Making Big Lattices Bigger:
Bloch's Theorem and
The Lattice Gluon Propagator (Part I)

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Color Confinement & Bloch Waves

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High computational cost **BUT**: infinite-volume limit as periodic-potential problem (by "cloning" the gauge configuration), simplified by analogy with Bloch's theorem $\Rightarrow$ physical insight as well as technical tool?

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In Landau gauge

$$D^{ab}_{\mu\nu}(p) = \sum_x e^{-2i\pi k\cdot x} \langle A^a_\mu(x)\, A^b_\nu(0)\rangle$$

$$= \delta^{ab}\left(g_{\mu\nu} - \frac{p_\mu\, p_\nu}{p^2}\right) D(p^2)$$

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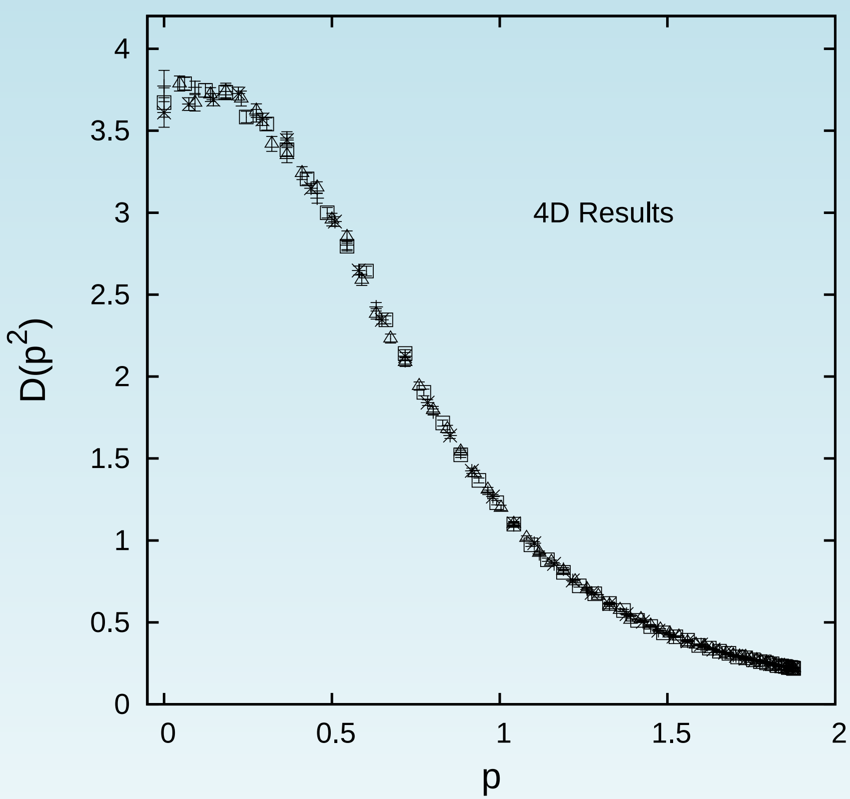
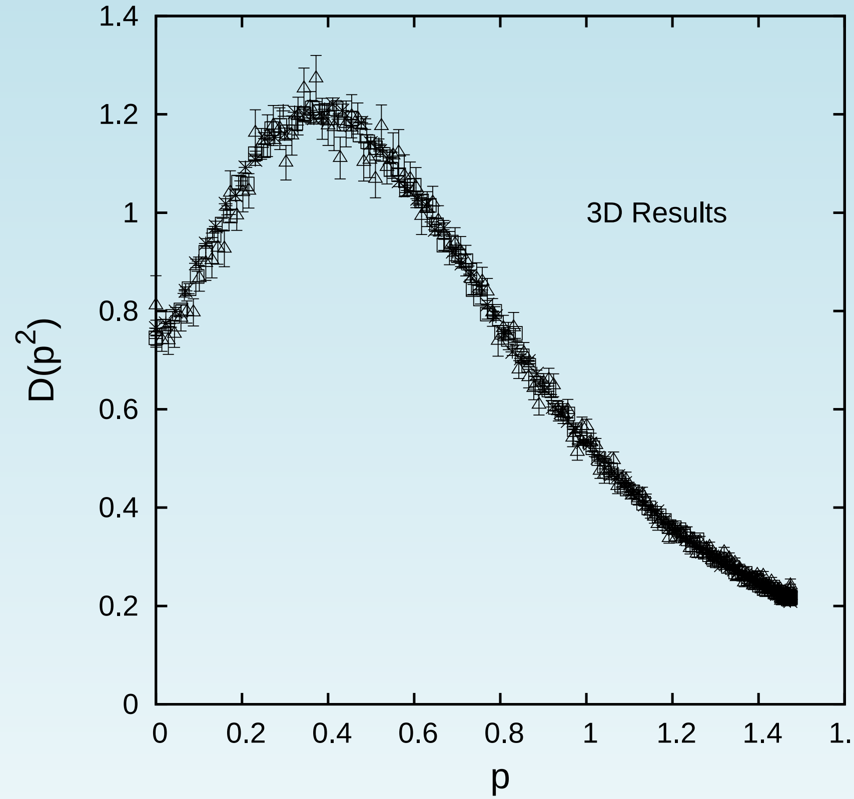
Now (2024): Gluon propagator, Quo Vadis?

