Bloch Waves in Minimal Landau Gauge and the Infinite-Volume Limit of Lattice Gauge Theory

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By exploiting the similarity between Bloch’s theorem for electrons in crystalline solids and the problem of Landau gauge-fixing in Yang-Mills theory on a “replicated” lattice, one is able to obtain essentially infinite-volume results from numerical simulations performed on a relatively small lattice. This approach, proposed by D. Zwanziger in [1], corresponds to taking the infinite-volume limit for Landau-gauge field configurations in two steps: firstly for the gauge transformation alone, while keeping the lattice volume finite, and secondly for the gauge-field configuration itself. The solutions to the gauge-fixing condition are then given in terms of Bloch waves. Applying the method to data from Monte Carlo simulations of pure SU(2) gauge theory in two and three space-time dimensions, we are able to evaluate the Landau-gauge gluon propagator for lattices of linear extent up to sixteen times larger than that of the simulated lattice. The approach is reminiscent of Fisher and Ruelle’s construction of the thermodynamic limit in classical statistical mechanics.

I. INTRODUCTION

Since 2007 [2, 3], we know that very large (physical) volumes are required in lattice simulations of Yang-Mills theories in minimal Landau gauge if one wishes to uncover the true infrared behavior of Green’s functions, a topic that has attracted much attention in the past two decades [4]. Indeed, due to the generation of a dynamical mass $m_g$ of a few hundred MeV in the gluon sector (see [5–7] and references therein), one must reach momenta $p$ as small as 50 MeV in order to generate a result similar to Bloch’s theorem for crystalline solids. An ideal crystalline solid in $d$ dimensions is (geometrically) defined by a Bravais lattice [10]: an infinite set of points $\vec{R} = n_\mu \vec{a}_\mu$, where $n_\mu \in \mathbb{Z}$ (with $\mu = 1, \ldots, d$), $\vec{a}_\mu$ are $d$ linearly independent vectors, and the sum over repeated indices is understood. For Bloch’s theorem one also considers an electrostatic potential $U(\vec{r})$, due to the ions of the solid, with the periodicity of the Bravais lattice, i.e. $U(\vec{r}) = U(\vec{r} + \vec{R})$ for any Bravais-lattice vector $\vec{R}$. The corresponding Hamiltonian $\mathcal{H}$ for a single electron is then invariant under translations by $\vec{R}$ — represented by the operators $\mathcal{T}(\vec{R})$ — and we can choose the eigenstates $\psi(\vec{r})$ of $\mathcal{H}$ to be also eigenstates of $\mathcal{T}(\vec{R})$. Now, since

$$\mathcal{T}(\vec{R}) \mathcal{T}(\vec{R}^\prime) = \mathcal{T}(\vec{R} + \vec{R}^\prime) = \mathcal{T}(\vec{R}) \mathcal{T}(\vec{R}^\prime), \quad (1)$$

the corresponding setup allows one to prove a result similar to Bloch’s theorem for crystalline solids. As a consequence, even though one deals with gauge transformations on the extended lattice, the numerical gauge fixing is actually done on the original (small) lattice. The obtained gauge transformation is then used to evaluate a Landau-gauge gluon propagator for lattices of linear extent up to sixteen times larger than that of the simulated lattice. The approach is reminiscent of Fisher and Ruelle’s construction of the thermodynamic limit in classical statistical mechanics.

II. BLOCH WAVES

An ideal crystalline solid in $d$ dimensions is (geometrically) defined by a Bravais lattice [10]: an infinite set of points $\vec{R} = n_\mu \vec{a}_\mu$, where $n_\mu \in \mathbb{Z}$ (with $\mu = 1, \ldots, d$), $\vec{a}_\mu$ are $d$ linearly independent vectors, and the sum over repeated indices is understood. For Bloch’s theorem one also considers an electrostatic potential $U(\vec{r})$, due to the ions of the solid, with the periodicity of the Bravais lattice, i.e. $U(\vec{r}) = U(\vec{r} + \vec{R})$ for any Bravais-lattice vector $\vec{R}$. The corresponding Hamiltonian $\mathcal{H}$ for a single electron is then invariant under translations by $\vec{R}$ — represented by the operators $\mathcal{T}(\vec{R})$ — and we can choose the eigenstates $\psi(\vec{r})$ of $\mathcal{H}$ to be also eigenstates of $\mathcal{T}(\vec{R})$. Now, since

