# Pure gauge theory on the lattice 

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## 1 Gauge fields in the Euclidean continuum

Gauge fields are an important concept in a special type of quantum field theory, the so-called gauge field theory, where matter fields such as electrons interact with each other via forces mediated by gauge fields. In quantum electrodynamics (QED), the force mediator is the photon field, often denoted as $A_{\mu}(x)$ with $\mu$ a Lorentz index. It appears in the QED action $S=\int d^{4} x \mathcal{L}(x)$ with

$$
\begin{equation*}
\mathcal{L}=-\frac{1}{4} F_{\mu \nu}(x) F^{\mu \nu}(x)-\bar{\psi}(x) \gamma^{\mu} D_{\mu} \psi(x)-m \bar{\psi}(x) \psi(x) \tag{1}
\end{equation*}
$$

in terms of the covariant derivative and electromagnetic field strength tensor

$$
\begin{equation*}
D_{\mu}=\partial_{\mu}+i e A_{\mu}, \quad F_{\mu \nu}(x)=\partial_{\mu} A_{\nu}(x)-\partial_{\nu} A_{\mu}(x)=D_{\mu} A_{\nu}(x)-D_{\nu} A_{\mu}(x) . \tag{2}
\end{equation*}
$$

In the equations above, $\psi(x)$ denotes the electron field, $m$ its mass and $e$ the unit charge. Inserting Eq. (2) into Eq. (1) we find a term like $-i e \bar{\psi}(x) \gamma^{\mu} A_{\mu} \psi(x)$ which dictates the interaction between electrons and photons. In other words, $e$ quantifies the strength of electromagnetic gauge interaction, and thus can be viewed as the gauge coupling strength.

Sometimes it is more convenient to have the gauge coupling as an overall factor of the gauge part, we can achieve this by rescaling the gauge field

$$
\begin{equation*}
A_{\mu}(x) \rightarrow \frac{1}{e} A_{\mu}(x) \tag{3}
\end{equation*}
$$

This is allowed because the gauge field itself is not an observable, we have the freedom to do the above rescaling without changing the physical observables.

After the rescaling, $\mathcal{L}$ then becomes

$$
\begin{equation*}
\mathcal{L}=-\frac{1}{4 e^{2}} F_{\mu \nu}(x) F^{\mu \nu}(x)-\bar{\psi}(x) \gamma^{\mu}\left[\partial_{\mu}-i q A_{\mu}(x)\right] \psi(x)-m \bar{\psi}(x) \psi(x) \tag{4}
\end{equation*}
$$

with $q=-1$ for the electron.
It is easy to see that the above Lagrangian is invariant under the following transformation

$$
\begin{equation*}
\psi^{\prime}(x)=e^{i \omega(x) q} \psi(x), \quad \bar{\psi}^{\prime}(x)=e^{-i \omega(x) q} \bar{\psi}(x), \quad A_{\mu}^{\prime}(x)=A_{\mu}(x)+\partial_{\mu} \omega(x), \tag{5}
\end{equation*}
$$

where $\omega(x)$ is a real function of $x$. The phase factor $\Omega(x)=e^{i \omega(x)}$ forms a group, the $U(1)$ (1-dim. unitary) gauge group. This is a symmetry group under which the QED action is invariant. It is worth
noting that if $\omega(x)$ is a constant independent of $x$ (called a global symmetry because the symmetry transformation is the same everywhere), $A_{\mu}(x)$ will remain unchanged under the transformation above, and so does the interaction term itself $\bar{\psi}(x) \gamma^{\mu} A_{\mu}(x) \psi(x)$. In other words, the interaction is not needed to maintain global gauge symmetry. However, when the symmetry becomes local or when $\omega(x)$ depends on the spacetime coordinate $x$, as in Eq. (5), then the interaction term must be present with $A_{\mu}(x)$ transforming as in Eq. (5) to ensure local guage symmetry, i.e., local gauge symmetry dictates interactions.