Gluon Propagator at "Infinite" Volume

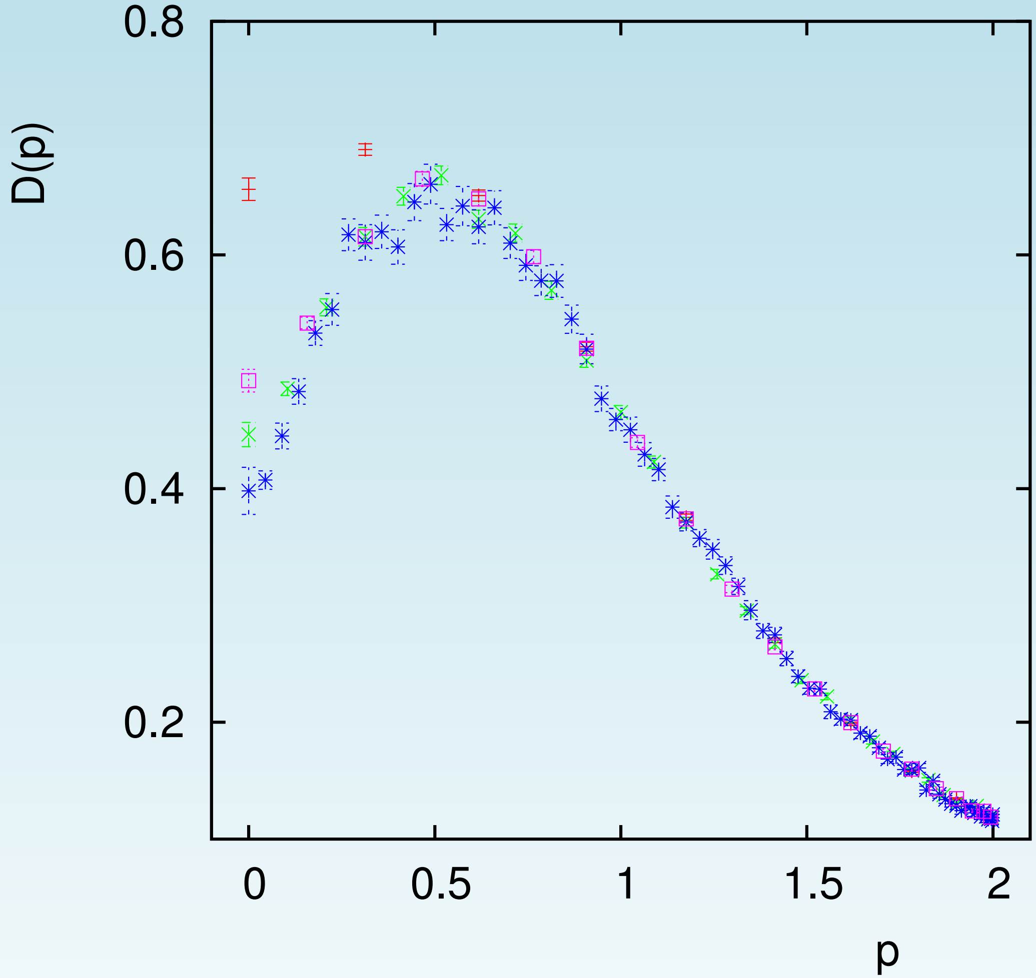
Attilio Cucchieri & T.M. (2008)





Gluon propagator $D(p^2)$ as a function of the lattice momenta p (both in physical units) for the pure-$SU(2)$ case in $d = 4$ (left), for volumes of up to 128^4 (lattice extent ~ 27 fm) and $d = 3$ (right), for volumes of up to 320^3 (lattice extent ~ 85 fm)

Gluon Propagator: Volume Effects



Gluon propagator vs. lattice momentum for $V = 20^3$, 40^3, 60^3 and 140^3

How are the data obtained?

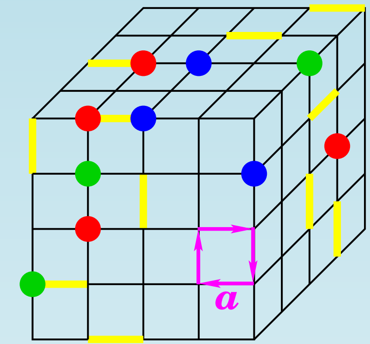
The Lattice

1) Quantization by path integrals $\Rightarrow$ configurations with "weight" $e^{i\,S/\hbar}$

2) Euclidean formulation (imaginary time) $\Rightarrow$ weight becomes $e^{-S/\hbar}$

