Wilson Loop

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0.1 Wilson $Loop^1$

After we have produced the pure gauge configurations, we can make some physical measurements on these configurations. The physical observables have to be gauge-invariant. A prototype of a gauge-invariant object, made from only the gauge fields, is the trace of a product of link variables along a closed loop

$$L[U] = tr \left[\prod_{(n,\mu)\in\mathcal{L}} U_{\mu}(n) \right]$$
(0.1.1)

Here L is a closed loop of links on the lattice and the product in (0.1.1) runs over all these links. The Wilson loop which we introduce now is of that type.

A Wilson loop $W_{\mathcal{L}}$ is made from four pieces, two so-called Wilson lines $S(\mathbf{m},\mathbf{n},n_t)$, $S(\mathbf{m},\mathbf{n},0)$, and two temporal transporters $T(\mathbf{n},n_t)$, $T(\mathbf{m},n_t)$. The Wilson line $S(\mathbf{m},\mathbf{n},n_t)$ connects the two spatial points m and n along some path $\mathcal{C}_{m,n}$ with all link variables restricted to time argument n_t ,

$$S(\boldsymbol{m}, \boldsymbol{n}, n_t) = \prod_{(\boldsymbol{k}, j) \in \mathcal{C}_{m,n}} U_j(\boldsymbol{k}, n_t). \qquad (0.1.2)$$

The temporal transporter $T(\mathbf{n}, n_t)$ is a straight line of n_t link variables in time direction, all situated at spatial position \mathbf{n} ,

$$T(\boldsymbol{n}, n_t) = \prod_{j=0}^{n_t - 1} U_4(\boldsymbol{n}, j).$$
(0.1.3)

Attaching the four pieces to each other gives a closed loop \mathcal{L} ,

$$\mathcal{L}: \quad (\boldsymbol{m}, n_t) \xrightarrow{S} (\boldsymbol{n}, n_t) \xrightarrow{T^{\dagger}} (\boldsymbol{n}, 0) \xrightarrow{S^{\dagger}} (\boldsymbol{m}, 0) \xrightarrow{T} (\boldsymbol{m}, n_t). \quad (0.1.4)$$

The Wilson loop WL is obtained by taking the trace,

$$W_{\mathcal{L}}[U] = \operatorname{tr}\left[S\left(\boldsymbol{m}, \boldsymbol{n}, n_{t}\right) T\left(\boldsymbol{n}, n_{t}\right)^{\dagger} S(\boldsymbol{m}, \boldsymbol{n}, 0)^{\dagger} T\left(\boldsymbol{m}, n_{t}\right)\right] = \operatorname{tr}\left[\prod_{(k, \mu) \in \mathcal{L}} U_{\mu}(k)\right]$$
(0.1.5)

If the piece of loop $C_{m,n}$ used in $S(\mathbf{m},\mathbf{n},n_t)$ is a straight line we speak of a planar Wilson loop. Note that this can be the case only if \mathbf{m} and \mathbf{n} fall on a common coordinate axis. Otherwise the Wilson loop is called nonplanar. Figure 0.1 shows an example of a planar and a nonplanar loop.

 $^{^1{\}rm Most}$ of the content is excerpted from Gattringer C, Lang C.B., Quantum Chromodynamics on the Lattice: An Introductory Presentation, Lect. Notes Phys. 78 (Springer, Berlin Heidelberg 2010)



Figure 1: Examples for a planar (left-hand side plot) and a nonplanar (righthand side) Wilson loop. The horizontal direction is time

0.1.1 Physical interpretation of the Wilson loop

Due to the gauge symmetry, We can choice a gauge for gauge field $A_{\mu}(x)$

$$A_4(x) = 0, (0.1.6)$$

i.e., the aforementioned temporal gauge. So the temporal transporters become trivial,

$$T(\boldsymbol{n}, n_t) = \prod_{j=0}^{n_t - 1} U_4(\boldsymbol{n}, j) = \mathscr{V}, \qquad (0.1.7)$$

and we obtain the following chain of identities

$$\langle W_{\mathcal{L}} \rangle = \langle W_{\mathcal{L}} \rangle_{\text{temp}} = \left\langle \text{tr} \left[S \left(\boldsymbol{m}, \boldsymbol{n}, n_t \right) S \left(\boldsymbol{m}, \boldsymbol{n}, 0 \right)^{\dagger} \right] \right\rangle_{\text{temp}},$$
 (0.1.8)

where in the first step we have used the fact that the expectation value of a gauge-invariant observable remains unchanged when fixing the gauge. In the second step we used $W_{\mathcal{L}}[U] = \operatorname{tr} \left[S(\boldsymbol{m}, \boldsymbol{n}, n_t) S(\boldsymbol{m}, \boldsymbol{n}, 0)^{\dagger} \right]$, which follows from the definition of the Wilson loop in (0.1.5) and the triviality of the temporal transporter in temporal gauge (0.1.7).

