Trivializing maps, the Wilson flow and the HMC algorithm

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Abstract

In lattice gauge theory, there exist field transformations that map the theory to the trivial one, where the basic field variables are completely decoupled from one another. Such maps can be constructed systematically by integrating certain flow equations in field space. The construction is worked out in some detail and it is proposed to combine the Wilson flow (which generates approximately trivializing maps for the Wilson gauge action) with the HMC simulation algorithm in order to improve the efficiency of lattice QCD simulations.

1. Introduction

The Nicolai map transforms interacting supersymmetric theories to non-interacting ones [1]. Supersymmetry is considered to be essential for the existence of these field transformations in view of the fact that their Jacobian is exactly cancelled by the fermion partition function.

In lattice gauge theory, a natural question to ask is whether there are field transformations that map the theory to its strong-coupling limit. In particular, if there are no matter fields, one is looking for substitutions

\[ U = \mathcal{F}(V) \quad (1.1) \]

of the gauge field \( U \) in the functional integral whose Jacobian cancels the gauge-field action. Similarly to the Nicolai map, this kind of transformation maps the theory to a solvable one, but supersymmetry is not required and the Jacobian plays a different rôle.
Fig. 1. The proposed simulation algorithm for lattice QCD updates the gauge field $U$ in three steps, following the arrows in this diagram, where the Hamilton function used in the HMC step has the standard kinetic term and includes the Jacobian of the field transformation $\mathcal{F}$ (cf. subsect. 2.4).

On a finite lattice, and if the gauge group is compact and connected, the existence of such trivializing maps is guaranteed by a general theorem on volume forms on compact manifolds (see ref. [2], Theorem 1.26, for example). One may be inclined to assume that these transformations are too complicated to be of any use. However, as explained later in this paper, it is possible to build up trivializing maps by integrating flows in field space, whose generators satisfy certain partial differential equations. The latter are quite tractable and can, to some extent, be solved analytically in the pure gauge theory. An application of trivializing maps, which can then be envisaged, is the acceleration of lattice QCD simulations.

The fact that the efficiency of the available simulation algorithms is unpredictable has always been a weakness of numerical lattice QCD. Already a while ago, empirical studies of the SU(3) gauge theory by Del Debbio, Panagopoulos and Vicari [3] showed that the autocorrelation times of observables related to the topological charge of the gauge field tend to be large and appear to grow exponentially with the inverse of the lattice spacing. Moreover, Schaefer, Sommer and Virotta [4] recently found that the situation is, in this respect, essentially unchanged when the sea quarks are included in the simulations.

The rapid slowdown of the simulations at small lattice spacings may conceivably be overcome by combining approximately trivializing maps with the HMC simulation algorithm [5] (see fig. 1). Since the transformation moves the theory closer to the strong-coupling limit, where the HMC algorithm is known to be highly efficient, the autocorrelation times are, in general, expected to be reduced in this way. Evidently, for the combined algorithm to work out in practice, approximately trivializing maps must be found which are fairly simple and programmable. One of the goals of the present paper is thus to provide a solution to this problem.
2. Field transformations

Most concepts developed in this paper are expected to be widely applicable, but as explained above, the case of immediate interest is lattice QCD. In the following, the gauge group is therefore taken to be SU(3). Since the quarks will play a spectator rôle, they will be added to the theory only in sect. 6, where the proposed simulation algorithm for lattice QCD is discussed.

2.1 Field space

The lattice theory is set up on a finite hypercubic lattice \( \Lambda \) with periodic boundary conditions. For notational convenience, the lattice spacing is set to unity. As usual, the gauge field variables \( U(x, \mu) \in SU(3) \) are assumed to reside on the links \( (x, \mu) \) of the lattice (where \( x \in \Lambda \) and \( \mu = 0, \ldots, 3 \)). The expectation value of any observable \( \mathcal{O}(U) \) is then given by the functional integral

\[
\langle \mathcal{O} \rangle = \frac{1}{Z} \int D[U] \mathcal{O}(U) e^{-S(U)}
\]

over the space of gauge fields. In this expression, \( S(U) \) denotes the gauge-field action, \( Z \) the partition function and \( D[U] \) the product of the normalized \( SU(3) \)-invariant integration measures of the link variables \( U(x, \mu) \).

From a purely mathematical point of view, the space of lattice gauge fields is a power of \( SU(3) \) and therefore a compact connected manifold. Field transformations are invertible maps of this manifold onto itself. Such transformations will always be required to be differentiable in both directions and orientation-preserving (here and below, “differentiable” means “infinitely often continuously differentiable”).

2.2 Right-invariant differential operators

Since the link variables \( U(x, \mu) \) take values in a Lie group, it is natural to express differentiations with respect to them through a basis \( \partial^a_{x,\mu} \), \( a = 1, \ldots, 8 \), of differential operators that are invariant under the right-action of the group. The action of these operators on a differentiable function \( f(U) \) of the gauge field is given by

\[
\partial^a_{x,\mu} f(U) = \frac{d}{dt} f(U_t) \bigg|_{t=0}, \quad U_t(y, \nu) = \begin{cases} 
e^t T^a U(x, \mu) & \text{if } (y, \nu) = (x, \mu), \\ U(y, \nu) & \text{otherwise}, \end{cases}
\]

where \( T^a \) are the \( SU(3) \) generators (see appendix A). In particular, \( \partial^a_{x,\mu} \) transforms according to the adjoint representation under the left-action of \( SU(3) \).
The operators $\partial^a_{x,\mu}$ go along with a basis of 1-forms on the field manifold,

$$\theta^a_{x,\mu} = -2 \text{tr}\{dU(x,\mu)U(x,\mu)^{-1}T^a\},$$

such that

$$df(U) = \sum_{x,\mu} \theta^a_{x,\mu} \partial^a_{x,\mu} f(U)$$

for all functions $f(U)$.

### 2.3 Jacobian matrix

For any given gauge field $V(y,\nu)$, the transformation (1.1) produces another field $U(x,\mu) = [\mathcal{F}(V)](x,\mu)$. When considering such transformations, one needs to distinguish differentiations with respect to $V$ from those with respect $U$. The associated 1-forms must also be distinguished. In the following, all symbols carrying a hat represent quantities and operations referring to $V$.

