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, we show that large-volume results can be reproduced by simulations performed on much smaller lattices. This approach, proposed by Zwanziger [Nucl. Phys. **B412**, 657 (1994)], corresponds to taking the infinite-volume limit for Landau-gauge field configurations in two steps: first for the gauge transformation alone, while keeping the lattice volume finite, and second 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 16 times larger than that of the simulated lattice. This approach is reminiscent of the Fisher-Ruelle construction of the thermodynamic limit in classical statistical mechanics.

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Introduction.—Since 2007 [1,2], we have known that very large (physical) volumes are required in lattice simulations of Yang-Mills theories in the 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 [3]. Indeed, due to the generation of a dynamical mass m_g of a few hundred MeV in the gluon sector (see Refs. [4–6] and references therein), one must reach momenta p as small as 50 MeV in order to generate data at $p \ll m_g$, allowing a good description of gluonic correlation functions in the infrared limit. Since the smallest momentum on a lattice with N points per direction is $2a^{-1} \sin(\pi/N)$, where a is the lattice spacing, the above requisite implies an unfeasibly large lattice side of about 250 points (for $a \approx 0.1$ fm). Alternatively, one needs good control of the extrapolation of the data to infinite volume. A step in this direction was the consideration of exact (upper and lower) bounds for gluon and ghost propagators [7,8], which can help in extrapolating the numerical data to large lattice volumes.

In this work, following Zwanziger's idea [9], we present a new approach, based on taking the infinite-volume limit for a Landau-gauge transformation applied to a (replicated) thermalized field configuration at a given volume V. 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 extended gauge transformation is then used to obtain a Landau-gauge-fixed gluon-field configuration and to evaluate the gluon propagator in momentum space $D(p^2)$.

The Letter is organized as follows. In the next section, we briefly review Bloch's theorem and discuss the idea presented in Ref. [9]. We then show our preliminary numerical results and, in the last section, we draw our conclusions.

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 $n_\mu \in \mathcal{Z}$ (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

$$\mathcal{T}(\vec{R})\mathcal{T}(\vec{R}') = \mathcal{T}(\vec{R}')\mathcal{T}(\vec{R}) = \mathcal{T}(\vec{R} + \vec{R}'), \tag{1}$$

$\mathcal{T}(\vec{R})$ has eigenvalues $\exp(i\vec{k} \cdot \vec{R}) = \exp(2\pi i k_\nu n_\nu)$, i.e., $\mathcal{T}(\vec{R})\psi(\vec{r}) = \psi(\vec{r} + \vec{R}) = \exp(i\vec{k} \cdot \vec{R})\psi(\vec{r})$. Here $\vec{k} = k_\nu \vec{b}_\nu$ is a vector of the reciprocal lattice: $k_\nu \in \mathcal{Z}$ (with $\nu = 1, \ldots, d$) and $\vec{a}_\mu \cdot \vec{b}_\nu = 2\pi\delta_{\mu\nu}$, usually restricted to the first Brillouin zone. As a consequence, the eigenstates $\psi(\vec{r})$ can be written as Bloch waves

$$\psi_{\vec{k}}(\vec{r}) = \exp(i\vec{k} \cdot \vec{r}) h_{\vec{k}}(\vec{r}), \tag{2}$$

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

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 Λ_x with volume $V = N^d$ and periodic boundary conditions (PBCs). Then, following Ref. [9], we extend Λ_x by replicating it m times along each direction, yielding an extended lattice Λ_z, with lattice volume $m^d V$ and PBCs [11]. We indicate the points of Λ_z with

$$\vec{z} = \vec{x} + \vec{y}N, \tag{3}$$

where $\vec{x} \in \Lambda_x$ and $\vec{y}$ belongs to the *replica lattice* Λ_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 Λ_z; i.e., we consider the minimizing functional

$$\mathcal{E}_U[g] = -\frac{\Re\mathrm{Tr}}{dN_c m^d V} \sum_{\mu=1}^{d} \sum_{\vec{z}\in\Lambda_z} g(\vec{z}) U_\mu(\vec{z}) g(\vec{z}+\hat{e}_\mu)^\dagger, \tag{4}$$

where $g(\vec{z})$ are $\mathrm{SU}(N_c)$ matrices, $\hat{e}_\mu$ is a unit vector in the μ direction, $\Re\mathrm{Tr}$ indicates the real part of the trace and † 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 Λ_z. Note that for $\{g(\vec{z})\}$ we take PBCs on Λ_z.