The temporal gauge used in (0.1.8) makes explicit that the Wilson loop is the correlator of two Wilson lines $S(\mathbf{m},\mathbf{n},n_t)$ and $S(\mathbf{m},\mathbf{n},0)$ situated at time slices n_t and 0. Thus we can interpret this correlator using the equation

$$\lim_{T \to \infty} \left\langle O_2(t) O_1(0) \right\rangle_T = \sum_n \left\langle 0 \left| \widehat{O}_2 \right| n \right\rangle \left\langle n \left| \widehat{O}_1 \right| 0 \right\rangle e^{-tE_n}$$

where we inserting the unit operator of the vectors of a complete orthonormal basis as

$$\mathscr{V} = \sum_{n} \left| e_n \right\rangle \left\langle e_n \right|$$

in the left-hand side of the equation. Accordingly, the correlator behaves for

large total temporal extent T of our Euclidean lattice as (a, b are summed)

$$\left\langle \operatorname{tr}\left[S\left(\boldsymbol{m},\boldsymbol{n},\boldsymbol{n},\boldsymbol{n}_{t}\right)S(\boldsymbol{m},\boldsymbol{n},0)^{\dagger}\right]\right\rangle_{\operatorname{temp}} = \sum_{k}\left\langle 0\left|\widehat{S}(\boldsymbol{m},\boldsymbol{n})_{ab}\right|k\right\rangle\left\langle k\left|\widehat{S}(\boldsymbol{m},\boldsymbol{n})_{ba}^{\dagger}\right|0\right\rangle e^{-tE_{k}}$$

$$(0.1.9)$$

where the Euclidean time argument t is related to n_t via $t = a n_t$ with a being the lattice spacing. The sum in (0.1.9) runs over all states $|k\rangle$ that have a non-vanishing overlap with $\hat{S}(\mathbf{m}, \mathbf{n})^{\dagger}|0\rangle$

In the next paragraph we will argue that the states $|k\rangle$ with non-vanishing overlap are states describing a static quark-antiquark pair located at spatial positions **m** and **n**. Thus in (0.1.9) the term with the lowest energy E_1 is expected to be the state describing our static quark-antiquark pair. Higher states could be, e.g., this pair plus additional particle-antiparticle combinations with the quantum numbers of the vacuum. The energy E_1 is thus identified with the energy of the quark-antiquark pair, which is the static potential V(r)at spatial quark separation r,

$$E_1 = V(r) \quad \text{with} \quad r = a|\boldsymbol{m} - \boldsymbol{n}| \tag{0.1.10}$$

Combining (0.1.8), (0.1.9), and (0.1.10) we obtain

$$\langle W_{\mathcal{L}} \rangle \propto e^{-tV(r)} \left(1 + \mathcal{O} \left(e^{-t\Delta E} \right) \right) = e^{-n_t a V(r)} \left(1 + \mathcal{O} \left(e^{-n_t a \Delta E} \right) \right)$$
 (0.1.11)

Thus we find that we can calculate the static quark-antiquark potential from the large- n_t behavior of the Wilson loop. The corrections in (0.1.11) are exponentially suppressed, where ΔE is the difference between V(r) and the first excited energy level of the quark-antiquark pair.

We stress that Wilson loops are oriented. However, reversing the orientation, which on an algebraic level is complex conjugation, simply corresponds to the interchange of quark and antiquark. Thus both orientations serve equally well for a determination of the potential V(r).