We can rewrite the gauge transformation in Eq. (5) in terms of $\Omega(x)$

$$
\begin{equation*}
\psi^{\prime}(x)=\Omega^{q}(x) \psi(x), \quad \bar{\psi}^{\prime}(x)=\Omega^{* q}(x) \bar{\psi}(x), \quad A_{\mu}^{\prime}(x)=A_{\mu}(x)+i \Omega(x) \partial_{\mu} \Omega^{*}(x) \tag{6}
\end{equation*}
$$

and the covariant derivative $D_{\mu}=\partial_{\mu}-i q A_{\mu}$ acting on $\psi(x)$ transforms just like $\psi(x)$ itself

$$
\begin{equation*}
D_{\mu}^{\prime} \psi^{\prime}(x)=\left[\partial_{\mu}-i q A_{\mu}^{\prime}(x)\right] \psi^{\prime}(x)=\Omega^{q}(x) D_{\mu} \psi(x), \tag{7}
\end{equation*}
$$

so that the combination $\bar{\psi}^{\prime} \gamma^{\mu} D_{\mu}^{\prime} \psi^{\prime}=\bar{\psi} \gamma^{\mu} D_{\mu} \psi$ is gauge invariant. Another interesting feature of the QED gauge group is that it implies charge shall be quantized. This can be seen from the requirement that $\omega \rightarrow \omega+2 \pi$ shall give the same value for the fields.

Now let us turn to quantum chromodynamics (QCD). The QCD action is very much similar to the QED one except that now we generalize the symmetry group to a bigger group, the 3-dim. special unitary group or $S U(3)$, whose elements are $3 \times 3$ unitary matrices with the determinant 1 . In other words, the phase factor dictating gauge transformations, $\Omega(x)$, now becomes matrix-valued with

$$
\begin{equation*}
\Omega(x)=e^{i \omega^{k}(x) t_{k}} \tag{8}
\end{equation*}
$$

where $t_{k}, k=1 \ldots 8$ are a complete set of Hermitian traceless $3 \times 3$ matrices. The properties of such matrices imply that $\Omega^{-1}=\Omega^{\dagger}$ and

$$
\begin{equation*}
\operatorname{Tr} t_{k}=0 \rightarrow \operatorname{det} \Omega=e^{\operatorname{Tr} \ln \Omega}=1 \tag{9}
\end{equation*}
$$

The matrices $t_{k}$ are also called the generators of the group (in a given representation). A standard choice of them is $t_{k}=1 / 2 \lambda_{k}$ with

$$
\begin{align*}
& \lambda_{i}=\left(\begin{array}{ccc}
\sigma_{i} & & 0 \\
& & 0 \\
0 & 0 & 0
\end{array}\right), \text { for } i=1,2,3, \quad \lambda_{4}=\left(\begin{array}{ccc}
0 & 0 & 1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{array}\right), \quad \lambda_{5}=\left(\begin{array}{ccc}
0 & 0 & -i \\
0 & 0 & 0 \\
i & 0 & 0
\end{array}\right), \\
& \lambda_{6}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
0 & 0 & 1 \\
0 & 1 & 0
\end{array}\right), \quad \lambda_{7}=\left(\begin{array}{ccc}
0 & 0 & 0 \\
0 & 0 & -i \\
0 & i & 0
\end{array}\right), \quad \lambda_{8}=\frac{1}{\sqrt{3}}\left(\begin{array}{ccc}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -2
\end{array}\right), \tag{10}
\end{align*}
$$

where $\sigma_{i}$ are the Pauli matrices

$$
\sigma_{1}=\left(\begin{array}{ll}
0 & 1  \tag{11}\\
1 & 0
\end{array}\right), \quad \sigma_{2}=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right), \quad \sigma_{1}=\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)
$$

The matrices $\lambda_{k}$ are the well-known Gell-Mann matrices, and they satisfy

$$
\begin{equation*}
\operatorname{Tr}\left(t_{k} t_{l}\right)=\frac{1}{2} \delta_{k l}, \quad\left[t_{k}, t_{l}\right]=i f_{k l m} t_{m} \tag{12}
\end{equation*}
$$

where $f_{k l m}$ are called the structure constants of the group $S U(3)$. They are totally antisymmetric with respect to the interchange of any two indices.

