nu(h; \vec{x}_2) \right\rangle. \tag{56}$$

Then, the associated (double) Fourier transform $D^{bc}_{\mu\nu}(\vec{k}_1,\vec{k}_2)$ is diagonal in momentum space, see Equation (24), i.e.,

$$\begin{aligned} D^{bc}_{\mu\nu}(\vec{k}_1,\vec{k}_2) &= \sum_{\vec{x}_1,\vec{x}_2} D^{bc}_{\mu\nu}(\vec{x}_1-\vec{x}_2)\, \exp\left\{ -\frac{2\pi i}{N}\left[\vec{k}_1\cdot\left(\vec{x}_1+\frac{\hat{e}_\mu}{2}\right)+\vec{k}_2\cdot\left(\vec{x}_2+\frac{\hat{e}_\nu}{2}\right)\right]\right\} \\ &= \sum_{\vec{x},\vec{x}_2} D^{bc}_{\mu\nu}(\vec{x})\, \exp\left\{ -\frac{2\pi i}{N}\left[\vec{k}_1\cdot\left(\vec{x}+\frac{\hat{e}_\mu}{2}\right)+\left(\vec{k}_2+\vec{k}_1\right)\cdot\vec{x}_2+\vec{k}_2\cdot\frac{\hat{e}_\nu}{2}\right]\right\} \\ &= V\,\delta(\vec{k}_1+\vec{k}_2,\vec{0})\sum_{\vec{x}} D^{bc}_{\mu\nu}(\vec{x})\, \exp\left\{ -\frac{2\pi i}{N}\left[\vec{k}_1\cdot\left(\vec{x}+\frac{\hat{e}_\mu}{2}\right)+\vec{k}_2\cdot\frac{\hat{e}_\nu}{2}\right]\right\} \\ &= V\,\delta(\vec{k}_1,-\vec{k}_2)\sum_{\vec{x}} D^{bc}_{\mu\nu}(\vec{x})\, \exp\left[-\frac{2\pi i}{N}\,\vec{k}_1\cdot\left(\vec{x}+\frac{\hat{e}_\mu}{2}-\frac{\hat{e}_\nu}{2}\right)\right], \end{aligned} \tag{57}$$

where we defined $\vec{x} \equiv \vec{x}_1 - \vec{x}_2$ (with $\vec{x},\vec{x}_1,\vec{x}_2 \in \Lambda_x$) and we used Equation (27). Thus, after setting $\vec{k} \equiv \vec{k}_1 = -\vec{k}_2$, we can write

$$D^{bc}_{\mu\nu}(\vec{k},-\vec{k}) = V\sum_{\vec{x}} D^{bc}_{\mu\nu}(\vec{x})\, \exp\left[-\frac{2\pi i}{N}\left(\vec{k}\cdot\vec{x}+\frac{k_\mu-k_\nu}{2}\right)\right] \equiv V\,D^{bc}_{\mu\nu}(\vec{k}) \tag{58}$$

and

$$D^{bc}_{\mu\nu}(\vec{x}) = \left\langle A^b_\mu(h;\vec{x})\,A^c_\nu(h;\vec{0})\right\rangle = \frac{1}{V}\sum_{\vec{k}\in\widetilde{\Lambda}_x} D^{bc}_{\mu\nu}(\vec{k})\, \exp\left[\frac{2\pi i}{N}\left(\vec{k}\cdot\vec{x}+\frac{k_\mu-k_\nu}{2}\right)\right], \tag{59}$$

as can be seen by substituting the rightmost expression above into Equation (58) and using Equation (27). This defines, in a natural way, the inverse Fourier transform for the gluon propagator. Note that it is also in agreement with the corresponding definition given in the case of the gauge field in Equation (29) since it is equivalent to

$$\begin{aligned} D^{bc}_{\mu\nu}(\vec{k},-\vec{k}) &= \sum_{\vec{x},\vec{x}_2}\left\langle A^b_\mu(h;\vec{x}+\vec{x}_2)\,A^b_\mu(h;\vec{x}_2)\right\rangle \exp\left\{-\frac{2\pi i}{N}\left[\vec{k}\cdot(\vec{x}+\vec{x}_2-\vec{x}_2)+\frac{k_\mu-k_\nu}{2}\right]\right\} \\ &= \left\langle \widetilde{A}^b_\mu(h;\vec{k})\,\widetilde{A}^c_\nu(h;-\vec{k})\right\rangle, \end{aligned} \tag{60}$$

where we substitute (56) into Equation (58), apply the translation $\vec{x}+\vec{x}_2 \to \vec{x}$ (with $\vec{x}_2$ fixed) before summing over $\vec{x} \in \Lambda_x$, and use (24).

At the same time, due to global color invariance and to the transversality condition (31), the Landau-gauge propagator must be given by (see Ref. [23])

$$D^{bc}_{\mu\nu}(\vec{x}) = \frac{\delta^{bc}}{V}\left\{D(\vec{0})\,\delta_{\mu\nu}+\sum_{\substack{\vec{k}\in\widetilde{\Lambda}_x\\ \vec{k}\neq\vec{0}}} D(\vec{k})\,\exp\left(\frac{2\pi i}{N}\,\vec{k}\cdot\vec{x}\right)P_{\mu\nu}(\vec{k})\exp\left[\frac{\pi i\left(k_\mu-k_\nu\right)}{N}\right]\right\}, \tag{61}$$

where $\vec{0}$ is the wave-number vector with all null components, $\delta_{\mu\nu}$ stands for the Kronecker delta function of the lattice directions and

$$P_{\mu\nu}(\vec{k}) \equiv \left[\delta_{\mu\nu} - \frac{p_\mu(\vec{k})\,p_\nu(\vec{k})}{p^2(\vec{k})}\right] \tag{62}$$

is the usual transverse projector, see Equation (32). In particular, note that

$$D^{bb}_{\mu\mu}(\vec{x}) \;=\; \frac{D(\vec{0}\,)}{V} \;+\; \sum_{\substack{\vec{k}\in\widetilde{\Lambda}_x \\ \vec{k}\neq\vec{0}}} \frac{D(\vec{k}\,)}{V}\,\exp\left(\frac{2\pi i}{N}\,\vec{k}\cdot\vec{x}\right) P_{\mu\mu}(\vec{k}\,), \tag{63}$$

where the repeated indices do not imply summation. Then, the scalar function $D(\vec{0}\,)$ can be evaluated, for example, using Equations (27) and (63), yielding[13]

$$\begin{aligned} D(\vec{0}\,) \;&\equiv\; \frac{1}{d\,(N_c^2-1)} \sum_{b,\,\mu} \sum_{\vec{x}} D^{bb}_{\mu\mu}(\vec{x}) \;=\; \frac{1}{\mathcal{N}} \sum_{b,\mu} \sum_{\vec{x},\,\vec{x}_2} \left\langle A^b_\mu(h;\vec{x}+\vec{x}_2)\, A^b_\mu(h;\vec{x}_2) \right\rangle \\ &=\; \frac{1}{\mathcal{N}} \sum_{b,\,\mu} \left\langle \left[\sum_{\vec{x}} A^b_\mu(h;\vec{x}) \right]^2 \right\rangle, \end{aligned} \tag{64}$$

where we also use Equation (56) and, in the last step, we apply again the translation $\vec{x}+\vec{x}_2 \,\to\, \vec{x}$ (with $\vec{x}_2$ fixed). As always, in the sums, we have $\mu = 1, \ldots, d$, the color index b takes values $1, \ldots, N_c^2-1$ and $\vec{x}, \vec{x}_2 \in \Lambda_x$. We also define the normalization factor $\mathcal{N} \equiv d(N_c^2-1)V$. Similarly, we have

$$\begin{aligned} D(\vec{k}\,) \;&\equiv\; \frac{1}{(d-1)\,(N_c^2-1)} \sum_{b,\mu} \sum_{\vec{x}} D^{bb}_{\mu\mu}(\vec{x})\, \exp\left(-\frac{2\pi i}{N}\,\vec{k}\cdot\vec{x}\right) \\ &=\; \frac{1}{\mathcal{N}'} \sum_{b,\mu} \sum_{\vec{x},\vec{x}_2} \left\langle A^b_\mu(h;\vec{x}+\vec{x}_2)\, A^b_\mu(h;\vec{x}_2) \right\rangle \exp\left[-\frac{2\pi i}{N}\,\vec{k}\cdot(\vec{x}+\vec{x}_2-\vec{x}_2)\right] \\ &=\; \frac{1}{\mathcal{N}'} \sum_{b,\mu} \left\langle \sum_{\vec{x}} A^b_\mu(h;\vec{x})\, \exp\left(-\frac{2\pi i}{N}\,\vec{k}\cdot\vec{x}\right) \sum_{\vec{x}_2} A^b_\mu(h;\vec{x}_2)\, \exp\left(\frac{2\pi i}{N}\,\vec{k}\cdot\vec{x}_2\right) \right\rangle \end{aligned} \tag{65}$$

$$=\; \frac{1}{\mathcal{N}'} \sum_{b,\mu} \left\langle \left[\sum_{\vec{x}} A^b_\mu(h;\vec{x}) \cos\left(\frac{2\pi}{N}\vec{k}\cdot\vec{x}\right) \right]^2 + \left[\sum_{\vec{x}} A^b_\mu(h;\vec{x}) \sin\left(\frac{2\pi}{N}\vec{k}\cdot\vec{x}\right) \right]^2 \right\rangle, \tag{66}$$

where we use one more time the translation $\vec{x}+\vec{x}_2 \;\to\; \vec{x}$ and we define $\mathcal{N}' \equiv (d-1)(N_c^2-1)V$.

Let us remark that the above expressions, obtained in the lattice formulation, are essentially the same as in the continuum, with only a few subtleties. In particular, in the continuum, the scalar quantities $D(\vec{0}\,)$ and $D(\vec{k}\,)$ depend only on the magnitude k of the wave-number vector $\vec{k}$ (or of the corresponding momentum $p \propto k$) and are usually denoted by $D(0)$ and $D(k)$. This notation is also very often employed in lattice studies. Here, however, we prefer to keep explicitly the dependence of the gluon propagator on the components of $\vec{k}$ for two (related) reasons. Firstly, due to the breaking of the rotational symmetry [24], it is no longer true that the lattice results for the gluon propagator are just a function of k. Secondly, when representing $D(\vec{k}\,)$ as a function of $p^2(\vec{k}\,)$, see Equation (35), it is necessary to consider all the components of $\vec{k}$—and not simply its magnitude k—since p^2 is not proportional to k^2. Let us also recall [25] that the factor $d-1$ in the denominator of the expression for $D(\vec{k}\,)$ comes from

$$\sum_{\mu=1}^{d} P_{\mu\mu}(\vec{k}\,) \;=\; d-1 \tag{67}$$

and tells us that, for each value of b, there are only $d-1$ linearly independent components $\widetilde{A}^b_\mu(h;\vec{k}\,)$ due to the Landau-gauge-fixing condition, see Equation (31). At the same time, the factor d in the denominator of the expression for $D(\vec{0})$ reflects the fact that the same equation does not impose any constraint on the gauge field for $\vec{k} = \vec{0}$. Also note that Equation (66) is invariant[14] under the reflection $\vec{k} \to -\vec{k}$ or, more generally, under the reflection $\vec{k} \to -\vec{k} + N\hat{e}_\mu$.

The gluon-propagator functions $D(\vec{0})$ and $D(\vec{k})$ can also be written in terms of the momentum-space gauge field $\widetilde{A}^b_\mu(h;\vec{k})$, see Equation (24), yielding

$$D(\vec{0}) = \frac{1}{\mathcal{N}} \sum_{b,\mu} \left\langle \widetilde{A}^b_\mu(h;\vec{0})^2 \right\rangle = \frac{1}{2\mathcal{N}} \sum_{\mu} \mathrm{Tr} \left\langle \widetilde{A}_\mu(h;\vec{0})^2 \right\rangle \tag{68}$$

and, see Equation (65),

$$\begin{aligned} D(\vec{k}) &= \frac{1}{\mathcal{N}'} \sum_{b,\mu,\vec{x},\vec{x}_2} \left\langle A^b_\mu(h;\vec{x}) \exp\left[-\frac{2\pi i}{N}\left(\vec{k}\cdot\vec{x}+\frac{k_\mu}{2}\right)\right] A^b_\mu(h;\vec{x}_2) \exp\left[\frac{2\pi i}{N}\left(\vec{k}\cdot\vec{x}_2+\frac{k_\mu}{2}\right)\right]\right\rangle \\ &= \frac{1}{\mathcal{N}'} \sum_{b,\mu} \left\langle \widetilde{A}^b_\mu(h;\vec{k})\, \widetilde{A}^b_\mu(h;-\vec{k}) \right\rangle = \frac{1}{2\mathcal{N}'} \sum_{\mu} \mathrm{Tr} \left\langle \widetilde{A}_\mu(h;\vec{k})\, \widetilde{A}_\mu(h;-\vec{k}) \right\rangle, \end{aligned} \tag{69}$$

where we use (8) and the definition

$$\widetilde{A}_\mu(h;\vec{k}) \equiv \sum_{b=1}^{N_c^2-1} t^b\, \widetilde{A}^b_\mu(h;\vec{k}), \tag{70}$$

in analogy with Equation (13). At the same time, Equation (24) implies that

$$\widetilde{A}_\mu(h;\vec{k}) = \sum_{b=1}^{N_c^2-1} t^b \sum_{\vec{x}\in\Lambda_x} A^b_\mu(h;\vec{x}) \exp\left[-\frac{2\pi i}{N}\left(\vec{k}\cdot\vec{x} + \frac{k_\mu}{2}\right)\right]. \tag{71}$$

Then, given that the generators t^b of the SU(N_c) group are chosen to be Hermitian and the components $A^b_\mu(h;\vec{x})$ are real—see the comment below Equation (7) [or Equation (15)]—we have

$$\left[\widetilde{A}_\mu(h;\vec{k})\right]^\dagger = \widetilde{A}_\mu(h;-\vec{k}). \tag{72}$$

Thus, we can also write Equation (69) as

$$D(\vec{k}) = \frac{1}{2\mathcal{N}'} \sum_{\mu=1}^{d} \mathrm{Tr} \left\langle \widetilde{A}_\mu(h;\vec{k}) \left[\widetilde{A}_\mu(h;\vec{k})\right]^\dagger \right\rangle. \tag{73}$$

Finally, when considering a global gauge transformation v, $\widetilde{A}_\mu(h;\vec{k})$ transforms—see Equations (13), (51) and (71)—as

$$\widetilde{A}_\mu(h;\vec{k}) \to v\, \widetilde{A}_\mu(h;\vec{k})\, v^\dagger, \tag{74}$$

so that the scalar functions $D(\vec{0})$ and $D(\vec{k})$ are invariant under such (global) gauge transformations. In other words, the Landau-gauge gluon propagator has the same invariance of the minimal-Landau-gauge condition and of the quantities (42)–(44), shown in the last section.

3. Minimal Landau Gauge on the Extended Lattice

Here we define the extended-lattice version of the gauge-fixing problem presented in the previous section, highlighting the similarities with Bloch's theorem and discussing the corresponding result for the minimal Landau gauge in Yang–Mills theory. More specifically, after describing the setup, we review, in Section 3.1, the statement of the theorem in solid-state physics, summarizing its demonstration. Then, in Section 3.2, we outline the analogous result for the gauge-fixing case, while in Section 3.3 we present its proof. Our notation for Cartan sub-algebras and other mathematical details that are relevant in the gauge-theory case are given in Appendix A.

Following refs. [1,5], we consider a thermalized link configuration $\{U_\mu(\vec{x})\}$, for the $SU(N_c)$ gauge group in d dimensions, defined on a lattice Λ_x with volume $V = N^d$ and PBCs. Then, we extend this configuration by replicating it m times along each direction, yielding a configuration on the extended lattice Λ_z, with lattice volume $m^d V$. We parametrize the sites of Λ_z by

$$\vec{z} \equiv \vec{x} + N\,\vec{y}, \tag{75}$$

where $\vec{x} \in \Lambda_x$ and $\vec{y}$ belongs to the *index lattice*[15] $\{\Lambda_y\colon\, y_\mu = 0, 1, \ldots, m-1\}$, so that the components z_μ take values $1, 2, \ldots, mN$. We also denote by $\Lambda_x^{(\vec{y})}$ each of the m^d (identical) replicas of the original lattice Λ_x, specified by the $\vec{y}$ index coordinates. By construction, $\{U_\mu(\vec{z})\}$ is invariant under translations by N in any direction.

Then, as was performed in the previous section for the original lattice Λ_x, we impose the minimal-Landau-gauge condition on Λ_z, i.e., we minimize the functional

$$\mathcal{E}_U[g] \;\equiv\; \frac{\Re\,\mathrm{Tr}}{N_c\, d\, m^d\, V} \sum_{\mu=1}^{d} \sum_{\vec{z}\in\Lambda_z} \left[\, 1\!\!1 - U_\mu(g;\vec{z})\,\right], \tag{76}$$

$$U_\mu(g;\vec{z}) \;\equiv\; g(\vec{z})\, U_\mu(\vec{z})\, g(\vec{z}+\hat{e}_\mu)^\dagger \tag{77}$$

with respect to the gauge transformation $\{g(\vec{z})\}$, while keeping the link configuration $\{U_\mu(\vec{z})\}$ fixed. Here, $g(\vec{z})$ are $SU(N_c)$ matrices subject to PBCs on the extended lattice Λ_z, i.e.,

$$g(\vec{z} + mN\hat{e}_\mu) \;=\; g(\vec{z}). \tag{78}$$

The resulting gauge-fixed field configuration is, of course, transverse on Λ_z, and it is also invariant under a translation by $mN\hat{e}_\mu$. Indeed, as mentioned above, by construction of Λ_z, we have $U_\nu(\vec{z} + N\hat{e}_\mu) = U_\nu(\vec{z}) = U_\nu(\vec{z} + mN\hat{e}_\mu)$ for $\mu, \nu = 1, \ldots, d$. Then, from Equations (77) and (78), we get

$$U_\nu(g;\vec{z} + mN\hat{e}_\mu) \;=\; U_\nu(g;\vec{z}). \tag{79}$$

We thus have invariance under a translation by $mN\hat{e}_\mu$ —i.e., PBCs on Λ_z—for the transformed gauge field. On the other hand, the original invariance under a translation by $N\hat{e}_\mu$ is lost after the gauge-fixing process since the gauge transformation $\{g(\vec{z})\}$ does not have it.

3.1. Bloch's Theorem for a Crystalline Solid

As explained in Ref. [1], the extended-lattice problem defined above on Λ_z is very similar to the setup usually considered in the proof of Bloch's theorem [26] for an (ideal) crystalline solid in d dimensions. Indeed, the index lattice Λ_y corresponds to a finite cubic Bravais lattice, with m unit cells in each direction, equipped with PBCs. Equivalently, this Bravais lattice is a simple cubic lattice, with cells indexed by vectors $\vec{y} \in \Lambda_y$. At the same time, the original lattice Λ_x may be viewed as a primitive cell of the Bravais lattice. Let us recall that, in state-solid physics, the primitive cell is defined as the d-dimensional volume spanned by the (orthogonal) primitive vectors $l\hat{e}_\mu$, where l is the length of the cell, i.e., a vector $\vec{r}$ restricted to the primitive cell is written as $l\sum_{\mu=1}^{d} r_\mu \hat{e}_\mu$, with $r_\mu \in [0, 1)$. Finally, the thermalized lattice configuration $\{U_\mu(\vec{z})\}$, invariant under translation by $N\,\vec{y} = N\sum_{\mu=1}^{d} y_\mu \hat{e}_\mu$ with $\vec{y} \in \Lambda_y$, corresponds (for example) to a periodic electrostatic potential $U(\vec{r}\,)$, invariant under translations by any vector $\vec{R} = l\,\sum_{\mu=1}^{d} R_\mu \hat{e}_\mu$ of the Bravais lattice, where the integer components R_μ take values $0, 1, \ldots, m-1$.

Bloch's theorem states that the solution of the Schrödinger equation for this problem, i.e., the wave function $\psi(\vec{r}\,)$ for an electron in such a periodic potential, can be expressed as a combination of so-called Bloch states—or *Bloch waves*—given by a plane wave (over the whole lattice) modulated by a function, which is obtained as a (periodic) solution to the restricted unit-cell problem. More precisely, let us denote by $\psi(\vec{r}\,)$ any function defined on the considered crystalline cubic lattice and by $L = lm$ the physical size of the lattice. Then, the use of PBCs, i.e., the condition $\psi(\vec{r}\,) = \psi(\vec{r} + L\hat{e}_\mu)$ for any direction μ, implies that $\psi(\vec{r}\,)$ can be (Fourier) expanded in plane waves $\exp\,(2\pi i\,\vec{k}\cdot\vec{r}/L)$ with

$$\exp\left(2\pi i\,\frac{\vec{k}\cdot L\hat{e}_\mu}{L}\right) \;=\; \exp\left(2\pi i\,k_\mu\right) \;=\; 1. \tag{80}$$

This tells us that the components of $\vec{k}$ are integer numbers (i.e., $k_\mu \in \mathcal{Z}$) and that, when they are restricted to the first Brillouin zone, we have[16] $k_\mu \in [-m/2, m/2)$, yielding discrete Fourier momenta $\widetilde{k}_\mu \equiv 2\pi k_\mu/(lm) \in [-\pi/l, \pi/l)$. Then, with this restriction, the allowed plane waves have components $k_\mu + mK_\mu$, with $K_\mu \in \mathcal{Z}$, i.e., they can be written as $\exp\,[2\pi i\,(\vec{k} + m\,\vec{K})\cdot\vec{r}/L\,]$. Here, the vector $m\,\vec{K}/L = \sum_{\mu=1}^{d} K_\mu \hat{e}_\mu / l$ corresponds to the so-called reciprocal lattice, i.e., it is such that

$$\exp\left(2\pi i\,\frac{m\,\vec{K}}{L}\cdot\vec{R}\right) \;=\; \exp\left(2\pi i\,\sum_{\mu=1}^{d} K_\mu\,R_\mu\right) \;=\; 1 \tag{81}$$

for any translation vector $\vec{R}$ of the Bravais lattice, yielding

$$\exp\left[2\pi i\left(\frac{\vec{k} + m\,\vec{K}}{L}\right)\cdot\vec{R}\,\right] \;=\; \exp\left(2\pi i\,\frac{\vec{k}}{L}\cdot\vec{R}\right) \;=\; \exp\left(2\pi i\,\sum_{\mu=1}^{d} \frac{k_\mu\,R_\mu}{m}\right), \tag{82}$$

with $\vec{k}$ in the first Brillouin zone.

With this setup, one can prove Bloch's theorem (see the first proof in Ref. [26]) by using the properties of the translation operator

$$\mathcal{T}(\vec{R}\,)\,\psi(\vec{r}\,) \;=\; \psi(\vec{r} + \vec{R}\,). \tag{83}$$

In particular, we need to recall the relation

$$\mathcal{T}(\vec{R}\,)\,\mathcal{T}(\vec{R}^{\,\prime}\,) \;=\; \mathcal{T}(\vec{R}^{\,\prime}\,)\,\mathcal{T}(\vec{R}\,) \;=\; \mathcal{T}(\vec{R} + \vec{R}^{\,\prime}\,), \tag{84}$$

valid for all vectors $\vec{R}$ and $\vec{R}^{\,\prime}$ on the Bravais lattice. Hence, the translation operators form an Abelian group, with the trivial identity element $\mathcal{T}(\vec{0}\,)$ and the inverse element $\mathcal{T}^{-1}(\vec{R}\,) = \mathcal{T}(-\vec{R}\,)$. At the same time, it is evident that any plane wave $\exp\,[2\pi i\,(\vec{k} + m\,\vec{K}\,)\cdot\vec{r}/L]$—with fixed $\vec{k}$ (restricted to the first Brillouin zone) and $\vec{K}$ as above—is an eigenfunction of $\mathcal{T}(\vec{R}\,)$ with eigenvalue $\exp\,(2\pi i\vec{k}\cdot\vec{R}/L)$, see Equation (82). Thus, in the most general case, we have the eigenvectors

$$\mathcal{T}(\vec{R}\,)\,\psi_{\vec{k}}(\vec{r}\,) \;=\; \psi_{\vec{k}}(\vec{r} + \vec{R}\,) \;=\; \exp\left(2\pi i\,\frac{\vec{k}}{L}\cdot\vec{R}\right)\psi_{\vec{k}}(\vec{r}\,) \tag{85}$$

with

$$\psi_{\vec{k}}(\vec{r}) \,=\, \sum_{\vec{K}} c_{\vec{k}}(\vec{K}) \, \exp\left[2\pi i \left(\frac{\vec{k} + m\,\vec{K}}{L}\right) \cdot \vec{r}\,\right], \tag{86}$$

where $\vec{k}$ is fixed and taken in the first Brillouin zone, while $\vec{K}$ refers to vectors of the reciprocal lattice. The last result is usually written as

$$\psi_{\vec{k}}(\vec{r}) \,=\, \exp\left(2\pi i \,\frac{\vec{k}}{L} \cdot \vec{r}\right) \sum_{\vec{K}} c_{\vec{k}}(\vec{K}) \exp\left(2\pi i \frac{m\,\vec{K}}{L} \cdot \vec{r}\right) \,\equiv\, \exp\left(2\pi i \,\frac{\vec{k}}{L} \cdot \vec{r}\right) u_{\vec{k}}(\vec{r}), \tag{87}$$

where the function $u_{\vec{k}}(\vec{r})$ trivially satisfies, see Equation (81), the condition

$$u_{\vec{k}}(\vec{r} + \vec{R}) \,=\, u_{\vec{k}}(\vec{r}) \,. \tag{88}$$

Hence, $u_{\vec{k}}(\vec{r})$ is effectively specified by vectors $\vec{r}$ in the primitive cell and may be obtained from a restricted version of the original problem.