The analogy of the above minimization problem with the setup for Bloch's theorem is evident: Λ_y is a finite Bravais lattice with PBCs 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 [9], 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

$$g(\vec{z}) = e^{i\Theta_\mu z_\mu/N} h(\vec{z}) = e^{i\Theta_\mu z_\mu/N} h(\vec{x}), \tag{5}$$

where we make explicit that $h(\vec{z}) \in \mathrm{SU}(N_c)$ 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 Θ_μ—having eigenvalues $2\pi n_\mu/m$ (with $n_\mu \in \mathcal{Z}$)—can be written as $\tau^a\theta^a_\mu$ (with $a = 1, \ldots, N_c - 1$), where the τ^a belong to a Cartan subalgebra of the $\mathrm{SU}(N_c)$ 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

$$\mathcal{E}_U[g] = -\frac{\Re\mathrm{Tr}}{dN_c V} \sum_{\mu=1}^{d} e^{-i\Theta_\mu/N} Q_\mu, \tag{6}$$

$$Q_\mu = \sum_{\vec{x}\in\Lambda_x} h(\vec{x}) U_\mu(\vec{x}) h(\vec{x}+\hat{e}_\mu)^\dagger, \tag{7}$$

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

The proof of Eq. (5) is quite similar—see Appendix F of Ref. [9]—to the proof of Bloch's theorem. Indeed, the minimizing problem, Eq. (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 redefinition of the origin for Λ_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

$$\mathcal{T}(N\hat{e}_\mu) g(\vec{z}) = g(\vec{z}+N\hat{e}_\mu) = \lambda_\mu g(\vec{z}), \tag{8}$$

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

$$g(\vec{z}) = \exp(i\Theta_\mu y_\mu) g(\vec{x}), \tag{9}$$

where the gauge transformation $g(\vec{x})$ is defined on the first lattice Λ_x of Λ_z (corresponding to $y_\mu = 0$, $\forall\mu$). Thus, Eq. (5) is immediately obtained if one writes

$$g(\vec{x}) \equiv \exp(i\Theta_\mu x_\mu/N) h(\vec{x}), \tag{10}$$

yielding Eqs. (6) and (7). Moreover, due to the PBCs for Λ_z, we need to impose the conditions $[\exp(i\Theta_\mu)]^m = \mathbb{1}$, where $\mathbb{1}$ is the identity matrix. Clearly, these conditions are satisfied if the eigenvalues of the matrices Θ_μ are of the type $2\pi n_\mu/m$, with $n_\mu \in \mathcal{Z}$. In the SU(2) case, considered here, a Cartan subalgebra is one dimensional and, by taking the third Pauli matrix σ_3 as the Cartan generator, one can write [9] the most general gauge transformation, Eq. (5), as $\Theta_\mu = 2\pi(v^\dagger\sigma_3 v)n_\mu/m$ with $v \in \mathrm{SU}(2)$.

Before presenting the numerical results obtained with the new approach described above, let us discuss the hypothesis of uniqueness for the gauge transformation $\{g(\vec{z})\}$, which is essential for Eq. (8) to be valid. In Ref. [9] the gauge fixing on Λ_z 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 unique (see proof in the Appendix A of the same reference), the implicit assumption made in Ref. [9] is that the gauge transformation $\{g(\vec{z})\}$ that connects the unfixed, thermalized configuration $\{U_\mu(\vec{z})\}$ to the (gauge-fixed) absolute minimum $\{U^{(g)}_\mu(\vec{z})\}$ 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