In QCD, the force mediator is called gluons. There are eight gluons in total, in accordance with the degrees of freedom inherited in the gauge group. In contrast with the photon field which does not carry electric charge and is denoted as $A^{\mu}(x)$, the gluon carries color charge, and can be denoted as $A_{a b}^{\mu}(x)$ with $a, b=1,2,3$ the color indices. In other words, the gluon fields are matrix-valued. Traditionally, the colors are called red, blue and green. For given $x$ and $\mu$, the field $A_{a b}^{\mu}(x)$ is a traceless, Hermitian $3 \times 3$ matrix at each spacetime point $x$.

Now the fermion field transforms as

$$
\begin{equation*}
\psi(x) \rightarrow \psi^{\prime}(x)=\Omega(x) \psi(x), \quad \bar{\psi}(x) \rightarrow \bar{\psi}^{\prime}(x)=\bar{\psi}(x) \Omega^{\dagger}(x) \tag{13}
\end{equation*}
$$

This also implies how the gauge field transforms. To see this, let us consider the fermion part of the Lagrangian (leave aside the gauge invariant mass term for the moment), which changes as

$$
\begin{equation*}
\bar{\psi}(x) \gamma^{\mu}\left(\partial_{\mu}+i g A_{\mu}\right) \psi(x) \rightarrow \bar{\psi}(x) \Omega^{\dagger}(x) \gamma^{\mu}\left(\partial_{\mu}+i g A_{\mu}^{\prime}\right) \Omega(x) \psi(x) \tag{14}
\end{equation*}
$$

where $A_{\mu}^{\prime}$ denotes the transformed gauge field. For the above Lagrangian to be invariant, we need

$$
\begin{equation*}
A_{\mu}^{\prime}(x)=\Omega(x) A_{\mu}(x) \Omega^{\dagger}(x)+i\left(\partial_{\mu} \Omega(x)\right) \Omega^{\dagger}(x) \tag{15}
\end{equation*}
$$

From this, we can also read off the transformation property of the covariant derivative

$$
\begin{equation*}
D_{\mu}(x) \rightarrow D_{\mu}^{\prime}(x)=\Omega(x) D_{\mu}(x) \Omega^{\dagger}(x) \tag{16}
\end{equation*}
$$

In analogy to QED, we can define the field strength tensor as

$$
\begin{equation*}
F_{\mu \nu}(x)=D_{\mu} A_{\nu}(x)-D_{\nu} A_{\mu}(x)=\partial_{\mu} A_{\nu}(x)-\partial_{\nu} A_{\mu}(x)+i g\left[A_{\mu}(x), A_{\nu}(x)\right] \tag{17}
\end{equation*}
$$

It is easy to check that it transforms in the same way as the covariant derivative. We can then construct the gauge part of the Lagrangian as

$$
\begin{equation*}
L_{g}=\frac{1}{2} \operatorname{Tr}\left[F^{\mu \nu}(x) F_{\mu \nu}(x)\right] \tag{18}
\end{equation*}
$$

If we do the same rescaling of the gauge field as in $\mathrm{QED}, A_{\mu}(x) \rightarrow 1 / g A_{\mu}(x)$, we then have

$$
\begin{equation*}
L_{g}=\frac{1}{2 g^{2}} \operatorname{Tr}\left[F^{\mu \nu}(x) F_{\mu \nu}(x)\right] \tag{19}
\end{equation*}
$$

The gauge field $A_{\mu}(x)$ can be expanded in terms of its color components

$$
\begin{equation*}
A_{\mu}(x)=\sum_{i=1}^{8} A_{\mu}^{i}(x) T_{i} \tag{20}
\end{equation*}
$$

with $T_{i}$ an appropriate matrix representation, we then have

$$
\begin{align*}
& F_{\mu \nu}(x)=\sum_{i=1}^{8} F_{\mu \nu}^{i}(x) T_{i} \\
& F_{\mu \nu}^{i}(x)=\partial_{\mu} A_{\nu}^{i}(x)-\partial_{\nu} A_{\mu}^{i}(x)-f_{i j k} A_{\mu}^{j}(x) A_{\nu}^{k}(x) \tag{21}
\end{align*}
$$