The proof of Bloch's theorem is as follows. The Hamiltonian $\mathcal{H}$ for the crystalline solid is, by hypothesis, invariant under a translation by $\vec{R}$, i.e., $\mathcal{H}$ commutes with $\mathcal{T}(\vec{R})$. Then, one can choose the eigenstates $\psi_{\vec{k}}(\vec{r})$ of $\mathcal{T}(\vec{R})$ to also be eigenstates of $\mathcal{H}$, i.e.,

$$\mathcal{H}\,\psi_{\vec{k}}(\vec{r}) \,=\, \lambda_{\vec{k}}\,\psi_{\vec{k}}(\vec{r}). \tag{89}$$

Equivalently, by using Equation (87), one can define [26]

$$\mathcal{H}\,\psi_{\vec{k}}(\vec{r}) \,=\, \lambda_{\vec{k}}\,\exp\left(2\pi i \,\frac{\vec{k}}{L} \cdot \vec{r}\right) u_{\vec{k}}(\vec{r}) \,\equiv\, \exp\left(2\pi i \,\frac{\vec{k}}{L} \cdot \vec{r}\right) \mathcal{H}_{\vec{k}}\, u_{\vec{k}}(\vec{r}) \tag{90}$$

and consider, instead of the original problem (89) on the Bravais lattice and with the Hamiltonian $\mathcal{H}$, the new problem

$$\mathcal{H}_{\vec{k}}\, u_{\vec{k}}(\vec{r}) \,=\, \lambda_{\vec{k}}\, u_{\vec{k}}(\vec{r}), \tag{91}$$

which is restricted to a single primitive cell and subject to the BCs (88). In the general case, one expects the last eigenvalue problem to have infinite solutions (indexed by n), i.e., we can write

$$\mathcal{H}_{\vec{k}}\, u_{\vec{k},n}(\vec{r}) \,=\, \lambda_{\vec{k},n}\, u_{\vec{k},n}(\vec{r}) \,. \tag{92}$$

Clearly, $\mathcal{H}_{\vec{k}}$ depends[17] on the (discretized) components $\widetilde{k}_\mu \equiv 2\pi k_\mu/(lm) \in [-\pi/l, \pi/l)$. Hence, when one considers the infinite-volume limit $m \to +\infty$, the new Hamiltonian depends on the (now continuous) parameters $\widetilde{k}_\mu$ and one expects the energy levels $\lambda_{\vec{k},n}$ to be also a continuous function of these parameters. Then, for each n, these values constitute a so-called energy band, leading to the description of the solid in terms of a band structure.

3.2. Bloch's Theorem for the Gauge-Fixing Problem

The above setup applies—in a rather straightforward manner—also to the gauge link configuration on the extended lattice Λ_z. The main difference is that, here, the primitive cell, i.e., the original lattice Λ_x, is also discretized, since it is given by the vectors $\vec{x} = a \sum_{\mu=1}^{d} x_\mu \hat{e}_\mu$, where a is the *lattice spacing* and the components x_μ take integer values in $[1, N]$. Thus, in the above formulae for the crystalline solid, we just have to substitute the magnitude l with Na (and, therefore, L with mNa). Then, after setting the lattice spacing equal to 1, as usually performed in lattice gauge theory, we find that the vectors of the Bravais lattice become $\vec{R} = N \sum_{\mu=1}^{d} R_\mu \hat{e}_\mu$, with $R_\mu = 0, 1, \ldots, m-1$. Finally, by combining the original lattice Λ_x with the index lattice Λ_y, we recover our notation for Λ_z, identifying the components R_μ with y_μ and $\vec{r}$ with $\vec{z} = \vec{x} + N\vec{y}$. In particular, we find that the generic plane waves $\exp\left[2\pi i \vec{k}' \cdot \vec{z} / (mN)\right]$ are written in terms of wave-number vectors with components $k'_\mu = k_\mu + m\, K_\mu$, as above. However, as stressed before (see note 5), instead of the symmetric interval around 0 usually taken for the first Brillouin zone, here we consider integers k_μ in the interval $[0, m-1]$ and K_μ in $[0, N-1]$.

In analogy with the Bloch theorem described in the previous section, one can prove (see Appendix F of Ref. [5] and Section 3.3 below) that the gauge transformation $g(\vec{z})$ that minimizes the functional $\mathcal{E}_U[g]$—see Equations (76) and (77)—defined for the extended lattice through $\vec{z} = \vec{x} + N\vec{y}$ can be written as

$$g(\vec{z}) \;=\; \exp\left(i \sum_{\mu=1}^{d} \frac{\Theta_\mu\, z_\mu}{N} \right) h(\vec{x}), \tag{93}$$

where $h(\vec{x}) = h(\vec{x} + N\vec{y})$ has the periodicity of the original lattice Λ_x and the matrices Θ_μ belong to a Cartan sub-algebra of the $su(N_c)$ Lie algebra, i.e., they commute. In Appendix A we discuss the main properties of these matrices, which can be written as

$$\Theta_\mu \;=\; \sum_{b=1}^{N_c-1} \theta_\mu^b\, t_C^b, \tag{94}$$

where θ_μ^b ($\mu = 1, \ldots, d$) are real parameters and the matrices t_C^b are the generators of the Cartan sub-algebra of $su(N_c)$, which has dimension $N_c - 1$.

As a result of Equation (93) above and the cyclicity of the trace, the minimizing functional $\mathcal{E}_U[g]$ in Equation (76) becomes

$$\mathcal{E}_U[g] \;=\; \frac{\Re\,\mathrm{Tr}}{N_c\, d\, m^d\, V} \sum_{\mu=1}^{d} \sum_{\vec{z} \in \Lambda_z} \left[\mathbb{1} \,-\, U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} \right], \tag{95}$$

which is independent of $\vec{y}$. Thus, we can write

$$\mathcal{E}_U[g] \;\equiv\; \mathcal{E}_{U,\Theta}[h] \;=\; \frac{\Re\,\mathrm{Tr}}{N_c\, d\, V} \sum_{\mu=1}^{d} \sum_{\vec{x} \in \Lambda_x} \left[\mathbb{1} \,-\, U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} \right] \tag{96}$$

and define

$$\mathcal{E}_{U,\Theta}[h] \;\equiv\; \frac{\Re\,\mathrm{Tr}}{N_c\, d} \sum_{\mu=1}^{d} \left[\mathbb{1} \,-\, Z_\mu(h)\, \frac{e^{-i\frac{\Theta_\mu}{N}}}{V} \right], \tag{97}$$

where

$$Z_\mu(h) \;\equiv\; \sum_{\vec{x} \in \Lambda_x} U_\mu(h;\vec{x}) \tag{98}$$

is the zero mode of the (gauge-transformed) link variable $U_\mu(h;\vec{x})$ in a given direction, and it is evident that the numerical minimization can now be carried out on the original lattice Λ_x. At the same time, imposing PBCs on Λ_z in Equation (93), we see that the expression (with no summation over the index μ)

$$\exp\left(i\, \frac{\Theta_\mu\, z_\mu}{N} \right), \tag{99}$$

evaluated for $z_\mu = mN$, should be equal to

$$\exp\left(im\Theta_\mu\right) \;=\; \left[\, \exp\left(i\Theta_\mu\right) \right]^m \;=\; \mathbb{1}. \tag{100}$$

Thus, the matrices Θ_μ have eigenvalues of the type $2\pi n_\mu/m$, where n_μ is an integer. Equivalently, the matrices $\exp(i\Theta_\mu)$ have eigenvalues $\exp(2\pi i n_\mu/m)$.

By comparing Equation (93) with Equation (87), and also Equation (100) with Equation (80), it is evident that the matrices Θ_μ play the role of the momentum $\vec{k}$ in the crystalline-solid problem. It is also interesting to observe that, from the numerical point of view, the minimizing functional (97) and (98) can be interpreted as the usual minimizing functional (2) on the lattice Λ_x, using a periodic gauge transformation $h(\vec{x})$, together with an "extended" (i.e., nonperiodic) gauge transformation $\exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, x_\nu/N\right)$. The functional $\mathcal{E}_{U,\Theta}[h]$, however, still depends (implicitly) on the size m of the index lattice Λ_y through Equation (100). One should also note that the substitution of the original minimizing function $\mathcal{E}_U[g]$, which considers the gauge transformation $g(\vec{z})$ on the extended lattice Λ_z, with the modified minimizing function $\mathcal{E}_{U,\Theta}[h]$, which is restricted to the original lattice Λ_x and depends on the Θ_μ matrices (see again Equations (97) and (98)), is completely analogous to the substitution of the eigenvalue problem (89) with the problem (91). The main difference is that, while the vector $\vec{k}$ is fixed in the Hamiltonian $\mathcal{H}_{\vec{k}}$, the matrices Θ_μ are chosen by the minimization algorithm (see Section 6 below). On the other hand, one could also consider—in analogy with the usual condensed matter approach—a given (fixed) set of matrices Θ_μ and look (for example) at the different[18] "Gribov copies" corresponding to different solutions $\{h(\vec{x})\}$ of the small-lattice problem (96) defined by fixed Θ_μ's.

We should note here that we are using the same notation as in Section 2 for the solution $\{h(\vec{x})\}$, meaning a periodic gauge transformation—i.e., effectively restricted to the small lattice Λ_x—that solves the optimization problem defined by the minimizing functional on Λ_x. However, one must remember that, in the extended-lattice problem, the corresponding functional does not depend only on $\{U_\mu(\vec{x})\}$ and $\{h(\vec{x})\}$, but also on $\{\Theta_\mu\}$. In fact, as it is evident from Equation (93), here the gauge transformation $h(\vec{x})$ is *not* just the restriction of $g(\vec{z})$ to the small lattice Λ_x, but it is the solution to the modified small-lattice problem (96). Hence, if we want to relate the two objects, we might say that the transformation $\{h(\vec{x})\}$ in Section 2 is the minimum of $\mathcal{E}_{U,\Theta}[h]$ with all matrices Θ_μ trivially given by $\mathbb{1}$. This distinction will be made clearer in the next few sections.

3.3. *Proof of Equation (93)*

Expression (83) can of course be applied also to the lattice setup considered in Section 3.2. For example, the translation operator $\mathcal{T}(N\hat{e}_\mu)$ acts on $U_\nu(\vec{z})$ and $g(\vec{z})$ by shifting them to the site $\vec{z}+N\hat{e}_\mu$, i.e.,

$$\mathcal{T}(N\hat{e}_\mu)\, U_\nu(\vec{z}) \;=\; U_\nu(\vec{z}+N\hat{e}_\mu), \tag{101}$$

$$\mathcal{T}(N\hat{e}_\mu)\, g(\vec{z}) \;=\; g(\vec{z}+N\hat{e}_\mu). \tag{102}$$

Moreover, the use of PBCs, see Equations (78) and (79), implies that

$$\mathcal{T}(mN\hat{e}_\mu) \,=\, \left[\,\mathcal{T}(N\hat{e}_\mu)\,\right]^{m} \,=\, \mathbb{1}, \tag{103}$$

where $\mathbb{1}$ is the identity operator. Also, with our setup, the effect of $\mathcal{T}(N\hat{e}_\mu)$ in Equation (101) is simply that of the identity.

In order to prove Equation (93), a key point is that the minimizing problem for the extended lattice, defined by the functional in Equation (76), is invariant if we consider a shift of the lattice sites $\vec{z}$ by N in any direction μ since this amounts to a simple redefinition of the origin for the extended lattice Λ_z. This implies that, if $g(\vec{z})$ is a solution of the minimizing problem satisfying the BCs (78), then $g'(\vec{z}) \,=\, g(\vec{z}+N\hat{e}_\mu)$ is (trivially) a solution too, satisfying the same BCs. Moreover, these two solutions select the same local minimum within the first Gribov region. At the same time, as already stressed above, due to cyclicity of the trace, $\mathcal{E}_U[g]$ is invariant under global gauge transformations v, and the same is true for the quantities introduced in Equations (42)–(44), when applied to the extended lattice Λ_z. Note that this corresponds to left multiplication[19] of the solution to the gauge-fixing problem by a fixed group element, mapping $\{g(\vec{z})\}$ onto $\{v\, g(\vec{z})\}$. Thus, the gauge transformation $\{g(\vec{z})\}$—i.e., a given minimum solution—is always determined modulo a global (left) transformation, and (with our setup) remains a solution under translations by N in any direction.

The above observation needs some comments. In particular, we recall that, in Ref. [5], the proof of Equation (93) is presented only for the absolute minima (of the minimizing functional) that belong to the interior of the so-called fundamental modular region. Indeed, as shown in Appendix A of the same reference, these minima are unique, i.e., non degenerate, implying that the gauge transformation $\{g(\vec{z})\}$ connecting the (unfixed) thermalized configuration $\{U_\mu(\vec{z})\}$ to the (gauge-fixed) absolute minimum $\{U_\mu(g;\vec{z})\}$ is unique, modulo a global gauge transformation. However, as stressed at the end of the *Bloch waves* section of Ref. [1], even in the case of local minima one can make the (reasonable) hypothesis that a specific realization of one of these minima also corresponds to a specific and unique transformation $\{g(\vec{z})\}$ (up to a global transformation) when considering a given configuration $\{U_\mu(\vec{z})\}$. Indeed, this has been verified numerically (see Ref. [27]) for small lattice volumes and for the local minima of the minimizing functional (2). We thus assume, as in Ref. [1], that the local minima of $\mathcal{E}_U[g]$ also define unique gauge transformations. In other words, here we are considering truly degenerate local minima, i.e., connected by a nontrivial gauge transformation, as different minima. Also, we assume that—at least for numerical simulations on finite lattice volumes—these degenerate minima will not have identical values of the quantities characterizing the minimum solution, such as $\mathcal{E}, \Delta\mathcal{E}, (\nabla A)^2$ and Σ_Q, described[20] in Section 2 (see also Section 4.3 below). As a matter of fact, at the numerical level, the only degeneracy that can likely occur is the trivial one, i.e., when the corresponding link configurations are related by a global gauge transformation.

Based on the above discussion, we proceed to prove Equation (93) by writing

$$\mathcal{T}(N\hat{e}_\mu)\, g(\vec{z}) \,=\, \left[\, \mathcal{T}(\hat{e}_\mu)\,\right]^N g(\vec{z}) \,=\, g(\vec{z}+N\hat{e}_\mu) \,=\, g'(\vec{z}) \,=\, s_\mu\, g(\vec{z}), \tag{104}$$

where s_μ is a $\vec{z}$-independent SU(N_c) matrix. This is the main hypothesis considered in Refs. [1,5] and it is supported by our arguments above, i.e., that a shift of $\{g(\vec{z})\}$ by N along a given direction μ produces an equivalent solution, and can therefore be parametrized as left multiplication by a fixed element s_μ of the group. Then, due to Equation (84), we have that the s_μ's are commuting SU(N_c) matrices, i.e., they can be written as $\exp(i\Theta_\mu)$, with Θ_μ given in Equation (94). Also, due to the PBCs for Λ_z, we need to impose the condition (103). Hence, the relations

$$\mathcal{T}(mN\hat{e}_\mu)\, g(\vec{z}) \,=\, \left[\, \mathcal{T}(N\hat{e}_\mu)\,\right]^m g(\vec{z}) \,=\, s_\mu^m\, g(\vec{z}) \tag{105}$$

and

$$\mathcal{T}(mN\hat{e}_\mu)\, g(\vec{z}) \,=\, g(\vec{z}+mN\hat{e}_\mu) \,=\, g(\vec{z}) \tag{106}$$

yield

$$s_\mu^m \,=\, \mathbb{1}. \tag{107}$$

We stress that the action of the translation operator $\mathcal{T}(N\hat{e}_\mu)$ in Equation (104), i.e., the matrix $s_\mu = \exp(i\Theta_\mu)$, depends on the solution $\{g(\vec{z})\}$ to which it is applied, i.e., the parametrization of the matrices Θ_μ is determined by the considered solution of the gauge-fixing problem, see also the comment below Equation (110).

The above Equation (104) is the matrix analogue of the eigenvalue Equation (85) [for $\vec{R} = N\hat{e}_\mu$ and $l \to N$, so that $L \to mN$]. Indeed, instead of the wave function $\psi_{\vec{k}}(\vec{r})$, Equation (104) applies to a solution $\{g(\vec{z})\}$ of the minimizing problem $\mathcal{E}_U[g]$, corresponding to a specific local minimum. Also, on the r.h.s. of the equation, the matrix s_μ appears[21] instead of the phase $\exp(2\pi i\, k_\mu/m)$, i.e., the corresponding eigenvalue in Equation (85). Moreover, the action of the translation operators $\mathcal{T}(N\hat{e}_\mu)$ in Equation (104) can likewise be expressed in terms of phase factors, if we write the gauge transformation $g(\vec{z})$ as

$$g(\vec{z}) \,=\, \sum_{i,j=1}^{N_c} g^{ij}(\vec{z})\, \mathbf{W}^{ij}, \tag{108}$$

where the matrices $\mathbf{W}^{ij} = w_i w_j^\dagger$ are defined in Appendix A.2 of Appendix A and $g^{ij}(\vec{z})$ denotes the coefficient of $\mathbf{W}^{ij}$ in the expansion of $g(\vec{z})$. Then, we immediately find[22]

$$\mathcal{T}(N\hat{e}_\mu)\, g(\vec{z}) \,=\, s_\mu\, g(\vec{z}) \,=\, \exp(i\Theta_\mu)\, g(\vec{z}) \,=\, \sum_{i,j=1}^{N_c} e^{2\pi i n_\mu^i/m}\, g^{ij}(\vec{z})\, \mathbf{W}^{ij}, \tag{109}$$

with integer n_μ^i, so that each coefficient $g^{ij}(\vec{z})\,\mathbf{W}^{ij}$ gains a phase factor $\exp(2\pi i\, n_\mu^i/m)$. These factors are the usual eigenvalues τ_μ of the translation operator $\mathcal{T}(N\hat{e}_\mu)$ that satisfy the relation $(\tau_\mu)^m = 1$, implying that they can be written as $\tau_\mu = \exp\left(2\pi i\, k'_\mu/m\right)$ with $k'_\mu \in \mathcal{Z}$. In particular, in the first Brillouin zone, we have $\tau_\mu = \exp(2\pi i\, k_\mu/m)$ with $k_\mu = k'_\mu$ (mod m).

The above result

$$g(\vec{z} + N\hat{e}_\mu) \,=\, \exp(i\Theta_\mu)\, g(\vec{z}) \tag{110}$$

is already equivalent to one of the usual formulations of the Bloch theorem (see Equation (8.6) in Ref. [26]). Indeed, by paraphrasing the statement in Ref. [28], we can say that

> *For any solution $g(\vec{z})$ of the minimizing problem $\mathcal{E}_U[g]$ there exists a set of commuting matrices Θ_μ such that the translation by a vector $N\hat{e}_\mu$ is equivalent to multiplying the solution by the factor* $\exp(i\Theta_\mu)$.

This provides a way to construct the solution $g(\vec{z})$—at a point $\vec{z}$ of the extended lattice Λ_z—as the successive application of $\exp(i\Theta_\mu)$ to $g(\vec{x})$, which is the same solution but restricted to the primitive cell Λ_x. Hence, by taking into account the displacement, from point $\vec{x}$, along each direction μ—given by the indices y_μ—we can write

$$g(\vec{z}) \,=\, g(\vec{x} + N\vec{y}) \,=\, \exp\left(i \sum_{\nu=1}^{d} \Theta_\nu\, y_\nu\right) g(\vec{x})\,. \tag{111}$$

We stress that the above expression tells us that the extended-lattice solution $g(\vec{z})$ is obtained by successive "block-rotations" of the primitive-cell portion of the solution $g(\vec{x})$: each time we move to a neighboring cell along the direction μ, the solution picks up a factor $\exp(i\Theta_\mu)$. As a consequence, by substituting Equation (111) into the expressions (76) and (77) and in analogy with the discussion presented in Section 3.2 above, the minimization problem is broken down (due to cyclicity of the trace) into m^d copies of the minimization problem[23]

$$\frac{\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{\mu=1}^{d} \sum_{\vec{x}\in\Lambda_x} \left[\mathbb{1} \,-\, g(\vec{x})\, U_\mu(\vec{x})\, g(\vec{x} + \hat{e}_\mu)^\dagger \right]. \tag{112}$$

For each of these copies, it corresponds to the minimization of the original functional for the lattice Λ_x, i.e., the expression in Equation (2) [with $g(\vec{x})$ instead of $h(\vec{x})$] but with the boundary condition (see Equation (110) with $\vec{z} = \vec{x}$),

$$g(\vec{x} + N\hat{e}_\mu) \;=\; \exp(i\Theta_\mu)\, g(\vec{x})\,. \tag{113}$$

Thus, the function $g(\vec{x})$ is *not* a solution to the usual gauge-fixing problem restricted to the primitive cell Λ_x—which would correspond to a periodic function under translations by N in all directions—but is closely related to it by the above rotations.

We now note that the BCs (113) may be incorporated automatically if we write, in analogy with the usual proof of the Bloch theorem [26,28],

$$g(\vec{x}) \;=\; \exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) h(\vec{x}), \tag{114}$$

where $h(\vec{x})$ is a solution to the gauge-fixing problem restricted to Λ_x, redefined[24] in terms of a modified gauge-transformed link configuration $\{U_\mu(h;\vec{x})\exp(-i\Theta_\mu/N)\}$, see Equation (96). In this way, the condition (113) is clearly satisfied. Moreover, it is straightforward to verify that the function $h(\vec{x})$ is periodic on Λ_x. Indeed, by inverting (114), i.e., by writing

$$h(\vec{x}) \;=\; \exp\left(-i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) g(\vec{x}), \tag{115}$$

we have that

$$\begin{aligned} h(\vec{x} + N\hat{e}_\mu) \;&=\; \exp\left(-i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) \exp\left(-i\Theta_\mu\right) g(\vec{x} + N\hat{e}_\mu) \\ &=\; \exp\left(-i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) g(\vec{x}) \;=\; h(\vec{x}), \end{aligned} \tag{116}$$

where we use (113) and the fact that the matrices Θ_ν commute with each other. Therefore, the above Equation (114) provides the desired solution to the modified minimization problem on Λ_x, written in terms of the periodic function $h(\vec{x})$, up to choice of parameters for the Θ_μ matrices, which are also fixed by the minimization problem.[25]

This completes our proof of Equation (93), which may also be written as

$$g(\vec{z}) \;=\; \exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, z_\nu}{N} \right) h(\vec{z}), \tag{117}$$

where the function $h(\vec{z})$ is defined on the extended lattice but has periodicity under translations by N in all directions, i.e., it is a "clone" of the primitive-cell solution $h(\vec{x})$ above. Hence, as performed for the original Bloch theorem, we can write the solution $g(\vec{z})$ as a product of a "plane wave" by a (periodic) solution of a modified version of the primitive-cell problem.