The Jacobian matrix

$$[\mathcal{F}_s(V)](x,\mu; y,\nu)^{ab} = -2 \text{tr}\{\hat{\partial}^b_{y,\nu} U(x,\mu)U(x,\mu)^{-1}T^a\}$$

can be considered to be the kernel of a linear operator acting on link fields with values in $\mathfrak{su}(3)$. In particular,

$$\theta^a_{x,\mu} = \sum_{y,\nu}[\mathcal{F}_s(V)](x,\mu; y,\nu)^{ab} \hat{\theta}^b_{y,\nu}. \quad (2.6)$$

Since the functional integration measure $D[U]$ is proportional to the maximal product of these 1-forms, it follows that

$$D[U] = D[V] \det \mathcal{F}_s(V). \quad (2.7)$$

The Jacobian of the map (1.1) is thus $\det \mathcal{F}_s(V)$.

If the transformation satisfies

$$S(\mathcal{F}(V)) - \ln \det \mathcal{F}_s(V) = \text{constant}, \quad (2.8)$$

the substitution $U \rightarrow V$ of the integration variables in the functional integral maps the theory to the trivial one where the link variables are completely decoupled from
one another. The expectation values (2.1) are then given by

$$\langle O \rangle = \int D[V] O(F(V)).$$

(2.9)

Such trivializing maps thus contain the entire dynamics of the theory.

Although the remark is likely to remain an academic one, an intriguing observation is that the integral (2.9) can be simulated simply by generating uniformly distributed random gauge fields. Subsequent field configurations are uncorrelated in this case and there are therefore no autocorrelations in the data series for the observables $O$.

2.4 Transformation behaviour of the HMC algorithm

The HMC algorithm [5] operates on the phase space associated to the field manifold. In particular, the transition $V \rightarrow V'$ in fig. 1 requires the equations of motion derived from the Hamilton function

$$\hat{H}(\hat{\pi}, V) = \frac{1}{2} (\hat{\pi}, \hat{\pi}) + S(F(V)) - \ln \det F^*(V)$$

(2.10)

to be integrated, where $\hat{\pi}(x, \mu) \in \mathfrak{su}(3)$ is the canonical momentum of $V(x, \mu)$.

Although the complete update algorithm for the field $U$ described by fig. 1 looks different, it is in fact equivalent to the HMC algorithm with a non-standard Hamilton function. The equivalence can be established by noting that the transformation from $V$ to $U$ preserves the symplectic 2-form

$$\hat{\Omega} = \sum_{x, \mu} \{ \hat{\pi}^a(x, \mu) \hat{\theta}^a_{x, \mu} \},$$

(2.11)
i.e. $\Omega = \hat{\Omega}$, if the momenta of the fields are transformed according to

$$\hat{\pi}^b(y, \nu) = \sum_{x, \mu} [F_*(V)](x, \mu; y, \nu)^{ab} \pi^a(x, \mu).$$

(2.12)

The evolution of the transformed fields is then governed by the Hamilton function

$$H(\pi, U) = \frac{1}{2} (\pi, K(U)\pi) + S(U) - \ln \det F_*(V),$$

(2.13)

where

$$K(U) = F_*(V)^T F_*(V), \quad V = F^{-1}(U).$$

(2.14)
Note that the Jacobian in eq. (2.13) cancels when the momenta are integrated over in the functional integral. The algorithm outlined in fig. 1 thus amounts to applying the HMC algorithm with a modified Hamilton function of the kind considered long ago by Duane et al. [6].

3. Transformations generated by flow equations

Flows in field space build up field transformations from infinitesimal transformations. The latter are generally easier to work with than integral transformations, because they refer to the current field only. Moreover, the differentiability and invertibility of the generated transformations is automatically guaranteed.

3.1 Flows in field space

An infinitesimal field transformation,

\[ U \rightarrow U + \varepsilon Z(U)U + O(\varepsilon^2), \]

is generated by a link field \( [Z(U)](x, \mu) \) with values in \( \mathfrak{su}(3) \). The continuous composition of such transformations amounts to integrating a flow equation

\[ \dot{U}_t = Z_t(U_t)U_t \]

with respect to a fictitious time \( t \). A simple choice for the generator of the flow is

\[ [Z_t(U)]^a(x, \mu) = \partial^a_{x, \mu} \mathcal{W}_0(U), \]

\[ \mathcal{W}_0(U) = \sum_{x, \mu \neq \nu} \text{tr}\{U(x, \mu, \nu)\}, \]

where \( U(x, \mu, \nu) \) denotes the plaquette loop in the \( (\mu, \nu) \)-directions at the point \( x \). In the following, this flow will be referred to as the “Wilson flow”.

If \( Z_t(U) \) is a differentiable function of \( t \) and \( U \), the flow equation (3.2) has a unique solution \( U_t \) for any specified initial value \( U_0 = V \) and all \( t \in (-\infty, \infty) \). Moreover, the solution is differentiable with respect to \( t \) and \( V \) (for a proof of these statements, see ref. [7], for example). It should be emphasized that the existence of the solution for all times is non-trivial and can only be guaranteed, without further assumptions, because the field manifold is compact.
3.2 Integrated transformations

At fixed $t$, the field $U_t$ is a well-defined function of the initial field $V$. Through the integration of the flow equation, one thus obtains a differentiable transformation, $V \rightarrow U_t = \mathcal{F}_t(V)$, of the field space. The transformation is invertible and its inverse is differentiable, because the flow equation can be integrated backwards from $t$ to 0. Moreover, since the Jacobian $\det \mathcal{F}_{t,*}(V)$ is equal to unity at $t = 0$ and does not pass through zero at any time, the transformation is also orientation-preserving and thus fulfills all requirements for an acceptable map of field space.