The Lagrangian then becomes

$$
\begin{equation*}
L_{g}=\frac{1}{4 g^{2}} \sum_{i=1}^{8} F^{\mu \nu, i}(x) F_{\mu \nu}^{i}(x), \tag{22}
\end{equation*}
$$

which appears as eight copies of the QED gauge Lagrangian. However, there is a crucial difference coming from the last term in Eq. (21) that is not present in QED. When plugged into Eq. (22), it introduces cubic and quartic terms, implying that gluons interact among themselves. It is these gluon self-interactions that are responsible for asymptotic freedom and confinement in QCD.

## 2 Gauge fields on the lattice

Now we consider how to formulate gauge fields on the lattice, where the Euclidean spacetime is discretized. A spacetime point on a 4 -dimensional Euclidean lattice can be characterized by a set of numbers $n=\left(n_{1}, n_{2}, n_{3}, n_{4}\right)$ which are multiples of the lattice spacing $a$. In discretized spacetime, the fermion fields are placed at the lattice points so that we label them as $\psi(n)$. Their derivative can be discretized in different ways. A convenient choice is the symmetric combination

$$
\begin{equation*}
\partial_{\mu} \psi(x) \rightarrow \frac{\psi(n+\hat{\mu})-\psi(n-\hat{\mu})}{2 a}, \tag{23}
\end{equation*}
$$

where $\hat{\mu}$ denotes a unit vector along the direction $\mu$. As we mentioned earlier, local gauge invariance requires the existence of gauge fields and dictates their transformation properties. To see how this is realized on the lattice, let us begin with the discretized free fermion Lagrangian

$$
\begin{equation*}
\bar{\psi}(x) \partial_{\mu} \psi(x) \rightarrow \bar{\psi}(n) \sum_{\mu=1}^{4} \frac{\psi(n+\hat{\mu})-\psi(n-\hat{\mu})}{2 a}, \tag{24}
\end{equation*}
$$

which is no longer invariant under the discrete gauge transformation

$$
\begin{equation*}
\psi(n) \rightarrow \psi^{\prime}(n)=\Omega(n) \psi(n), \quad \bar{\psi}(n) \rightarrow \bar{\psi}^{\prime}(n)=\bar{\psi}(n) \Omega^{\dagger}(n) . \tag{25}
\end{equation*}
$$

For example,

$$
\begin{equation*}
\bar{\psi}(n) \psi(n+\hat{\mu}) \rightarrow \bar{\psi}^{\prime}(n) \psi^{\prime}(n+\hat{\mu})=\bar{\psi}(n) \Omega^{\dagger}(n) \Omega(n+\hat{\mu}) \psi(n+\hat{\mu}) \neq \bar{\psi}(n) \psi(n+\hat{\mu}) . \tag{26}
\end{equation*}
$$

If we want to restore gauge invariance, we need to introduce an extra field $U_{\mu}(n)$ to compensate for the gauge transformation above. This can be done if we insert $U(n)$ into the expression above forming $\bar{\psi}(n) U_{\mu}(n) \psi(n+\hat{\mu})$ and let $U_{\mu}(n)$ transform as

$$
\begin{equation*}
U_{\mu}(n) \rightarrow U_{\mu}^{\prime}(n)=\Omega(n) U_{\mu}(n) \Omega^{\dagger}(n+\hat{\mu}) . \tag{27}
\end{equation*}
$$

The field $U_{\mu}(n)$ links the fermion fields at different spacetime points $n$ and $n+\hat{\mu}$, and thus is called the link variable. It is oriented with the orientation specified by $\hat{\mu}$ (see Fig. 1). From Fig. 1 and Eq. (27) we can identify

$$
\begin{equation*}
U_{-\mu}(n+\hat{\mu})=U_{\mu}^{\dagger}(n) . \tag{28}
\end{equation*}
$$



Figure 1: Depiction of the link variable $U_{\mu}(n)$.