4. The Minimizing Problem Revisited

Using the analogue of Bloch's theorem, i.e., Equation (93), the gauge-transformed link variable (77) is given by

$$U_\mu(g;\vec{z}) \;=\; \exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, z_\nu}{N} \right) U_\mu(h;\vec{x}) \,\exp\left(-i\, \frac{\Theta_\mu}{N} \right) \,\exp\left(-i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, z_\nu}{N} \right), \tag{118}$$

with $h(\vec{x})$ discussed in the previous two sections and recalling the general expression for a gauge-transformed link, Equation (3). Since $h(\vec{x})$ satisfies PBCs with respect to the original lattice Λ_x, it is clear that $\{U_\mu(h;\vec{x})\}$ is also a periodic, gauge-transformed link configuration on Λ_x. Thus, the effect of the index lattice is completely encoded in the exponential factors and in the matrices Θ_μ. Let us stress that, even though we use the same notation[26] considered in Section 2, in the present case $\{U_\mu(h;\vec{x})\}$ is not transverse on Λ_x. Indeed, transversality[27] applies to $\{U_\mu(g;\vec{z})\}$, taken for the extended lattice Λ_z. By considering the relation (75) we can, however, rewrite the above result in a different way, i.e.,

$$U_\mu(g;\vec{z}) \;=\; U_\mu(g;\vec{x},\vec{y}) \;=\; \exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) U_\mu(l;\vec{x})\, \exp\left(-i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right), \tag{119}$$

where the $\vec{y}$ coordinates characterize the replicated lattice $\Lambda_x^{(\vec{y})}$ and we define a "local" version of the transformed gauge link

$$\begin{aligned} U_\mu(l;\vec{x}) \;&=\; l(\vec{x})\, U_\mu(\vec{x})\, l(\vec{x}+\hat{e}_\mu)^\dagger \\ &\equiv\; \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right)\left[U_\mu(h;\vec{x})\, \exp\left(-i\,\frac{\Theta_\mu}{N}\right)\right] \exp\left(-i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) \end{aligned} \tag{120}$$

where the gauge transformation restricted to Λ_x, see Equation (93), is given as

$$l(\vec{x}) \;=\; \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) h(\vec{x}). \tag{121}$$

Similarly, we can write[28]

$$U_\mu(l;\vec{x}-\hat{e}_\mu) \;\equiv\; \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right)\left[\exp\left(-i\,\frac{\Theta_\mu}{N}\right) U_\mu(h;\vec{x}-\hat{e}_\mu)\right] \exp\left(-i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right). \tag{122}$$

Let us point out that the quantity $l(\vec{x})$ is actually a redefinition of $g(\vec{x})$ in (114), which is however never extended to Λ_z. This is performed to single out the Λ_x portion of the solution $g(\vec{z})$ and will be important from now on in our analysis. In particular, we make use of the fact that both $l(\vec{x})$ and $h(\vec{x})$ "exist" only on Λ_x, and are therefore simply replicated identically to other cells $\Lambda_x^{(\vec{y})}$. We stress, however, that the properties of these two small-lattice gauge transformations differ: indeed, while $l(\vec{x})$ is the nonperiodic solution of the minimization problem defined by the original functional $\mathcal{E}_U[l]$ on Λ_x, see Equation (128) below, $h(\vec{x})$ is the periodic solution of the modified minimization problem (96), which depends on the Θ_μ's. Thus, $\{U_\mu(l;\vec{x})\}$ is transverse on Λ_x and $\{U_\mu(h;\vec{x})\}$ is not as already mentioned above.

The definition of $l(\vec{x})$ implies that, see Equation (113),

$$\begin{aligned} l(\vec{x}+N\hat{e}_\mu) \;&=\; \exp\left(i\Theta_\mu\right) \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) h(\vec{x}+N\hat{e}_\mu) \\ &=\; \exp\left(i\Theta_\mu\right) \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) h(\vec{x}) \;=\; \exp\left(i\Theta_\mu\right) l(\vec{x}), \end{aligned} \tag{123}$$

yielding

$$
\begin{aligned}
U_\mu(l;\vec{x}+N\hat{e}_\nu) &= l(\vec{x}+N\hat{e}_\nu)\,U_\mu(\vec{x}+N\hat{e}_\nu)\,l(\vec{x}+N\hat{e}_\nu+\hat{e}_\mu)^\dagger \\
&= \exp\left(i\Theta_\nu\right) l(\vec{x})\,U_\mu(\vec{x})\,l(\vec{x}+\hat{e}_\mu)^\dagger \exp\left(-i\Theta_\nu\right) \\
&= \exp\left(i\Theta_\nu\right) U_\mu(l;\vec{x}) \exp\left(-i\Theta_\nu\right), \qquad (124)
\end{aligned}
$$

which is reminiscent of the so-called twisted BCs [29] with constant transition matrices[29] $\Omega_\nu = \exp\left(i\Theta_\nu\right)$. One should also note that, if we expand the link variable $U_\mu(l;\vec{x})$ in terms of the $\mathbf{W}^{ij}$ matrices, as done in the previous section for the $g(\vec{z})$ matrices, we can rewrite Equation (124) as[30]

$$
U_\mu(l;\vec{x}+N\hat{e}_\nu) = \sum_{i,j=1}^{N_c} U_\mu^{ij}(l;\vec{x}+N\hat{e}_\nu)\,\mathbf{W}^{ij} = \sum_{i,j=1}^{N_c} e^{2\pi i(n_\nu^i - n_\nu^j)/m}\,U_\mu^{ij}(l;\vec{x})\,\mathbf{W}^{ij}, \qquad (125)
$$

where n_ν^i, n_ν^j are integers. Hence, the coefficients of $U_\mu(l;\vec{x})$ satisfy toroidal BCs (see Appendix A.3 in Ref. [16])

$$
U_\mu^{ij}(l;\vec{x}+N\hat{e}_\nu) \;=\; e^{2\pi i(n_\nu^i - n_\nu^j)/m}\,U_\mu^{ij}(l;\vec{x}), \qquad (126)
$$

which, depending on the values of n_ν^i and n_ν^j, include periodic as well as anti-periodic BCs, given respectively by $e^{2\pi i(n_\nu^i - n_\nu^j)/m} = 1$ and $e^{2\pi i(n_\nu^i - n_\nu^j)/m} = -1$.

The above Equation (119) implies that gauge-fixed configurations in different replicated lattices $\Lambda_x^{(\vec{y})}$ differ only by the exponential factors $\exp\left(\pm i\sum_{\nu=1}^d \Theta_\nu\,y_\nu\right)$, which correspond to a global gauge transformation within each $\Lambda_x^{(\vec{y})}$. Moreover, we have that $\{U_\mu(l;\vec{x})\}$ is transverse on each replicated lattice $\Lambda_x^{(\vec{y})}$. Indeed, by noting that

$$
\mathrm{Tr}\left[\,U_\mu(l;\vec{x})\,\right] \;=\; \mathrm{Tr}\left[\,U_\mu(h;\vec{x})\,\exp\left(-i\,\frac{\Theta_\mu}{N}\right)\right], \qquad (127)
$$

we can rewrite Equation (96) as

$$
\mathcal{E}_U[g] \;=\; \mathcal{E}_{U,\Theta}[h] \;=\; \mathcal{E}_U[l] \;\equiv\; \frac{\Re\,\mathrm{Tr}}{N_c\,d\,V}\sum_{\mu=1}^{d}\sum_{\vec{x}\in\Lambda_x}\left[\,\mathbb{1} \,-\, U_\mu(l;\vec{x})\,\right] \qquad (128)
$$

and, therefore, $\{U_\mu(l;\vec{x})\}$ is transverse[31] when the functional $\mathcal{E}_U[l]$ is minimized.

We can summarize these results by saying that, with the consideration of the extended lattice Λ_z, we trade the periodic transverse link configuration $\{U_\mu(h;\vec{x})\}$ on the original lattice Λ_x—in the small-lattice problem—with the nonperiodic, but still transverse, link configuration $\{U_\mu(l;\vec{x})\}$, also defined on Λ_x.[32] Moreover, this transverse link configuration is replicated on each $\Lambda_x^{(\vec{y})}$, indexed by the y_μ coordinates, and then globally rotated using the gauge transformation $\exp\left(i\sum_{\nu=1}^d \Theta_\nu\,y_\nu\right)$, see Equation (119), in such a way that PBCs are satisfied on Λ_z. One could visualize this lattice setup by making an analogy with some of the works by M.C. Escher, such as those called *Metamorphosis I, II* and *III* (see, for example, [30]), in which one starts from a simple geometrical form, e.g., a square, and replicates it several times on a plane by adding a small rotation (and a distortion) at each step. As already stressed in note 23, the description of the gauge-fixed configuration—in terms of $\{U_\mu(l;\vec{x})\}$ and of global rotations $\exp\left(i\sum_{\nu=1}^d \Theta_\nu\,y_\nu\right)$—naturally singles out domains, which can be characterized (for example) in terms of color magnetization as performed in Section 6.

The above observations have important consequences also for the type of Gribov copies that one can obtain when using the extended lattice Λ_z in our setup. Indeed, they are essentially given by the Gribov copies that can be found on the original lattice Λ_x where, however, the transverse link configuration $\{U_\mu(l;\vec{x})\}$ is now nonperiodic. As a consequence, the set of local minima generated by the usual small-lattice gauge-fixing procedure, i.e., by the gauge transformation $\{h(\vec{x})\}$ as in Section 2, are (in principle) not related to the local minima generated by the new gauge-fixing approach, i.e., by the gauge transformation $\{l(\vec{x})\}$. In fact, one should recall that $\{h(\vec{x})\}$ in the extended problem is also (implicitly) determined by the Θ_ν matrices, and vice versa, through the minimization process. Moreover, due to the extra freedom allowed by the Bloch waves (see note 25), we expect

$$\mathcal{E}_U[l] \,=\, \mathcal{E}_{U,\Theta}[h] \,\leq\, \mathcal{E}_U[h] \tag{129}$$

for a fixed (thermalized) gauge-link configuration $\{U_\mu(\vec{x})\}$. At the same time, not much can be said about a comparison of different Gribov copies due to the $\{l(\vec{x})\}$ gauge transformation and those obtained by gauge fixing a configuration that is directly thermalized on the extended lattice Λ_z, i.e., which has (at any step) an invariance under translation by $mN\hat{e}_\mu$ only.

4.1. The Transversality Condition

We turn now to the constraints imposed by the minimization of the functional $\mathcal{E}_U[l]$. Our goal is to obtain expressions for observables constructed from the transformed gauge links $U_\mu(l;\vec{x})$, both to characterize the transversality condition, i.e., to obtain the gauge-fixing criteria from the minimizing functional $\mathcal{E}_U[l]$, and to define the quantities that will be measured in our simulations. However, since we want to explore the similarities between the minimization problem on the extended lattice and the original problem on the small lattice Λ_x (as addressed in Section 2), we also express our results in terms of the periodic transformation $\{h(\vec{x})\}$, stressing that it now refers to the modified minimization condition depending on the matrices Θ_μ. To this end, we note that these matrices (detailed in Appendix A) are conveniently parametrized in terms of an $SU(N_c)$ matrix v and a set of integers $\{n_\mu^j\}$ characterizing the plane waves.

We first recall that, see Equations (97) and (98),

$$\begin{aligned}\mathcal{E}_U[g] \,=\, \mathcal{E}_U[l] \quad &= \quad \mathcal{E}_{U,\Theta}[h] \\ &= \quad \frac{\Re\,\mathrm{Tr}}{N_c\,d}\sum_{\mu=1}^{d}\left\{\mathbb{1}\,-\,\left[\sum_{\vec{x}\in\Lambda_x} h(\vec{x})\,U_\mu(\vec{x})\,h^\dagger(\vec{x}+\hat{e}_\mu)\right]\frac{e^{-i\frac{\Theta_\mu}{N}}}{V}\right\}\end{aligned} \tag{130}$$

and that, when the matrices Θ_μ are written in the basis $\{\mathbf{W}^{ij} = w_i\,w_j^\dagger = v^\dagger\,\mathbf{M}^{ij}\,v\}$ introduced in Appendix A.2, we have, see Equation (A25),

$$e^{-i\frac{\Theta_\mu}{N}} \,=\, v^\dagger\,T_\mu(mN;\{n_\mu^j\})\,v, \tag{131}$$

where the diagonal matrix $T_\mu(mN;\{n_\mu^j\})$ has elements

$$T_\mu{}^{jj} \,\equiv\, \exp\left(-2\pi i\,\frac{n_\mu^j}{m\,N}\right). \tag{132}$$

Then, from the above equations it is evident that, when analyzing the consequences of the gauge-fixing condition, we have to treat differently the gauge transformations $h(\vec{x})$ and v, which depend on real parameters,[33] and the transformation $T(mN;\{n_\mu^j\})$, which is defined in terms of the integer parameters n_μ^j. In particular, the minimizing functional (130) is quadratic with respect to the matrix elements $h_{ij}(\vec{x})$ (see also Appendix C.3 in Ref. [31]) and v_{ij}, and has to satisfy the (also quadratic) constraints $h(\vec{x})\, h^\dagger(\vec{x}) = v\, v^\dagger = \mathbb{1}$. At the same time, $\mathcal{E}_{U,\Theta}[h]$ depends nonlinearly on the (integer) parameters n_μ^j, which are subject to the linear constraint (A32). Thus, the minimizing problem we are interested in is a mixed-integer nonlinear optimization problem, which can be formulated as [32]

$$\min_{x,n} f(x,n) \tag{133}$$

with

$$f : \left[\mathcal{R}^{d_r} \times \mathcal{Z}^{d_i} \right], \quad x \in \Omega_r \subset \mathcal{R}^{d_r}, \text{ and } n \in \Omega_i \subset \mathcal{Z}^{d_i}, \tag{134}$$

where the subsets Ω_r and Ω_i (respectively of dimensions d_r and d_i) are determined by the constraints imposed on the real variables x and on the integer variables n. It is important to stress that, in these cases, the determination of the global minimum is, in general, an NP-hard problem.

In order to obtain an explicit expression for the stationarity condition imposed by the minimization of $\mathcal{E}_{U,\Theta}[h]$, let us first examine the case in which the matrices Θ_μ are fixed. For this, we can repeat the analysis carried out in Section 2 and consider the gauge transformation $h(\vec{x}) \to R(\tau;\vec{x})\, h(\vec{x})$ with the one-parameter subgroup (7). Hence, we obtain, see Equation (130),

$$\begin{aligned} \mathcal{E}_{U,\Theta}[h]'(0) &= \frac{\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{b,\mu,\vec{x}} -i \left[\gamma^b(\vec{x})\, t^b\, U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} - e^{-i\frac{\Theta_\mu}{N}} U_\mu(h;\vec{x}) \gamma^b(\vec{x}+\hat{e}_\mu)\, t^b \right] \\ &= \frac{2\,\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{b,\mu,\vec{x}} \frac{\gamma^b(\vec{x})\, t^b}{2\, i} \left[U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} - e^{-i\frac{\Theta_\mu}{N}} U_\mu(h;\vec{x}-\hat{e}_\mu) \right], \end{aligned} \tag{135}$$

which should be compared to Equation (9). Here, as usual, $\vec{x} \in \Lambda_x$, the color index b takes values $1,\ldots,N_c^2-1$ and $\mu = 1,\ldots,d$. The above expression is also equal to

$$\frac{2\,\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{b,\mu,\vec{x}} \frac{\gamma^b(\vec{x})}{2\, i}\, e^{i \sum_\nu \frac{\Theta_\nu x_\nu}{N}} \left[t^b\, U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} - e^{-i\frac{\Theta_\mu}{N}} U_\mu(h;\vec{x}-\hat{e}_\mu) t^b \right] e^{-i \sum_\nu \frac{\Theta_\nu x_\nu}{N}}, \tag{136}$$

since the external factors $\exp\left(\pm i \sum_{\nu=1}^d \Theta_\nu\, x_\nu / N\right)$ are simplified by using the cyclicity of the trace. Then, the first derivative of the minimizing functional—with respect to $\{h(\vec{x})\}$ and considering fixed Θ_μ's—can be written in terms of the link variables $U_\mu(l;\vec{x})$, see Equation (120), as

$$\begin{aligned} \mathcal{E}_{U,\Theta}[h]'(0) &= \frac{2\,\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{b,\mu,\vec{x}} \frac{\gamma^b(\vec{x})}{2\, i} \left[\tilde{t}^{\,b}(\vec{x})\, U_\mu(l;\vec{x}) - U_\mu(l;\vec{x}-\hat{e}_\mu)\, \tilde{t}^{\,b}(\vec{x}) \right] \\ &= \frac{2\,\Re\, \mathrm{Tr}}{N_c\, d\, V} \sum_{b,\mu,\vec{x}} \frac{\gamma^b(\vec{x})\, \tilde{t}^{\,b}(\vec{x})}{2\, i} \left[U_\mu(l;\vec{x}) - U_\mu(l;\vec{x}-\hat{e}_\mu) \right], \end{aligned} \tag{137}$$

where we define the new set of Hermitian and traceless generators[34]

$$\tilde{t}^{\,b}(\vec{x}) \equiv \exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) t^b \exp\left(-i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right). \tag{138}$$

Now, we impose the stationarity condition $\mathcal{E}_{U,\Theta}[h]^{'}(0) = 0$, which must hold for any set of parameters $\gamma^b(\vec{x})$. Clearly, this means that, for each lattice site $\vec{x}$ and color index b, we have the condition

$$\Re\,\mathrm{Tr}\sum_{\mu=1}^{d}\frac{\tilde{t}^{\,b}(\vec{x})}{2\,i}\left[U_\mu(l;\vec{x})\;-\;U_\mu(l;\vec{x}-\hat{e}_\mu)\right]\;=\;0\,. \tag{139}$$

In analogy with Equations (10) and (23), let us define

$$A_\mu(l;\vec{x}) \;\equiv\; \frac{1}{2\,i}\left[U_\mu(l;\vec{x})\;-\;U_\mu^\dagger(l;\vec{x})\right]_{\text{traceless}} \tag{140}$$

$$=\; \frac{1}{2\,i}\left[U_\mu(l;\vec{x})-U_\mu^\dagger(l;\vec{x})\right]\;-\;\mathbb{1}\,\frac{\mathrm{Tr}}{2\,i\,N_c}\left[U_\mu(l;\vec{x})-U_\mu^\dagger(l;\vec{x})\right] \tag{141}$$

and

$$(\nabla\cdot A)(l;\vec{x})\;\equiv\;\sum_{\mu=1}^{d}\left[A_\mu(l;\vec{x})-A_\mu(l;\vec{x}-\hat{e}_\mu)\right]. \tag{142}$$

We can now write the minimization condition (139) above in terms of color components of the gauge-field gradient, using the site-dependent generators in Equation (138) as

$$\left(\nabla\cdot A^b\right)(l;\vec{x})\;=\;\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{(\nabla\cdot A)(l;\vec{x})}{2}\right]\;=\;0\qquad\forall\;\vec{x},b\quad, \tag{143}$$

by noting, see Equation (141), that

$$\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x})}{2}\right]=\mathrm{Tr}\left\{\tilde{t}^{\,b}(\vec{x})\left[\frac{U_\mu(l;\vec{x})\;-\;U_\mu^\dagger(l;\vec{x})}{4\,i}\right]\right\}=\Re\,\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{U_\mu(l;\vec{x})}{2\,i}\right] \tag{144}$$

and

$$\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x}-\hat{e}_\mu)}{2}\right]\;=\;\Re\,\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{U_\mu(l;\vec{x}-\hat{e}_\mu)}{2\,i}\right]. \tag{145}$$

Hence, the $\mathcal{N}_p = V\,(N_c^2-1)$ constraints needed to characterize the stationary point of $\mathcal{E}_{U,\Theta}[h](\tau)$, with respect to the gauge transformation $\{h(\vec{x})\}$—obtained in Equation (139) and rewritten in Equation (143)—may be interpreted as a transversality condition for the color components of the gauge-transformed gauge field $A_\mu(l;\vec{x})$ as will be defined below. Actually, as already mentioned, to implement these conditions in practice, it is convenient[35] to write the above expressions in terms of $U_\mu(h;\vec{x})$ and Θ_μ. We then get, from Equation (144),

$$\begin{aligned}\mathrm{Tr}\left[\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x})}{2}\right]\;&=\;\mathrm{Tr}\left\{\frac{t^b}{4\,i}\left[U_\mu(h;\vec{x})\,e^{-i\frac{\Theta_\mu}{N}}\;-\;e^{i\frac{\Theta_\mu}{N}}\,U_\mu^\dagger(h;\vec{x})\right]\right\}\\ &=\;\Re\,\mathrm{Tr}\left[t^b\,\frac{U_\mu(h;\vec{x})\,e^{-i\frac{\Theta_\mu}{N}}}{2i}\right],\end{aligned} \tag{146}$$

using Equation (120) and the definition (138). In like manner, see Equations (122) and (145), we have

$$\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x}-\hat{e}_\mu)}{2}\,\Big] \;=\; \mathrm{Tr}\left\{\frac{t^b}{4\,i}\Big[\,e^{-i\frac{\Theta_\mu}{N}}\,U_\mu(h;\vec{x}-\hat{e}_\mu)-U^\dagger_\mu(h;\vec{x}-\hat{e}_\mu)\,e^{i\frac{\Theta_\mu}{N}}\,\Big]\right\}$$
$$=\;\Re\,\mathrm{Tr}\left[\,t^b\,\frac{e^{-i\frac{\Theta_\mu}{N}}\,U_\mu(h;\vec{x}-\hat{e}_\mu)}{2\,i}\,\right]. \tag{147}$$

Notice that, contrary to Equations (144) and (145), the expressions on the r.h.s. of Equations (146) and (147) are written in terms of the original (site-independent) generators $\{t^b\}$ and involve only $U_\mu(h;\vec{x})$ and Θ_μ. They are the natural choice to be employed in a numerical simulation. Of course, the above connection between the expressions in terms of $\{\tilde{t}^{\,b}(\vec{x})\}$ and of $\{t^{\,b}\}$ can also be seen directly after rewriting Equation (143) as

$$0\;=\;\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{(\nabla\cdot A)(l;\vec{x})}{2}\,\Big]\;=\;\mathrm{Tr}\left[\,t^b\,\frac{e^{-i\sum_\nu\frac{\Theta_\nu x_\nu}{N}}(\nabla\cdot A)(l;\vec{x})\,e^{i\sum_\nu\frac{\Theta_\nu x_\nu}{N}}}{2}\,\right], \tag{148}$$

where the r.h.s. is in agreement with Equation (135), see also Equations (120) and (122).