There is a useful compact expression for the Jacobian which is obtained starting from the equations

$$\frac{d}{dt} \ln \det \mathcal{F}_{t,*}(V) = \text{Tr}\{\dot{\mathcal{F}}_{t,*}(V) \mathcal{F}_{t,*}(V)^{-1}\}, \quad (3.5)$$

$$[\dot{\mathcal{F}}_{t,*}(V)](x, \mu; y, \nu)^{ab} = -2 \text{tr}\{\hat{\partial}_{y,\nu} \{[Z_t(U_t)](x, \mu)U_t(x, \mu)\}U_t(x, \mu)^{-1}T^a$$
$$- \hat{\partial}_{y,\nu} U_t(x, \mu)U_t(x, \mu)^{-1}[Z_t(U_t)](x, \mu)T^a\}. \quad (3.6)$$

Noting

$$\hat{\partial}_{y,\nu} = \sum_{x,\mu} [\mathcal{F}_{*}(V)](x, \mu; y, \nu)^{ab} \partial^a_{x,\mu}, \quad (3.7)$$

a few lines of algebra then lead to the formula

$$\ln \det \mathcal{F}_{t,*}(V) = \int_0^t ds \sum_{x,\mu} \{\partial^a_{x,\mu} [Z_s(U)]^a(x, \mu)\}_{U=U_s}. \quad (3.8)$$

In the case of the Wilson flow, for example, the contribution of the Jacobian to the action of the field $V$,

$$\ln \det \mathcal{F}_{t,*}(V) = -\frac{16}{3} \int_0^t ds \mathcal{W}_0(U_s), \quad (3.9)$$

is proportional to the integral of the Wilson plaquette action along the flow.
4. Trivializing maps

Somewhat surprisingly, trivializing maps can, to some extent, be constructed explicitly in the pure gauge theory. The construction is explained in this section, assuming that the gauge action $S(U)$ is a sum of Wilson loops (plaquettes, rectangles, etc.).

4.1 Trivializing flows

If the generator $Z_t(U)$ of the flow (3.2) is such that

$$\int_0^t ds \sum_{x,\mu} \{ \partial_a x,\mu [Z_s(U)]^a x,\mu \} U = U_s = tS(U_t) + C_t, \tag{4.1}$$

where $C_t$ may depend on $t$ but not on the fields, the associated integrated transformations satisfy

$$S(\mathcal{F}_t(V)) - \ln \det \mathcal{F}_{t,s}(V) = (1 - t)S(\mathcal{F}_t(V)) - C_t. \tag{4.2}$$

In particular, the transformation at $t = 1$ is then a trivializing map.

Equation (4.1) is a rather implicit condition on the generator of the flow. However, when differentiated with respect to $t$, it assumes a more tractable form,

$$\sum_{x,\mu} \{ \partial_a x,\mu [Z_t(U)]^a x,\mu - t\partial_a x,\mu S(U)[Z_t(U)]^a x,\mu \} = S(U) + \dot{C}_t, \tag{4.3}$$

which involves the generator at time $t$ only. Note that the differential condition (4.3) and the flow equation (3.2) imply eq. (4.1), i.e. it suffices to find a generator $Z_t(U)$ that satisfies eq. (4.3).

4.2 Existence of trivializing flows

Equation (4.3) is an inhomogeneous linear partial differential equation for the generator $Z_t(U)$. Since it is a scalar equation, one expects that there are many solutions. In the following, the solution will be obtained in the form

$$[Z_t(U)]^a x,\mu = -\partial_a x,\mu \bar{S}_t(U), \tag{4.4}$$

where the action $\bar{S}_t(U)$ is to be determined.
When inserted in eq. (4.3), the ansatz (4.4) leads to the Laplace equation

$$\mathcal{L}_t \tilde{S}_t = S + \dot{C}_t,$$

(4.5)

$$\mathcal{L}_t = \sum_{x, \mu} \left\{-\partial_{x, \mu}^a \partial_{x, \mu}^a + t (\partial_{x, \mu}^a S) \partial_{x, \mu}^a \right\}$$

(4.6)

(for simplicity, the argument $U$ is now often omitted). The operator $\mathcal{L}_t$ is elliptic and symmetric with respect to the scalar product

$$(\phi, \psi) = \int D[U] e^{-tS(U)} \phi(U)^* \psi(U).$$

(4.7)

$\mathcal{L}_t$ has therefore a complete set of differentiable eigenfunctions and a purely discrete spectrum with no accumulation points (see ref. [8], sect. 1.6, for example). Moreover, since

$$(\phi, \mathcal{L}_t \phi) = \sum_{x, \mu} (\partial_{x, \mu}^a \phi, \partial_{x, \mu}^a \phi) \geq 0,$$

(4.8)

the function $\phi(U) = 1$ is the only zero mode of $\mathcal{L}_t$ and all other eigenfunctions have eigenvalues separated from the origin by a strictly positive spectral gap.

Now if one chooses $C_t$ to be such that

$$\dot{C}_t = -(1, S)/(1, 1),$$

(4.9)

the zero-mode component is removed from the right-hand side of eq. (4.5) and

$$\tilde{S}_t = \mathcal{L}_t^{-1} (S + \dot{C}_t).$$

(4.10)

is then a well-defined expression that solves the equation. The differentiability of $\tilde{S}_t$ with respect to $t$ and $U$ essentially follows from the ellipticity of $\mathcal{L}_t$ (appendix E). A constructive proof of the existence of trivializing flows has thus been given.

4.3 Expansion in powers of $t$

The solution (4.10) is well defined but still quite implicit since it involves the inverse of an operator acting on functions of the gauge field. In this and the next subsection, the solution is worked out analytically in powers of $t$. 
When the series
\[ \tilde{S}_t = \sum_{k=0}^{\infty} t^k \tilde{S}^{(k)} \]  
(4.11)
is inserted in eq. (4.5), the matching of the terms of a given order in \( t \) leads to the recursion
\[ \mathfrak{L}_0 \tilde{S}^{(0)} = S + \dot{C}^{(0)} , \]  
(4.12)
\[ \mathfrak{L}_0 \tilde{S}^{(k)} = - \sum_{x,\mu} \partial_{x,\mu}^a S \partial_{x,\mu}^a \tilde{S}^{(k-1)} + \dot{C}^{(k)} , \quad k = 1, 2, \ldots , \]  
(4.13)
for the actions \( \tilde{S}^{(k)} \). The Laplacian \( \mathfrak{L}_0 \) coincides with the colour-electric part of the Hamilton operator in lattice gauge theory in 4 + 1 dimensions. In particular, its eigenfunctions are products of SU(3) representation functions of the link variables. Sums of Wilson loops and products of Wilson loops, for example, are eigenfunctions of \( \mathfrak{L}_0 \) or can easily (algebraically) be decomposed into eigenfunctions.