Then, the free fermion Lagrangian Eq. (24) can be turned into a gauge invariant expression

$$
\begin{equation*}
\bar{\psi}(x) \partial_{\mu} \psi(x) \rightarrow \bar{\psi}(n) \sum_{\mu=1}^{4} \frac{U_{\mu}(n) \psi(n+\hat{\mu})-U_{-\mu}(n) \psi(n-\hat{\mu})}{2 a} . \tag{29}
\end{equation*}
$$

This is sometimes called a naive discretization of the fermion action, because it is straightforward, but introduces unphysical poles in the lattice propagator of free fermions that do not exist in the continuum. Such unphysical poles have to be removed by adding extra terms to the lattice action so that the continuum theory can be recovered.

From the discussion above, $U_{\mu}(n)$ plays the same role on the lattice as that the gauge field plays in the continuum. It can be viewed as a discrete generalization of the latter. To see how they are related to each other, let us take the following quantity which transforms in the continuum in the same way as Eq. (27) (known as the gauge transporter)

$$
\begin{equation*}
U(x, y)=\mathcal{P} \exp \left[i \int_{C_{x, y}} d s^{\mu} A_{\mu}(s)\right] \tag{30}
\end{equation*}
$$

where $C_{x, y}$ is a path connecting the two points $x, y$, and $\mathcal{P}$ denotes the path-ordering. It means the following: if $s$ is a position along the path from $x$ to $y$, then fields with larger $s$ stand to the left of those with smaller $s$. The reason that the path ordering appears is that in QCD $A_{\mu}(x)$ is matrix-valued, the contribution $d s^{\mu} A_{\mu}(s)$ of different path segments do not commute. If we switch from QCD to QED, then $A_{\mu}(x)$ becomes a pure number, and the path ordering becomes irrelevant.

Under gauge transformation, $U(x, y)$ changes as

$$
\begin{equation*}
U(x, y) \rightarrow U^{\prime}(x, y)=\Omega(x) U(x, y) \Omega^{\dagger}(y) \tag{31}
\end{equation*}
$$

It is the same as Eq. (27) if we identify $n$ and $n+\hat{\mu}$ with $x$ and $y$. We can thus interpret the link variable $U(n)$ as a discrete version of the gauge transporter and define it in analogy with $U(x, y)$ as

$$
\begin{equation*}
U_{\mu}(n)=\exp \left[i a A_{\mu}(n)\right], \tag{32}
\end{equation*}
$$

where we have approximated the integral in Eq. (30) by the contribution of a small segment from $n$ to $n+\hat{\mu}$. This approximation is accurate to $O(a)$, and at this order the path ordering is irrelevant. Expanding to $O(a)$, it is easy to see that Eq. (29) with $U_{\mu}(n)$ defined in Eq. (32) recovers the continuum action in the $a \rightarrow 0$ limit.

Given the gauge transformation property of the link variable, we can form gauge invariant quantities from it which will be useful for constructing the gauge part of the QCD Lagrangian on the lattice. Since $\Omega(x)$ is a unitary matrix, we can choose a closed loop formed by link variables and take the trace, then the transformation matrices at the endpoints cancel, leaving us with a gauge invariant quantity. It turns


Figure 2: Depiction of the plaquette $U_{\mu \nu}(n)$ formed by four link variables.
out that to construct the gluon action it is sufficient to use the simplest closed loop formed by four link variables

$$
\begin{equation*}
U_{\mu \nu}(n)=U_{\mu}(n) U_{\nu}(n+\hat{\mu}) U_{-\mu}(n+\hat{\mu}+\hat{\nu}) U_{-\nu}(n+\hat{\nu})=U_{\mu}(n) U_{\nu}(n+\hat{\mu}) U_{\mu}^{\dagger}(n+\hat{\nu}) U_{\nu}^{\dagger}(n) . \tag{33}
\end{equation*}
$$