The Wilson loops we have introduced are not necessarily planar. In Fig. 0.1 we show two Wilson loops, a planar one (left-hand side plot) and a nonplanar loop (right-hand side). Both loops have n = 5 (the horizontal direction is time). The planar loop has r = 3a, the nonplanar loop has $r = \sqrt{3^2 + 1a} = \sqrt{10a}$. Thus with nonplanar Wilson loops we can calculate the potential V(r) not only at distances r that are integer multiples of a, but also at intermediate points. Nonplanar Wilson loops also allow one to study whether rotational invariance is eventually restored when approaching the continuum limit. We will show that the potential can be parameterized by

$$V(r) = A + \frac{B}{r} + \sigma r. \tag{0.1.12}$$

0.1.2 The static quark potential

In order to illustrate the properties of the potential we calculate the vacuum expectation value of the Wilson loop in the limit of strong coupling, i.e., large g (small β). More explicitly we compute

$$\langle W_{\mathcal{C}} \rangle = \frac{1}{Z} \int \mathcal{D}[U] \exp\left(-\frac{\beta}{3} \sum_{P} \operatorname{Re} \operatorname{tr}\left[\mathcal{V} - U_{P}\right]\right) \operatorname{tr}\left[\prod_{l \in \mathcal{C}} U_{l}\right]$$
(0.1.13)

For this calculation we use a simplified notation: The sum runs over all plaquettes P, where each plaquette is counted with only one of the two possible orientations. The product over l runs over all link variables contained in the contour C defining the Wilson loop. This expression can be rewritten as

$$\langle W_{\mathcal{C}} \rangle = \frac{1}{Z'} \int \mathcal{D}[U] \exp\left(\frac{\beta}{3} \sum_{P} \operatorname{Re} \operatorname{tr}[U_{P}]\right) \operatorname{tr}\left[\prod_{l \in \mathcal{C}} U_{l}\right]$$

$$= \frac{1}{Z'} \int \mathcal{D}[U] \exp\left(\frac{\beta}{6} \sum_{P} \left(\operatorname{tr}[U_{P}] + \operatorname{tr}\left[U_{P}^{\dagger}\right]\right)\right) \operatorname{tr}\left[\prod_{l \in \mathcal{C}} U_{l}\right]$$

$$(0.1.14)$$

In the first step we separate the constant factor $\exp(-\beta/3\sum_P \operatorname{Retr}[\mathbb{W}])$ from the Boltzmann factor $\exp(-S)$. Exactly the same constant factor appears in the partition function Z and we cancel the two factors in the numerator and the denominator. The partition function without this factor is denoted by Z'. In the second step we use

$$\operatorname{Re}\operatorname{tr}\left[U_{P}\right] = \frac{1}{2}\left(\operatorname{tr}\left[U_{P}\right] + \operatorname{tr}\left[U_{P}^{\dagger}\right]\right)$$
(0.1.15)

We stress that, hermitian conjugation of the plaquette variable U_P is equivalent to inverting the orientation of the plaquette. Thus in the second line of (0.1.14) we explicitly display both orientations of the plaquette variables U_P , which leads to an extra factor 1/2.

Some SU(3) integrals is usefull. Based on the invariance of the measure dU. The integrals which integrals over products of entries U_{ab} of group elements U in the fundamental representation as

$$\int_{\mathrm{SU}(3)} \mathrm{d}U U_{ab} = 0$$

$$\int_{\mathrm{SU}(3)} \mathrm{d}U U_{ab} U_{cd} = 0$$

$$\int_{\mathrm{SU}(3)} \mathrm{d}U U_{ab} \left(U^{\dagger}\right)_{cd} = \frac{1}{3} \delta_{ad} \delta_{bc}$$

$$\int_{\mathrm{SU}(3)} \mathrm{d}U U_{ab} U_{cd} U_{ef} = \frac{1}{6} \epsilon_{ace} \epsilon_{bdf}$$
(0.1.16)

The basic tool for analyzing these integrals is the following equation for integrals over functions f(U):

$$\int_{\mathrm{SU}(3)} \mathrm{d}Uf(U) = \int_{\mathrm{SU}(3)} \mathrm{d}Uf(VU) = \int_{\mathrm{SU}(3)} \mathrm{d}Uf(UW)$$