The solution of the recursion,
\[ \tilde{S}^{(0)} = \mathfrak{L}_0^{-1} S , \]  
(4.14)
\[ \tilde{S}^{(k)} = - \mathfrak{L}_0^{-1} \sum_{x,\mu} \partial_{x,\mu}^a S \partial_{x,\mu}^a \tilde{S}^{(k-1)} , \quad k = 1, 2, \ldots , \]  
(4.15)
is thus obtained in the form of sums of Wilson loops and products of Wilson loops. Note that, as already mentioned in subsect. 4.2, the constant function is the only zero mode of \( \mathfrak{L}_0 \). Since the smallest non-zero eigenvalue of \( \mathfrak{L}_0 \) is \( \frac{4}{3} \), the right-hand sides of eqs. (4.14),(4.15) are therefore unambiguously determined up to an irrelevant additive constant.

4.4 Calculation of \( \tilde{S}^{(0)} \) and \( \tilde{S}^{(1)} \) in the Wilson theory

For illustration, the first two terms of the series (4.11) are now worked out explicitly for the plaquette action [9]
\[ S_p(U) = -\frac{1}{6} \beta W_0(U) \]  
(4.16)
(where \( \beta = 6/g_0^2 \) denotes the inverse gauge coupling). A short calculation, using the completeness relation (A.5), shows that the leading term is
\[ \tilde{S}^{(0)} = -\frac{1}{32} \beta W_0 = \frac{3}{16} S_w . \]  
(4.17)
Fig. 2. Classes of loops and pairs of loops contributing to $\tilde{S}^{(1)}$ in the Wilson theory. The loops $5 - 7$ reside on a single plaquette of the lattice. All other loops occupy two plaquettes which can lie in a plane or be at right angles in three dimensions.

To this order and up to a rescaling of the time parameter $t$, the trivializing flow in the Wilson theory thus coincides with the Wilson flow.

The expression to be worked out at the next order is

$$\tilde{S}^{(1)} = -\frac{1}{192} \beta^2 \sum_{x,\mu} \partial^n_{x,\mu} \mathcal{W}_0 \partial^n_{x,\mu} \mathcal{W}_0.$$  \hspace{1cm} (4.18)

The Wilson loops and products of Wilson loops that can occur at this point derive from the contractions of two plaquette loops with a common link. Altogether there are then seven classes $\mathcal{C}_i$, $i = 1, \ldots, 7$, of loops and pairs of loops to consider (see fig. 2). By summing the traces of the associated Wilson loops, each class $\mathcal{C}_i$ defines an action

$$\mathcal{W}_i = \sum_{C \in \mathcal{C}_i} \text{tr}\{U(C)\} \quad \text{if} \quad i = 1, 2, 5, \hspace{1cm} (4.19)$$

$$\mathcal{W}_i = \sum_{\{C, C'\} \in \mathcal{C}_i} \text{tr}\{U(C)\}\text{tr}\{U(C')\} \quad \text{if} \quad i = 3, 4, 6, 7, \hspace{1cm} (4.20)$$

where $U(C)$ denotes the ordered product of the link variables along the loop $C$. The sums in these equations extend over all possible positions of the loops on the lattice. Loops with opposite orientation are considered to be different and are both included in the sums.
Using the identity (A.5) again, some algebra now yields
\[
\sum_{x,\mu} \partial_{x,\mu}^a \mathcal{W}_0 \partial_{x,\mu}^a \mathcal{W}_0 = \mathcal{W}_1 - \mathcal{W}_2 - \frac{1}{3} \mathcal{W}_3 + \frac{1}{3} \mathcal{W}_4 - 2 \mathcal{W}_5 + \frac{2}{3} \mathcal{W}_6 - \frac{4}{3} \mathcal{W}_7 \tag{4.21}
\]
up to an additive constant. Furthermore,
\[
\mathcal{L}_0 \mathcal{W}_1 = 8 \mathcal{W}_1, \tag{4.22}
\]
\[
\mathcal{L}_0 \mathcal{W}_2 = \frac{31}{3} \mathcal{W}_2 + \mathcal{W}_4, \tag{4.23}
\]
\[
\mathcal{L}_0 \mathcal{W}_3 = 11 \mathcal{W}_3 - \mathcal{W}_1, \tag{4.24}
\]
\[
\mathcal{L}_0 \mathcal{W}_4 = \frac{31}{3} \mathcal{W}_4 + \mathcal{W}_2, \tag{4.25}
\]
\[
\mathcal{L}_0 \mathcal{W}_5 = \frac{28}{3} \mathcal{W}_5 + 4 \mathcal{W}_6, \tag{4.26}
\]
\[
\mathcal{L}_0 \mathcal{W}_6 = \frac{28}{3} \mathcal{W}_6 + 4 \mathcal{W}_5, \tag{4.27}
\]
\[
\mathcal{L}_0 \mathcal{W}_7 = 12 \mathcal{W}_7 + \text{constant}. \tag{4.28}
\]
In the subspace of these functions, the operator $\mathcal{L}_0$ can be easily inverted and the result
\[
\tilde{S}^{(1)} = \frac{1}{192} \beta^2 \left\{ - \frac{4}{33} \mathcal{W}_1 + \frac{12}{119} \mathcal{W}_2 + \frac{1}{33} \mathcal{W}_3 - \frac{5}{119} \mathcal{W}_4 + \frac{3}{40} \mathcal{W}_5 \\
- \frac{1}{5} \mathcal{W}_6 + \frac{1}{9} \mathcal{W}_7 \right\} \tag{4.29}
\]
is thus obtained. Note that the smallness of the numerical coefficients in this formula is balanced, to some extent, by the number of loops per lattice point in the classes $C_i$ (which are equal to 120, 12 and 6 for $i = 1, \ldots, 4$, $i = 5,6$ and $i = 7$ respectively).