This is called a plaquette (see Fig. 2 for a depiction).
In terms of the plaquettes, a discrete gluon action can be constructed as

$$
\begin{equation*}
S_{g}=\frac{2}{g^{2}} \sum_{n} \sum_{\mu<\nu} \operatorname{Re} \operatorname{Tr}\left[1-U_{\mu \nu}(n)\right] . \tag{34}
\end{equation*}
$$

This is called the Wilson gauge action, which is the first lattice formulation of QCD gauge action. As one can explicitly check, the above discrete action reduces to the continuum counterpart in the $a \rightarrow 0$ limit.

## 3 Pure gauge theory on the lattice

Now let us focus on pure gauge theory where the fermions are absent. In QED, pure $U(1)$ gauge theory is trivial as photons do not interact with each other. In QCD, pure $S U(3)$ gauge theory has non-trivial dynamics because gluons carry color charges and interact among themselves. On the lattice, the physical observable for a pure gauge theory is calculated as following

$$
\begin{equation*}
\langle O\rangle=\frac{1}{Z} \int \mathcal{D}[U] e^{-S_{g}[U]} O[U], \tag{35}
\end{equation*}
$$

with

$$
\begin{equation*}
Z=\int \mathcal{D}[U] e^{-S_{g}[U]}, \quad \mathcal{D}[U]=\prod_{n} \prod_{\mu=1}^{4} d U_{\mu}(n), \tag{36}
\end{equation*}
$$

This is very much similar to the calculation of physical observables in a statistical system, where $Z$ plays the role of partition function of the system. In the above equation, $d U_{\mu}(n)$ represents a volume element in the group space associated with the link variable $U_{\mu}(n)$. In the case of QED or QCD, the total volume of the group space is finite and the functional $Z$ is well-defined on a finite lattice. In such a theory, gauge-fixing is not necessary for the non-perturbative calculation of observables. However, if the symmetry group is a different one such that it has an infinite group space, then one needs gauge-fixing to have a well-defined functional $Z$, which in some sense brings in a regulator for the infinite group


Figure 3: Depiction of integrating out the common link variable shared by two plaquettes.
space. Nevertheless, in practical calculations of physical observables it might not be necessary to do so because the infinite group space formally cancels in the ratio in Eq. (35).

From gauge invariance of the functional $Z$ and the action $S_{g}[U]$, we have

$$
\begin{equation*}
\mathcal{D}[U]=\mathcal{D}\left[U^{\prime}\right] \tag{37}
\end{equation*}
$$

or equivalently

$$
\begin{equation*}
d U_{\mu}(n)=d U_{\mu}^{\prime}(n) \tag{38}
\end{equation*}
$$

for $U_{\mu}^{\prime}(n)=\Omega(n) U_{\mu}(n) \Omega^{\dagger}(n+\hat{\mu})$. This implies some interesting properties of the functional integral above. For example,

$$
\begin{equation*}
\int d U \operatorname{Tr}[V U] \operatorname{Tr}\left[U^{\dagger} W\right]=\frac{1}{3} \operatorname{Tr}[V W], \tag{39}
\end{equation*}
$$

which allows one to integrate out the common link variable shared by two plaquettes, resulting in a trace of the product formed by the remaining link variables. This is shown in Fig. 3.

## 4 Numerical simulations of pure gauge theory

To calculate physical observables on the lattice, one usually needs to evaluate numerically the functional integral in Eq. (35). This can be done by generating the $N$ sample gauge configurations $U_{n}$ distributed with the probability $e^{-S_{g}\left[U_{n}\right]}$, calculating the observable for each $U_{n}$ and taking the averaged sum

$$
\begin{equation*}
\langle O\rangle=\frac{1}{N} \sum_{n} O\left[U_{n}\right]+\mathcal{O}(1 / \sqrt{N}) . \tag{40}
\end{equation*}
$$