3) Discrete space-time $\Rightarrow$ UV cut at $p \lesssim 1/a$ $\Rightarrow$ regularization

Also: finite-size lattices $\Rightarrow$ IR cut for small momenta $p \approx 1/L$



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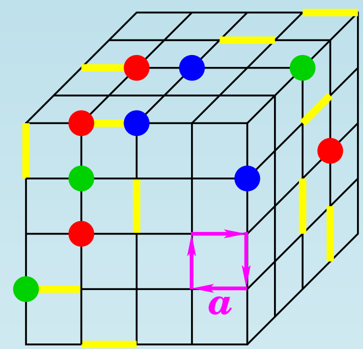

The Wilson action (1974)

$$S \;=\; -\frac{\beta}{3}\sum_{\square} \mathrm{ReTr}\, U_{\square}\,, \qquad \beta \;=\; 6/{g_0}^2$$

$\Rightarrow$ lattice parameter β is related to a, plaquettes $U_{\square}$ are oriented products of the gauge-link variables $U_\mu(x)$, which are SU(3) group elements

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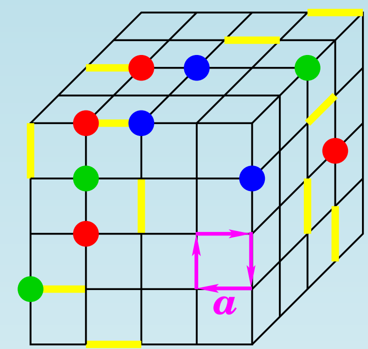

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Gauge transformation: $U_\mu(x) \to U^g_\mu(x) = g(x)\, U_\mu(x)\; g^\dagger(x+\mu)$

$\Rightarrow$ closed loops are gauge-invariant quantities (S is gauge-invariant)

Lattice Landau Gauge

Landau gauge is imposed on the lattice by minimizing the functional

$$\mathcal{E}[U;g] = \Re\,\mathrm{Tr}\sum_{x,\mu}[\mathbb{1} - U_\mu^g(x)]$$

with respect to $g(x) \in SU(N_c)$ for a fixed gauge configuration $U_\mu(x)$

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Taking $g(x) = e^{i\tau\gamma(x)}$ with $\gamma(x) = \gamma^b(x)\,T_b \in \mathfrak{su}(N_c)$ fixed and $\tau \to 0$

$$\mathcal{E}[U;g] \;\approx\; \mathcal{E}[U;\mathbb{1}] \;+\; \tau\,\mathcal{E}'[U;\mathbb{1}](b,x)\,\gamma^b(x) + (\tau^2/2)\,\gamma^b(x)\,\mathcal{E}''[U;\mathbb{1}](b,x;c,y)\,\gamma^c(y)$$

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At any local minimum (stationary solution) we have $\mathcal{E}' = 0 \;\forall\, \gamma^b(x)$

$\Rightarrow\; \left(\nabla\cdot A^b\right)(x) = 0 \;\forall\, x, b\,,$ where $A_\mu(\vec{x}) = \dfrac{1}{2\,i}\left[\,U_\mu(\vec{x}) - U^\dagger_\mu(\vec{x})\,\right]_{\mathrm{traceless}}$

Therefore, the (minimal) Landau gauge condition on the lattice reads

$$\left(\nabla\cdot A^b\right)(\vec{x}) = \sum_{\mu=1}^{d} A^b_\mu(\vec{x}) - A^b_\mu(\vec{x} - \hat{e}_\mu) = 0$$

Gauge-Related Lattice Features

- Gauge action written in terms of oriented plaquettes formed by the link variables $U_{x,\mu}$, which are group elements
- under gauge transformations: $U_{x,\mu} \to g(x)\, U_{x,\mu}\, g^{\dagger}(x+\mu)$, where $g \in SU(3) \Rightarrow$ closed loops are gauge-invariant
- integration volume is finite: no need for gauge-fixing
- when gauge fixing, procedure is incorporated in the simulation, no need to consider Faddeev-Popov matrix
- get FP matrix without considering ghost fields explicitly
- Lattice momenta given by $\hat{p}_\mu = 2\,\sin\left(\pi\, k_\mu / N\right)$ with $k_\mu = 0, 1, \ldots, N/2 \;\Leftrightarrow\; p_{min} \sim 2\pi/(a\,N) = 2\pi/L$, $p_{max} = 4/a$ in physical units