The elements V and W are arbitrary SU(3) matrices. This relation follows directly from the invariance of the measure dU = d(UV) = d(VU). you can use this tool to prove these integrals. In the form of (0.1.14) we can now discuss the expansion of the Wilson loop expectation value for strong coupling (small β). In particular we expand the Boltzmann factor of (0.1.14) in β using the Taylor expansion for the exponential function,

$$\exp\left(\frac{\beta}{6}\sum_{P}\left(\operatorname{tr}\left[U_{P}\right]+\operatorname{tr}\left[U_{P}^{\dagger}\right]\right)\right)=\sum_{i,j=0}^{\infty}\frac{1}{i!j!}\left(\frac{\beta}{6}\right)^{i+j}\left(\sum_{P}\operatorname{tr}\left[U_{P}\right]\right)^{i}\left(\sum_{P}\operatorname{tr}\left[U_{P}^{\dagger}\right]\right)^{j}$$

$$(0.1.17)$$

Note that in this expansion we have separated the contributions from clockwise oriented plaquettes U_P^{\dagger} and counter-clockwise oriented plaquettes U_P . This is important since for the leading term in the expansion only those plaquettes oriented oppositely to the Wilson loop contribute.

For the normalization factor Z' it is straightforward to determine the leading contribution in the small- β expansion. Already the first term with i = j = 0 in (0.1.14) gives a nonvanishing contribution to the integral and we obtain (using the normalization of the Haar measure)

$$Z' = \int \mathcal{D}[U] \exp\left(\frac{\beta}{6} \sum_{P} \left(\operatorname{tr}\left[U_{P}\right] + \operatorname{tr}\left[U_{P}^{\dagger}\right]\right)\right) = \int \mathcal{D}[U](1 + \mathcal{O}(\beta)) = 1 + \mathcal{O}\left(\beta^{2}\right)$$

$$(0.1.18)$$

The expansion of the numerator of (0.1.14) is less straightforward. If only the leading term in the expansion of the Boltzmann factor is kept, then the product of link variables building up the observable, $\prod_{l \in \mathcal{C}} U_l$, gives rise to integrals of the type (0.1.16) which all vanish. Thus, in order to find the leading nonvanishing term of the expansion we have to expand the Boltzmann factor in small β . This brings down additional link variables from the exponent and in this way we can saturate the integrals over the links to obtain nonvanishing contributions of the type 0.1.16.

If we consider the contour C of the Wilson loop to be a $n_r \times n_t$ rectangle of links, then the minimal area \mathcal{A}_C spanned by this contour contains $n_A = n_r n_t$ plaquettes (note that n_r, n_t, n_A are positive integers). The physical area \mathcal{A}_C is related to the extension of the Wilson loop in physical units an_r, an_t by $\mathcal{A}_C = a^2 n_A = an_r an_t$. According to the relationship

$$\int dUtr[VU]tr[U^{\dagger}W] = \frac{1}{3}tr[VW] \qquad (0.1.19)$$

, we find nonvanishing contributions only when each link variable $U_{\mu}(n)$ in the loop is paired with its conjugate partner $U_{\mu}(n)^{\dagger}$. since we have plaquettes in our action, this must continue until we have filled the contour C with n_A plaquettes obtained from the expansion of the Boltzmann factor. We depict this contribution in Fig. 2

Note that the plaquettes used for filling the contour have to have the opposite orientation of the Wilson loop. Only in this way the contributions at each link have the form of the integrand in (0.1.16). Since we need at least $n_A = n_r n_t$ plaquettes from the exponent, the necessary term in the expansion (0.1.17) of



Figure 2: Leading contribution in the strong coupling (small β) expansion of the Wilson loop. The outer, counter-clockwise-oriented rectangle is the Wilson loop, the smaller, clockwise-oriented squares are the single plaquette terms from the action

the exponential is of order n_A . Explicitly this leading term reads (note that from the two orientations in (0.1.17) only the one opposite to the Wilson loop contributes)

$$\int \mathcal{D}[U] \frac{1}{n_A!} \left(\frac{\beta}{6}\right)^{n_A} \left(\sum_P \operatorname{tr}\left[U_P^{\dagger}\right]\right)^{n_A} \operatorname{tr}\left[\prod_{l \in \mathcal{C}} U_l\right]$$
$$= \left(\frac{\beta}{6}\right)^{n_A} \int \mathcal{D}[U] \prod_{P \in \mathcal{A}_C} \operatorname{tr}\left[U_P^{\dagger}\right] \operatorname{tr}\left[\prod_{l \in \mathcal{C}} U_l\right]$$
$$= \operatorname{tr}[\mathbb{W}] \left(\frac{\beta}{6}\right)^{n_A} \left(\frac{1}{3}\right)^{n_A} = 3 \exp\left(n_A \ln\left(\frac{\beta}{18}\right)\right) \qquad (0.1.20)$$