Using the above results and in analogy with Section 2, we can define the color components of the gauge-transformed gauge field as

$$A^b_\mu(l;\vec{x})\;\equiv\;\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x})}{2}\,\Big]$$
$$=\;\Re\,\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{U_\mu(l;\vec{x})}{2\,i}\,\Big]\;=\;\Re\,\mathrm{Tr}\left[\,t^b\,\frac{U_\mu(h;\vec{x})\,e^{-i\frac{\Theta_\mu}{N}}}{2i}\,\right] \tag{149}$$

and

$$A^b_\mu(l;\vec{x}-\hat{e}_\mu)\;\equiv\;\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{A_\mu(l;\vec{x}-\hat{e}_\mu)}{2}\,\Big]\;=\;\Re\,\mathrm{Tr}\Big[\,\tilde{t}^{\,b}(\vec{x})\,\frac{U_\mu(l;\vec{x}-\hat{e}_\mu)}{2\,i}\,\Big]$$
$$=\;\Re\,\mathrm{Tr}\left[\,t^b\,\frac{e^{-i\frac{\Theta_\mu}{N}}\,U_\mu(h;\vec{x}-\hat{e}_\mu)}{2\,i}\,\right], \tag{150}$$

which imply the relations

$$A_\mu(l;\vec{x})\;=\;\sum_{b=1}^{N_c^2-1}A^b_\mu(l;\vec{x})\,\tilde{t}^{\,b}(\vec{x})\qquad\text{and}\qquad A_\mu(l;\vec{x}-\hat{e}_\mu)\;=\;\sum_{b=1}^{N_c^2-1}A^b_\mu(l;\vec{x}-\hat{e}_\mu)\,\tilde{t}^{\,b}(\vec{x}), \tag{151}$$

since $\{\tilde{t}^{\,b}(\vec{x})\}$ is a basis of the $su(N_c)$ Lie algebra. Then, Equation (143) can be written as

$$\sum_{\mu=1}^{d}\Big[A^b_\mu(l;\vec{x})-A^b_\mu(l;\vec{x}-\hat{e}_\mu)\Big]\;=\;0\qquad\forall\;\vec{x},b \tag{152}$$

and it is also equivalent to the transversality condition

$$(\nabla\cdot A)(l;\vec{x})\;=\;\sum_{\mu=1}^{d}\Big[A_\mu(l;\vec{x})-A_\mu(l;\vec{x}-\hat{e}_\mu)\Big]\;=\;0\qquad\forall\;\vec{x}\quad. \tag{153}$$

One should stress that the above expressions are valid only "locally", i.e., when evaluating the lattice divergence of the gauge field at site $\vec{x}$, and that they have to be modified accordingly when moving to the next site, e.g., when evaluating $\Big(\nabla \cdot A^b\Big)(l;\vec{x}+\hat{e}_\mu)$. In particular, we consider a new set of generators $\{\tilde{t}^b(\vec{x})\}$ for each site $\vec{x}$, where the divergence is evaluated, and these generators are used both to define $A^b_\mu(l;\vec{x})$ and $A^b_\mu(l;\vec{x}-\hat{e}_\mu)$, in terms of the matrices $U_\mu(l;\vec{x})$ and $U_\mu(l;\vec{x}-\hat{e}_\mu)$. Indeed, the lattice divergence is just a simple (backward) discretization of the usual continuum divergence and, when written explicitly for the color components of the gauge field, it should be based on the same generators at points $\vec{x}$ and $\vec{x}-\hat{e}_\mu$, namely $\{\tilde{t}^b(\vec{x})\}$. This is the origin of the different expressions obtained for the gauge field at site $\vec{x}$ and at site $\vec{x}-\hat{e}_\mu$—respectively Equations (144) and (145), or Equations (146) and (147)—considering that the generators $\tilde{t}^b(\vec{x})$ are defined as a function of $\vec{x}$, and that the generators t^b do not generally commute with the matrices Θ_μ. At the same time, note that the combination $U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}}$ or, equivalently, $e^{-i\frac{\Theta_\mu}{N}}\, U_\mu(h;\vec{x})$, also appears in the minimizing functional (96), which enforces the transversality condition on the lattice Λ_x but applied to this modified link configuration, see the comment below Equation (114).

Of course, as performed in Section 5, a more natural approach would be to consider an expansion in the basis $\{\mathbf{W}^{ij}\}$, which is constructed using the common eigenvectors of the matrices Θ_μ. Then the matrices Θ_μ are diagonal, see Equation (A24), and we obtain a unique definition of the gauge-field components at $\vec{x}$ and $\vec{x}-\hat{e}_\mu$. Here, however, we work with the color components in order to obtain expressions that can be easily compared with those presented in Section 2. Indeed, all the expressions above clearly reduce to the ones in Section 2 in the trivial case $\Theta_\mu = \mathbb{1}$ for all μ.

As for the minimization with respect to the matrices Θ_μ, it does not introduce any other constraint, even though—when varying the parameters v_{ij} and n^j_μ (see Equations (131) and (132))—we need to verify the inequalities imposed by the considered definition of local minimum, see Equations (133) and (134). This becomes evident if we consider the stationarity condition for the whole (extended) lattice Λ_z, i.e.,

$$\begin{aligned} 0 \;=\; (\nabla\cdot A)(g;\vec{z}) \;&=\; (\nabla\cdot A)(g;\vec{x}+\vec{y}N) \\ &=\; \sum_{\mu=1}^{d} A_\mu(g;\vec{x}+\vec{y}N) \;-\; A_\mu(g;\vec{x}+\vec{y}N-\hat{e}_\mu), \end{aligned} \tag{154}$$

which enforces the $\mathcal{N}_{p,m} = V m^d (N_c^2-1)$ constraints expected[36] from the minimization of $\mathcal{E}_U[g]$. At the same time, we know that

$$\begin{aligned} A_\mu(g;\vec{z}) \;&=\; A_\mu(g;\vec{x}+\vec{y}N) \\ &\equiv\; \frac{1}{2\,i}\Big[U_\mu(g;\vec{x}+\vec{y}N) - U^\dagger_\mu(g;\vec{x}+\vec{y}N)\Big]_{\text{traceless}} \qquad (155) \\ &=\; \exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right)\left[\frac{U_\mu(l;\vec{x}) - U^\dagger_\mu(l;\vec{x})}{2\,i}\right]_{\text{traceless}} \exp\left(-i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) \qquad (156) \\ &=\; \exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) A_\mu(l;\vec{x})\,\exp\left(-i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) \qquad (157) \end{aligned}$$

where we use Equations (119), (120) and (140), and similarly[37] for $A_\mu(g;\vec{z}-\hat{e}_\mu) = A_\mu(g;\vec{x}+\vec{y}N-\hat{e}_\mu)$. Hence, we find that

$$(\nabla\cdot A)(g;\vec{z}) \;=\; \exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right)\,(\nabla\cdot A)(l;\vec{x})\;\exp\left(-i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) \tag{158}$$

and it is evident that Equation (154) does not add any information to Equation (153).

In summary, the transversality condition for the lattice gauge field $A_\mu(g;\vec{z})$ defined in (155) is imposed by requiring the small-lattice field $A_\mu(l;\vec{x})$, defined in (140), to be transverse. This can be verified by using the expressions in Equations (143), (152) or (153).

4.2. The Limit $m \to +\infty$

We consider now the limit of m going to infinity, i.e., when the eigenvalues $\exp(2\pi i \bar{n}_\mu / m)$ of the matrices $\exp(i\Theta_\mu)$—with $\bar{n}_\mu = n_\mu \pmod{m} \in [0, m-1]$—can be written as $\exp(2\pi i \epsilon_\mu)$ with the real (continuous) parameters $\epsilon_\mu \equiv \bar{n}_\mu / m$ taking values in the interval $[0,1)$. Then, as noticed in Ref. [5], the minimization process imposes also the stationarity condition with respect to variation of the Θ_μ matrices. In this case, it is convenient to consider Equation (130) with the matrices Θ_μ written in terms of the Cartan generators $\{t^b_C\}$, as in Equation (94). Next, we can consider small variations of the parameters θ^b_μ, i.e., write the matrices

$$\Theta'_\mu = \sum_{b=1}^{N_c-1} t^b_C \left(\theta^b_\mu + \tau\, \eta^b_\mu \right) = \Theta_\mu + \tau \sum_{b=1}^{N_c-1} t^b_C\, \eta^b_\mu, \tag{159}$$

where η^b_μ are general parameters and τ is small, so that

$$e^{-i\frac{\Theta'_\mu}{N}} \approx e^{-i\frac{\Theta_\mu}{N}} \left(\mathbb{1} - i\,\frac{\tau}{N} \sum_{b=1}^{N_c-1} t^b_C\, \eta^b_\mu \right). \tag{160}$$

Hence, by imposing a null first variation of the minimizing functional with respect to τ, as above, we must have, see Equations (97) and (98),

$$0 = \frac{\Re\,\mathrm{Tr}}{N_c\, d} \sum_{\mu=1}^{d} \left[i\, Z_\mu(h)\, \frac{e^{-i\frac{\Theta_\mu}{N}}}{V\, N} \sum_{b=1}^{N_c-1} t^b_C\, \eta^b_\mu \right] = \frac{\Re\,\mathrm{Tr}}{N_c\, d\, N\, V} \sum_{\mu,b} t^b_C\, \eta^b_\mu \left[i\, Z_\mu(h)\, e^{-i\frac{\Theta_\mu}{N}} \right] \tag{161}$$

and we find

$$0 = \Re\,\mathrm{Tr} \left\{ t^b_C \left[i\, Z_\mu(h)\, e^{-i\frac{\Theta_\mu}{N}} \right] \right\} = \frac{1}{2}\, \mathrm{Tr} \left\{ i\, t^b_C \left[Z_\mu(h)\, e^{-i\frac{\Theta_\mu}{N}} - e^{i\frac{\Theta_\mu}{N}}\, Z^\dagger_\mu(h) \right] \right\} \tag{162}$$

for all μ and b since the equality must hold for any set of parameters $\{\eta^b_\mu\}$. Finally, using Equation (98) we obtain

$$0 = \mathrm{Tr} \left\{ \frac{t^b_C}{2i} \sum_{\vec{x} \in \Lambda_x} \left[U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} - e^{i\frac{\Theta_\mu}{N}}\, U^\dagger_\mu(h;\vec{x}) \right] \right\}, \tag{163}$$

which can be written as,[38] see Equation (146),

$$Q^b_\mu(l) \equiv \sum_{\vec{x} \in \Lambda_x} A^b_\mu(l;\vec{x}) = 0. \tag{164}$$

At the same time, we can define, see Equation (140),

$$Q_\mu(l) \equiv \sum_{\vec{x} \in \Lambda_x} A_\mu(l;\vec{x}) \tag{165}$$

so that

$$Q^b_\mu(l) = \frac{\mathrm{Tr}}{2} \left[t^b_C\, Q_\mu(l) \right], \tag{166}$$

where we use Equation (149) and the definition (138).

The above gauge-fixing condition tells us that the color components of the gauge field $A_\mu(l;\vec{x})$, corresponding to the generators t_C^b of the Cartan sub-algebra, have zero constant mode in the infinite-volume limit $m \to +\infty$, yielding

$$\sum_{b=1}^{N_c-1} Q_\mu^b(l)\, t_C^b \;=\; 0. \tag{167}$$

Then, using the result obtained at the end of Appendix A.2 of Appendix A, see Equations (A44)–(A46), which relates the coefficients m^i—in the expansion of a matrix M_C of the Cartan sub-algebra, such as the (null) expression in Equation (167), relative to the generators t_C^i—with its coefficients a^{jj} in the basis of the matrices $\mathbf{W}^{jj}$, we can also write, see Equation (164),

$$Q_\mu^{jj}(l) \;=\; \sum_{i=1}^{N_c-1} Q_\mu^i(j) \left[R^{ij}\,\xi^j \;-\; R^{i(j-1)}\,\xi^{j-1} \right] \;=\; 0 \tag{168}$$

for the coefficients $Q_\mu^{jj}(l)$ of $Q_\mu(l)$, which implies

$$\sum_{j=1}^{N_c} Q_\mu^{jj}(l)\, \mathbf{W}^{jj} \;=\; 0\,. \tag{169}$$

We will comment again on this outcome in Section 5.4. For the moment we only stress that the condition (164)—or (167) — is weaker than the one presented in Ref. [5], which, however, has been obtained considering the absolute minimum of the minimizing functional $\mathcal{E}_{U,\Theta}[h]$. Per contra, here we prefer to focus on a minimizing condition that can be verified in a numerical simulation, given that—in the general case—we have access only to the local minima of $\mathcal{E}_{U,\Theta}[h]$.

4.3. Convergence of the Numerical Minimization

The numerical convergence of a gauge-fixing algorithm can be checked, also when using the extended lattice Λ_z, by considering the three quantities defined in Equations (42)–(44). Moreover, as for the minimizing functional $\mathcal{E}_U[l] = \mathcal{E}_{U,\Theta}[h]$, they can be evaluated on the original lattice Λ_x, (essentially) without the need to consider the whole extended lattice Λ_z. For the quantity $\Delta\mathcal{E}$, this has already been proven in Equation (97). In the case of $(\nabla A)^2$ we can write, as in Equation (52),

$$\begin{aligned}
(\nabla A)^2 \;&\equiv\; \frac{\mathrm{Tr}}{2\,(N_c^2-1)\,m^d\,V} \sum_{\vec{z}\in\Lambda_z} \Big[(\nabla\cdot A)(g;\vec{z}) \Big]^2 \\
&=\; \frac{1}{m^d} \sum_{\vec{y}\in\Lambda_y} \left\{ \frac{\mathrm{Tr}}{2\,(N_c^2-1)\,V} \sum_{\vec{x}\in\Lambda_x} \Big[(\nabla\cdot A)(g;\vec{x}+\vec{y}N) \Big]^2 \right\}
\end{aligned} \tag{170}$$

and use the expression for $(\nabla\cdot A)(g;\vec{x}+\vec{y}N)$ reported in the previous section, see Equation (158). Then, due to the trace, it is clear that the exponential factors $\exp\left(\pm i \sum_{\nu=1}^d \Theta_\nu y_\nu\right)$ cancel for each site $\vec{x}$. In particular—after evaluating the trace—there is no dependence on the $\vec{y}$ coordinates in Equation (170) and we have

$$(\nabla A)^2 \;=\; \frac{\mathrm{Tr}}{2\,(N_c^2-1)\,V} \sum_{\vec{x}\in\Lambda_x} \Big[(\nabla\cdot A)(l;\vec{x}) \Big]^2 \;=\; \frac{1}{(N_c^2-1)\,V} \sum_{\vec{x}\in\Lambda_x} \sum_{b=1}^{N_c^2-1} \Big[\Big(\nabla\cdot A^b\Big)(l;\vec{x}) \Big]^2, \tag{171}$$

with $\left(\nabla \cdot A^b\right)(l;\vec{x})$ defined in Section 4.1. The above result is, of course, expected since the gauge-fixed gauge configuration $\{A_\mu(l;\vec{x})\}$ is transverse on each replicated lattice, for any lattice site $\vec{x}$.

Finally, see Equations (44) and (53), for the quantity

$$\begin{aligned}
\Sigma_Q &= \frac{1}{mN} \sum_{\mu=1}^{d} \sum_{b=1}^{N_c^2-1} \sum_{z_\mu=1}^{mN} \left[Q_\mu^b(g;z_\mu) - \widehat{Q}_\mu^b(g) \right]^2 \Big/ \sum_{\mu=1}^{d} \sum_{b=1}^{N_c^2-1} \left[\widehat{Q}_\mu^b(g) \right]^2 \\
&= \frac{1}{mN} \sum_{\mu=1}^{d} \sum_{z_\mu=1}^{mN} \mathrm{Tr} \left[Q_\mu(g;z_\mu) - \widehat{Q}_\mu(g) \right]^2 \Big/ \sum_{\mu=1}^{d} \mathrm{Tr} \left[\widehat{Q}_\mu(g) \right]^2 ,
\end{aligned} \tag{172}$$

we define

$$Q_\mu^b(g;z_\mu) \equiv \sum_{\substack{z_\nu \\ \nu\neq\mu}} A_\mu^b(g;\vec{z}) \qquad \text{and} \qquad \widehat{Q}_\mu^b(g) \equiv \frac{1}{mN} \sum_{z_\mu=1}^{mN} Q_\mu^b(g;z_\mu), \tag{173}$$

in analogy with Section 2.1. On the other hand, similarly to Equation (15), we can write

$$Q_\mu^b(g;z_\mu) = \Re \, \mathrm{Tr} \sum_{\substack{z_\nu \\ \nu\neq\mu}} \frac{U_\mu(g;\vec{z})\, t^b}{2\,i} \tag{174}$$

so that we can use the expression

$$Q_\mu^b(g;z_\mu) = \Re \, \mathrm{Tr} \left[\frac{Q_\mu(g;z_\mu)\, t^b}{2\,i} \right] \tag{175}$$

with, see Equation (119),

$$Q_\mu(g;z_\mu = x_\mu + N y_\mu) = \sum_{\substack{z_\nu \\ \nu\neq\mu}} U_\mu(g;\vec{z}) = \sum_{\substack{y_\nu=1,m \\ \nu\neq\mu}} \exp\left(i \sum_{\rho=1}^{d} \Theta_\rho \, y_\rho \right) Q_\mu(l;x_\mu) \exp\left(-i \sum_{\rho=1}^{d} \Theta_\rho \, y_\rho \right) \tag{176}$$

and

$$Q_\mu(l;x_\mu) \equiv \sum_{\substack{x_\nu=1,N \\ \nu\neq\mu}} U_\mu(l;\vec{x}). \tag{177}$$

Then, it is evident from the above equations that, in the evaluation of Σ_Q, we do not need a full loop over the extended lattice Λ_z, but it suffices to consider a loop over Λ_x (see the last equation), followed by a loop over Λ_y, see the r.h.s. of Equation (176). Thus, the computational cost is still of order V (if $m^d \lesssim V$). Let us stress that the quantities $Q_\mu(l;x_\mu)$ are not constant on Λ_x since the transverse gauge-fixed link configuration $\{U_\mu(l;\vec{x})\}$ is nonperiodic and, therefore, when repeating the steps in Equation (47), the second term is different from zero, see also Equations (48) and (49). As a consequence, we cannot expect to write Σ_Q by averaging only over the fluctuations $\left[Q_\mu^b(l;x_\mu) - \widehat{Q}_\mu^b(l)\right]^2$, where

$$Q_\mu^b(l;x_\mu) \equiv \sum_{\substack{x_\nu \\ \nu\neq\mu}} A_\mu^b(l;\vec{x}) \qquad \text{and} \qquad \widehat{Q}_\mu^b(l) \equiv \frac{1}{N} \sum_{x_\mu=1}^{N} Q_\mu^b(l;x_\mu). \tag{178}$$

On the contrary, the quantities $Q_\mu^b(g;z_\mu)$ in Equation (175) are independent of z_μ since $U_\mu(g;\vec{z})$ is periodic in Λ_z and the gauge field $A_\mu(g;\vec{z})$ is transverse. Therefore, for the evaluation of Σ_Q, we need to consider the global rotations $\exp\left(i \sum_{\rho=1}^{d} \Theta_\rho y_\rho\right)$, on each replicated lattice $\Lambda_x^{(\vec{y})}$, see Equation (176), and we cannot avoid the double sum, i.e., the sum over the y_ν coordinates in Equation (176) and the sum over the x_ν coordinates in Equation (177).

5. Link Variables in Momentum Space and the Gluon Propagator

The formulae discussed in Section 2.2 for the gluon propagator in momentum space $D(\vec{k})$—when the usual lattice Λ_x is considered—clearly apply also to the case of the extended lattice Λ_z, simply by exchanging the sum over $\vec{x} \in \Lambda_x$ with the sum over $\vec{z} \in \Lambda_z$ and, correspondingly, the sum over $\vec{k} \in \widetilde{\Lambda}_x$ with the sum over $\vec{k}' \in \widetilde{\Lambda}_z$, i.e., the wave-number vectors have now components $k'_\mu = 0, 1, \ldots, mN-1$ (when restricted to the first Brillouin zone). However, in order to understand the impact of the extended lattice on the evaluation of the gluon propagator (see Section 5.4 below), it is useful to first evaluate the Fourier transform

$$\widetilde{U}_\mu(g;\vec{k}') \equiv \sum_{\vec{z}\in\Lambda_z} U_\mu(g;\vec{z}) \exp\left[-\frac{2\pi i}{m\,N}\left(\vec{k}'\cdot\vec{z}\right)\right] \tag{179}$$

of $U_\mu(g;\vec{z})$, for $\mu = 1, \ldots, d$. Notice that this definition is based on the extended lattice, differing from the small-lattice definition (25) in the range of the sum and in the exponential factor. Also, it is natural to consider the coefficients[39]

$$U_\mu^{ij}(g;\vec{z}) \equiv w_i^\dagger\, U_\mu(g;\vec{z})\, w_j \qquad\qquad (\text{with} \quad i,j = 1,2,\ldots,N_c) \tag{181}$$

in the basis of the common eigenvectors w_j of the Cartan generators and of the matrices Θ_μ, see Equations (A21), (A29) and (A30). More exactly, we use

$$\exp\left(-i\,\Theta_\mu\right) w_j = \exp\left[-\frac{2\pi i}{m}\, n_\mu^j\right] w_j \tag{182}$$

as well as

$$w_i^\dagger \exp\left(i\,\Theta_\mu\right) = w_i^\dagger \exp\left[\frac{2\pi i}{m}\, n_\mu^i\right], \tag{183}$$

and find, see also Equations (75) and (119),

$$\begin{aligned} U_\mu^{ij}(g;\vec{z}) &= w_i^\dagger \exp\left(i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) U_\mu(l;\vec{x}) \exp\left(-i\sum_{\nu=1}^{d}\Theta_\nu\, y_\nu\right) w_j \\ &= \exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(n_\nu^j - n_\nu^i\right) y_\nu\right] w_i^\dagger\, U_\mu(l;\vec{x})\, w_j \\ &\equiv \exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(n_\nu^j - n_\nu^i\right) y_\nu\right] U_\mu^{ij}(l;\vec{x}) \end{aligned} \tag{184}$$

where, recalling Equation (120) and that the Θ_μ's commute with each other,

$$\begin{aligned} U_\mu^{ij}(l;\vec{x}) &= w_i^\dagger \exp\left(i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) U_\mu(h;\vec{x}) \exp\left(-i\,\frac{\Theta_\mu}{N} - i\sum_{\nu=1}^{d}\frac{\Theta_\nu\, x_\nu}{N}\right) w_j \\ &= \exp\left\{-\frac{2\pi i}{m\,N}\left[\sum_{\nu=1}^{d}\left(n_\nu^j - n_\nu^i\right) x_\nu + n_\mu^j\right]\right\} w_i^\dagger\, U_\mu(h;\vec{x})\, w_j \\ &= \exp\left\{-\frac{2\pi i}{m\,N}\left[\sum_{\nu=1}^{d}\left(n_\nu^j - n_\nu^i\right) x_\nu + n_\mu^j\right]\right\} U_\mu^{ij}(h;\vec{x}). \end{aligned} \tag{185}$$

Then, we obtain

$$\widetilde{U}^{ij}_\mu(g;\vec{k}') \equiv w_i^\dagger\, \widetilde{U}_\mu(g;\vec{k}')\, w_j \tag{186}$$

$$= \sum_{\vec{z}\in\Lambda_z} U^{ij}_\mu(g;\vec{z}) \exp\left[-\frac{2\pi i}{m\,N}\left(\vec{k}'\cdot\vec{z}\right)\right] \tag{187}$$

$$= \widetilde{U}^{ij}_\mu\left(l;\frac{\vec{k}'}{m}\right) \sum_{\vec{y}\in\Lambda_y} \exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(k'_\nu + n^j_\nu - n^i_\nu\right) y_\nu\right] \tag{188}$$

$$= \widetilde{U}^{ij}_\mu\left(l;\frac{\vec{k}'}{m}\right) \prod_{\nu=1}^{d}\left\{\sum_{y_\nu=0}^{m-1} \exp\left[-\frac{2\pi i}{m}\left(k'_\nu + n^j_\nu - n^i_\nu\right) y_\nu\right]\right\}, \tag{189}$$

where we use Equations (179) and (184). We also introduce the coefficients of the Fourier transform $\widetilde{U}_\mu(l;\vec{k}'/m)$ of the matrix $U_\mu(l;\vec{x})$ on the Λ_x lattice, see Equation (25), given by

$$\widetilde{U}^{ij}_\mu\left(l;\frac{\vec{k}'}{m}\right) = \sum_{\vec{x}\in\Lambda_x} U^{ij}_\mu(l;\vec{x}) \exp\left[-\frac{2\pi i}{m\,N}\left(\vec{k}'\cdot\vec{x}\right)\right]$$

$$= \sum_{\vec{x}\in\Lambda_x} U^{ij}_\mu(h;\vec{x}) \exp\left\{-\frac{2\pi i}{m\,N}\left[\sum_{\nu=1}^{d}\left(k'_\nu + n^j_\nu - n^i_\nu\right) x_\nu + n^j_\mu\right]\right\}, \tag{190}$$

where we make use of the expression (185). Thus, from Equations (27) and (189), we find that $\widetilde{U}^{ij}_\mu(g;\vec{k}')$ is zero unless the quantity $k'_\nu + n^j_\nu - n^i_\nu$ is a multiple of m, for every direction ν, and in this case we have

$$\widetilde{U}^{ij}_\mu(g;\vec{k}') = m^d\, \widetilde{U}^{ij}_\mu\left(l;\frac{\vec{k}'}{m}\right). \tag{191}$$

In order to better understand the above result, we note that the integers k'_ν can be written as

$$k'_\nu = k_\nu + K_\nu\, m, \tag{192}$$

where $k_\nu \in [0, m-1]$ and $K_\nu \in \mathcal{Z}$. This is the decomposition we choose for representing the wave numbers of the Fourier momenta on the extended lattice for the gauge-fixing problem, as explained at the beginning of Section 3.2, and it is completely analogous to the one introduced for the crystalline-solid problem in Section 3.1. In particular, for $\vec{k}'$ in the first Brillouin zone, corresponding to $k'_\nu \in [0, mN-1]$, we have K_ν in the interval $[0, N-1]$.[40] Indeed, this implies that the vector with components $2\pi k'_\nu/(mN)$ becomes the sum of two terms, $2\pi k_\nu/(mN)$ and $2\pi K_\nu/N$, with the latter one—corresponding to $2\pi\vec{K}/N$ (with $K_\nu = 0, 1, \ldots, N-1$)—belonging to the reciprocal lattice since $\exp\left(2\pi i\,\vec{K}\cdot\vec{R}/N\right) = 1$ for any translation vector $\vec{R} = N\vec{y} = N\sum_{\mu=1}^{d} y_\mu \hat{e}_\mu$. At the same time, the former one—i.e., $2\pi\vec{k}/(mN)$ (with $k_\nu = 0, 1, \ldots, m-1$)—is generated by the translation operator $\mathcal{T}$. In fact, as already noted in Section 3.3, the coefficients $g^{ij}(\vec{z})$ of $g(\vec{z})$ in the $\mathbf{W}^{ij}$ basis become multiplied by the phase $\exp\left(2\pi i n^i_\mu/m\right)$ under a translation by $\vec{R} = N\hat{e}_\mu$, see Equation (109), in agreement with the above observation if we identify k_μ with n^i_μ.