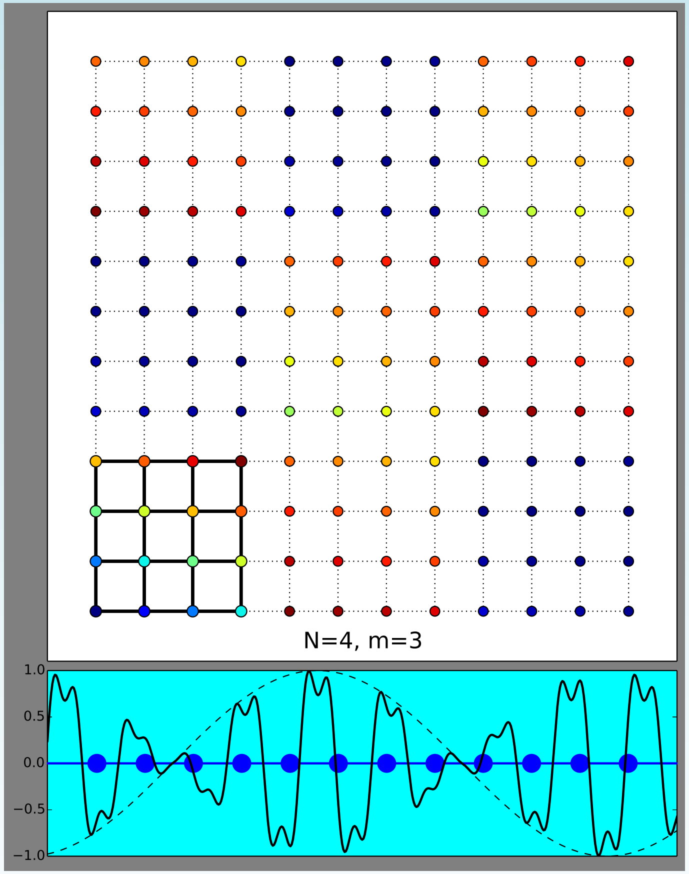
3-Step Code

```
main() {
/* set parameters: beta, number of configurations NC,
                   number of thermalization sweeps NT */
     read_parameters();
/* {U} is the link configuration */
     set_initial_configuration(U);
/* cycle over NC configurations */
     for (int c=0; c < NC; c++) {
          thermalize(U,beta,NT);
          gauge_fix(U,g);
          evaluate_propagators(U[g]);
     }
}
```

Algorithms: Heat-Bath and Micro-canonical (thermalization), overrelaxation and simulated annealing (gauge fixing), conjugate gradient and Fourier transform (propagators, etc.).

Large Lattices via Bloch's Theorem

Perform thermalization step on small lattice, then replicate it and use Bloch's theorem from condensed-matter physics to obtain gauge-fixing step for much larger lattice (A. Cucchieri, TM, PRL 2017)



Two-step Infinite-Volume Limit

Zwanziger suggests (NPB 1994) taking the infinite-volume limit in two steps

1) first, considering the $V \to +\infty$ limit for the gauge transformation $g(x)$

2) then, taking the same limit for the gluon field [i.e. the link variables $\{U_\mu(x)\}$]

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$\Rightarrow$ $g(x)$ sees infinite volume while the one for $U_\mu(x)$ is still finite

The Extended Lattice

Setup:

1. Consider a d-dimensional link configuration $\{U_\mu(\vec{x})\} \in$ SU(N_c), defined on a lattice Λ_x with volume $V = N^d$ and periodic boundary conditions (PBC)

2. Replicate this configuration m times along each direction, yielding an extended lattice Λ_z with volume $m^d V$ and PBC

3. Indicate the points of Λ_z with $\vec{z} = \vec{x} + \vec{y}N$, where $\vec{x} \in \Lambda_x$ and $\vec{y}$ is a point on the index lattice Λ_y

4. By construction, $\{U_\mu(\vec{z})\}$ in Λ_z is invariant under translations by N (in any direction)

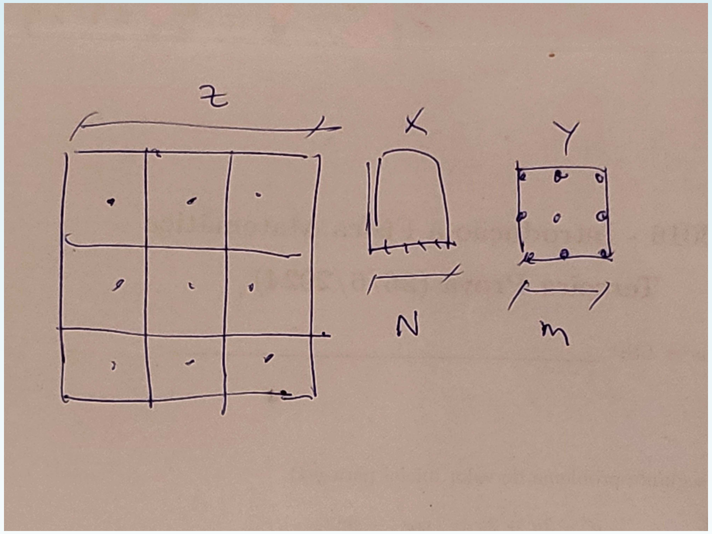
The Extended Gauge Transformation

Impose the minimal-Landau-gauge condition on Λ_z, i.e. consider the minimizing functional

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

where $g(\vec{z})$ has periodicity mN, i.e. $g(\vec{z} + mN\hat{e}_\mu) = g(\vec{z})$ (PBC in Λ_z)

The two limits: first take $m \to +\infty$ and then $N \to +\infty$



Bloch's Theorem (I)

For an ideal crystalline solid in d dimensions, one considers an electrostatic potential $U(\vec{r})$ with the periodicity of the Bravais lattice, i.e. $U(\vec{r}) = U(\vec{r} + \vec{R})$ for any vector $\vec{R} = N\vec{a}_\mu$.