In the first step of (0.1.20) we expand the n_{A^-} th power over the sum of plaquette variables with the correct orientation $\left(U_P^{\dagger}\right)$. We keep only the terms where each of the n_A plaquettes P inside the minimal area $\mathcal{A}_{\mathcal{C}}$ is occupied by the matching U_P^{\dagger} . There are exactly n_A ! such products and thus the factor $1/n_A$! is canceled. All other terms in the expansion of the n_A -th power vanish since they give rise to integrals of the type (0.1.16). In the second step we evaluate the nonvanishing term using the integral (0.1.19). We glue together the plaquette variables inside the Wilson loop first into rows and then these rows into the full inner block of Fig. 2. Another gauge integral ties this block to the oppositely oriented outer contour of the Wilson loop. One finds that these steps give rise to the factor $(1/3)^{n_A}$ in 0.1.20. Combining (0.1.18) and (0.1.20) we find

$$\langle W_{\mathcal{C}} \rangle = 3 \exp\left(n_A \ln\left(\frac{\beta}{18}\right)\right) (1 + \mathcal{O}(\beta)) = 3 \exp\left(n_r n_t \ln\left(\frac{\beta}{18}\right)\right) (1 + \mathcal{O}(\beta))$$
(0.1.21)

According to (0.1.11) this expression has to be compared to the asymptotic form, i.e., for large $t = an_t$ we have

$$\langle W_{\mathcal{C}} \rangle \propto \exp\left(-an_t V(r)\right)$$
 (0.1.22)

Thus, we conclude that in the strong coupling limit (note that $r = an_r$)

$$V(r) = \sigma r \tag{0.1.23}$$

where the string tension σ is given by the leading order expression

$$\sigma = -\frac{1}{a^2} \ln\left(\frac{\beta}{18}\right) (1 + \mathcal{O}(\beta)) \tag{0.1.24}$$

We remark that it is relatively easy to produce higher corrections to the string tension. However, since the strong coupling expansion does not play a central role in modern lattice gauge theory (we will soon see that we are actually interested in approaching weak coupling), we will not discuss the calculation of higher terms and the convergence properties of this series. Instead, we stress once more that with a relatively simple expansion we have extracted from the lattice formulation a linearly rising potential. Below we discuss that such a term in the potential gives rise to the important feature of confinement. However, before we come to the discussion of the physical implications, let us first present the argument for the presence of the Coulomb-type term in the parameterization (0.1.12) of the static QCD potential.

Let us briefly sketch the physical implications of the static QCD potential, in particular the role of the linear term. The linearly rising term in the potential between a static quark-antiquark pair implies that the energy keeps rising linearly as one tries to pull the two constituents apart. Thus the quark and the antiquark are confined in a strongly bound meson state. Similarly, as we show later, also a combination of three quarks is bound, forming a baryon. The phenomenon that only color neutral combinations like hadrons are observable objects is one possible definition of confinement.

The physical mechanism which leads to the linearly rising term is the formation of a flux tube between the two sources. In QED, where we have no self-interaction of the gauge field, the field lines between a source and a sink spread out in space. In QCD the strong self-interaction of the gluons prevents this behavior, and the field is squeezed into a narrow tube or string producing the linear rise. Direct experimental evidence for the linearly rising potential is seen when the mass of hadrons is plotted as a function of their total spin and a linear behavior is found . Since for a linearly rising potential the energy rises linearly with the angular momentum, this experimental finding confirms the linear term in (0.1.12). So far our discussion is based only on the static potential obtained from pure gluodynamics. Certainly also the quarks, which we have not yet included in our discussion, play an important role. In the full theory with dynamical quarks, processes of particle-antiparticle creation and annihilation become important. In particular if the quark and antiquark are pulled sufficiently far apart, the energy becomes large enough to create a quark-antiquark pair, which may recombine with the two initial constituents to form two mesons. This phenomenon is called string breaking and can be studied on the lattice.

To summarize, we find that lattice QCD is very friendly to confinement. This property can easily be proven in the strong coupling limit, but it is also relatively simple to extract the QCD potential in a numerical calculation at weaker coupling.