4.5 Miscellaneous remarks
(a) **Higher orders.** The actions $\tilde{S}^{(k)}$, $k \geq 2$, can be computed algebraically following the steps taken in the previous subsection. Since all loops generated by contracting a plaquette loop with the loops at order $k - 1$ must be considered, the work required for the calculation is however rapidly growing with $k$.
(b) **Locality and convergence.** The series (4.11) is an expansion in local terms whose footprint on the lattice increases proportionally to the order $k$. At the values of $t$, where the expansion converges, the action $\tilde{S}_t$ is then guaranteed to be local as well.
The norm estimates in appendix E imply a lower bound on the convergence radius of the series, but this bound is rather poor and vanishes in the infinite-volume limit. It seems nevertheless plausible that the series has a non-zero convergence radius in this limit, because the inverse of the operator \( \mathcal{L}_t \) in eq. (4.10) is likely to remain bounded in a complex neighbourhood of \( t = 0 \). An analysis that takes the locality properties of \( \mathcal{L}_t \) into account will however be required to show this.

(c) \textit{Truncation of the expansion}. If all terms in the series (4.11) of order \( k \geq n \) are dropped, one obtains an approximately trivializing flow that satisfies eq. (4.2) up to an additive correction of order \( t^{n+1} \). An at least partial cancellation of the action is achieved in this case as long as \( t \) is sufficiently small for the correction to be strongly suppressed.

(d) \textit{Smoothing property}. The Wilson flow satisfies

\[
\frac{d}{dt} S_w(U_t) = -\frac{2}{16} \sum_{x, \mu} \{ \partial_{x, \mu} S_w(U) \partial_{x, \mu} S_w(U) \}_{U=U_t} \leq 0
\]  

(4.30)

and therefore lowers the Wilson action as \( t \) increases. To leading order in \( t \), the trivializing flow constructed in this section for the Wilson theory thus has a smoothing effect on the gauge field. On the other hand, if the flow is followed in the reverse direction, the gauge field tends to become rougher.

(e) \textit{Topological charge sectors}. In lattice QCD, the topological (instanton) sectors are not a property of the field manifold alone, but are expected to emerge dynamically when the continuum limit is approached. The fact that trivializing maps completely “straighten out” the sectors is therefore not in conflict with the topological properties of the field space.

(f) \textit{Renormalization group}. By composing the trivializing map \( U = \mathcal{F}_1(V) \) in the Wilson theory with its inverse at another value of the gauge coupling, one obtains a group of transformations whose only effect on the action is a shift of the coupling. The locality properties of these transformations are not transparent, however, and could be quite different from the ones of a Wilsonian “block spin” transformation.

5. \textbf{Numerical integration of the Wilson flow}

The discussion in sect. 1 now suggests to combine the HMC algorithm with the field transformations generated by the trivializing flow constructed in the previous sec-
tion. In particular, if the Wilson gauge action is used, the transformations generated by the Wilson flow may lead to an algorithm with improved sampling efficiency.

5.1 Forward integration

There is a wide range of numerical integration methods that can in principle be used to integrate the Wilson flow (see ref. [10], for example). The Euler scheme discussed in the following performs the integration in time steps of size $\epsilon$ and updates the link variables one after another according to

$$U(x, \mu) \rightarrow U'(x, \mu) = e^{[Z(U)](x, \mu)} U(x, \mu),$$

(5.1)

where

$$[Z(U)](x, \mu) = T^a \partial_{x, \mu} W_0(U).$$

(5.2)

Starting from the gauge field $U_t$ at time $t$, the field at time $t + \epsilon$ is thus obtained by running through all links $(x, \mu)$ on the lattice and updating the link variable residing there. Note that the ordering of the links matters, since the old value of $U(x, \mu)$ is replaced by the new one before going to the next link.

The generator of the flow is explicitly given by

$$[Z(U)](x, \mu) = - \sum_{\nu \neq \mu} \mathcal{P}\{U(x, \mu)U(x + \hat{\mu}, \nu)U(x + \hat{\nu}, \mu)^{-1}U(x, \nu)^{-1}$$

$$+ U(x, \mu)U(x + \hat{\mu} - \hat{\nu}, \nu)^{-1}U(x - \hat{\nu}, \mu)^{-1}U(x - \hat{\nu}, \nu)^{-1}U(x, \mu)\},$$

(5.3)

where $\hat{\mu}$ denotes the unit vector in direction $\mu$ and

$$\mathcal{P}\{M\} = \frac{1}{2} (M - M^\dagger) - \frac{1}{4} \text{tr}(M - M^\dagger)$$

(5.4)

projects any $3 \times 3$ matrix $M$ to $\text{su}(3)$. The Euler integration of the Wilson flow thus amounts to applying a number of "stout smearing" steps [11], except that the link variables are here updated one by one rather than all at once.

5.2 Backward integration

The application of $n$ Euler sweeps maps the initial field $V = U_0$ to the field $U = U_{n\epsilon}$ at time $t = n\epsilon$. If $t$ is held fixed and $n$ is taken to infinity, this map converges to the transformation obtained by integrating the Wilson flow exactly. However, the HMC algorithm may potentially be combined with the map defined by the Euler integrator
at fixed $n$ and $\epsilon$. For this proposition to be a viable option, the transformation must be invertible, i.e. one must be able to trace back the Euler integration by inverting the link update steps one by one in the reverse order.

The question is thus whether eq. (5.1) has a unique solution $U(x, \mu)$ given $U'(x, \mu)$ (and keeping all other link variables fixed). As explained in appendix D, the answer is affirmative, for arbitrary values of the field variables, if

$$|\epsilon| < \frac{1}{8}. \quad (5.5)$$

Moreover, in this range of $\epsilon$, the solution $U(x, \mu) = e^{-\epsilon X} U'(x, \mu)$ can be obtained through the fixed-point iteration

$$X_0 = 0,$$

$$X_{n+1} = \left\{ [Z(U)](x, \mu) \right\}_{U(x, \mu)=e^{-\epsilon X_n U'(x, \mu)}, \quad n = 0, 1, 2, \ldots}, \quad (5.7)$$

which converges to $X_*$ at an exponential rate.