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first Brillouin zone. As a consequence, the eigenstates \( \psi(\vec{r}) \) can be written as Bloch waves

\[
\psi_G(\vec{r}) = \exp(i\vec{k} \cdot \vec{r}) h_G(\vec{r}),
\]

where the functions \( h_G(\vec{r}) \) have the periodicity of the Bravais lattice, i.e. \( h_G(\vec{r} + \vec{R}) = h_G(\vec{r}) \).

Let us now consider a thermalized link configuration \( \{U_\mu(\vec{x})\} \), for the SU(\( N_c \)) gauge group in \( d \) dimensions, defined on a lattice \( \Lambda_x \) with volume \( V = N^d \) and periodic boundary conditions (PBC). Then, following Ref. \( \text{[1]} \), we extend \( \Lambda_x \) by replicating it \( m \) times along each direction, yielding an extended lattice \( \Lambda_z \), with lattice volume \( m^dV \) and PBC. Let us note that a similar idea has been recently used in Ref. \( \text{[11]} \) in order to include infinite-volume QED effects into a finite QCD system. We indicate the points of \( \Lambda_x \) with

\[
\vec{z} = \vec{x} + \vec{y}N,
\]

where \( \vec{x} \in \Lambda_x \) and \( \vec{y} \) belongs to the replica lattice \( \Lambda_y \), \( y_\mu = 0, \ldots, m - 1 \). By construction, \( \{U_\mu(\vec{z})\} \) is invariant under translation by \( N \) in any direction.

We now impose the minimal-Landau-gauge condition on \( \Lambda_z \), i.e. we consider the minimizing functional

\[
\mathcal{E}_U[g] = -\frac{\Re \text{ Tr}}{dN_c m^dV} \sum_{\mu=1}^d \sum_{\vec{z} \in \Lambda_z} g(\vec{z}) U_\mu(\vec{z}) g(\vec{z} + \hat{e}_\mu)^\dagger,
\]

(4)

where \( g(\vec{z}) \) are SU(\( N_c \)) matrices, \( \hat{e}_\mu \) is a unit vector in the \( \mu \) direction, \( \Re \text{ Tr} \) indicates the real part of the trace and \( \dagger \) stands for the Hermitian conjugate. Also, the minimization is done with respect to the gauge transformation \( \{g(\vec{z})\} \), with the link configuration \( \{U_\mu(\vec{z})\} \) kept fixed. The resulting gauge-fixed field configuration is transverse on \( \Lambda_z \). Note that for \( \{g(\vec{z})\} \) we take PBC on \( \Lambda_z \), i.e. \( g(\vec{z}) = g(\vec{z} + mN\hat{e}_\mu) \) for \( \mu = 1, \ldots, d \).

The analogy of the above minimization problem with the setup for Bloch’s theorem is evident: \( \Lambda_y \) is a finite Bravais lattice with PBC and the thermalized lattice configuration \( \{U_\mu(\vec{z})\} \) corresponds to the periodic electrostatic potential \( U(\vec{r}) \). It is then not surprising that one can prove \( \text{[1]} \), in analogy with Eq. (2), that the gauge transformation \( g(\vec{z}) \) that yields a given local minimum of \( \mathcal{E}_U[g] \) can be written as

\[
g(\vec{z}) = e^{i\Theta_\mu z_\mu/N} h(\vec{z}) = e^{i\Theta_\mu z_\mu/N} h(\vec{x}),
\]