0.2 data analysis²

The statistical analysis of the measured observables is the important final step of a Monte Carlo simulation. This analysis should also provide one with the information how many updating sweeps have to be discarded before configurations in equilibrium are produced and how many sweeps are necessary between two measurements. The final product of the statistical analysis is the average value which one quotes for an observable and an estimate for the corresponding statistical error.

Since in our case the data sample is the result of a (computer-)time series in our Monte Carlo simulation there is high chance that the observables are in fact correlated. This so-called autocorrelation leads to a nonvanishing *autocorrelation function*, which we define as

$$C_X(X_i, X_{i+t}) = \langle (X_i - \langle X_i \rangle) (X_{i+t} - \langle X_{i+t} \rangle) \rangle = \langle X_i X_{i+t} \rangle - \langle X_i \rangle \langle X_{i+t} \rangle$$

$$(0.2.1)$$

For a Markov chain in equilibrium the autocorrelation function depends only on the (computer time) separation t and we write

$$C_X(t) = C_X(X_i, X_{i+t})$$
 (0.2.2)

Note that $C_X(0) = \sigma_X^2$. In a typical situation the normalized correlation function Γ_X exhibits exponential behavior asymptotically for large t:

$$\Gamma_X(t) \equiv \frac{C_X(t)}{C_X(0)} \sim \exp\left(-\frac{t}{\tau_{X,\exp}}\right)$$
(0.2.3)

and one calls $\tau_{X, \exp}$ the exponential autocorrelation time for X. The complete expression for $\Gamma_X(t)$ involves a sum over several such terms. In (0.2.3) we consider only the asymptotically leading term with the largest autocorrelation time.

²Most of the content is excerpted from Gattringer C, Lang C.B., Quantum Chromodynamics on the Lattice: An Introductory Presentation, Lect. Notes Phys. 78 (Springer, Berlin Heidelberg 2010)

This number provides information on how strongly subsequent measurements are correlated. The exponential autocorrelation time τ_{\exp} is the supremum of the values $\tau_{X,\exp}$ for all possible observables X :

$$\tau_{\exp} = \sup_{X} \tau_{X,\exp} \tag{0.2.4}$$

Autocorrelations lead to systematic errors which are $\mathcal{O}(\exp(-t/\tau_{\exp}))$ if the computer time between subsequent measurements is t.

For uncorrelated data, the variance of that estimator is

$$\sigma_{\hat{X}}^{2} = \left\langle (\hat{X} - \langle X \rangle)^{2} \right\rangle = \left\langle \left(\frac{1}{N} \sum_{i=1}^{N} (X_{i} - \langle X \rangle) \right)^{2} \right\rangle$$
$$= \frac{1}{N^{2}} \left\langle \sum_{i,j=1}^{N} (X_{i} - \langle X \rangle) (X_{j} - \langle X \rangle) \right\rangle = \frac{1}{N} \left\langle X^{2} \right\rangle - \left\langle X \right\rangle^{2} + \frac{1}{N^{2}} \sum_{i \neq j} \left\langle X_{i} X_{j} \right\rangle$$
(0.2.5)

But for correlated random variables X_i the terms with $i \neq j$ in the second line of (0.2.5) do not vanish and one can continue this equation to obtain for the correlated case

$$\sigma_{\hat{X}}^{2} = \frac{1}{N^{2}} \sum_{i,j=1}^{N} C_{X}(|i-j|) = \frac{1}{N^{2}} \sum_{t=-(N-1)}^{N-1} \sum_{k=1}^{N-|t|} C_{X}(|t|)$$
$$= \sum_{t=-N}^{N} \frac{N-|t|}{N^{2}} C_{X}(|t|) = \frac{C_{X}(0)}{N} \sum_{t=-N}^{N} \Gamma_{X}(|t|) \left(1 - \frac{|t|}{N}\right)$$
(0.2.6)
$$\approx \frac{\sigma_{X}^{2}}{N} 2 \left(\frac{1}{2} + \sum_{t=1}^{N} \Gamma_{X}(|t|)\right) \equiv \frac{\sigma_{X}^{2}}{N} 2\tau_{X, \text{ int}}$$

where we have introduced the integrated autocorrelation time

$$\tau_{X, \text{ int }} = \frac{1}{2} + \sum_{t=1}^{N} \Gamma_X(t).$$
 (0.2.7)

This definition is motivated by the observation that for exponential behavior

$$\tau_{X, \text{ int }} = \frac{1}{2} + \sum_{t=1}^{N} \Gamma_X(|t|) \approx \int_0^\infty \mathrm{d}t \mathrm{e}^{-t/\tau} = \tau(\text{ for large } \tau).$$
 (0.2.8)

In the last step of (0.2.6) we have neglected the factor 1 - |t|/N which is justified for large enough N due to the exponential suppression of $\Gamma_X(|t|)$.