In appendix D it is also shown that the Jacobian of the transformation (5.1) is strictly positive in the range (5.5). The field transformations obtained through the Euler integration of the Wilson flow are therefore orientation-preserving diffeomorphisms of the field manifold, as required for acceptable maps of field space.

5.3 Jacobian matrix of the Euler integrator

The Euler step (5.1) amounts to applying the field transformation

$$[\mathcal{E}_{x,\mu}(U)](y, \nu) = \begin{cases} e^{\epsilon[Z(U)](x, \mu)} U(x, \mu) & \text{if } (y, \nu) = (x, \mu), \\ U(y, \nu) & \text{otherwise}, \end{cases} \quad (5.8)$$

to the current gauge field. An Euler sweep is then the composition product of these transformations over all links $(x, \mu)$. It is straightforward to show that the Jacobian matrix of a composed transformation is the product of the Jacobian matrices of the factors. The Jacobian matrix of the Euler integrator is therefore an ordered product of the Jacobian matrices

$$[\mathcal{E}_{x,\mu,*}(U)](y, \nu; z, \rho)^{ac} = -2 \text{tr} \left\{ \partial_\rho [\mathcal{E}_{x,\mu}(U)](y, \nu) [\mathcal{E}_{x,\mu}(U)](y, \nu)^{-1} T^a \right\} \quad (5.9)$$

of the one-link transformations (5.8).

The matrix (5.9) can be expressed through the derivative

$$[Z_*(U)](y, \nu; z, \rho)^{bc} = \partial_\rho [Z(U)]^b(y, \nu) \quad (5.10)$$
of the generator of the Wilson flow. Explicitly, one finds that

\[
\left[ \mathcal{E}_{x,\mu,*}(U) \right](y, \nu; z, \rho)^{ac} = \delta^{ac} \delta_{yz} \delta_{\nu\rho} + \delta_{xy} \delta_{\mu\nu} \left\{ (e^{\text{Ad}X} - 1)^{ac} \delta_{yz} \delta_{\nu\rho} \right. \\
+ \epsilon J(-X)^{ab} [Z(U)](y, \nu; z, \rho)^{bc} \left\} \right. \\
X = \epsilon[Z(U)](x, \mu), \quad (5.11)
\]

where use was made of the SU(3) formulae listed in appendix A and B.

5.4 Jacobian of the integrated transformations

The Euler integrator generates a sequence of fields

\[
V = U_0 \rightarrow U_\epsilon \rightarrow U_{2\epsilon} \rightarrow \ldots \rightarrow U_{n\epsilon} = U
\]

by sweeping through the lattice \( n \) times and updating the link variables one by one in a specified order. In the following, the intermediate field configurations obtained starting from \( U_{k\epsilon} \) and updating the link variables on all links that come before \((x, \mu)\) will be denoted by \( U_{k\epsilon,[x,\mu]} \). In particular, \( U_{k\epsilon,[x,\mu]} = U_{k\epsilon} \) if \((x, \mu)\) is the first link and

\[
U_{k\epsilon,[y,\nu]} = \mathcal{E}_{x,\mu}(U_{k\epsilon,[x,\mu]})
\]

if \((y, \nu)\) follows \((x, \mu)\) in the chosen link order.

Since the transformation \( V \rightarrow U = \mathcal{F}_{n\epsilon}(V) \) is a composition product of one-link update steps, its Jacobian

\[
\det \mathcal{F}_{n\epsilon,*}(V) = \prod_{k=0}^{n-1} \prod_{x,\mu} \det \mathcal{E}_{x,\mu,*}(U_{k\epsilon,[x,\mu]})
\]

factorizes into the product of the Jacobians of the steps. The latter coincide with the determinants of certain real \(8 \times 8\) matrices given explicitly in appendix C.

6. Proposed simulation algorithm for lattice QCD

With respect to the QCD simulation algorithms used to date, the combination of the transformations obtained through the Euler integration of the Wilson flow and the
HMC algorithm is expected to sample the topological sectors more quickly and to be generally more efficient. The use of the Wilson flow is suggested if the gauge action coincides with the Wilson plaquette action. For other actions, the appropriate flow can be easily constructed following the lines of sect. 4.

6.1 Choice of the parameters

The parameters of the Euler integrator are the integration step size $\epsilon$ and the number $n$ of Euler sweeps that are applied. One also needs to choose a definite ordering of the links of the lattice.

The step size $\epsilon$ should be positive and not larger than, say, 1/16 so that the invertibility of the Euler integrator is guaranteed within a safe margin. Some tuning of the integration time $n\epsilon$ will certainly be required in order to maximize the efficiency of the algorithm. Note that the unit of time differs from the one used in subsect. 4.4, i.e. setting $t = 1$ there corresponds to an integration time $n\epsilon = \beta/32$.

The ordering of the links can be chosen arbitrarily. One may, for example, first visit the links $(x,0)$ on all even points $x$, then the links $(x,0)$ on all odd points, then the links $(x,1)$ on all even points, and so on. This ordering is well suited for parallel processing, since the link variables in a given direction on the even (odd) sites are decoupled from one another and can therefore be updated in parallel.

6.2 Force calculation

At the beginning of an update cycle, the current gauge field $U$ is transformed to the field $V = \mathcal{F}_{n\epsilon}^{-1}(U)$ by applying $n$ backward Euler sweeps to $U$. The force that drives the molecular-dynamics evolution of $V$ is then given by

$$F(z,\rho)^c = \partial_{z^c} \{ S(\mathcal{F}_{n\epsilon}(V)) - \ln \det \mathcal{F}_{n\epsilon,*}(V) \}, \quad (6.1)$$

where the action $S(U)$ now includes the usual sea-quark pseudo-fermion actions (for simplicity, the dependence on the pseudo-fermion fields is suppressed).