(5)

where we make explicit that \( h(\vec{z}) \in \text{SU}(N_c) \) is invariant under a shift by \( N \), i.e. \( h(\vec{z} + N\hat{e}_\mu) = h(\vec{z}) \). Here, the vectors \( \vec{z} \) and \( \vec{x} \) are related through Eq. (3) and the matrices \( \Theta_\mu \) —having eigenvalues \( 2\pi n_\mu/m \) (with \( n_\mu \in \mathbb{Z} \))—can be written as \( \tau^a\theta^a_\mu \) (with \( a = 1, \ldots, N_c - 1 \)), where the \( \tau^a \) belong to a Cartan sub-algebra of the SU(\( N_c \)) Lie algebra. It is important to note that, due to Eq. (5) and to cyclicity of the trace, the minimizing functional \( \mathcal{E}_U[g] \) in Eq. (4) becomes

\[
\mathcal{E}_U[g] = -\frac{\Re \text{ Tr}}{dN_c V} \sum_{\mu=1}^d e^{-i\Theta_\mu/N} Q_\mu,
\]

(6)

\[
Q_\mu = \sum_{\vec{z} \in \Lambda_z} h(\vec{x}) U_\mu(\vec{z}) h(\vec{x} + \hat{e}_\mu)^\dagger,
\]

(7)

e.i. the numerical minimization, which now includes extended gauge transformations, can still be carried out on the original lattice \( \Lambda_x \).

The proof of Eq. (6) is quite similar—see Appendix F of Ref. \( \text{[1]} \)—to the proof of Bloch’s theorem. Indeed, the minimizing problem (4) is clearly invariant if we consider a shift of the lattice sites \( \vec{z} \) by \( N \) in any direction \( \hat{e}_\mu \), since this amounts to a simple redefinition of the origin for \( \Lambda_z \). Note also that, due to cyclicity of the trace, \( \mathcal{E}_U[g] \) is invariant under (left) global transformations and thus \( \{g(\vec{z})\} \) is determined modulo a global transformation. As a result, if \( \{g(\vec{z})\} \) is unique (see discussion below), we must have

\[
T(N\hat{e}_\mu) g(\vec{z}) = g(\vec{z} + N\hat{e}_\mu) = \lambda_\mu g(\vec{z}),
\]

(8)

where \( \lambda_\mu \) is a \( \vec{z} \)-independent SU(\( N_c \)) matrix. At the same time, by using the relation (1) for the translation operators, we obtain that the \( \lambda_\mu \)'s are commuting matrices, i.e. they can be written as \( \exp(i\Theta_\mu) = \exp(i\tau^a\theta^a_\mu) \), where the \( \tau^a \) matrices are Cartan generators. Then, by using Eq. (3) and applying Eq. (8) iteratively, we find

\[
g(\vec{z}) = \exp(i\Theta_\mu y_\mu) g(\vec{x}),
\]

(9)

where the gauge transformation \( g(\vec{x}) \) is defined on the first lattice \( \Lambda_x \) of \( \Lambda_z \) (corresponding to \( y_\mu = 0 \) for all directions \( \mu \)). Thus, Eq. (5) is immediately obtained if one writes

\[
g(\vec{x}) \equiv \exp(i\Theta_\mu x_\mu/N) h(\vec{x}),
\]

(10)
yielding Eqs. (1) and (7). Moreover, due to the PBC for \( \Lambda_z \), we need to impose the conditions \( \exp(i\Theta_\mu)^m = 1 \), where \( 1 \) is the identity matrix. Clearly, these conditions are satisfied if the eigenvalues of the matrices \( \Theta_\mu \) are of the type \( 2\pi n_\mu/m \), with \( n_\mu \in \mathbb{Z} \).

In the SU(2) case, considered here, a Cartan sub-algebra is one-dimensional and, by taking the third Pauli matrix \( \sigma_3 \) as the Cartan generator, one can write
the most general gauge transformation \( \Theta_\mu = 2\pi(v^\dagger \sigma_3 v) n_\mu/m \) with \( v \in SU(2) \).