The same observation applies to the integers[41] n^j_ν and n^i_ν such that we can write

$$n^j_\nu \equiv \bar{n}^j_\nu + m\,\widetilde{n}^j_\nu, \tag{193}$$

with $\bar{n}^j_\mu \in [0, m-1]$ and $\widetilde{n}^j_\nu \in \mathcal{Z}$ (and similarly for n^i_ν). This implies that the quantity

$$\chi_\nu \;\equiv\; k_\nu \,+\, \bar{n}^j_\nu \,-\, \bar{n}^i_\nu \;=\; \mathrm{mod}\big(k'_\nu,\, m\big) \,+\, \mathrm{mod}\Big(n^j_\nu \,-\, n^i_\nu,\, m\Big), \tag{194}$$

where the difference $\bar{n}^j_\nu - \bar{n}^i_\nu$ is a fixed integer in the interval $[-m+1, m-1]$, must be an integer multiple of m, in order to produce a nonzero value in Equation (189). Therefore, since k_ν is non-negative and smaller than m, we may have[42]

$$\chi_\nu \;=\; \begin{cases} 0 & \text{if } \bar{n}^j_\nu - \bar{n}^i_\nu \le 0, \\ m & \text{if } \bar{n}^j_\nu - \bar{n}^i_\nu \text{ is positive}. \end{cases} \tag{196}$$

Clearly, in both cases there is only one value of $k_\nu \;=\; \chi_\nu - (\bar{n}^j_\nu - \bar{n}^i_\nu)$ that makes $k'_\nu + n^j_\nu - n^i_\nu$ an integer multiple of m, i.e., such that

$$k'_\nu \,+\, n^j_\nu \,-\, n^i_\nu \;=\; m\left(K_\nu \,+\, \frac{\chi_\nu}{m} \,+\, \widetilde{n}^j_\nu \,-\, \widetilde{n}^i_\nu\right), \tag{197}$$

with χ_ν / m equal to 0 or 1. It is also evident that, for any direction ν, this result does not depend on the value of K_ν and we have, for any given vector $\vec{K}$, a set of nonzero coefficients. In this sense, for the purpose of determining which coefficients $\widetilde{U}^{ij}_\mu(g;\vec{k}')$ are nonzero, see Equation (189), we can think of χ_ν as a "function" of $\bar{n}^j_\nu - \bar{n}^i_\nu$ as detailed above (see also note 42), in such a way that momenta $\vec{k}' \,=\, \vec{k} + m\vec{K}$ corresponding to nonzero coefficients will have general $\vec{K}$ and specific combinations for $\vec{k}$, determined from (194). Thus, if we define

$$\widetilde{U}^{ij}_\mu\left(l;\, \frac{\vec{k}'}{m}\right) \;\equiv\; \widetilde{U}^{ij}_\mu(l;\vec{k},\vec{K}), \tag{198}$$

we can collect these nonzero coefficients—with different values of $\vec{k}$—in families indexed by the vectors $\vec{K}$. Finally, when the relation (197) is satisfied (for any direction ν—with a suitable choice for k'_ν—and with $\chi_\nu / m = 0, 1$) we can write, see Equation (190),

$$\widetilde{U}^{ij}_\mu\left(l;\, \frac{\vec{k}'}{m}\right) \;=\; \exp\left(-\frac{2\pi i\, n^j_\mu}{m\, N}\right) \sum_{\vec{x}\in\Lambda_x} U^{ij}_\mu(h;\vec{x})\, \exp\left[-\frac{2\pi i}{N}\, \sum_{\nu=1}^{d}\left(K_\nu \,+\, \frac{\chi_\nu}{m} \,+\, \widetilde{n}^j_\nu \,-\, \widetilde{n}^i_\nu\right)x_\nu\right]. \tag{199}$$

Thus, considering the above result and Equation (191), we see that, if the Fourier transform $\widetilde{U}_\mu(g;\vec{k}')$ of the link variables on the extended lattice Λ_z, evaluated for the wave-number vector $\vec{k}'$, is nonzero, i.e., if Equation (197) is verified, then its evaluation is always reduced to a Fourier transform on the original lattice Λ_x for a modified wave-number vector, with components $K_\nu + \chi_\nu / m + \widetilde{n}^j_\nu - \widetilde{n}^i_\nu$. It is important to stress again that—while we can choose $\vec{K}$ freely—the vector $\vec{\chi}$ depends on the considered indices i and j of the coefficients.

5.1. The Diagonal Elements

The results obtained in the previous section greatly simplify when[43] $i = j$, i.e., when $n^j_\nu - n^i_\nu = 0$, so that the coefficients $\widetilde{U}^{jj}_\mu(g;\vec{k}')$ are nonzero for, see Equation (194),

$$\chi_\nu \;=\; k_\nu \;=\; 0, \tag{200}$$

yielding $k'_\nu = 0,\, m,\, 2m,\, \ldots,\, (N-1)\, m = K_\nu\, m$. Then, we find, see Equation (199),

$$\widetilde{U}^{jj}_\mu\left(l;\, \frac{\vec{k}'}{m}\right) = \exp\left(-\frac{2\pi i\, n^j_\mu}{m\, N}\right) \sum_{\vec{x}\in\Lambda_x} U^{jj}_\mu(h;\vec{x})\, \exp\left(-\frac{2\pi i}{N}\vec{K}\cdot\vec{x}\right) = \exp\left(-\frac{2\pi i\, n^j_\mu}{m\, N}\right) \widetilde{U}^{jj}_\mu(h;\vec{K}), \tag{201}$$

where

$$\widetilde{U}^{jj}_{\mu}(h;\vec{K}) \equiv \sum_{\vec{x}\in\Lambda_x} U^{jj}_{\mu}(h;\vec{x}) \exp\left[-\frac{2\pi i}{N}\left(\vec{K}\cdot\vec{x}\right)\right] \tag{202}$$

is the usual Fourier transform[44] (on the original lattice Λ_x) of $U^{jj}_{\mu}(h;\vec{x})$, see Equation (25). At the same time, the components of the lattice momenta are given by

$$p_{\nu}(\vec{k}') \equiv 2 \sin\left(\frac{\pi k'_{\nu}}{mN}\right) = 2 \sin\left(\frac{\pi K_{\nu}}{N}\right), \tag{203}$$

i.e., they coincide exactly[45] with the values allowed on the original Λ_x lattice, see Equation (32) with k_{ν} substituted by K_{ν}.

One should also note that the case $i = j$ is the only one relevant for the evaluation of the minimizing functional—see (in this order) Equations (128), (A29), (A26), (190) and (202)—since

$$\begin{aligned}\mathcal{E}_U[l] &= 1 - \frac{\Re\,\mathrm{Tr}}{N_c\, d\, V}\sum_{\mu,\vec{x}} U_{\mu}(l;\vec{x}) = 1 - \frac{\Re\,\mathrm{Tr}}{N_c\, d\, V}\sum_{\mu,\vec{x}}\sum_{i,j=1}^{N_c} U^{ij}_{\mu}(l;\vec{x})\,\mathbf{W}^{ij} \\ &= 1 - \sum_{\mu,\vec{x}}\sum_{j=1}^{N_c}\frac{\Re\, U^{jj}_{\mu}(l;\vec{x})}{N_c\, d\, V} = 1 - \frac{\Re}{N_c\, d\, V}\sum_{\mu}\sum_{j=1}^{N_c}\exp\left(-\frac{2\pi i\, n^j_{\mu}}{m\,N}\right)\widetilde{U}^{jj}_{\mu}(h;\vec{0}),\end{aligned} \tag{205}$$

where $\mu = 1,\dots,d$ and $\vec{x} \in \Lambda_x$.

5.2. Fixed Wave-Number Vectors

The above results clarify for which values of $\vec{k}'$ a given coefficient $\widetilde{U}^{ij}_{\mu}(g;\vec{k}')$ is nonzero. Now we can invert the question and try to understand which coefficients are nonzero for a given (chosen) momentum $\vec{k}'$. Indeed, note that, in a numerical evaluation of the gluon propagator using lattice simulations, the considered momenta $\vec{k}'$ are usually fixed a priori. The integers n^i_{ν}, on the other hand, will be selected to minimize the functional $\mathcal{E}_U[l]$ and we can analyze which combinations are expected to produce a nonzero value for the propagator. For example, if (at least) one component k'_{ν} of $\vec{k}'$ is equal to zero, it is evident that only the diagonal elements (i.e., $i = j$) are usually different from zero, given that the factor, see Equation (189),

$$\sum_{y_{\nu}=0}^{m-1} \exp\left[-\frac{2\pi i}{m}\left(n^j_{\nu} - n^i_{\nu}\right) y_{\nu}\right] = \sum_{y_{\nu}=0}^{m-1} \exp\left[-\frac{2\pi i}{m}\left(\bar{n}^j_{\nu} - \bar{n}^i_{\nu}\right) y_{\nu}\right] \tag{206}$$

is always equal to zero for $i \neq j$, unless[46] $\bar{n}^i_{\nu} = \bar{n}^j_{\nu}$, see again Equation (26). This result is even stronger when $k'_{\nu} = 0$ for more than one direction, i.e., it would be even more unlikely in this case to have a nonzero coefficient when $i \neq j$. Thus, when evaluating the zero-momentum gluon propagator, one should recall that, except in a fortuitous event with $\bar{n}^i_{\nu} = \bar{n}^j_{\nu}$ for all $\nu = 1,\dots,d$, when $i \neq j$, usually the only nonzero coefficients of the zero-momentum link variables are the diagonal ones (i.e., $i = j$), given by, see Equations (191) and (201) with $\vec{K} = \vec{0}$,

$$\widetilde{U}^{jj}_{\mu}(g;\vec{0}') = m^d \exp\left(-\frac{2\pi i\, n^j_{\mu}}{m\,N}\right)\widetilde{U}^{jj}_{\mu}(h;\vec{0}). \tag{207}$$

For the same reason, if the vector $\vec{k}'$ has (for example) all equal components, i.e.,

$$k'_{\nu} = k + K\,m \qquad\qquad \text{for } \nu = 1,2,\dots,d, \tag{208}$$

where k and K are fixed integers with values (respectively) in $[0, m-1]$ and $[0, N-1]$, then a nondiagonal coefficient $\widetilde{U}^{ij}_{\mu}(g;\vec{k}')$ (with $i \neq j$) could be nonzero only in the unlikely event that, for all $\nu = 1, \ldots, d$, the differences $\bar{n}^j_\nu - \bar{n}^i_\nu$ are either equal to $-k$ or to $m-k$ so that the value of $\chi_\nu = k_\nu + \bar{n}^j_\nu - \bar{n}^i_\nu = k + \bar{n}^j_\nu - \bar{n}^i_\nu$, see Equation (196), is either 0 or m for all directions ν. On the other hand, as seen in the previous section, all the diagonal elements are (always) different from zero for $k'_\nu = K\,m$ (i.e., $k = 0$) since the factors in Equation (189) become

$$\sum_{y_\nu=0}^{m-1} \exp\left(-\frac{2\pi i}{m}\,k'_\nu\,y_\nu\right) \;=\; \sum_{y_\nu=0}^{m-1} \exp\left(-2\pi i\,K_\nu\,y_\nu\right) \;=\; m. \tag{209}$$

5.3. Gauge Field in Momentum Space

We can now apply the outcomes obtained in the previous section to the evaluation of the gauge field, given in terms of the gauge-transformed gauge link, see Equations (10) and (140), as

$$\begin{aligned} A_\mu(g;\vec{z}) \;&\equiv\; \frac{1}{2\,i}\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right]_{\text{traceless}} \\ &=\; \frac{1}{2\,i}\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right] \;-\; \mathbb{1}\,\frac{\text{Tr}}{N_c}\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right] \end{aligned} \tag{210}$$

or of its coefficients $A^{ij}_\mu(g;\vec{z})$, in momentum space. As a first step, we need to consider how Equations (186)–(190) become modified when evaluating the Fourier transform of the coefficients,[47] see, for example, Equation (A30),

$$\left[U^\dagger_\mu(g;\vec{z})\right]^{ij} \;=\; w^\dagger_i\,U^\dagger_\mu(g;\vec{z})\,w_j \;=\; \left[w^\dagger_j\,U_\mu(g;\vec{z})\,w_i\right]^* \;=\; \left[U^{ji}_\mu(g;\vec{z})\right]^*. \tag{211}$$

In particular, using Equation (184) we can write

$$\left[U^\dagger_\mu(g;\vec{z})\right]^{ij} \;=\; \exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(n^j_\nu - n^i_\nu\right)y_\nu\right]\left[U^{ji}_\mu(l;\vec{x})\right]^*, \tag{212}$$

with, see Equation (185),

$$\left[U^{ji}_\mu(l;\vec{x})\right]^* \;=\; \exp\left\{-\frac{2\pi i}{m\,N}\left[\sum_{\nu=1}^{d}\left(n^j_\nu - n^i_\nu\right)x_\nu \;-\; n^i_\mu\right]\right\}\left[U^{ji}_\mu(h;\vec{x})\right]^*. \tag{213}$$

Then, the difference

$$\left[U_\mu(g;\vec{z}) \;-\; U^\dagger_\mu(g;\vec{z})\right]^{ij} \tag{214}$$

is simply given, see Equations (184) and (212), by

$$\exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(n^j_\nu - n^i_\nu\right)y_\nu\right]\left[U^{ij}_\mu(l;\vec{x}) \;-\; U^{ji}_\mu(l;\vec{x})^*\right]. \tag{215}$$

Thus, if we write, in analogy with Equation (24),

$$\widetilde{A}_\mu(g;\vec{k}') \;\equiv\; \sum_{\vec{z}\in\Lambda_z} A_\mu(g;\vec{z})\,\exp\left[-\frac{2\pi i}{m\,N}\left(\vec{k}'\cdot\vec{z} \;+\; \frac{k'_\mu}{2}\right)\right], \tag{216}$$

and similarly for the coefficients $\widetilde{A}^{ij}_\mu(g;\vec{k}')$, we find that, see Equations (188), (210), (215) and (A30),

$$\widetilde{A}^{ij}_\mu(g;\vec{k}') = \sum_{\vec{z}\in\Lambda_z} \frac{\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right]^{ij} - \delta^{ij}\frac{\mathrm{Tr}}{N_c}\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right]}{2i}\, e^{-\frac{2\pi i}{mN}\left(\vec{k}'\vec{z} + \frac{k'_\mu}{2}\right)}$$
$$\propto \sum_{\vec{y}\in\Lambda_y} \exp\left[-\frac{2\pi i}{m}\sum_{\nu=1}^{d}\left(k'_\nu + n^j_\nu - n^i_\nu\right) y_\nu\right], \tag{217}$$

which is again null, see Equation (197), unless the relation

$$k'_\nu + n^j_\nu - n^i_\nu = m\left(K_\nu + \frac{\chi_\nu}{m} + \widetilde{n}^j_\nu - \widetilde{n}^i_\nu\right) \tag{218}$$

is verified (for every direction ν) with $\chi_\nu/m = 0, 1$ determined by $\bar{n}^j_\nu - \bar{n}^i_\nu$, see Equation (195). In this case, the r.h.s. in Equation (217) is equal to m^d. Here we use the fact that the trace term is multiplied by the identity, see Equation (210), which has coefficients δ^{ij}. Also note that we are writing the gauge field in momentum space as a linear combination of the $(N_c \times N_c)$ matrices $\mathbf{W}^{ij} = w_i\, w^\dagger_j$ (with $i, j = 1, \ldots, N_c$) and that $\mathrm{Tr}\left(w_i\, w^\dagger_j\right) = \delta^{ij}$, see Equation (A26). Also, as detailed below, the trace term does not depend on $\vec{y}$, in agreement with the overall exponential factor in (217).

As for the second factor in Equation (215), it is equal to

$$\exp\left[-\frac{2\pi i}{m\,N}\sum_{\nu=1}^{d}\left(n^j_\nu - n^i_\nu\right)x_\nu\right]\left[e^{-\frac{2\pi i n^j_\mu}{mN}}\, U^{ij}_\mu(h;\vec{x}) - e^{\frac{2\pi i\, n^i_\mu}{mN}}\, U^{ji}_\mu(h;\vec{x})^*\right], \tag{219}$$

where we use Equations (185) and (213). At the same time, for the trace term in (210) and (217) we have, see Equations (119) and (120),

$$\frac{1}{2i}\,\mathrm{Tr}\left[U_\mu(g;\vec{z}) - U^\dagger_\mu(g;\vec{z})\right] = \frac{1}{2i}\,\mathrm{Tr}\left[U_\mu(l;\vec{x}) - U^\dagger_\mu(l;\vec{x})\right]$$
$$= \frac{1}{2i}\,\mathrm{Tr}\left[U_\mu(h;\vec{x})\, e^{-i\frac{\Theta_\mu}{N}} - e^{i\frac{\Theta_\mu}{N}}\, U^\dagger_\mu(h;\vec{x})\right]. \tag{220}$$

Hence, noting again $\mathrm{Tr}\left(\mathbf{W}^{ij}\right) = \delta^{ij}$, the above trace can be written as

$$\sum_{j=1}^{N_c}\frac{1}{2i}\left[U^{jj}_\mu(h;\vec{x})\, e^{-\frac{2\pi i n^j_\mu}{mN}} - e^{\frac{2\pi i n^j_\mu}{mN}}\, U^{jj}_\mu(h;\vec{x})^*\right] = \sum_{j=1}^{N_c}\Im\left[U^{jj}_\mu(h;\vec{x})\exp\left(\frac{-2\pi i\, n^j_\mu}{mN}\right)\right], \tag{221}$$

which can also be obtained by summing Equation (219) for $j = i$ and dividing the result by $2\,i$. This yields

$$A^{ij}_\mu(l;\vec{x}) = w^\dagger_i\, A_\mu(l;\vec{x})\, w_j = w^\dagger_i\, \frac{1}{2\,i}\left[U_\mu(l;\vec{x}) - U^\dagger_\mu(l;\vec{x})\right]_{\mathrm{traceless}} w_j$$
$$= \exp\left[-\frac{2\pi i}{mN}\sum_{\nu=1}^{d}(n^j_\nu - n^i_\nu)\, x_\nu\right]\left\{\frac{1}{2i}\left[U^{ij}_\mu(h;\vec{x})\, e^{-\frac{2\pi i n^j_\mu}{mN}}\right.\right.$$
$$\left.\left. - e^{\frac{2\pi i n^i_\mu}{mN}}\, U^{ji}_\mu(h;\vec{x})^*\right] - \frac{\delta^{ij}}{N_c}\sum_{l=1}^{N_c}\Im\left[U^{ll}_\mu(h;\vec{x})\, e^{\frac{-2\pi i n^l_\mu}{mN}}\right]\right\} \tag{222}$$

where we use Equations (219) and (221). Then, by recalling Equation (157), it is evident that the coefficient of proportionality in Equation (217) is given by

$$\widetilde{A}^{ij}_{\mu}\left(l; \frac{\vec{k}'}{m}\right) = \sum_{\vec{x}\in\Lambda_x} \exp\left[-\frac{2\pi i}{mN}\,\vec{k}'\cdot\left(\vec{x}+\frac{\hat{e}_{\mu}}{2}\right)\right] A^{ij}_{\mu}(l;\vec{x}), \tag{223}$$

which is the usual small-lattice definition of the Fourier transform of $A^{ij}_{\mu}(l;\vec{x})$, i.e., Equation (24), for the wave-number vector $\vec{k}'/m$. By collecting the above results, we end up with the expression[48]

$$\widetilde{A}^{ij}_{\mu}(g;\vec{k}') = m^d\,\widetilde{A}^{ij}_{\mu}\left(l; \frac{\vec{k}'}{m}\right) = m^d \sum_{\vec{x}\in\Lambda_x} e^{-\frac{2\pi i}{N}\left(\frac{\vec{k}'}{m}\right)\cdot\left(\vec{x}+\frac{\hat{e}_{\mu}}{2}\right)} A^{ij}_{\mu}(l;\vec{x}). \tag{225}$$

Therefore, besides the factor m^d and the modified wave-number vector $\vec{k}'/m$ with components, see Equations (193) and (218),

$$k'_{\mu} = m\left(K_{\mu} + \frac{\chi_{\mu}}{m} + \widetilde{n}^{j}_{\mu} - \widetilde{n}^{i}_{\mu}\right) - n^{j}_{\mu} + n^{i}_{\mu} = m\left(K_{\mu} + \frac{\chi_{\mu}}{m}\right) - \bar{n}^{j}_{\mu} + \bar{n}^{i}_{\mu}, \tag{226}$$

the only difference—with respect to the computation on the original lattice Λ_x, see Equations (12) and (24)—is represented by the phase factors in Equation (222), which are a direct consequence of the dependence of the gauge transformation on the Θ_{μ} matrices.

Finally, as already stressed in Appendix A.2, see comment below Equation (A27), the N_c^2 coefficients entering the linear combination of the $\mathbf{W}^{ij} = w_j\, w_i^{\dagger}$ matrices are not all independent, when considering an element of the $su(N_c)$ Lie algebra. Moreover, with our convention, the gauge field is Hermitian. Then, if we write

$$A_{\mu}(l;\vec{x}) = \sum_{i,j=1}^{N_c} \mathbf{W}^{ij} A^{ij}_{\mu}(l;\vec{x}) \tag{227}$$

we obtain, see Equation (A35), that the coefficients $A^{ij}_{\mu}(l;\vec{x})$ are complex numbers such that

$$A^{ij}_{\mu}(l;\vec{x})^{*} = A^{ji}_{\mu}(l;\vec{x}), \tag{228}$$

which can be verified directly from Equation (222). The above result gives, see Equation (225),

$$\widetilde{A}^{ij}_{\mu}(g;\vec{k}')^{*} = m^d\,\widetilde{A}^{ij}_{\mu}(l;\vec{k}'/m)^{*} = m^d\,\widetilde{A}^{ji}_{\mu}(l;-\vec{k}'/m) = \widetilde{A}^{ji}_{\mu}(g;-\vec{k}'). \tag{229}$$

At the same time, we have

$$\begin{aligned}\left[\widetilde{A}_{\mu}(l;\vec{k}'/m)\right]^{\dagger} &= \sum_{i,j=1}^{N_c} \widetilde{A}^{ij}_{\mu}(l;\vec{k}'/m)^{*}\,\mathbf{W}^{ij\,\dagger} \\ &= \sum_{i,j=1}^{N_c} \widetilde{A}^{ji}_{\mu}(l;-\vec{k}'/m)\,\mathbf{W}^{ji} = \widetilde{A}_{\mu}(l;-\vec{k}'/m)\end{aligned} \tag{230}$$

and

$$\left[\widetilde{A}_{\mu}(g;\vec{k}')\right]^{\dagger} = m^d\left[\widetilde{A}_{\mu}(l;\vec{k}'/m)\right]^{\dagger} = m^d\,\widetilde{A}_{\mu}(l;-\vec{k}'/m) = \widetilde{A}_{\mu}(g;-\vec{k}'), \tag{231}$$

i.e., Equation (72) is verified also on the extended lattice Λ_z.