Computing $\tau_{X, \text{ int}}$ in a realistic situation one has to cut off sum (0.2.7) at a value of t where the values of $\Gamma(t)$ become unreliable. Usually one then assumes exponential behavior for the part not explicitly taken into account in the sum. Still, the determination of τ_{exp} or even τ_{int} is a delicate business.

Usually one needs at least 1000τ data values for estimates of τ itself. In order to judge whether the measured autocorrelation time is reliable, one therefore should start with small size lattices and high statistics and work oneself up to larger sizes, carefully checking the behavior and reliability of C(t).

If it is too expensive to compute the autocorrelation time - and unfortunately this is often the case in Monte Carlo calculations for quantum field theory problems - there are simpler statistical methods for obtaining at least some estimate for the correlation of the data.

Data blocking methods: One divides the data into sub-blocks of data of size K, computes the block mean values, and considers them as new variables X_i . The variance of these blocked X_i then should decrease like 1/K if the original data were independent. One repeats this for a sequence of different values for K. As soon as the 1/K behavior is observed for large enough K one may consider these block variables as statistically independent. Once the data (or the block results) can be considered independent, one may determine the expectation values of the observables of interest and their errors. Often, however, the number of data is too small to get a reliable estimate of the variance of the computed expectation values. Another obstacle may be that error propagation is unreliable or impossible to determine. There are two efficient and easy-to-use methods dealing with both problems. Both assume that the data are not correlated.

Statistical bootstrap: Given a set of N data, assume that we are interested in some observable θ which may be estimated from that set. This observable can also be, e.g., the result of a fit based on all N raw data. Let us call the value of the observable obtained from the original data set $\hat{\theta}$. One recreates from the sample repeatedly other samples by choosing randomly N data out of the original set. This costs essentially nothing, since we just recycle the original data set for the building of new sets. Let us assume we have done this Ktimes and thus have K sets of N data values each. Of course some values will enter more than once in the new sets. For each of these sets one computes the observable θ resulting in values θ_k with $k = 1, \ldots, K$. Then one determines

$$\widetilde{\theta} \equiv \frac{1}{K} \sum_{k=1}^{K} \theta_k, \quad \sigma_{\widetilde{\theta}}^2 \equiv \frac{1}{K} \sum_{k=1}^{K} \left(\theta_k - \widetilde{\theta} \right)^2$$

These are estimators for $\langle \theta \rangle$ and σ_{θ}^2 . They are not unbiased and therefore $\theta \neq \hat{\theta}$ for finite K. The difference is called bias and gives an idea on how far away the result may be from the true $\langle \theta \rangle$. As final result for the observable one quotes $\langle \theta \rangle = \tilde{\theta} \pm \sigma_{\tilde{\theta}}$

Jackknife: We start with a data set of size N and an observable θ like for the statistical bootstrap. The value of the observable computed for the original set is again called $\hat{\theta}$. One now constructs N subsets by removing the n th entry of the original set (n = 1, ..., N) and determines the value θ_n for each set. Then

$$\sigma_{\widehat{\theta}}^2 \equiv \frac{N-1}{N} \sum_{n=1}^{N} \left(\theta_n - \widehat{\theta}\right)^2$$

The square root of the variance gives an estimate for the standard deviation of $\hat{\theta}$. For the final result one quotes either $\langle \theta \rangle = \hat{\theta} \pm \sigma_{\hat{\theta}}$ or replaces $\hat{\theta}$ by the unbiased estimator. The bias may be determined from

$$\widetilde{\theta} \equiv \frac{1}{N} \sum_{n=1}^{N} \theta_n$$

leading to $\hat{\theta} - (N-1)(\tilde{\theta} - \hat{\theta})$ as the unbiased estimator for $\langle \theta \rangle$.