Ingredients:

1. The Hamiltonian $\mathcal{H}$ for a single electron is invariant under translations by $\vec{R}$
2. Translation operators $\mathcal{T}(\vec{R})$ commute, i.e.

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

3. We can choose the eigenstates $\psi(\vec{r})$ of $\mathcal{H}$ to be also eigenstates of $\mathcal{T}(\vec{R})$

Bloch's Theorem (II)

4. The eigenvalues $c(\vec{R})$ of $\mathcal{T}(\vec{R})$ are $\exp(i\vec{k}\cdot\vec{R}) = \exp(2\pi i\, k_\nu\, n_\nu)$, where $\vec{k} = k_\nu \vec{b}_\nu$ is a vector of the reciprocal lattice (i.e. $\vec{a}_\mu \cdot \vec{b}_\nu = 2\pi\delta_{\mu\nu}$)

5. Since

$$\mathcal{T}(\vec{R})\,\psi(\vec{r}) = \psi(\vec{r}+\vec{R}) = \exp(i\vec{k}\cdot\vec{R})\,\psi(\vec{r})\ ,$$

the eigenstates $\psi(\vec{r})$ can be written as Bloch waves

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

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

Analogy with Gauge Transformation

Correspondence:

1. $\Lambda_y \Longleftrightarrow$ finite Bravais lattice with PBC
2. $\{U_\mu(\vec{z})\} \Longleftrightarrow$ periodic electrostatic potential $U(\vec{r})$

One can prove that:

- $g(\vec{z})$ can be written as $g(\vec{z}) = \exp\left(i\Theta_\mu\, z_\mu/N\right) h(\vec{z})$
- $h(\vec{z})$ has periodicity N, i.e. $h(\vec{z} + N\hat{e}_\mu) = h(\vec{z}) \;\Rightarrow\; h(\vec{x})$
- The matrices $\Theta_\mu = \theta^a_\mu \lambda^a_{\mathrm{C}}$ (with $a = 1, \ldots, N_c - 1$) have eigenvalues $2\pi n_\mu/m$, with $n_\mu \in \mathcal{Z}$
- The matrices λ^a_{C} are elements of a Cartan sub-algebra of the SU(N_c) Lie algebra

The New Minimizing Functional

Due to the expression for $g(\vec{z})$ and to the cyclicity of the trace, the minimizing functional becomes

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

where

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

i.e. the numerical minimization may still carried out on the original lattice Λ_x and used to write the solution for the extended lattice, as for the case of Bloch waves

$\Rightarrow$ More on this later

The Proof: Ingredients (I)

1. The original minimizing problem is invariant under translations $\mathcal{T}(N\hat{e}_\mu)$
2. Due to the cyclicity of the trace, the minimizing functional $\mathcal{E}_U[g]$ is invariant under global (left) gauge transformations, i.e. $g(\vec{z}) \to v\, g(\vec{z})$, with $v \in$ SU(N_c)
3. If the sought gauge transformation $\{g(\vec{z})\}$ is unique, then $g(\vec{z})$ and $g(\vec{z} + N\hat{e}_\mu)$ can differ only by a global transformation, i.e.

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

where $v_\mu \in$ SU(N_c) is a $\vec{z}$-independent matrix

The Proof: Ingredients (II)

4. Since the translation operators commute, the v_μ matrices are commuting matrices, i.e. they can be written as $\exp(i\Theta_\mu) = \exp(i\theta_\mu^a \lambda_{\mathrm{C}}^a)$, where the λ_{C}^a matrices are Cartan generators

5. Then

$$g(\vec{z} + \vec{y}N) = \mathcal{T}(N\vec{y})\, g(\vec{z}) = \exp(i\Theta_\mu y_\mu)\, g(\vec{z})$$

   and the proof is complete if we define

$$g(\vec{z}) \equiv \exp(i\Theta_\mu z_\mu / N)\, h(\vec{x})$$

6. Due to the PBC for Λ_z, we need to impose the condition $[\exp(i\Theta_\mu)]^m = \mathbb{1} \Longrightarrow$ the eigenvalues of the matrices Θ_μ are of the type $2\pi n_\mu / m$, with $n_\mu \in \mathcal{Z}$

Numerical Simulations

In the SU(N_c) case:

1. generate a thermalized d-dimensional link configuration $U_\mu(x)$ with periodicity N, i.e. $V = N^d$ with PBC
2. minimize $\mathcal{E}_U[h, \Theta_\mu]$ with respect to $h(x)$ and Θ_μ using two alternating steps:
   a) the matrices Θ_μ are kept fixed and one updates the matrices $h(\vec{x})$ by sweeping through the lattice
   b) the matrices Q_μ are kept fixed and one minimizes $\mathcal{E}_U[h, \Theta_\mu]$ with respect to the matrices Θ_μ, belonging to the corresponding Cartan sub-algebra
3. evaluate the gluon propagator using the extended gauge-fixed link variables $U_\mu^{(g)}(\vec{z}) = g(\vec{z})\, U_\mu(\vec{z})\, g(\vec{z} + \hat{e}_\mu)^\dagger$

The SU(2) Case

In the $SU(2)$ case (one-dimensional Cartan sub-algebra) we can write

$$\Theta_\mu \equiv (v^\dagger \sigma_3 v) \alpha_\mu$$

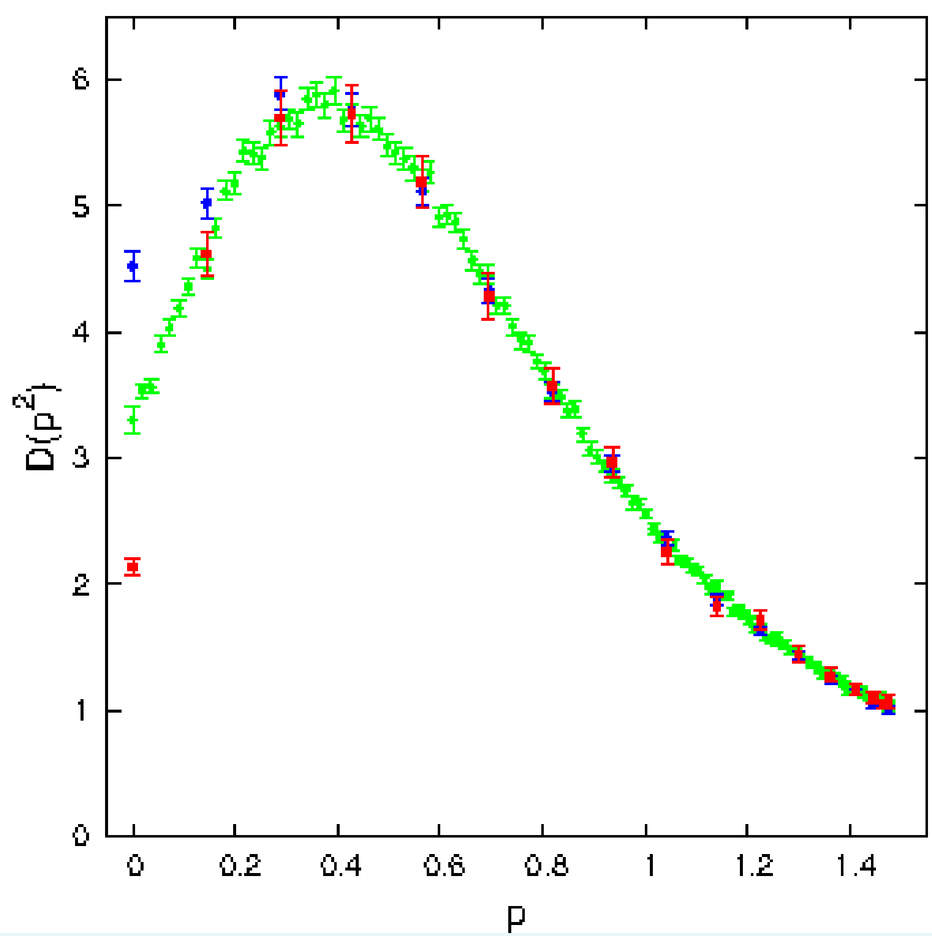
with $v \in$ SU(2) and eigenvalues $\pm\alpha_\mu = \pm 2\pi n_\mu / m$

Then, in the new minimizing functional

$$\exp\left(-i\Theta_\mu/N\right) \, = \, v^\dagger \, \exp[-2\pi i \sigma_3 n_\mu/(mN)] \, v$$

Also, the matrices Q_μ are proportional to SU(2) matrices

Results: $3D$ Gluon Propagator



The gluon propagator $D(p^2)$ as a function of the lattice momentum p at $\beta = 3.0$ for the Λ_x lattice volumes $V = 32^3$ ($+$) and 256^3 ($*$) and for the Λ_z lattice volume $V = 32^3 \times 8^3 = 256^3$ ($\Box$)

Back to the Minimizing Problem

As mentioned earlier, the minimizing problem is simplified as a consequence of $g(\vec{z}) = \exp\left(i\Theta_\mu z_\mu/N\right) h(\vec{x})$, since the solution for the extended-lattice problem is obtained from minimizing a similar functional on the small one