5.4. Gluon Propagator on the Extended Lattice

In order to evaluate the gluon propagator on Λ_z, it is convenient to start from Equations (68) and (69), which now are written as

$$D(\vec{0}') = \frac{\mathrm{Tr}}{2\,\mathcal{N}\,m^d} \sum_{\mu=1}^{d} \left\langle \left[\widetilde{A}_\mu(g;\vec{0}') \right]^2 \right\rangle \tag{232}$$

and

$$D(\vec{k}') = \frac{\mathrm{Tr}}{2\,\mathcal{N}'\,m^d} \sum_{\mu=1}^{d} \left\langle \widetilde{A}_\mu(g;\vec{k}')\, \widetilde{A}_\mu(g;-\vec{k}') \right\rangle, \tag{233}$$

where the normalization factors $\mathcal{N}$ and $\mathcal{N}'$ are defined in Section 2.2. At the same time, one can easily evaluate the trace after expanding the gauge-field matrices in the basis $\mathbf{W}^{ij} = w_i\, w_j^\dagger$, yielding

$$\begin{aligned} D(\vec{k}') &= \frac{1}{2\,\mathcal{N}'\,m^d} \sum_{\mu=1}^{d} \sum_{i,j=1}^{N_c} \left\langle \widetilde{A}^{ij}_\mu(g;\vec{k}')\, \widetilde{A}^{ji}_\mu(g;-\vec{k}') \right\rangle \\ &= \frac{m^d}{2\,\mathcal{N}'} \sum_{\mu=1}^{d} \sum_{i,j=1}^{N_c} \left\langle \widetilde{A}^{ij}_\mu(l;\vec{k}'/m) \widetilde{A}^{ji}_\mu(l;-\vec{k}'/m) \right\rangle \\ &= \frac{m^d}{2\,\mathcal{N}'} \sum_{\mu=1}^{d} \sum_{i,j=1}^{N_c} \left\langle \left| \widetilde{A}^{ij}_\mu(l;\vec{k}'/m) \right|^2 \right\rangle, \end{aligned} \tag{234}$$

where we use (in this order) Equations (A27), (225) and (229). However, as discussed above—in order to be different from zero—each coefficient $\widetilde{A}^{ij}_\mu(l;\vec{k}'/m)$ requires a specific value for the wave-number vector $\vec{k}$ and, hence, for the wave-number vector $\vec{k}' = \vec{k} + m\vec{K}$, for a given $\vec{K}$, see Equations (194), (218) and (226). Conversely, for fixed $\vec{k}$, only some of the coefficients entering the expression (234) contribute to the gluon propagator. On the other hand, for each choice of $\vec{k}$, we have the freedom to choose among N^d different vectors $\vec{K}$. In particular, as shown in Section 5.2, if we consider $k'_\nu = m\,K_\nu$, with K_ν either equal to zero or to a fixed value K in the interval $[1, N-1]$, then (most likely) the gluon propagator is given by

$$D(\vec{k}') \approx \frac{m^d}{2\,(d-1)\,(N_c^2-1)\,V} \sum_{\mu=1}^{d} \sum_{j=1}^{N_c} \left\langle \left| \widetilde{A}^{jj}_\mu(l;\vec{K}) \right|^2 \right\rangle, \tag{235}$$

i.e., only the diagonal elements contribute to it, with a null vector $\vec{\chi}$, see again Equation (194). At the same time, from Equation (203), we also know that the corresponding gluon propagator can be considered a function of the lattice momenta with components

$$p_\nu(\vec{k}') = 2\,\sin\left(\frac{\pi\,K_\nu}{N}\right) = \begin{cases} 0, \text{ or,} \\ 2\,\sin\left(\frac{\pi K}{N}\right). \end{cases} \tag{236}$$

This observation is in agreement with our findings in Ref. [1], where indeed momenta $\vec{k}'$ of the type $(k', 0, 0, \ldots, 0)$, $(k', k', 0, \ldots, 0)$, $\ldots$, $(k', k', k', \ldots, k')$, with $k' = k + mK$, have produced nonzero results only for $k = 0$. From Equation (235) it is also evident that, in order to compare a result obtained on the extended lattice Λ_z with a result obtained on the original lattice Λ_x, we have to consider $D(\vec{k}')/m^d$, which is again in agreement with the findings presented in the same reference.

Similarly, for the case of zero momentum, we have

$$D(\vec{0}) \,=\, \frac{m^d}{2\,\mathcal{N}} \sum_{\mu=1}^{d} \sum_{i,j=1}^{N_c} \Big\langle \, \Big| \, \widetilde{A}_\mu^{ij}(l;\vec{0}\,) \, \Big|^2 \, \Big\rangle \tag{237}$$

and each matrix element appearing on the r.h.s. is nonzero, see Equation (194), only if $\bar{n}_\nu^i = \bar{n}_\nu^j$ (for any $\nu = 1, \ldots, d$). Thus, also in this case, the main contribution to the gluon propagator comes from the diagonal coefficients, i.e.,

$$D(\vec{0}) \,\approx\, \frac{m^d}{2\,d\,(N_c^2-1)\,V} \sum_{\mu=1}^{d} \sum_{j=1}^{N_c} \Big\langle \, \widetilde{A}_\mu^{jj}(l;\vec{0}\,)^2 \, \Big\rangle, \tag{238}$$

where we use the result, see below Equation (A35), that the coefficients $A_\mu^{jj}(l;\vec{x}\,)$ are real. Note that the above approximation should become more and more valid in the limit of $m \to +\infty$, given that the probability of having $\bar{n}_\nu^i = \bar{n}_\nu^j$ is equal to $1/m$, if we imagine that both $\bar{n}_\nu^i$ and $\bar{n}_\nu^j$ have equal probability of taking one of the possible values $0, 1, \ldots, m-1$. Moreover, using Equation (223) we can write

$$\widetilde{A}_\mu^{jj}(l;\vec{0}\,) = \sum_{\vec{x}\in\Lambda_x} A_\mu^{jj}(l;\vec{x}\,), \tag{239}$$

which are the jj coefficients of the matrix $Q_\mu(l)$, defined in Equation (165), so that

$$\widetilde{A}_\mu^{jj}(l;\vec{0}\,) \,=\, w_j^\dagger \, Q_\mu(l) \, w_j \,=\, Q_\mu^{jj}(l). \tag{240}$$

Therefore, Equation (168) [see also Equation (164)] implies that all gauge-fixed configurations (on the extended lattice Λ_z, for $m \to +\infty$) should be characterized by a gauge field with almost null zero-mode coefficients $\widetilde{A}_\mu^{jj}(l;\vec{0}\,)$ and, consequently, by a strongly suppressed zero-momentum gluon propagator $D(\vec{0}\,)$. This result was already proven in Ref. [5] for the case of an absolute minimum of the minimizing functional $\mathcal{E}_U[g]$. Here, we have shown that it applies also to any local minimum of $\mathcal{E}_U[g]$, in agreement with our numerical findings in Ref. [1]. However, as already suggested in the caption of Figure 1 of the same reference, this suppression is simply a peculiar effect of the extended gauge transformations in the limit of large m—as shown above—and not a physically significant result. To further support this conclusion, we recall that null zero modes for the gauge fields in minimal Landau gauge are also obtained on a finite lattice with free boundary conditions (FBCs) [33]. In the present work, the BCs for the link variables $U_\mu(l;\vec{x}\,)$ are given by Equation (124), i.e., they are not free but they are more general than the usual PBCs. In particular, as $m \to +\infty$, we find that the toroidal BCs (126) applied to the coefficients of the link variables yield

$$\begin{aligned} U_\mu^{ij}(l;\vec{x}+N\vec{e}_\nu) \quad &= \quad e^{\frac{2\pi i}{m}\left(n_\mu^j - n_\mu^i\right)} \, U_\mu^{ij}(l;\vec{x}\,) \,=\, e^{\frac{2\pi i}{m}\left(\bar{n}_\mu^j - \bar{n}_\mu^i\right)} \, U_\mu^{ij}(l;\vec{x}\,) \\ &\to \quad e^{2\pi i\left(\epsilon_\mu^j - \epsilon_\mu^i\right)} \, U_\mu^{ij}(l;\vec{x}\,), \end{aligned} \tag{241}$$

where the real parameters $\epsilon_\mu^j, \epsilon_\mu^i \in [0,1)$ have already been defined in Section 4.2, and we use Equation (193). Clearly, for each direction μ and for each coefficient (with indices i and j), there are—in principle—different BCs, even though they are not completely independent of each other. Hence, the BCs considered for the gauge field $U_\mu(l;\vec{x}\,)$ are somewhat in between the PBCs for the gauge field $U_\mu(h;\vec{x}\,)$ and the FBCs of Ref. [33], and it seems reasonable to us that one finds the zero modes of the nonperiodic gauge field $U_\mu(l;\vec{x})$ to be (much) more suppressed than those of the periodic gauge field $U_\mu(h;\vec{x})$.

6. Numerical Simulations and Conclusions

Numerical simulations can be easily implemented using the Bloch setup considered in this work (see also Ref. [1]). To this end, one just needs to generate a thermalized d-dimensional link configuration $\{U_\mu(x)\}$ with periodicity N, i.e., for a lattice volume $V = N^d$ with PBCs. As for the minimization of the functional $\mathcal{E}_U[g] = \mathcal{E}_{U,\Theta}[h]$, defined in Equations (3), (97) and (98), it can be performed recursively, using two alternating steps:

(a) The matrices Θ_μ are kept fixed as one updates the matrices $h(\vec{x})$ by sweeping through the lattice using a standard gauge-fixing algorithm [18–22]. In particular, one can again consider a single-site update (37), where the matrix $r(\vec{x})$ should satisfy the inequality (40) with, see Equation (135),

$$w(\vec{x}) \equiv \sum_{\mu=1}^{d} \Big[U_\mu(h;\vec{x})\, e^{-i\Theta_\mu/N} + U_\mu^\dagger(h;\vec{x}-\hat{e}_\mu)\, e^{i\Theta_\mu/N} \Big], \tag{242}$$

which should be compared to Equation (39).

(b) The matrices $Z_\mu(h)$ are kept fixed in Equation (97), as one selects the matrices Θ_μ, belonging to the Cartan sub-algebra, see Equation (94), in such a way that they minimize the quantities

$$-\Re\, \mathrm{Tr}\, \frac{e^{-i\Theta_\mu/N}}{V}\, Z_\mu(h) \tag{243}$$

and satisfy the condition (100) as in Equation (A25). We note that, for this minimization step, one usually does not employ a simple multiplicative update as in Equation (37). The main problem is that the minimizing functional is quadratic in the matrix v. On the other hand, the dependence on the integer parameters n_μ^j is rather trivial.

From the above discussion, it is also evident that, contrary to the situation described in Section 2.1 (for the implementation of the usual minimal-Landau-gauge condition), the organization of the numerical algorithm is slightly more complicated when considering the extended lattice Λ_z. Indeed, since the gauge transformation $h(\vec{x})$ and its update $r(\vec{x})$ do not commute (in general) with the Θ_μ matrices, it is no longer true that we can write the single-site update as

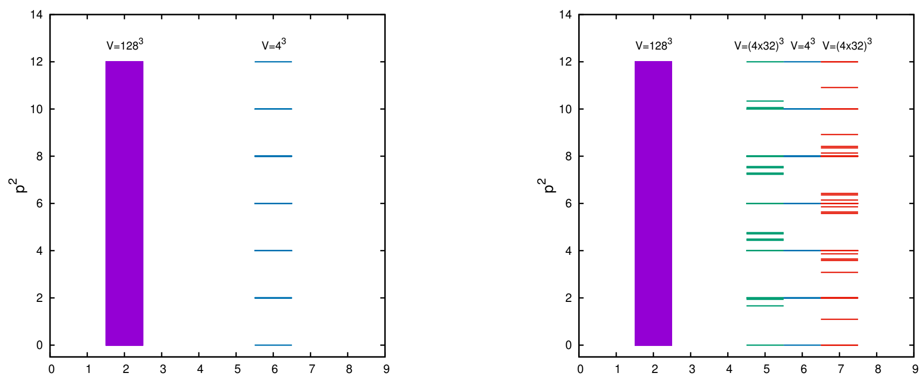
$$\exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) h(\vec{x}) \;=\; l(\vec{x}) \;\to\; r(\vec{x})\, l(\vec{x}). \tag{244}$$

Instead, we need to consider the update

$$l(\vec{x}) \;\to\; \exp\left(i \sum_{\nu=1}^{d} \frac{\Theta_\nu\, x_\nu}{N} \right) r(\vec{x})\, h(\vec{x}), \tag{245}$$

which preserves the Bloch-function structure. Thus, we can still make use of the multiplicative updates reported in Equation (41) but, besides the link configuration $\{U_\mu(h;\vec{x})\}$, we need to store (separately) the matrices Θ_μ. In fact, Equation (95) illustrates that it is sufficient (and necessary) to know $\{U_\mu(h;\vec{x})\}$ and $\{\Theta_\mu\}$ in order to carry out the minimization process. Let us notice that, as is the case for the usual minimizing functional, $\mathcal{E}_{U,\Theta}[h]$ is bounded from below. Hence, any iterative algorithm that ensures minimization at each step is expected to converge. Indeed, we did not encounter any convergence problems in our tests of the method.

More details about the numerical implementation of this algorithm will be discussed in a future work. Here, we only present the numerical checks we have performed to confirm the results obtained in Section 5. In particular, in Figures 1 and 2 we show the "spectrum" of the gluon propagator or, to be more specific, the allowed momenta, i.e., the momenta for which a nonzero gluon propagator $D(\vec{k})$ is obtained. To this end we recall that—when considering Λ_x—the lattice momenta $p^2(\vec{k}) = \sum_{\mu=1}^{d} p_\mu^2(\vec{k})$ have components $p_\mu(\vec{k}) = 2\sin\left(\pi k_\mu / N\right)$, see Equations (32) and (35), where N is the lattice side and, due to the symmetry of $p^2(\vec{k})$ under the reflection $\vec{k} \to -\vec{k} + N\hat{e}_\mu$ (see Section 2.2), we just need to consider $k_\mu = 0, 1, \ldots, N/2$ (when N is even). Then, it is easy to verify that, for $N = 4$ and $d = 3$, there are only seven different momenta (with degeneracy). Similarly, for $N = 8$ and $d = 3$, there are 25 different momenta (with degeneracy). These momenta—which we call here original momenta—are shown (in blue) in the right column of plots (a) and (b) of Figures 1 and 2, respectively for the $N = 4$ and $N = 8$ case. At the same time, for $N = 128$ (and again $d = 3$), there are about 45,000 different momenta (with degeneracy), which are shown (in magenta) in the left column of plots (a) and (b) of both figures.[49] Finally, on the right column of plot (b) of Figures 1 and 2 we show, in green and in red, the allowed momenta obtained by considering two different configurations for, respectively, the lattice $V = (4 \times 32)^3$ and $V = (8 \times 16)^3$, using the Bloch-wave setup described above. As one can easily see, the allowed momenta always include the original momenta, as well as other momenta that are configuration-dependent. Moreover, we considered the condition $k'_\nu + n^j_\nu - n^i_\nu \propto m$, see Equation (197), which should be satisfied by the allowed momenta. This was checked using one configuration for the lattice volumes $V = (16 \times 8)^3$ and $V = (32 \times 4)^3$, and two configurations for each of the setups $V = (8 \times 16)^3$ and $V = (4 \times 32)^3$. In total, for these six configurations, we found that there were slightly more than 16,000 allowed momenta. Of these, a little less than 6000 are the lattice momenta that can be considered also on the small (original) lattice. In all cases, we checked that Equation (197) is indeed verified for the nonzero values of the gluon propagator.



(**a**) (**b**)

Figure 1. In plot (**a**), on the left, we show the original momenta for the lattices $V = 128^3$ (**left** column) and $V = 4^3$ (**right** column). The same momenta are reported in plot (**b**), on the right, together with the allowed momenta, obtained by considering two different configurations for the lattice setup $V = (4 \times 32)^3$, i.e., with $N = 4$ and $m = 32$. All simulations were performed using the SU(2) gauge group at $\beta = 3.0$.

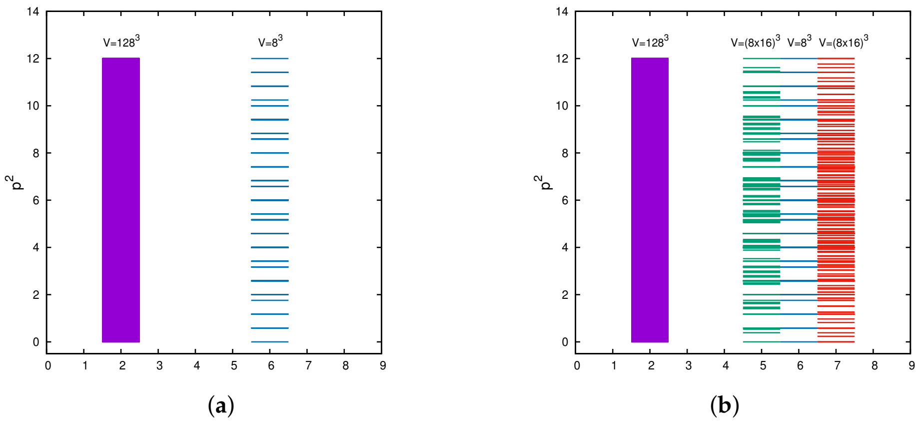


Figure 2. In plot (**a**), on the left, we show the original momenta for the lattices $V = 128^3$ (**left** column) and $V = 8^3$ (**right** column). The same momenta are reported in plot (**b**), on the right, together with the allowed momenta, obtained by considering two different configurations for the lattice setup $V = (8 \times 16)^3$, i.e., with $N = 8$ and $m = 16$. All simulations were performed using the SU(2) gauge group at $\beta = 3.0$.

We also stress that the explanation presented in Section 5.4 about the suppression of $D(\vec{0})$, in the limit $m \to \infty$, is essentially in agreement with the intuitive argument presented in Ref. [1]. To see this, using Equations (222) and (239), we can write

$$\widetilde{A}^{jj}_{\mu}(l;\vec{0}) = \sum_{\vec{x}\in\Lambda_x} \left\{ \frac{1}{2i} \left[U^{jj}_{\mu}(h;\vec{x}) e^{-\frac{2\pi i n^j_\mu}{mN}} - e^{\frac{2\pi i n^j_\mu}{mN}} U^{jj}_{\mu}(h;\vec{x})^* \right] - \frac{1}{N_c} \sum_{l=1}^{N_c} \Im \left[U^{ll}_{\mu}(h;\vec{x}) \, e^{\frac{-2\pi i n^l_\mu}{mN}} \right] \right\}, \tag{246}$$

i.e., we are evaluating the diagonal jj coefficients of the matrix, see Equation (98),

$$\begin{aligned} & \frac{1}{2i} \left[Z_\mu(h) \, e^{-i\frac{\Theta_\mu}{N}} - e^{i\frac{\Theta_\mu}{N}} \, Z^\dagger_\mu(h) \right] - \mathbb{1} \, \frac{\Im \, \mathrm{Tr}}{N_c} \left[Z_\mu(h) e^{-i\frac{\Theta_\mu}{N}} \right] \\ = \; & \frac{1}{2i} \left[Z_\mu(h) \, v^\dagger \, T_\mu \, v - v^\dagger \, T^\dagger_\mu \, v \, Z^\dagger_\mu(h) \right] - \mathbb{1} \, \frac{\Im \, \mathrm{Tr}}{N_c} \left[Z_\mu(h) \, v^\dagger \, T_\mu \, v \right], \end{aligned} \tag{247}$$

where T_μ is a shorthand notation for the diagonal matrices $T_\mu(mN;\{n^j_\mu\})$, see Equations (131) and (132). Hence, with $w_j = v^\dagger \, \hat{e}_j$, we end up with the expression

$$\begin{aligned} \widetilde{A}^{jj}_{\mu}(l;\vec{0}) & = \hat{e}^\dagger_j \, \frac{v \, Z_\mu(h) \, v^\dagger \, T_\mu \; - \; T^\dagger_\mu \, v \, Z^\dagger_\mu(h) v^\dagger}{2\,i} \, \hat{e}_j - \frac{\Im \, \mathrm{Tr}}{N_c} \left[Z_\mu(h) \, v^\dagger \, T_\mu \, v \right] \\ & = \hat{e}^\dagger_j \, \frac{V_\mu \; - \; V^\dagger_\mu}{2\,i} \, \hat{e}_j - \frac{\Im \, \mathrm{Tr}}{N_c} \, V_\mu, \end{aligned} \tag{248}$$

where we define $V_\mu \equiv v \, Z_\mu(h) \, v^\dagger \, T_\mu$. At the same time, in order to impose the gauge-fixing condition, we need to maximize the quantity, see Equation (97),

$$\Re \; \mathrm{Tr} \sum_{\mu=1}^{d} Z_\mu(h) \, e^{-i\frac{\Theta_\mu}{N}} = \Re \; \mathrm{Tr} \sum_{\mu=1}^{d} Z_\mu(h) \, v^\dagger \, T_\mu \, v = \Re \; \mathrm{Tr} \sum_{\mu=1}^{d} V_\mu \, . \tag{249}$$

Intuitively, this maximization can be easily achieved if one finds a global rotation v such that the (rotated) zero modes $v \, Z_\mu(h) \, v^\dagger$ become close to diagonal matrices. Then, given that in the limit $m \to \infty$ the discretized parameters n^j_μ / mN become continuous,[50] one should be able to use the diagonal matrices $T_\mu = T_\mu(mN;\{n^j_\mu\})$—whose elements are ${T_\mu}^{jj} = \exp\left(-2\pi i n^j_\mu / m \, N\right)$—to bring the matrices V_μ as close as possible to real diagonal matrices. As a consequence, both terms in Equation (248) should be close to zero, implying $\widetilde{A}^{ij}_{\mu}(l;\vec{0}\,) \approx 0$ and $D(\vec{0}\,) \approx 0$, see Equations (238). This is an artifact of the method and does not have a physical meaning. Let us recall that, as may be seen in Figure 1 of Ref. [1], the use of Bloch waves introduces a discontinuity in the gluon propagator at zero momentum, an effect that was previously not completely understood.

As we noted in Section 4, gauge-fixed link configurations within each replicated lattice $\Lambda_x^{(\vec{y})}$ are rotated, transformed by global group elements defined by the cell index $\vec{y}$, see Equation (119). The same applies to the gauge-fixed gauge-field configurations $\{A_\mu(l;\vec{x}\,)\}$, see Equation (157). It is then natural to consider, on each replicated lattice $\Lambda_x^{(\vec{y})}$, the average color magnetization $\vec{M}_\mu(\vec{y})$ with (color) components[51]

$$M^b_\mu(\vec{y}) \;=\; \frac{1}{V} \sum_{\vec{x}\in\Lambda_x} A^b_\mu(g;\vec{x}+\vec{y}N), \tag{251}$$

which is related to the gluon propagator at zero momentum since, see Equation (216),

$$\widetilde{A}^b_\mu(g;\vec{0}\,'\,) \;=\; V \sum_{\vec{y}\in\Lambda_y} M^b_\mu(\vec{y}), \tag{252}$$

so that Equation (232) implies by the expression

$$D(\vec{0}\,'\,) \;=\; \frac{\mathrm{Tr}}{2\,m^d\,\mathcal{N}} \sum_{\mu=1}^{d} \left\langle \left[\, \widetilde{A}_\mu(g;\vec{0}\,'\,) \,\right]^2 \right\rangle \;=\; \frac{V^2}{m^d\,\mathcal{N}} \sum_{\mu=1}^{d} \sum_{b=1}^{N_c^2-1} \left\langle \left[\, \sum_{\vec{y}\in\Lambda_y} M^b_\mu(\vec{y}) \,\right]^2 \right\rangle, \tag{253}$$

where $\mathcal{N} \equiv d(N_c^2-1)V$ has been defined in Section 2.2. We show in Figures 3 and 4 the vectors $\vec{M}_3(\vec{y})$ of the color magnetization, obtained in a simulation for the $SU(2)$ case and with lattice volume $V = (64\times 4)^3$ at $\beta = 3.0$. The vector components stand for the different values of the color index, i.e., $M^b_3(\vec{y})$, for $b = 1,2,3$. One can clearly see the effect of the Bloch waves. In particular, the average magnetization may appear "smooth" along a certain direction when moving from one cell to the next, but a suitably chosen projection reveals the modulated behavior as expected. For example, in Figure 4, $M^3_\mu(\vec{y})$ does not change when crossing a boundary, while $M^1_\mu(\vec{y})$ and $M^2_\mu(\vec{y})$ are rotated (see Figure 5). Thus, each cell $\Lambda_x^{(\vec{y})}$ may be seen as a domain, and the domain walls are characterized by the cell boundaries. As discussed in Ref. [35], the zero-momentum gluon propagator can be interpreted as a magnetic susceptibility. For $d = 3$ and 4, numerical simulations show—in the infinite-volume limit—zero magnetization and nonzero susceptibility. This can be associated to randomly oriented magnetization domains. Our setup, based on Bloch waves, allows us to "impose" such domains, while reproducing (see plots in Ref. [1]) the gluon-propagator results of the standard large-volume simulation. Of course, it would be very interesting to be able to characterize similar domain structures in a usual simulation.