Before presenting the numerical results obtained with the new approach described above, let us discuss the hypothesis of uniqueness for the gauge transformation \( \{g(z)\} \), which is essential for Eq. (8) to be valid. In Ref. [1] the gauge fixing on \( \Lambda \) is considered only for the absolute minima of the minimizing functional, belonging to the interior of the so-called fundamental modular region. Since these minima are proven to be unique (see Appendix A of the same reference), the implicit assumption made in [1] is that the gauge transformation \( \{g(z)\} \) that connects the unfixed, thermalized configuration \( \{U_\mu(z)\} \) to the (gauge-fixed) absolute minimum \( \{U_\mu^{(g)}(z)\} \) is also unique, modulo a global transformation, thus implying Eq. (8). However, the same hypothesis also applies to a specific local minimum. Indeed, even though local minima can be degenerate, a specific realization of one of these minima also requires a specific and unique \( \{g(z)\} \) (up to a global transformation) when starting from a given \( \{U_\mu(z)\} \).

III. NUMERICAL SIMULATIONS

From the practical point of view, the minimization of the functional \( \mathcal{E}_U[g] \), defined in Eqs. (6) and (7), can be done recursively, using two alternating steps: a) the matrices \( \Theta_\mu \) are kept fixed as one updates the matrices \( h(\vec{x}) \) by sweeping through the lattice using a standard gauge-fixing algorithm [12] and b) the matrices \( Q_\mu \) are kept fixed as one minimizes \( \mathcal{E}_U[g] \) with respect to the matrices \( \Theta_\mu \), belonging to the corresponding Cartan sub-algebra. After the gauge fixing is completed, one can evaluate the gauge-transformed link variables \( U_\mu^{(g)}(z) = g(z) U_\mu(z) g(z + \epsilon_\mu)^\dagger \). Then, considering Eqs. (9) and (10), and the invariance of the link configuration \( \{U_\mu(z)\} \) under translation by \( N \), it is clear that the dependence of \( U_\mu^{(g)}(z) \) on the \( y_\mu \) coordinates is rather trivial. As a consequence, the gluon propagator evaluated with extended gauge transformations is nonzero only for a subset of the lattice momenta available on the extended \( \Lambda z \) lattice [13].

Here we present data for the two- and the three-dimensional cases, for which it is feasible to simulate at considerably large lattice volumes (without the use of extended gauge transformations). This allows a comparison of the new approach with the traditional method at small momenta, for which finite-size effects are larger.

Indeed, such effects are strongest in the \( d = 2 \) case, since the gluon propagator is of the scaling type [7, 8, 14], i.e. \( \mathcal{D}(0) = 0 \) in the infinite-volume limit. The effects are also very large in the \( d = 3 \) case, for which the gluon propagator is of the massive type [3, 7] but with a clear and pronounced turnover point at small momenta [5, 7].

As one can see in Fig. 1, the results obtained for an extended lattice \( \Lambda z \) show very good agreement with the
IV. CONCLUSIONS

We have investigated an analogue of Bloch’s theorem for (lattice) Landau gauge-fixing [1], which arises because the Landau-gauge condition leaves a residual global transformation unfixed. We find that, at least in the gluon sector, numerical results for large lattice volumes can be reproduced by simulations at much smaller volumes with extended gauge transformations, thus reducing memory usage by a huge factor (at least up to 16d for d = 2, 3). The only limitation of the approach in its present form is that the allowed momenta are set by the discretization on the original (small) lattice Λx (see Fig. 1 and discussion in the previous section).

As observed for the limiting sequence of domains in the construction of infinite-volume statistical mechanics [15], our results show that the information encoded in a thermalized gauge-field configuration does not depend much on the (original) lattice volume V considered. As a consequence, the properties of Landau-gauge Green’s functions are essentially determined by the gauge-fixing procedure and, in this case, the size of the (extended) lattice volume matters! Let us note that another illustration of the nontrivial role of gauge-fixing is the fact that the lattice Landau-gauge gluon propagator at β = 0, i.e. for a completely random link configuration \{U_\mu(\vec{x})\}, shows qualitative agreement with the one at nonzero β [16].

More results and details of the numerical simulations presented here will be discussed elsewhere [13]. We also plan to extend our study of Green’s functions using extended gauge transformations to the ghost sector, investigating the impact on properties of the first Gribov region, and to the matter sector. A possible improvement of the approach is the use of continuous external momenta [17], which could make the method more attractive in the d = 4 case.

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