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For the gauge-transformed link variable $U_\mu^g(z)$ we have

$$U_\mu(g;\vec{z}) = e^{i\Theta_\nu z_\nu/N}\, U_\mu(h;\vec{x})\, e^{-i\Theta_\mu/N}\, e^{-i\Theta_\nu z_\nu/N}$$

$$= e^{i\Theta_\nu y_\nu} \left[e^{i\Theta_\nu x_\nu/N}\, U_\mu(h;\vec{x})\, e^{-i\Theta_\mu/N}\, e^{-i\Theta_\nu x_\nu/N} \right] e^{-i\Theta_\nu y_\nu}$$

where we used that $\vec{z} = \vec{x} + \vec{y}\vec{N}$

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where we used that $\vec{z} = \vec{x} + \vec{y}\vec{N}$

Note that the central (local) part of the above expression is the same for all “cells” and that different domains (=cells) are related by a global “rotation” (determined by $\vec{y}$), applied to each cell

Gauge-Configuration Domains

The local part of $U_\mu^g(z)$ is gauge-fixed (i.e. transverse) but is no longer periodic, while the original gauge configuration $U_\mu(z)$ was periodic, but not transverse

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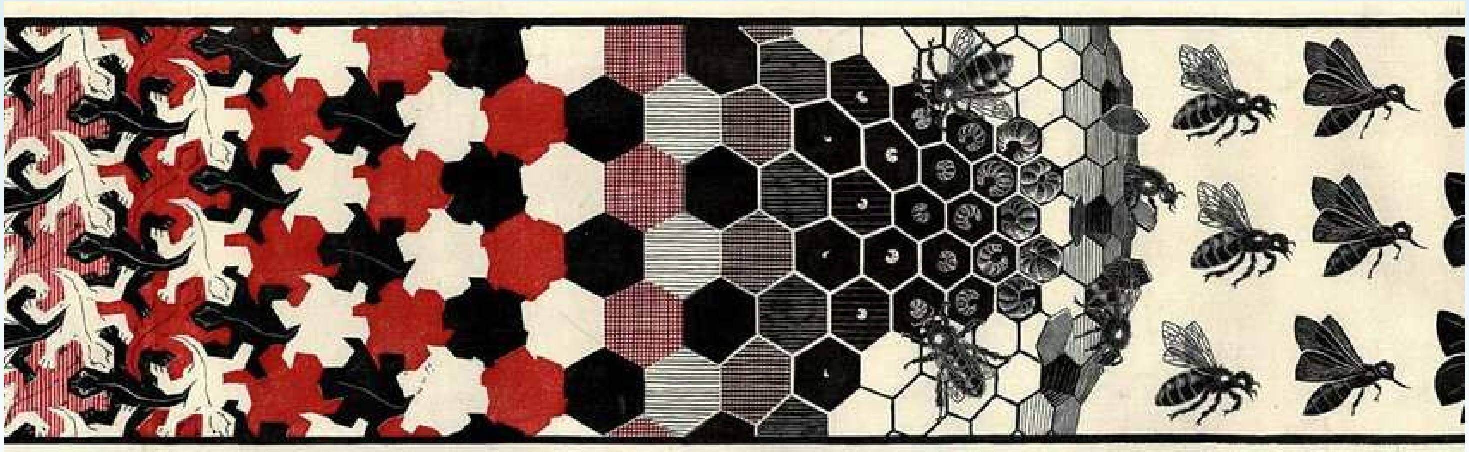
The local part of $U_\mu^g(z)$ is gauge-fixed (i.e. transverse) but is no longer periodic, while the original gauge configuration $U_\mu(z)$ was periodic, but not transverse

Gauge-field configurations within cells are rotated, transformed by global group elements defined by the cell index $\vec{y}$, in a manner reminiscent of Escher's work (Metamorphosis I, II, III), so that the full configuration on the extended lattice has the required $m \times N$ periodicity

A pattern of domains emerges!



Color Magnetization

One can define a (gluon-field) color magnetization

$$A_\mu^b \;=\; \frac{1}{N^d} \sum_{\vec{x}} A_\mu^b(\vec{x})$$

which is related to the gluon propagator at zero momentum as

$$D(0) \;=\; \frac{N^d}{d(N_c^2-1)} \sum_{b,\mu} \langle |A_\mu^b|^2 \rangle$$

Quantity $\mathcal{A} \;=\; \sum_{b,\mu} \langle |A_\mu^b| \rangle / d(N_c^2-1)$ considered by Zwanziger (in Landau gauge, this should vanish at least as fast as $1/N$).