Finally, we present our conclusions. Our main finding is that the gluon propagator $D(\vec{k}\,'\,)$ is nonzero only for the allowed momenta and, in these cases, its value comes from some of the coefficients $\widetilde{A}^{ij}_\mu(g;\vec{k}\,'\,)$, with all the other coefficients being equal to zero. Hence, we now completely understand the math behind the use of Bloch waves in minimal Landau gauge and we can perform the whole simulation (thermalization, gauge fixing and evaluation of the gluon propagator) in the small "unit cell" Λ_x. At the moment, we modified our numerical codes to incorporate the new results presented here and performed preliminary tests. These will be used to guide the thorough numerical investigation of the method for the evaluation of the gluon propagator. In this way, we hope to be able to produce large ensembles of data,[52] even considering small unit cells and large values of m. In particular, we want to find the minimum value of the lattice size N of Λ_x for which the momentum-space gluon propagator $D(\vec{k}')$, evaluated on Λ_z using the Bloch setup with a factor m, is still in agreement with numerical data obtained by working directly on a lattice of size mN (see results in Ref. [1]). More in general, we want to check the dependence of $D(\vec{k}')$ on N, while keeping the product mN fixed. Clearly, since we know that finite-size effects in the gluon propagator are relevant only in the infrared regime, it is essential to consider all allowed momenta in these numerical simulations. Indeed, the momenta given by the discretization on the original (small) lattice Λ_x are insufficient to adequately probe the infrared limit when N is small. Having more data should also help clarify the role of the $\{U_\mu(h,\Theta;\vec{x})\}$ "domains" and of the "magnetization" described above. Later on, we plan to extend this analysis to the ghost propagator. Furthermore, one may also try to relate the present approach to early studies of replicated lattices, which computed gauge-independent quantities such as the hadron spectrum [36,37].

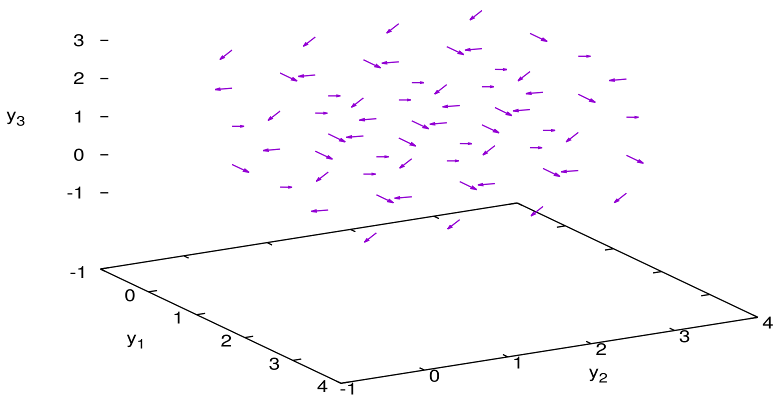


Figure 3. Average color "magnetization" $\vec{M}_3(\vec{y})$ on each replicated lattice $\Lambda_x^{(\vec{y})}$ for the pure-$SU(2)$ case and lattice volume $V = (64 \times 4)^3$, at $\beta = 3.0$. In this case, the index lattice Λ_y is a 4^3 lattice, and $\vec{y}$ has components $y_\mu = 0,1,2,3$ with $\mu = 1,2,3$. Also note that the color components $M_3^b(\vec{y})$ (with $b = 1,2$ and 3) are represented along the corresponding spatial directions $\mu = 1,2,3$.

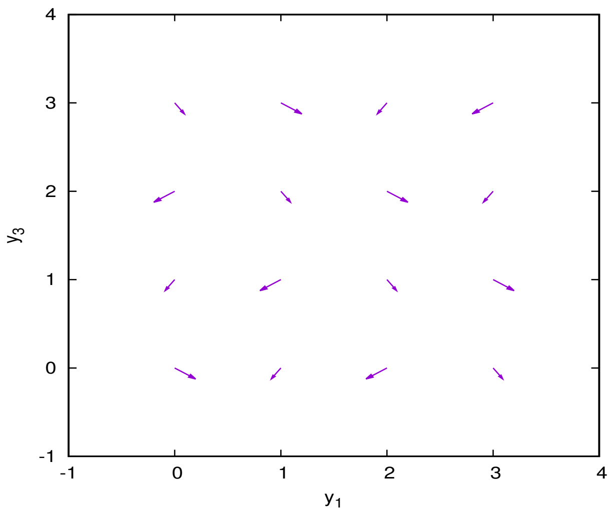


Figure 4. Average color "magnetization" $\vec{M}_3(\vec{y})$ on each replicated lattice $\Lambda_x^{(\vec{y})}$ for the pure-$SU(2)$ case and lattice volume $V = (64 \times 4)^3$, at $\beta = 3.0$. In this case, the index lattice Λ_y is a 4^3 lattice and $\vec{y}$ has components $y_\mu = 0,1,2,3$ with $\mu = 1,2,3$. Also note that the color components $M_3^b(\vec{y})$ (with $b = 1,2$ and 3) are represented along the corresponding spatial directions $\mu = 1,2,3$. Here we show the data presented in Figure 3 with coordinate $y_2 = 0$, projected on the $y_1 - y_3$ plane. Consequently, we are also showing only the $b = 1,3$ color components.

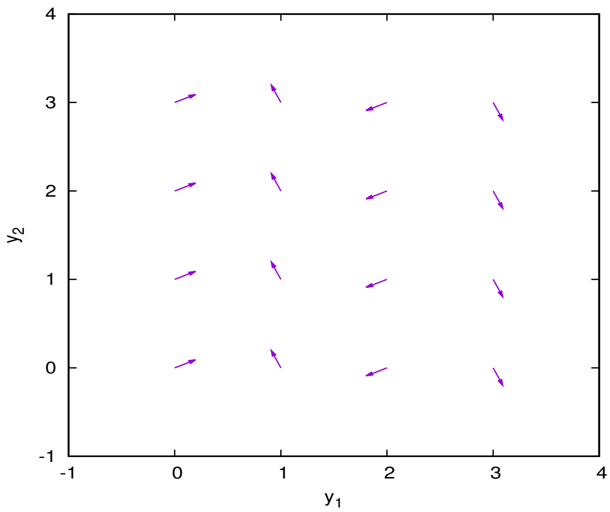


Figure 5. Average color "magnetization" $\vec{M}_3(\vec{y})$ on each replicated lattice $\Lambda_x^{(\vec{y})}$ for the pure-$SU(2)$ case and lattice volume $V = (64 \times 4)^3$, at $\beta = 3.0$. In this case the index lattice Λ_y is a 4^3 lattice, and $\vec{y}$ has components $y_\mu = 0, 1, 2, 3$ with $\mu = 1, 2, 3$. Also note that the color components $M_3^b(\vec{y})$ (with $b = 1, 2$ and 3) are represented along the corresponding spatial directions $\mu = 1, 2, 3$. Here we show the data presented in Figure 3 with coordinate $y_3 = 0$, projected on the $y_1 - y_2$. Consequently, we are also showing only the $b = 1, 2$ color components.

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Data Availability Statement: The raw data supporting the conclusions of this article will be made available by the authors on request.

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Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A. Cartan Sub-Algebra

In this appendix we discuss properties related to the matrices Θ_μ, introduced in Section 3.2, see Equation (94). Recall that these matrices belong to the Cartan sub-algebra of $su(N_c)$ and must satisfy the periodicity condition (100), which implies that their eigenvalues be given by $2\pi n_\mu / m$, where n_μ is an integer. We start by describing a general parametrization for the $N_c - 1$ generators of the Cartan sub-algebra in the SU(N_c) case [13,38,39], and then comment on possible advantages of other bases. We also compare our setup with that considered in Ref. [5]. As can be seen in Section 5, and in particular in Sections 5.3 and 5.4, some of these properties are central to obtain an analytic expression for the gluon propagator using the gauge-fixed configuration on the extended lattice Λ_z.

We recall that we have chosen the $N_c^2 - 1$ traceless generators t^b of the $su(N_c)$ Lie algebra to be Hermitian. Since the Cartan generators $\{t_C\}$ are mutually commuting, i.e., $[t_C^a, t_C^b] = 0$ (for $a, b = 1, \ldots, N_c - 1$), they can be simultaneously diagonalized. For example, in the SU(N_c) case, we can consider as diagonal Cartan generators (in the fundamental representation) the $N_c - 1$ linearly independent, $N_c \times N_c$ Hermitian and traceless matrices H^i $(i = 1, \ldots, N_c - 1)$ defined by [39]

$$H^i_{jk} \,=\, \xi^i\,\delta^{jk}\left[\delta^{ij} - \delta^{(i+1)j}\right], \tag{A1}$$

with ξ^i real and $j, k = 1, \ldots, N_c$. Note that, besides being diagonal, the matrix H^i only has nonzero elements in rows/columns i and $i+1$ and these two elements have opposite signs, enforcing the tracelessness condition. In particular, for $N_c = 2$, the matrix H^1 is given by ξ^1 times the third Pauli matrix σ_3. For the SU(3) case, after setting $\xi^1 = \xi^2 = 1$, we have

$$H^1 \,=\, \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad \text{and} \qquad H^2 \,=\, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{A2}$$

Since they are diagonal, the above generators H^i have—as common eigenvectors—the unit vectors[53] $\hat{e}_j$ [whose components are given by $(\hat{e}_j)_k \,=\, \delta^{jk}$], with eigenvalues $\lambda^i_j = \xi^i\left[\delta^{ij} - \delta^{(i+1)j}\right]$, where again $j = 1, \ldots, N_c$.

More in general, since the matrices H^i are diagonal, we may define the Cartan generators by any combination

$$D^i \,=\, \sum_{l=1}^{N_c-1} R^{il}\,H^l, \tag{A3}$$

where R is an invertible $(N_c-1) \times (N_c-1)$ matrix. For example, in the SU(3) case, with the Gell-Mann choice for the generators of the group algebra, the Cartan sub-algebra is spanned by the matrices $D^1 = H^1$ and $D^2 = (H^1 + 2H^2)/\sqrt{3}$—usually denoted by λ_3 and λ_8—instead of H^1 and H^2 given in Equation (A2). This corresponds to changing the basis with the matrix

$$R \,=\, \begin{pmatrix} 1 & 0 \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{3}} \end{pmatrix}. \tag{A4}$$

In order to generalize the above bases containing Pauli and Gell-Mann matrices to the SU(N_c) case (see Appendix A1 in Ref. [15]), we may consider[54] the matrices

$$D^i \,=\, \sqrt{\frac{2}{i(i+1)}}\left[\sum_{l=1}^{i} l\,H^l\right], \tag{A6}$$

with $i = 1, \ldots, N_c-1$. Note that, just as H^i, the matrices D^i are diagonal.[55] Their eigenvectors are also $\hat{e}_j$ but with eigenvalues[56]

$$\alpha^i_j \,=\, \sum_{l=1}^{N_c-1} R^{il}\,\lambda^l_j \,=\, R^{ij}\,\xi^j - R^{i(j-1)}\,\xi^{j-1}. \tag{A7}$$

Also, recall that, while j takes values from 1 to N_c, the indices of the matrix R^{il} and of the constants ξ^i only go from 1 to N_c-1. Thus, for $j = 1$ we have $\alpha^i_1 = R^{i1}\,\xi^1$ and for $j = N_c$ we find $\alpha^i_{N_c} = -R^{i(N_c-1)}\,\xi^{N_c-1}$.

Finally, it is rather evident [13,39] that, if H_C is a Cartan sub-algebra and v is any element of the Lie group, the conjugate $v^{-1}\,H_C\,v$ is another Cartan sub-algebra. Thus, for the SU(N_c) group, we can consider as matrices t^b_C the set $\{v^\dagger\,D^b\,v\}$, with common eigenvectors $\{w_j = v^\dagger\,\hat{e}_j$ for $j = 1, \ldots, N_c\}$—which are orthonormal since $w^\dagger_j\,w_k = \hat{e}^\dagger_j\,\hat{e}_k \,=\, \delta^{jk}$—and the eigenvalues α^b_j given above, where we switch back to the usual index b for the color degrees of freedom. This illustrates the expansion in Equation (94).

Appendix A.1. Comparison with Reference [5]

We note that Ref. [5] defines the Θ_μ matrices, belonging to a generic Cartan sub-algebra, as an expansion in terms of the generators t^b of the SU(N_c) algebra, i.e.,

$$\Theta_\mu \;=\; \sum_{b=1}^{N_c^2-1} \theta_\mu^b\, t^b, \tag{A8}$$

with real parameters θ_μ^b ($\mu = 1, \ldots, d$), subject to the condition

$$\left[\,\Theta_\mu,\, \Theta_\nu\,\right] \;=\; \sum_{b,c=1}^{N_c^2-1} \theta_\mu^b\, \theta_\nu^c \left[\, t^b,\, t^c \,\right] \;=\; 2\,i \sum_{a,b,c=1}^{N_c^2-1} f^{abc}\, \theta_\mu^b\, \theta_\nu^c\, t^a \;=\; 0, \tag{A9}$$

where we denote by f^{abc} the structure constants of the $su(N_c)$ Lie algebra. Now, since the matrices t^a are linearly independent, the above equality implies that

$$\sum_{b,c=1}^{N_c^2-1} f^{abc}\, \theta_\mu^b\, \theta_\nu^c \;=\; 0, \tag{A10}$$

for any $a = 1, \ldots, N_c^2 - 1$.

In the SU(2) case, for example, for which the Cartan sub-algebra is one dimensional and the structure constants f^{abc} are given by the completely anti-symmetric tensor ϵ^{abc}, we find that the above condition is equivalent to saying that the three-dimensional vectors $\vec{\theta}_\mu$ and $\vec{\theta}_\nu$ must be parallel[57] for any μ, ν. This can be easily achieved [5] with

$$\Theta_\mu \;=\; r_\mu \sum_{b=1}^{3} q^b\, t^b, \tag{A11}$$

where r_μ and q^b are real parameters. As a matter of fact, by factoring $\theta_\mu^b \;=\; r_\mu\, q^b$, i.e., by imposing that the vectors $\vec{\theta}_\mu$ are all proportional to the vector $\vec{q}$, it is evident that Equation (A10) is satisfied since $\sum_{b,c=1}^{3} f^{abc} q^b q^c = 0$. Note that matrices Θ_μ defined in this way are not necessarily diagonal. On the other hand, they are mutually commuting since they are proportional to the same matrix $\sum_{b=1}^{3}\, q^b\, t^b$. One can also write

$$\Theta_\mu \;=\; r_\mu\, v^\dagger\, \sigma_3\, v, \tag{A12}$$

where $v \in$ SU(2) and σ_3 is the third Pauli matrix, which is diagonal. Indeed, Equations (A11) and (A12) are completely equivalent.[58]

Hence, the above parametrization (A12) is clearly in agreement with the previously discussed setup, and we can say that the expansion used in Ref. [5] corresponds to a transformation $v^{-1}\, H_C\, v$ of the Cartan sub-algebra given by σ_3. Note that, using Equation (A12), the matrices Θ_μ trivially have eigenvectors

$$v^\dagger \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{A14}$$

and

$$v^\dagger \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{A15}$$

with eigenvalues $\pm\, r_\mu$.

In like manner, in the SU(3) case, which has rank two, we can write [5]

$$\Theta_\mu \,=\, r_{\mu,3} \sum_{b=1}^{8} q_3^b\, t^b \,+\, r_{\mu,8} \sum_{b=1}^{8} q_8^b\, t^b \tag{A16}$$

with real parameters $r_{\mu,3}$, $r_{\mu,8}$, q_3^b and q_8^b, i.e., we now factor $\theta_\mu^b = r_{\mu,3}\, q_3^b + r_{\mu,8}\, q_8^b$. This yields, see Equation (A10),

$$\sum_{b,c=1}^{8} f^{abc}\, q_3^b\, q_8^c \left(r_{\mu,3}\, r_{\nu,8} \,-\, r_{\mu,8}\, r_{\nu,3} \right) \,=\, 0, \tag{A17}$$

where we use the (obvious) relation $f^{abc} = -f^{acb}$. Clearly, since the above expression must be valid for any values of the parameters $r_{\mu,3}$ and $r_{\mu,8}$, we must select two commuting matrices

$$\widetilde{\lambda}_3 \,=\, \sum_{b=1}^{8} q_3^b\, t^b \qquad \text{and} \qquad \widetilde{\lambda}_8 \,=\, \sum_{c=1}^{8} q_8^c\, t^c \tag{A18}$$

to parametrize the expansion of Θ_μ so that

$$\frac{1}{2}\, \mathrm{Tr} \left\{ t^a \left[\widetilde{\lambda}_3, \widetilde{\lambda}_8 \right] \right\} \,=\, \sum_{b,c=1}^{8} f^{abc}\, q_3^b\, q_8^c \,=\, 0. \tag{A19}$$

Then, we recover again our definition for Θ_μ—in terms of diagonal matrices and the transformation $v^{-1}\, H_C\, v$—if we consider

$$\Theta_\mu \,=\, r_{\mu,3}\, \widetilde{\lambda}_3 \,+\, r_{\mu,8}\, \widetilde{\lambda}_8 \,=\, v^\dagger \left(r_{\mu,3}\, \lambda_3 \,+\, r_{\mu,8}\, \lambda_8 \right) v, \tag{A20}$$

where λ_3 and λ_8 are the two diagonal Gell-Mann matrices and $v \in$ SU(3).

Appendix A.2. New Basis for the Lie Algebra

As already noted above, the matrices Θ_μ—which belong to the Cartan sub-algebra and are written in terms of the basis $t_C^b = v^\dagger D^b v$ — have eigenvectors $w_j = v^\dagger\, \hat{e}_j$ (for $j = 1, \ldots, N_c$), with eigenvalues given by

$$\Theta_\mu\, w_j \,=\, \left[\sum_{b=1}^{N_c - 1} \theta_\mu^b\, \alpha_j^b \right] w_j \,\equiv\, \beta_\mu^j\, w_j \,=\, \frac{2\pi\, n_\mu^j}{m}\, w_j, \tag{A21}$$

where the parameters θ_μ^b refer to the expansion in Equation (94), α_j^b is defined in Equation (A7) and, in the last step, we impose the constraint (100), i.e., that n_μ^j be integers.

Then, it is natural to consider a new basis for Θ_μ, with matrices defined as an outer product of these eigenvectors, i.e.,

$$\mathbf{W}^{ij} \equiv w_i\, w_j^\dagger \,=\, v^\dagger\, \hat{e}_i\, \hat{e}_j^\dagger\, v \,\equiv\, v^\dagger\, \mathbf{M}^{ij}\, v, \tag{A22}$$

where the matrix element lm of $\mathbf{W}^{ij}$ is given by $(w_i)_l\, (w_j^\dagger)_m$ (for $l, m = 1, \ldots, N_c$). Similarly, we have also defined the $N_c \times N_c$ matrix $\mathbf{M}^{ij} = \hat{e}_i\, \hat{e}_j^\dagger$, whose elements are simply[59] $(\mathbf{M}^{ij})_{lm} = \delta^{il}\delta^{jm}$. In this way, considering $\Theta_\mu = \sum_{i,j} c_\mu^{ij}\, \mathbf{W}^{ij}$, we can left multiply Equation (A21) by $w_i^\dagger$ to obtain the expansion parameters

$$c_\mu^{ij} \,=\, w_i^\dagger\, \Theta_\mu\, w_j \,=\, \beta_\mu^i\, \delta^{ij} \,=\, \frac{2\pi\, n_\mu^i}{m}\, \delta^{ij} \tag{A23}$$

in the $\mathbf{W}^{ij}$ basis. As expected, they are nonzero only for $i = j$, since the eigenvectors w_i form an orthonormal set. Thus, we can write

$$\Theta_\mu = \sum_{j=1}^{N_c} \beta_\mu^j \, \mathbf{W}^{jj} = \sum_{j=1}^{N_c} \frac{2\pi \, n_\mu^j}{m} \, v^\dagger \, \mathbf{M}^{jj} \, v \tag{A24}$$

and

$$\exp\left(i \, \frac{\Theta_\mu}{N} \right) = v^\dagger \, \exp\left(\sum_{j=1}^{N_c} \frac{2\pi i \, n_\mu^j}{mN} \, \mathbf{M}^{jj} \right) v, \tag{A25}$$

which are important results for our analysis in Sections 3.3 and 4. Of course, when $v = \mathbb{1}$—or, equivalently, when considering the basis $\mathbf{M}^{ij}$—the matrices in Equations (A24) and (A25) are diagonal.

Let us stress that the matrices $\mathbf{W}^{ij}$ trivially satisfy the trace condition[60]

$$\mathrm{Tr}\left(\mathbf{W}^{ij}\right) = \mathrm{Tr}\left(w_i \, w_j^\dagger\right) = w_j^\dagger \, w_i = \delta^{ij} \tag{A26}$$

and the orthonormality relations

$$\mathrm{Tr}\left(\mathbf{W}^{ij} \, \mathbf{W}^{lm\,\dagger}\right) = \mathrm{Tr}\left(\mathbf{W}^{ij} \, \mathbf{W}^{ml}\right) = \mathrm{Tr}\left(w_i \, w_j^\dagger \, w_m \, w_l^\dagger\right) = \delta^{jm} \, \mathrm{Tr}\left(w_i \, w_l^\dagger\right) = \delta^{jm} \, \delta^{il}, \tag{A27}$$

where we use[61] $\mathbf{W}^{lm\,\dagger} = \mathbf{W}^{ml}$, the orthonormality of the w's and (A26). Hence, the N_c^2 matrices $\mathbf{W}^{ij}$ are indeed a basis for any $N_c \times N_c$ matrix, which is—as seen in Section 5—the most natural one to consider when analyzing the impact of the index lattice on the evaluation of the gluon propagator. On the other hand, elements of the (real) SU(N_c) Lie group—as well as of the corresponding $su(N_c)$ Lie algebra—are written in terms of $N_c^2 - 1$ real independent parameters. Therefore, when using this basis, the N_c^2 coefficients entering the linear combination of the $\mathbf{W}^{ij}$ matrices are not all independent. As a matter of fact, a generic matrix

$$A = \sum_{i,j=1}^{N_c} A^{ij} \, \mathbf{W}^{ij}, \tag{A29}$$

where the coefficients A^{ij} are given, see Equation (A23), by

$$A^{ij} = w_i^\dagger \, A \, w_j, \tag{A30}$$

is (in general) not traceless due to Equation (A26). Thus, for the $su(N_c)$ Lie algebra, we have to enforce the constraint

$$0 = \mathrm{Tr}\, A = \sum_{j=1}^{N_c} A^{jj}, \tag{A31}$$

yielding the relation, see Equation (A24),

$$0 = \sum_{j=1}^{N_c} \beta_\mu^j = \frac{2\pi}{m} \sum_{j=1}^{N_c} n_\mu^j \tag{A32}$$

for the Θ_μ matrices. Of course, this condition is automatically satisfied if the β_μ^j eigenvalues are given, see Equations (A7) and (A21), by

$$\beta_\mu^j = \sum_{b=1}^{N_c-1} \theta_\mu^b \, \alpha_j^b = \sum_{b=1}^{N_c-1} \theta_\mu^b \left[R^{bj} \, \xi^j - R^{b(j-1)} \, \xi^{j-1} \right], \tag{A33}$$

which implies

$$\sum_{j=1}^{N_c} \beta_\mu^j = \sum_{j=1}^{N_c-1} \sum_{b=1}^{N_c-1} \theta_\mu^b R^{bj} \xi^j - \sum_{j=2}^{N_c} \sum_{b=1}^{N_c-1} \theta_\mu^b R^{b(j-1)} \xi^{j-1} = 0. \tag{A34}$$

Indeed, when written in terms of the coefficients θ_μ^b, see Equation (94), the matrices Θ_μ depend on $d\,(N_c-1)$ free parameters; on the other hand, when they are written using the n_μ^j coefficients, see Equation (A24), we have $d\,N_c$ free parameters, subject to the d constraints (A32).