In the following we explain how to generate gauge configurations with the desired distribution probability $e^{-S_{g}\left[U_{n}\right]}$. The general idea is Metropolis algorithm which has been introduced in the harmonic oscillator practice. Start from some configuration $U$ and choose the candidate configuration $U^{\prime}$ by changing one link variable $U_{\mu}(n) \rightarrow U_{\mu}^{\prime}(n)$, then compute the change of the action $\Delta S=S\left[U^{\prime}\right]-S[U]$. The candidate configuration $U^{\prime}$ is accepted with the probability $\min \{1, \exp -\Delta S\}$. In four dimensions this link is shared by six plaquettes. Only these six plaquettes are affected when making the change. Their contribution to the action is

$$
\begin{equation*}
S\left[U_{\mu}^{\prime}(n)\right]=\frac{\beta}{N} \sum_{i=1}^{6} \operatorname{Re} \operatorname{tr}\left[1-\mathrm{U}_{\mu}^{\prime}(\mathrm{n}) \mathrm{P}_{\mathrm{i}}\right] \tag{41}
\end{equation*}
$$

where $P_{i}$ are products of the other three gauge link variables that build up the plaquettes together with $U_{\mu}^{\prime}(n)$. These products are called staples. In Fig. 4, the updated link variable and the affected plaquettes are illustrated in three dimensions. In this figure, when the link variable in red is updated, there are


Figure 4: Illustration of the staples in three dimensions.
four plaquettes are affected and the corresponding staples are shown in blue. In four dimensions, there are six staples and the sum of them is

$$
\begin{equation*}
A=\sum_{i=1}^{6} P_{i}=\sum_{\mu \neq \nu}\left[U_{\nu}(n+\hat{\mu}) U_{\mu}^{\dagger}(n+\hat{\nu}) U_{\nu}^{\dagger}(n)+U_{\nu}^{\dagger}(n+\hat{\mu}-\hat{\nu}) U_{\mu}^{\dagger}(n-\hat{\nu}) U_{\nu}(n-\hat{\nu})\right] . \tag{42}
\end{equation*}
$$

The change of action is

$$
\begin{equation*}
\Delta S=S\left(U_{\mu}^{\prime}(n)\right)-S\left(U_{\mu}(n)\right)=-\frac{\beta}{3} \operatorname{Retr}\left[\left(\mathrm{U}_{\mu}^{\prime}(\mathrm{n})-\mathrm{U}_{\mu}(\mathrm{n})\right) \mathrm{A}\right] \tag{43}
\end{equation*}
$$

The metroplolis algorithm with single link variable updates consists of the following steps:

1. Start from some configuration, choose a site $n$ and a direction $\mu$ and a candidate value $U_{\mu}^{\prime}(n)$ according to some symmetric selection probability $T_{0}$.
2. Compute the sum of the six staples and from this the change of the action $\Delta S$ according to Eq. 43. Accept the new variable $U_{\mu}^{\prime}(n)$ if $r<\exp (-\Delta S)$, where r is a random number uniformly distributed in $[0,1)$. Otherwise, reject it.
3. Repeat these step from the beginning.

The Metropolis algorithm described above is not very efficient since it only moves a very small step in the Markov Chain in each update. To achieve a more efficient way to generate configurations for a pure gauge theory, one can combine heatbath and overrelaxation algorithms.

In the heatbath algorithm, the candidate $\operatorname{link} U_{\mu}^{\prime}(n)$ is chosen according to the local probability distribution density:

$$
\begin{equation*}
d P(U)=d U \exp \left(\frac{\beta}{3} \operatorname{Re} \operatorname{tr}[\mathrm{UA}]\right) \tag{44}
\end{equation*}
$$

where $A$ is the sum of the staples as in Eq. 42, $d U$ denotes the integration measure of the $S U(3)$ gauge group. Every link on the lattice is visited in turn and a new value for the link variable is selected according to the above distribution. A change of all links of the lattice is called a sweep. A new configuration is obtained after one sweep.