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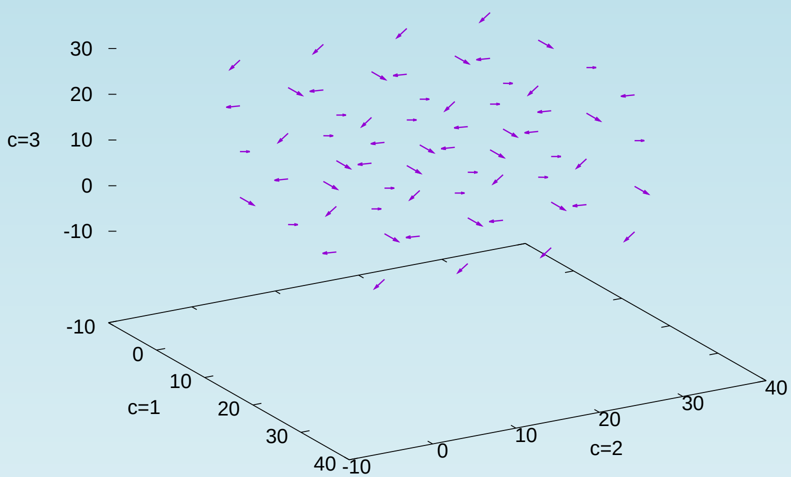
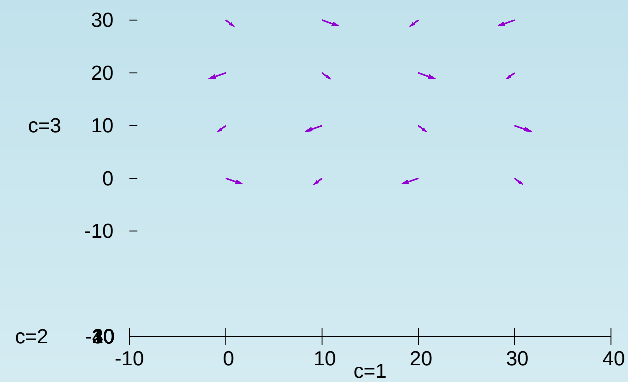
$\Rightarrow$ Let us look for the average color magnetization in each cell and try to relate it to the domains mentioned above

Average Cell Magnetization



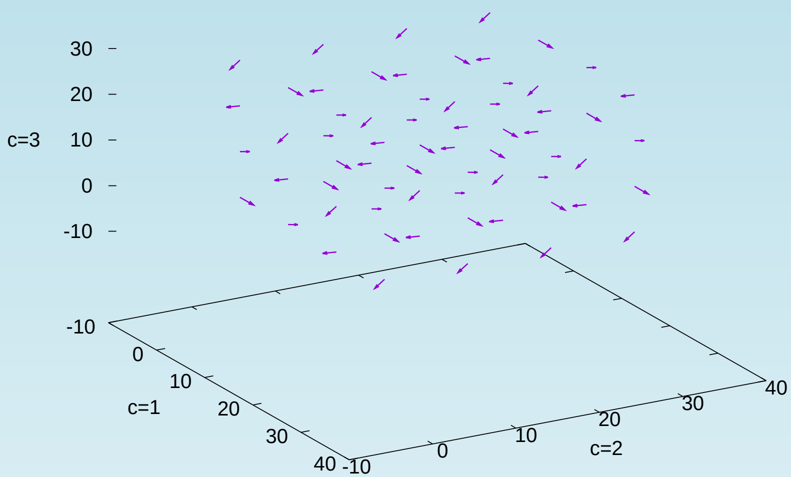


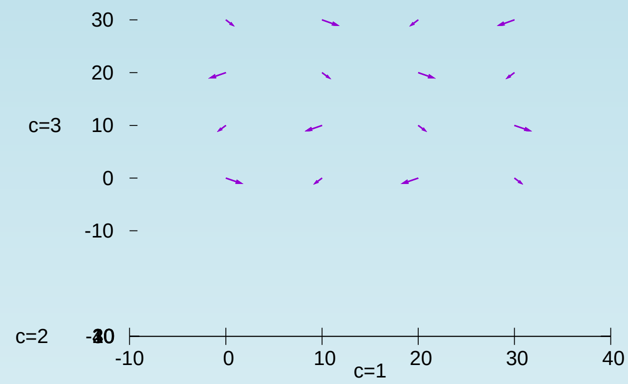
Average color "magnetization" in each cell

$$M^c_\mu(\vec{y}) \,=\, \frac{1}{N^d} \sum_{\vec{x}} A^c_\mu(\vec{z})$$

for the pure-$SU(2)$ case and lattice volume $V = (60 \times 4)^3$

Average Cell Magnetization





Average color "magnetization" in each cell

$$M_{\mu}^{c}(\vec{y}) = \frac{1}{N^d} \sum_{\vec{x}} A_{\mu}^{c}(\vec{z})$$

for the pure-$SU(2)$ case and lattice volume $V = (60 \times 4)^3$

A new type of domain wall?

Conclusions

- Numerical results (in the gluon sector) obtained using large lattice volumes can also be obtained using small lattice volumes with extended gauge transformations
- From the physical point of view:
  1. the information encoded in a thermalized configuration does not depend much on the lattice volume V
  2. the properties of the Landau-gauge Green's functions are essentially set by the gauge-fixing procedure and the size of V matters!
- Limitation: the allowed momenta seem to be fixed by the lattice discretization on the original lattice Λ_x, no way to obtain "big-volume" momenta? $\Rightarrow$ see Attilio's talk
- Interesting properties regarding "magnetization" domains!