Besides being traceless, an element of the SU(N_c) Lie algebra should also be (with our convention) Hermitian. Hence, if we impose $A^\dagger = A$ in Equation (A29), we find

$$\left(A^{ij}\right)^* = A^{ji}, \tag{A35}$$

given that $\left(\mathbf{W}^{ij}\right)^\dagger = \mathbf{W}^{ji}$, see note 61. (Here, * denotes complex conjugation.) The last result, together with Equation (A31), implies that the diagonal coefficients A^{jj} are real and that only N_c-1 of them are independent. At the same time, from Equation (A35), we find that there are only $N_c\,(N_c-1)/2$ independent complex off-diagonal elements, yielding a total of $(N_c-1)+(N_c^2-N_c) = N_c^2-1$ free real parameters (as expected). We stress that the coefficients A^{ij} are *not* the matrix elements of A, which are given by the expression

$$A_{lm} = \sum_{i,j=1}^{N_c} \left(\mathbf{W}^{ij}\right)_{lm} A^{ij} \tag{A36}$$

with

$$\left(\mathbf{W}^{ij}\right)_{lm} = \sum_{k,n=1}^{N_c} \left(v^\dagger\right)_{lk} \left(\mathbf{M}^{ij}\right)_{kn} v_{nm} = \left(v^\dagger\right)_{li} v_{jm} = v_{il}^* \, v_{jm}, \tag{A37}$$

so that one has (as always for a Hermitian matrix)

$$\begin{aligned} A_{lm}^* &= \sum_{i,j=1}^{N_c} \left(\mathbf{W}^{ij}\right)_{lm}^* \left(A^{ij}\right)^* = \sum_{i,j=1}^{N_c} \left[\, v_{il}^* \, v_{jm} \,\right]^* \left(A^{ij}\right)^* \\ &= \sum_{i,j=1}^{N_c} v_{jm}^* \, v_{il} \, A^{ji} = \sum_{j,i=1}^{N_c} \left(\mathbf{W}^{ji}\right)_{ml} A^{ji} = A_{ml}. \end{aligned} \tag{A38}$$

Finally, Equation (A24) tells us that we can easily relate the Cartan sub-algebra, defined by the diagonal matrices in Equations (A1) and (A3) above, with the matrices $\mathbf{M}^{jj}$ (or the matrices $\mathbf{W}^{jj}$). Indeed, given that $(\mathbf{M}^{jj})_{lm} = \delta^{jl}\delta^{jm}$, we can write (for $i = 1, \ldots, N_c-1$)

$$H^i = \xi^i \left[\mathbf{M}^{ii} - \mathbf{M}^{(i+1)(i+1)} \right] \tag{A39}$$

so that

$$D^i = \sum_{j=1}^{N_c-1} R^{ij} \, \xi^j \left[\mathbf{M}^{jj} - \mathbf{M}^{(j+1)(j+1)} \right] \tag{A40}$$

and

$$t_C^i = v^\dagger D^i v = \sum_{j=1}^{N_c-1} R^{ij} \, \xi^j \left[\mathbf{W}^{jj} - \mathbf{W}^{(j+1)(j+1)} \right]. \tag{A41}$$

In particular, if we set $\xi^j = 1$ in Equation (A40) and we use the matrix R defined in Equation (A5), the matrices D^i recover the generalized diagonal Gell-Mann matrices, see

Equation (A6). It is interesting that, using the matrices $\mathbf{M}^{ij}$, we can easily define also the generalized nondiagonal Gell-Mann matrices (see again Appendix A1 in Ref. [15])

$$t^b = \mathbf{M}^{ij} + \mathbf{M}^{ji} \tag{A42}$$

and

$$t^b = -i\left(\mathbf{M}^{ij} - \mathbf{M}^{ji}\right), \tag{A43}$$

with $i, j = 1, \ldots, N_c$ and $i < j$. Note that there are $N_c(N_c-1)/2$ symmetric matrices (A42), $N_c(N_c-1)/2$ anti-symmetric matrices (A43), and N_c-1 diagonal matrices $t_C^i = D^i$, for a total of $N_c^2 - 1$ (Hermitian and traceless) generators.

The above results imply that the (generic) matrix

$$M_C \equiv \sum_{i=1}^{N_c-1} m^i\, t_C^i = \sum_{i=1}^{N_c-1} m^i \sum_{j=1}^{N_c-1} R^{ij}\, \xi^j \left[\mathbf{W}^{jj} - \mathbf{W}^{(j+1)(j+1)}\right], \tag{A44}$$

which is in the Cartan sub-algebra, can also be written as

$$M_C = \sum_{j=1}^{N_c} a^{jj}\, \mathbf{W}^{jj} \tag{A45}$$

with[62]

$$a^{jj} = \sum_{i=1}^{N_c-1} m^i \left[R^{ij}\, \xi^j - R^{i(j-1)}\, \xi^{j-1}\right]. \tag{A46}$$

However, one should stress that, on the l.h.s. of the above equation, the index j takes (integer) values in the interval $[1, N_c]$, while, on the r.h.s., the indices j and $j-1$ of R and of ξ are always restricted to the interval $[1, N_c - 1]$. This implies the relations

$$a^{11} = \sum_{i=1}^{N_c-1} m^i\, R^{i1}\, \xi^1 \tag{A47}$$

$$a^{22} = \sum_{i=1}^{N_c-1} m^i \left(R^{i2}\, \xi^2 - R^{i1}\, \xi^1\right) \tag{A48}$$

$$a^{33} = \sum_{i=1}^{N_c-1} m^i \left(R^{i3}\, \xi^3 - R^{i2}\, \xi^2\right) \tag{A49}$$

$$\ldots \tag{A50}$$

$$a^{(N_c-1)(N_c-1)} = \sum_{i=1}^{N_c-1} m^i \left[R^{i(N_c-1)}\, \xi^{N_c-1} - R^{i(N_c-2)}\, \xi^{N_c-2}\right] \tag{A51}$$

$$a^{N_c N_c} = -\sum_{i=1}^{N_c-1} m^i\, R^{i(N_c-1)}\, \xi^{N_c-1}, \tag{A52}$$

which trivially ensure the constraint (A31).

Notes

1 We stress that, in order to have periodicity for the original and for the gauge-transformed link configurations, we only need the gauge transformation to be periodic up to a *global* center element z_μ per direction (see [7]). We do not consider this possibility here.

2 One can easily show that the minimum value of $\mathcal{E}_U[h]$ is equal to zero, corresponding to $U_\mu(h;\vec{x}) = \mathbb{1}$.

3 Usually, in order to simplify the notation, the gauge-fixed link configuration $\{U_\mu(h;\vec{x})\}$ is redefined simply as $\{U_\mu(\vec{x})\}$. Here, however, we prefer to keep the dependence on the gauge transformation $\{h(\vec{x})\}$ explicit, for better comparison of the setup on the original lattice Λ_x with that attained on the extended lattice Λ_z (see Sections 3–5).

4 Equivalently, one could note, in Equation (9), that

$$\Re\,\mathrm{Tr}\Big[t^b U_\mu(h;\vec{x})/i\Big] \;=\; \Re\,\mathrm{Tr}\Big[t^b U_\mu(h;\vec{x})/i\Big]^\dagger \;=\; \Re\,\mathrm{Tr}\Big[-t^b U_\mu^\dagger(h;\vec{x})/i\Big]. \tag{17}$$

This allows us to write

$$\mathcal{E}_U[h]'(0) \;=\; \sum_{b,\,\mu,\,\vec{x}} \frac{2\,\gamma^b(\vec{x})}{N_c\,d\,V}\,\Re\,\mathrm{Tr}\left\{ t^b \left[\frac{U_\mu(h;\vec{x}) - U_\mu^\dagger(h;\vec{x})}{4\,i} - \frac{U_\mu(h;\vec{x}-\hat{e}_\mu) - U_\mu^\dagger(h;\vec{x}-\hat{e}_\mu)}{4\,i} \right] \right\}, \tag{18}$$

which naturally suggests the definition (10), see also Equation (15), for the (gauge-transformed) gauge field.

5 One could also take $k_\mu = -N/2, -N/2+1, \ldots, N/2-1$ for even N and $k_\mu = -(N-1)/2, -(N-3)/2, \ldots, (N-1)/2$ for odd N or, equivalently, $k_\mu = -\lfloor N/2 \rfloor, -\lfloor N/2 \rfloor + 1, \ldots, \lceil (N/2) - 1 \rceil$ for general N, where $\lfloor x \rfloor$ is the largest integer less than or equal to x and $\lceil x \rceil$ is the smallest integer greater than or equal to x. This convention, however, would make the formulae—and the corresponding numerical code—more cumbersome (see also notes 16 and 40).

6 Of course, it should be specified in all formulae that the gauge field relative to the lattice point $\vec{x}$ is actually evaluated at $\vec{x} + \hat{e}_\mu/2$, e.g., by writing $U_\mu(h;\vec{x}) \equiv \exp\left[i\,A_\mu(h;\vec{x}+\hat{e}_\mu/2)\right]$. This is especially relevant when considering the Fourier transform, as in Equation (24), and in the (lattice) weak-coupling expansion [17]. Here, however, in order to keep the notation simpler, we do not indicate this explicitly.

7 Note that the inequality (40) is linear in the updating matrix $r(\vec{x})$. This makes the minimization problem within the chosen approach rather simple.

8 Of course, in a numerical simulation, one should verify that these transformations of the link variables do not spoil their unitarity due to accumulation of roundoff errors.

9 Note that, compared to Refs. [19–21], here we have slightly changed the definition of Σ_Q, in order to have a quantity that is invariant under global gauge transformations.

10 This proof is equivalent to the usual proof that a continuity equation implies a conserved charge.

11 This, of course, implies that $\Delta\mathcal{E}$ is also invariant under global gauge transformations.

12 Here, in order to simplify the notation, we do not make explicit the dependence of the gluon propagator on the gauge transformation $\{h(\vec{x})\}$.

13 The formulae reported here are those usually employed in lattice numerical simulations. However, it is evident that, in the evaluation of these scalar functions, one could also make use of the off-diagonal Lorentz components of $D^{bb}_{\mu\nu}(\vec{x})$. The evaluation of these (off-diagonal) components can be useful for analyzing the breaking of rotational symmetry on the lattice [14].

14 The same invariance applies to the magnitude of the lattice momenta $p^2(\vec{k})$, see Equations (32) and (35).

15 Note that in [1] we referred to Λ_y as the "replica" lattice.

16 Here, in order to simplify the notation, we consider an even value for the integer m. For m odd, the integers k_μ take values in the interval $[-(m-1)/2, (m-1)/2]$. (See also note 5).

17 In particular, the explicit form of $\mathcal{H}_{\vec{k}}$ corresponds to a "shifted" kinetic term (by the momentum $\vec{k}$) plus the periodic potential $U(\vec{r})$, defined for the primitive cell [26].

18 Let us notice that the usual Gribov copies are defined for the extended lattice Λ_z by general local minima, obtained for different values of $\{\Theta_\mu\}$ and $\{h(\vec{x})\}$.

19 In this sense, right multiplication by v does *not* produce an equivalent solution, since $\{g(\vec{z})\}$ is not necessarily a solution to the gauge-fixing problem defined by applying a global gauge transformation v to the original link configuration, i.e., in general $\{g(\vec{z})\}$ does not minimize the functional $\mathcal{E}$ when the link configuration is $v\,U_\mu(\vec{z})\,v^\dagger$.

20 Clearly, these quantities are unaffected by a shift of the origin. Also, as discussed above, they are invariant under global gauge transformations. On the other hand, we are not considering here the possibility that nontrivially different solutions might have all identical numerical values for these quantities, when performing a numerical simulation.

21 Based on this analogy, it is natural that the matrices s_μ be characteristic of the considered solution $\{g(\vec{z})\}$.

22 Here, we used the definition $g^{ij}(\vec{z}) = w_i^\dagger\, g(\vec{z})\, w_j$, as in Equation (A30), and the property (A21) of the matrices Θ_μ. See also Equations (182) and (183).

23 At the same time, the gauge-fixed link configuration $\{U_\mu(g;\vec{z})\}$ can also be visualized as made up of m^d domains, related by block-rotations (see discussion in Sections 4 and 6).

24 This is discussed in detail in the next section.

25 But this is precisely what enlarges the set of solutions and allows a more efficient way to deal with the extended-lattice problem. As said at the end of the previous section, an approach closer to the one usually employed in condensed matter theory would require to consider a given (fixed) set of matrices Θ_μ and use the minimization procedure only to determine $h(\vec{x})$.

26 See also the comment in the last paragraph of Section 3.2.

27 Here we mean the property (20)–(21), i.e., the fact that the Landau-gauge condition—applied to the lattice gauge fields defined by the gauge-link configuration and now written for the (gauge-fixed) links on Λ_z—is satisfied. One of the goals of this section is to understand what this implies for the gauge field when restricted to the original lattice Λ_x.

28 Note that in Equations (120) and (122) the external factors, i.e., $\exp\left(\pm i \sum_{\nu=1}^{d} \Theta_\nu \, x_\nu / N\right)$, are the same. The implied expressions for $U_\mu(h;\vec{x})$ and $U_\mu(h;\vec{x}-\hat{e}_\mu)$ are clearly compatible with each other and in principle there is no need to define them separately. This is performed for later convenience since these expressions are used for the (gauge-fixed) gauge field entering the transversality condition. See, in Section 4.1, Equations (143), (152) or (153), and note 37.

29 However, in that case, one needs to satisfy the relation $\Omega_\mu \, \Omega_\nu = z_{\mu\nu} \, \Omega_\nu \, \Omega_\mu$, where the constants $z_{\mu\nu}$ are elements of the center of the group. Then, since the Θ_ν are commuting matrices, we have (in our case) the trivial condition $z_{\mu\nu} = 1$ for any μ and ν, i.e., no twist.

30 The proof follows the same steps explained in note 22.

31 We will address the transversality condition in detail in the next section. See also note 27.

32 Or, equivalently, with the periodic and not transverse configuration $\{U_\mu(h;\vec{x})\}$ obtained from the modified minimization problem (96), determined by the Θ_μ's.

33 The matrix elements of $h(\vec{x})$ and v are complex when considering the $\mathrm{SU}(N_c)$ gauge group. Here, we will consider separately the real and imaginary parts of $h_{ij}(\vec{x})$ and v_{ij}.

34 This is a similarity transformation which preserves the orthogonality relation (8) and the structure constants f^{abc} of the $su(N_c)$ Lie algebra. Moreover, it does not change the Cartan generators $\{t_c^b\}$ (see Appendix A), which trivially commute with the Θ_μ matrices.

35 See also the beginning of Section 6, where it is stressed that, in the numerical code, it is more natural to save the values of $U_\mu(h;\vec{x})$ and Θ_μ, instead of the values of $U_\mu(l;\vec{x})$.

36 Clearly, the value of $\mathcal{N}_{p,m}$ is independent of the way in which we write the gauge transformation $\{g(\vec{z})\}$, i.e., as a Bloch function or as a general transformation, as long as $g(\vec{z}) \in \mathrm{SU}(N_c)$.

37 Clearly, similar expressions hold for $A_\mu(g;\vec{x}+\vec{y}N-\hat{e}_\mu)$, which can be written in terms of $U_\mu(l;\vec{x}-\hat{e}_\mu)$ or of $A_\mu(l;\vec{x}-\hat{e}_\mu)$, see Equations (122) and (140).

38 We stress that, even though we are using here the same index b to denote the color components with respect to the generators t^b of the Lie algebra, the constraint in Equation (163) is written in terms of color components with respect to the Cartan generators t_c^b. The same holds for the color components of $Q_\mu(l)$ and $A_\mu(l;\vec{x})$ in the Equations (164) and below.

39 Equivalently, we can say that we write the matrix $U_\mu(g;\vec{z})$ as a linear combination of the matrices $\mathbf{W}^{ij} = w_i \, w_j^\dagger = v^\dagger \, \mathbf{M}^{ij} \, v$, introduced in Appendix A.2. This yields

$$U_\mu(g;\vec{z}) \;=\; \sum_{i,j=1}^{N_c} U_\mu^{ij}(g;\vec{z}) \, \mathbf{W}^{ij} \;=\; v^\dagger \left\{ \sum_{i,j=1}^{N_c} U_\mu^{ij}(g;\vec{z}) \, \mathbf{M}^{ij} \right\} v. \tag{180}$$

40 One should also note that, if instead of the nonsymmetric interval $[0, mN-1]$ one contemplates the symmetric interval $k'_\nu \in [-(mN/2), (mN/2)-1]$ for mN even (see note 5 for the general case), this decomposition applies with $k_\nu \in [-(m/2), (m/2)-1]$ and $K_\nu \in [-(N-1)/2, (N-1)/2]$, at least for m even and N odd, and with slightly different formulae for m odd and/or N even. Thus, the use of the nonsymmetric interval (around the origin) makes our notation much simpler and straightforward.

41 Here, we suppose that the integers n_ν^j and n_ν^i have been fixed, either by the numerical minimization of $\mathcal{E}_{U,\Theta}[h]$ or set a priori (as in the case of fixed matrices Θ_μ).

42 Of course, the values of k_ν and χ_ν also depend on the (considered) indices i, j. Here, however, in order to simplify the notation, we do not make this dependence explicit. More specifically, we could define

$$\chi_\nu \;=\; \frac{\mathrm{sgn}(\bar{n}_\nu^j - \bar{n}_\nu^i) \left[1 + \mathrm{sgn}(\bar{n}_\nu^j - \bar{n}_\nu^i)\right]}{2} \, m, \tag{195}$$

after the phases n_ν^j have been chosen, and then pick k_ν given by Equation (194) for every ν, in order to obtain nonzero coefficients $\widetilde{U}_\mu^{ij}(g;\vec{k}'/m)$ in Equation (189). In the above expression we indicate with $\mathrm{sgn}(x)$ the sign function, which has values ± 1 or zero according to whether $x \lesseqgtr 0$.

43 Here, we call "diagonal" the coefficients with $i = j$—when using the basis $\{\mathbf{W}^{ij}\}$ — even though these coefficients do not necessarily contribute to the diagonal elements of the corresponding matrix, given that $(\mathbf{W}^{jj})_{lm} = v^*_{jl}\, v_{jm}$, see Equation (A37). On the other hand, all entries of the matrix $\mathbf{M}^{jj} = v\,\mathbf{W}^{jj}\,v^\dagger = \hat{e}_j\,\hat{e}_j^\dagger$ are null with the exception of the diagonal entry with indices jj (which is equal to one).

44 We stress that this is the result expected from condensed matter physics, where the Fourier transform of the periodic potential $U(\vec{r})$ is nonzero only when considering wave-number vectors on the reciprocal lattice (see the second proof of Bloch's theorem in Ref. [26]).

45 On the other hand, this result applies only approximately when considering a generic coefficient $\widetilde{U}^{ij}_\mu(g;\vec{k}')$ for which $k_\nu \neq 0$. As a matter of fact, if $\pi k_\nu \ll mN$ (recall that $k_\nu \in [0, m-1]$), we have

$$p_\nu(\vec{k}') \,\equiv\, 2\,\sin\left(\frac{\pi\,k'_\nu}{mN}\right) \,=\, 2\,\sin\left[\frac{\pi\,(k_\nu + K_\nu m)}{mN}\right] \,\approx\, 2\,\sin\left(\frac{\pi\,K_\nu}{N}\right). \tag{204}$$

46 Recall that $\bar{n}^j_\nu$ and $\bar{n}^i_\nu$ take values $0, 1, \ldots, m-1$, so that their difference is an integer number in the interval $[-m+1, m-1]$.

47 Note that $U_\mu(g;\vec{z})$ is a unitary matrix, which is written here in terms of the basis $\{\mathbf{W}^{ij}\}$.

48 Of course, once the nonzero coefficients $\widetilde{A}^{ij}_\mu(g;\vec{k}')$ have been evaluated, one can also obtain the color components $\widetilde{A}^b_\mu(g;\vec{k}')$ with respect to the generators $\{t^b\}$ using the relation

$$\widetilde{A}^b_\mu(g;\vec{k}') \,=\, \sum_{i,j=1}^{N_c} \widetilde{A}^{ij}_\mu(g;\vec{k}')\,\frac{\mathrm{Tr}}{2}\left(t^b\,\mathbf{W}^{ij}\right). \tag{224}$$

49 Of course, in this case the plot resembles a "continuum spectrum".

50 By looking at the matrix elements ${T_\mu}^{jj}$, it is clear that the integers n^j_μ can always be limited to the interval $[0, mN-1]$. Then, in the limit $m \to +\infty$, the parameters n^j_μ/mN are real numbers belonging to the interval $[0, 1)$.

51 Following Ref. [34] one can prove that the quantity

$$\mathcal{M} \,=\, \frac{1}{d\,(N_c^2-1)m^d}\sum_{b,\mu}\left\langle\,\left|\sum_{\vec{y}} M^b_\mu(\vec{y})\right|\,\right\rangle \tag{250}$$

should vanish—in Landau gauge and in the infinite-volume limit—at least as fast as the inverse lattice side. The volume dependence of $\mathcal{M}$ has been analyzed in detail in two, three and four space-time dimensions in Ref. [35].

52 To this end, it may be useful to move part of the simulation from CPUs to GPUs. For example, this may allow a systematic investigation of the gluon propagator's dependence on the possible choices for the Θ_μ matrices, as well as a more detailed study of the zero-momentum discontinuity of the propagator at large values of m.

53 Let us point out that this is the same notation as the one used in the main text for the unit vectors in the d-dimensional Euclidean space, but clearly we refer here to color indices (in the fundamental representation).

54 Equivalently, we can use Equation (A3) with the matrix

$$R \,=\, \begin{pmatrix} 1 & 0 & 0 & 0 & \ldots \\ \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{3}} & 0 & 0 & \ldots \\ \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{3}{\sqrt{6}} & 0 & \ldots \\ \frac{1}{\sqrt{10}} & \frac{2}{\sqrt{10}} & \frac{3}{\sqrt{10}} & \frac{4}{\sqrt{10}} & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}, \tag{A5}$$

i.e., with matrix elements $R^{il} = l\,\sqrt{\frac{2}{i(i+1)}}$ for $l \leq i$ and $R^{il} = 0$ otherwise.

55 For the choice in Equation (A6) we have the matrix elements $D^i_{jj} = \sqrt{\frac{2}{i(i+1)}}\,\xi^1$ for $j = 1$, $D^i_{jj} = \sqrt{\frac{2}{i(i+1)}}\left[j\xi^j - (j-1)\xi^{j-1}\right]$ for $j = 2, \ldots, i$, $D^i_{jj} = -i\,\xi^i\sqrt{\frac{2}{i(i+1)}}$ for $j = i+1$, and $D^i_{jj} = 0$ otherwise.

56 We recall that each vector α_j, with components α^i_j, corresponds to a *weight* (of the Cartan generators) [13,38,39].

57 Indeed, in this case, considering the vector components θ^a_μ and θ^a_ν, with $a = 1, 2, 3$, the expression in Equation (A10) corresponds to $\vec{\theta}_\mu \times \vec{\theta}_\nu = 0$, where $\times$ indicates the usual cross product.

58 This is a general result: any element of the $su(N_c)$ Lie algebra is conjugate to an element of a Cartan sub-algebra (see, for example, [39] and references therein). In the case of the SU(2) group, one can check this directly if t^c are the three Pauli matrices σ_c.

Indeed, by writing v as $v_0 \mathbb{1} + i\vec{\sigma} \cdot \vec{v}$, where $\mathbb{1}$ is the 2×2 identity matrix and $v_0^2 + \vec{v}^2 = 1$, one recovers Equation (A11)—starting from Equation (A12)—by using the relation

$$\sigma_i \sigma_j = \mathbb{1}\, \delta^{ij} + i \sum_{k=1}^{3} \epsilon^{ijk} \sigma_k . \tag{A13}$$

59 In other words, all the entries of $\mathbf{M}^{ij}$ are null with the exception of the entry with indices i, j, which is equal to 1.

60 Of course, similar expressions apply to the basis $\mathbf{M}^{ij} = \hat{e}_i \, \hat{e}_j^\dagger$.

61 The property

$$\mathbf{W}^{ij\,\dagger} = \mathbf{W}^{ji} \tag{A28}$$

can be seen directly from the definition (A22). Thus, we see that each matrix $\mathbf{W}^{ij}$ is *not* Hermitian, unless $i = j$.

62 A linear relation among the coefficients a^{jj} and m^i is, of course, expected for any change of basis in the Cartan sub-algebra.

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