The heatbath algorithm suffers critical slowing down, becoming less efficient as the lattice spacing is decreased. Acceleration can be achieved by the overrelaxation algorithm, in which the candidate link $U_{\mu}^{\prime}(n)$ is chosen such that the action in Eq. 41 is preserved. Such a change is always accepted according to the acceptance rule in the Metropolis algorithm. However, the overrelaxation algorithm is not ergodic, it has to be used in combination with an ergodic algorithm such as the heatbath.

So far we have left out the details of the the representation of the link variables and the generation of a candidate link in the three algorithms described above. For interested students, we refer to chapter 4 of the reference [1].

During this course, we will use the pre-installed Chroma application to generate a set of configurations for the $S U(3)$ pure gauge theory with the action defined in Eq. 34. Chroma takes inputs from an XML file. The input file for generating configurations is presented in Fig. 5. One can see that the input file consists of many nested tags. Here we explain some of the tags. The outer most tag is <purgaug> . This is the name of program we will run. Within this tag, there are 3 tags at the first indentation:
<Cfg>: This tag sets the details of configuration we are reading. Within this, <cfg_type> is the type of configuration. Here WEAK_FIELD means a slightly perturbed unit gauge, this is the start configuration. In this case, the tag <cfg_file> is ignored.
<MCControl>: This tag contains the Monte Carlo parameters. Within this tag, <RNG> sets the random seeds. <NWarmupUpdates> is the number of sweeps the algorithm needs to do before reach equilibrium. This number is usually determined by checking how a set of observables change with the number of sweeps. When the curves of the observables reach a plateau, the system approaches equilibrium. Fig. 6 shows how the value of Wilson plaquette changes with the number of sweeps. <SaveInterval> is the number of sweeps to be skipped before saving a configuration. This number is needed because the configurations generated subsequently in a Markov Chain will be correlated. In order to obtain statistically independent configurations, certain number of sweeps should be skipped before taking one for measurements. This number can be determined by computing the autocorrelation length.
<HBItr>: Inside this tag, <GaugeAction> defines the gauge action, here the action is Wilson gauge action and the value of $\beta$ is 6.0. <HBParams> is the algorithm parameters. In this practice, we use Heatbath algorithm combined with Overrelaxation. <nOver> is the number of overrelaxation sweeps and <NMaxHB> is the number of Heatbath sweeps.

## References

[1] C. Gattringer and C. B. Lang, "Quantum chromodynamics on the lattice," Lect. Notes Phys. 788, 1 (2010). doi:10.1007/978-3-642-01850-3
[2] J. Smit, "Introduction to quantum fields on a lattice: A robust mate," Cambridge Lect. Notes Phys. 15, 1 (2002).

```
<purgaug>
    <Cfg>
        <cfg_type>WEAK_FIELD</cfg_type>
        <cfg_file>dummy</cfg_file>
    </Cfg>
    <MCControl>
        <RNG>
            <Seed>
                <elem>11</elem>
                <elem>0 </elem>
                <elem>0 </elem>
                <elem>0 </elem>
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        </RNG>
        <StartUpdateNum>0</StartUpdateNum>
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        <SavePrefix>./beta6_xi3_2432_</SavePrefix>
        <SaveVolfmt>SINGLEFILE</SaveVolfmt>
    </MCControl>
    <HBItr>
        <GaugeAction>
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                <beta>6.0</beta>
            <AnisoParam>
                <anisoP>false</anisoP>
                    <t_dir>3</t_dir>
                    <xi_0>1.0</xi_0>
                    <nu>1.0</nu>
                </AnisoParam>
                <GaugeState>
                    <Name>SIMPLE_GAUGE_STATE</Name>
                    <GaugeBC>
                        <Name>PERIODIC_GAUGEBC</Name>
                    </GaugeBC>
            </GaugeState>
        </GaugeAction>
        <HBParams>
            <nOver>3</nOver>
            <NmaxHB>1</NmaxHB>
        </HBParams>
        <nrow>24 24 24 32</nrow>
    </HBItr>
</purgaug>
```

Figure 5: Input file for generating configurations.


Figure 6: History of the values of Wilson plaquette.