Each time the force is to be calculated, the current field $V$ must be transformed to $U$ again by applying $n$ forward Euler sweeps (see fig. 3). The fields $U_0, U_\epsilon, \ldots, U_{n\epsilon}$ generated in this process should be stored in memory so that they will be available when the force is propagated from $U$ to $V$. Note that the intermediate fields

$$U_{k\epsilon,[x,\mu]}(y,\nu) = \begin{cases} U_{k\epsilon}(y,\nu) & \text{if } (y,\nu) \geq (x,\mu), \\ U_{k\epsilon+\epsilon}(y,\nu) & \text{otherwise,} \end{cases} \quad (6.2)$$

are then also available.
Fig. 3. The proposed algorithm evolves the field $V$ using the standard HMC algorithm (thick line). The force that drives the molecular-dynamics evolution is obtained by forward integration of the Wilson flow and subsequent backward propagation of the derivatives of the action and the Jacobian of the flow ($n = 3$ in this figure).

The factorization (5.14) of the Jacobian implies

$$F(z, \rho)^c = \partial_{z,\rho}^c S(U_{n\epsilon}) - \sum_{k=0}^{n-1} \sum_{x,\mu} \partial_{z,\rho}^c \ln \det \mathcal{E}_{x,\mu,\epsilon}(U_{k\epsilon, [x,\mu]}). \quad (6.3)$$

Moreover,

$$\partial_{z,\rho}^c S(U_{n\epsilon}) = \sum_{y,\nu} \partial_{y,\nu}^a S(U) \bigg|_{U = U_{n\epsilon}} \mathcal{F}_{n\epsilon,\ast}(y, \nu; z, \rho)^{ac}, \quad (6.4)$$

and there is a similar formula for the other terms in eq. (6.3) involving the Jacobian matrices of the transformations $V \rightarrow U_{k\epsilon, [x,\mu]}$. All these matrices, as well as the one in eq. (6.4), are products of the Jacobian matrices of the one-link transformations (5.8). The force can therefore be computed recursively as follows:

1. Set $U = U_{n\epsilon}$ and $F(z, \rho)^c = \partial_{z,\rho}^c S(U)$.
2. For $k$ from $n-1$ to $0$, run through all links $(x, \mu)$ in reverse order, set $U = U_{k\epsilon, [x,\mu]}$ and update the force according to

$$F(z, \rho)^c \rightarrow \sum_{y,\nu} F(y, \nu)^a [\mathcal{E}_{x,\mu,\epsilon}(U)](y, \nu; z, \rho)^{ac} - \partial_{z,\rho}^c \ln \det \mathcal{E}_{x,\mu,\epsilon}(U). \quad (6.5)$$

Note that the field $U$ backtracks the forward integration of the Wilson flow in the course of the recursion. Since the Jacobian matrix $\mathcal{E}_{x,\mu,\epsilon}(U)$ differs from unity only
on the links sharing a plaquette with \((x, \mu)\), the total computational effort required for the propagation (6.5) of the force is expected to be similar to the one required for \(n\) applications of a nearest-neighbour gauge-covariant difference operator to the force field.

### 6.3 Domain-decomposed algorithm

Field transformations can also be combined with the DD-HMC algorithm [12]. Only the so-called active link variables are transformed in this case, but the transformations may depend on the inactive field components.

In the pure gauge theory, it is then again possible to construct trivializing flows. They operate on the active link variables and contract the gauge action in each domain to a constant (i.e. an expression depending on the inactive link variables only). These flows are not the same as the ones constructed in sect. 4, but can be obtained by solving the differential equations derived there. In particular, the trivializing flow for the Wilson action is, to leading order, a slightly modified Wilson flow, where the plaquettes containing \(\nu\) active links are given the weight \(4/\nu\).

### 7. Concluding remarks

Trivializing maps and flows in field space have here been discussed with a particular application in mind. The underlying concepts are fairly general, however, and may have other uses in rigorous constructive work, numerical perturbation theory or in connection with renormalizable smoothing techniques, for example.

Whether the proposed combination of the Wilson flow and the HMC algorithm does indeed sample the topological sectors in lattice QCD more efficiently than the simulation algorithms used so far remains to be determined. As the lattice spacing is taken to smaller and smaller values, the quark fields may eventually have to be included in the flow and perhaps also the next-to-leading order correction discussed in sect. 4. Trivializing maps in the presence of matter fields is, in any case, a subject that deserves to be studied in its own right.

In the course of this work, I profited from many discussions with Filippo Palombi and Stefan Schaefer of various questions related to the slow topology-switching in current lattice QCD simulations. I also wish to thank Stefan Schaefer, Rainer Sommer and Francesco Virotta for sharing some of their simulation results before publication.
Appendix A. SU(3) notation

A.1 Group generators
The Lie algebra $\text{su}(3)$ of SU(3) may be identified with the space of all anti-hermitian traceless $3 \times 3$ matrices. With respect to a basis $T^a$, $a = 1, \ldots, 8$, of such matrices, the elements $X \in \text{su}(3)$ are given by

\[ X = X^a T^a, \quad (A.1) \]

where $(X^1, \ldots, X^8) \in \mathbb{R}^8$ (repeated group indices are automatically summed over).

The generators $T^a$ are assumed to satisfy the normalization condition

\[ \text{tr}\{T^a T^b\} = -\frac{1}{2} \delta^{ab}. \quad (A.2) \]

The structure of the Lie algebra is then encoded in the commutators

\[ [T^a, T^b] = f^{abc} T^c, \quad (A.3) \]

while the completeness of the generators implies

\[ \{T^a, T^b\} = -\frac{1}{3} \delta^{ab} + i d^{abc} T^c, \quad (A.4) \]

\[ T^a_{\alpha\beta} T^a_{\gamma\delta} = -\frac{1}{2} \left\{ \delta_{\alpha\delta} \delta_{\beta\gamma} - \frac{1}{3} \delta_{\alpha\beta} \delta_{\gamma\delta} \right\}. \quad (A.5) \]

It follows from these equations that the structure constants $f^{abc}$ and the tensor $d^{abc}$ are both real. Moreover, $f^{abc}$ is totally anti-symmetric in the indices and $d^{abc}$ totally symmetric and traceless.