In a practical implementation both, statistical bootstrap and jackknife, may be combined with blocking by organizing the data in blocks and constructing subsets by removing blocks instead of only single values.

0.3 Code

The input of calculating wilson loop in chroma as

1	xml version = "1.0"?
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3	<param/>
4	$< \! { m InlineMeasurements} >$
5	$<\!\!\mathrm{elem}\!>$
6	<name>WILSLP</name>
7	$<\!\! m Frequency\! >\!\!2<\!\!/ m Frequency\! >$
8	<param/>
9	$<\!\!\mathrm{version}\!>\!\!3<\!\!/\!\mathrm{version}\!>$
10	$<\!\!\mathrm{kind}\!>\!\!7\!<\!\!/\mathrm{kind}\!>$
11	$<$ j_decay $>$ 3 $j_decay>$
12	$<\!{ m t_dir}\!>\!\!3<\!/{ m t_dir}>$
13	$<\!\mathrm{GaugeState}\!>$
14	<name>SIMPLE_GAUGE_STATE</name>
15	$<\!\!\mathrm{GaugeBC}\!\!>$
16	<name>PERIODIC_GAUGEBC</name>
17	$<\!\!/{ m Gauge BC}\!>$
18	$<\!/{ m GaugeState}>$
19	$<\!\!/\mathrm{Param}\!>$
20	$<\!\!\mathrm{NamedObject}\!>$
21	$<$ gauge_id $>$ default_gauge_field $gauge_id>$
22	$<\!\!/{ m NamedObject}\!>$
23	$<\!\!/ ext{elem}\!>$
24	$$
25	$<\!\!\mathrm{nrow}\!>\!\!24$ 24 24 $32\!<\!/\mathrm{nrow}\!>$
26	$<\!\!/\mathrm{Param}\!>$
27	<rng></rng>
28	$<\!\!\mathrm{Seed}\!>$
29	$<\!\! ext{elem}\!>\!\!11<\!\!/ ext{elem}\!>$
30	$<\!\! ext{elem}\!>\!\!11<\!\!/ ext{elem}\!>$

31	<elem $>11elem>$
201	
32	<elem $>$ 0 $elem>$
33	$<\!\!/{ m Seed}\!>$
34	$<\!\!/\mathrm{RNG}\!>$
35	
36	$<\!\!\mathrm{Cfg}\!>$
37	$<\!\mathrm{cfg_type}\!>\!\!\mathrm{SZINQIO}\!<\!\!/\mathrm{cfg_type}\!>$
38	$<$ cfg_file>conf_path
39	$<\!\!/\mathrm{Cfg}\!>$
40	

41 </chroma>

Parameter "kind" is used to control which kinds of wilson loop are calculated. there are three kinds of wilson loop: (1) "space-like" planar wilson loops in the directions perpendicular to j_decay that have equal length, (2) "timelike" planar Wilson loops with time direction j_decay and space directions the perpendicular ones that have equal length and (3) off-axis "time-like" wilson loops along 3 particular paths in the space directions that have equal length. the "kind" binary-combined YES/NO [1/0] of the three options. e.g. kind = 2 gives planar t-like, kind=6 is planar + off-axis: sqrt(2), sqrt(5), sqrt(3).We've calculated all three cases here.

The results are stored in output.xml. We can use the elementtree which is a python package to read the results in .xml files. The result of wilson loop can be stored in a three-dimensional array, such as (conf, tlength, rlength). We can apply bootstrap or jackknife methods to estimate errors. The three wilson loops are ploted in Fig 3. Each line in the Fig represents the vary of wilson loop with t at given distance r. According to the Eq. 0.1.11, when t is large, Wilson loop decays exponentially with t. Since we take logarithmic coordinates, each line is approximately as straight line .We can use the following formula to obtain the potential with different r which is simily in meson mass calculation:

$$V(t,r) = \log(\frac{W(t,r)}{W(t+1,r)}).$$

We show the potential V(t,r) in Fig. 4. When t is large enough, V(t,r) is close to the static potential of quark-antiquark. Finally, we obtain the vary of static potential with distance r as shown in Fig. 5.



Figure 3: The wilson loops vary with t dimentions. Each line represents a different distance r.



Figure 4: The potential V(t,r) obtained by wilson loops.



Figure 5: The static quark potential V(r) vary with distance r.