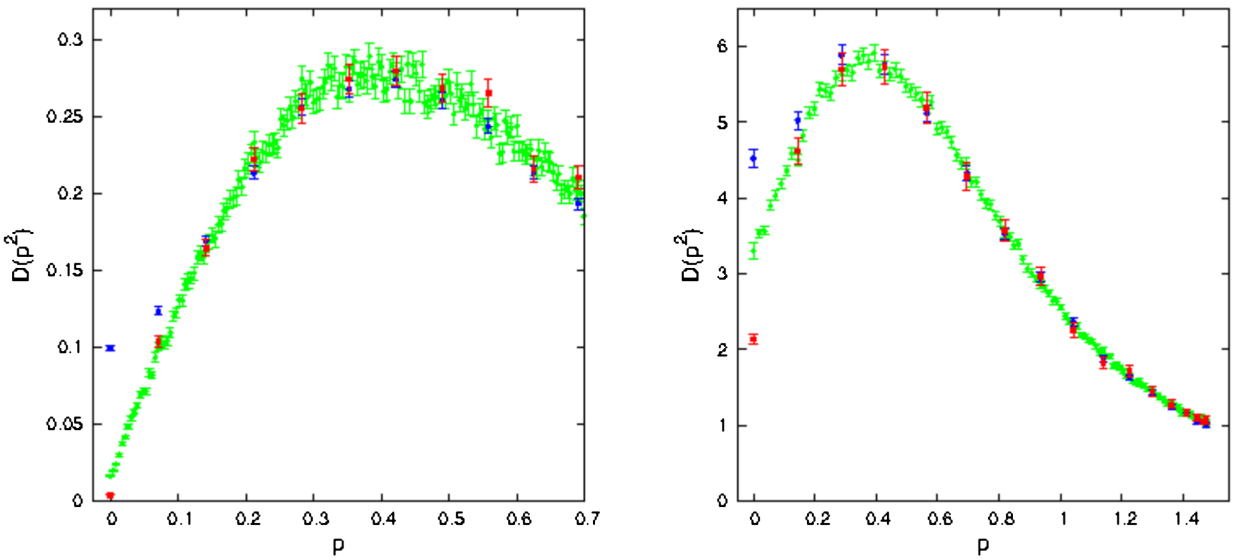

FIG. 1. The gluon propagator $D(p^2)$ as a function of the lattice momentum p. Left: $d = 2$ case with $\beta = 10.0$, considering original Λ_x lattice volumes 80^2 (filled circle) and 1280^2 (filled diamond), and an extended Λ_z lattice volume $80^2 \times 16^2 = 1280^2$ (filled square). Right: $d = 3$ case with $\beta = 3.0$, considering original Λ_x lattice volumes 32^3 (filled circle) and 256^3 (filled diamond) and an extended Λ_z lattice volume $32^3 \times 8^3 = 256^3$ (filled square). Note that the data for $\Lambda_x = 1280^2$ at $\beta = 10.0$ and for $\Lambda_x = 256^3$ at $\beta = 3.0$ are, essentially, infinite-volume results [2,4,6,7,14]. We also note that the strong suppression of $D(0)$ is a peculiar effect of the extended gauge transformations [13].

minima also requires a specific and unique $\{g(\vec{z})\}$ (up to a global transformation) when starting from a given $\{U_\mu(\vec{z})\}$.

Numerical simulations.—The numerical minimization of the functional $\mathcal{E}_U[g]$, defined in Eqs. (6) and (7), can be done recursively, using two alternating steps: (i) 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 [12] and (ii) the matrices Q_μ are kept fixed as one minimizes $\mathcal{E}_U[g]$ with respect to the matrices Θ_μ, belonging to the corresponding Cartan subalgebra. After the gauge fixing is completed, one can evaluate the gauge-transformed link variables $U_\mu^{(g)}(\vec{z}) = g(\vec{z}) U_\mu(\vec{z}) g(\vec{z} + \hat{e}_\mu)^\dagger$. Then, considering Eqs. (9) and (10), and the invariance of $U_\mu(\vec{z})$ under translation by N, it is clear that the dependence of $U_\mu^{(g)}(\vec{z})$ on the y_μ 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 Λ_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 [6,7,14], i.e., $D(0) = 0$ 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 [2,6] but with a clear and pronounced turnover point at small momenta [4,6].

As one can see in Fig. 1, the results obtained for an extended lattice Λ_z show very good agreement with the ones obtained with the traditional method for the same lattice volume, while the results from the corresponding original lattice Λ_x deviate considerably from the large-lattice results in the infrared limit.

Conclusions.—We have investigated an analogue of Bloch's theorem for (lattice) Landau gauge fixing [9], which arises because the Landau-gauge condition leaves a residual global transformation unfixed. The chosen procedure also resembles the limiting sequence of domains in the Fisher-Ruelle construction of infinite-volume statistical mechanics [15]. We find that, at least in the gluon sector, large-lattice data are reproduced by simulations at much smaller volumes with extended gauge transformations, thus reducing memory usage by a huge factor (at least up to 16^d 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 Λ_x (see Fig. 1 and discussion in the previous section).

Our work suggests that there are two different mass scales in the theory, one related to the thermalization and another to the gauge fixing, the latter being much smaller than the former. Typically, in the four-dimensional SU(3) case, the two scales would correspond to $m_g \sim 500$ MeV and to the lowest glueball mass, i.e., ~ 1500 MeV. The present numerical approach, although introduced in Ref. [9] for analytic reasons, seems suitable to handle both scales, by using the original (small) lattice Λ_x for thermalization and the extended (large) lattice Λ_z for gauge fixing. This also supports the suggestion that the IR properties of Landau-gauge Green's functions be essentially determined by the gauge-fixing procedure [16].

More results and details of the numerical simulations presented here will be discussed elsewhere [13]. We also plan to extend this study to the ghost and matter sectors, and to investigate its impact on properties of the Gribov region. 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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