A.2 Adjoint representation
The representation space of the adjoint representation of $\text{su}(3)$ is the Lie algebra itself, i.e. the elements $X$ of $\text{su}(3)$ are represented by linear transformations

\[ \text{Ad} X : \text{su}(3) \rightarrow \text{su}(3), \quad (A.6) \]

\[ \text{Ad} X \cdot Y = [X, Y] \quad \text{for all } Y \in \text{su}(3). \quad (A.7) \]

The action of Ad $X$ on the group generators is given by

\[ \text{Ad} X \cdot T^b = T^a (\text{Ad} X)^{ab}, \quad (A.8) \]
where

\[(\text{Ad } X)^{ab} = -f^{abc} X^c \]  

(A.9)

is a real antisymmetric $8 \times 8$ matrix.

A.3 Matrix norms

The natural scalar product in $\mathfrak{su}(3)$ is

\[(X, Y) = X^a Y^a = -2 \operatorname{tr} \{XY\}. \]  

(A.10)

In particular, $\|X\| = (X, X)^{1/2}$ is a possible definition of the norm of $X \in \mathfrak{su}(3)$.

Another useful matrix norm derives from the square norm

\[\|v\|_2 = \{|v_1|^2 + |v_2|^2 + |v_3|^2\}^{1/2} \]  

(A.11)

of complex colour vectors $v$. If $A$ is any complex $3 \times 3$ matrix, one defines

\[\|A\|_2 = \max_{\|v\|_2=1} \|Av\|_2. \]  

(A.12)

This norm satisfies

\[\|A + B\|_2 \leq \|A\|_2 + \|B\|_2, \quad \|AB\|_2 \leq \|A\|_2 \|B\|_2, \]  

(A.13)

for all matrices $A, B$. Moreover, if $A$ is hermitian or antihermitian, $\|A\|_2$ is equal to the maximum of the absolute values of its eigenvalues.

Appendix B. Properties of the SU(3) exponential function

B.1 Lipschitz bound

For any $X, Y \in \mathfrak{su}(3)$, the relation

\[\|e^X - e^Y\|_2 = \|1 - e^{-X}e^Y\|_2 \]  

(B.1)

follows from the fact that $e^X$ is unitary. Using the identity

\[1 - e^{-X}e^Y = \int_0^1 ds e^{-sX}(X - Y)e^{sY} \]  

(B.2)
and the subadditivity (A.13) of the norm, the Lipschitz bound
\[ \|e^X - e^Y\|_2 \leq \|X - Y\|_2 \] (B.3)
is then obtained.

**B.2 Differential of the exponential map**

Let \( X \) be an element of the Lie algebra \( \mathfrak{su}(3) \). A linear mapping \( J(X) : \mathfrak{su}(3) \mapsto \mathfrak{su}(3) \) is then defined by
\[
J(X) \cdot Y = e^{-X} \left. \frac{d}{dt} e^{X+ty} \right|_{t=0} \quad \text{for all } Y \in \mathfrak{su}(3).
\] (B.4)

\( J(X) \) is referred to as the differential of the exponential map. Scaling the exponents by a parameter \( s \), as above, one obtains the representation
\[
J(X) \cdot Y = \int_0^1 ds e^{-sX} Ye^{sX}
\] (B.5)
and thus the expansion
\[
J(X) = 1 + \sum_{k=1}^{\infty} \frac{(-1)^k}{(k + 1)!} (\text{Ad } X)^k
\] (B.6)
which is absolutely convergent for any \( X \in \mathfrak{su}(3) \).

The action of \( J(X) \) on the group generators \( T^a \) is given by
\[
J(X) \cdot T^b = T^a J(X)^{ab},
\] (B.7)
where \( J(X)^{ab} \) is a real \( 8 \times 8 \) matrix. Note that
\[
J(X)^T = J(-X) = e^{\text{Ad } X} J(X), \quad J(X)\text{Ad } X = 1 - e^{-\text{Ad } X}.
\] (B.8)

Moreover, eq. (B.5) implies
\[
\|J(X) \cdot Y\|_2 \leq \|Y\|_2
\] (B.9)
for all \( X,Y \in \mathfrak{su}(3) \).
Appendix C. Jacobian of the Euler step

The Jacobian matrix (5.11) of the Euler step is equal to unity except for some non-zero elements along the row \((y, \nu) = (x, \mu)\). Its determinant therefore coincides with the determinant of the \((x, \mu; x, \mu)\)-element

\[
A^{ac} = \left\{ (e^{A_{d}X})^{ac} + \epsilon J(-X)^{ab}[Z_{*}(U)](x, \mu; x, \mu)^{bc} \right\}_{X = \epsilon[Z(U)](x, \mu)} \tag{C.1}
\]
of the matrix.

The derivative \([Z_{*}(U)](x, \mu; x, \mu)^{bc}\) can be worked out explicitly in terms of the plaquette sum

\[
M = \sum_{\nu \neq \mu} \{ U(x, \mu)U(x + \hat{\mu}, \nu)U(x + \hat{\nu}, \mu)^{-1}U(x, \nu)^{-1} +
\]

\[
U(x, \mu)U(x + \hat{\mu} - \hat{\nu}, \nu)^{-1}U(x - \hat{\nu}, \mu)^{-1}U(x - \hat{\nu}, \nu) \}. \tag{C.2}
\]

A few lines of algebra then lead to the expression

\[
A^{ac} = B^{ac} + \frac{1}{2}\epsilon C^{ab} \left\{ \text{id}^{bcd} \text{tr}\{T^{d}(M + M^{\dagger})\} - \frac{1}{3} \delta^{bc} \text{tr}\{M + M^{\dagger}\} \right\} \tag{C.3}
\]

where

\[
B = \frac{1}{2}(e^{A_{d}X} + 1), \tag{C.4}
\]

\[
C = J(-X), \quad X = -\epsilon \mathcal{P}\{M\}. \tag{C.5}
\]

In particular,

\[
\det A = 1 - \frac{4}{3}\epsilon \text{tr}\{M + M^{\dagger}\} + \mathcal{O}(\epsilon^{2}), \tag{C.6}
\]
as expected from eq. (3.9).
Appendix D. Inversion of the Euler step

D.1 Basic norm bounds

For any complex $3 \times 3$ matrix $M$, the inequality
\[
\|P\{M\}\|_2 \leq \frac{2}{3}\|M\|_2
\]  
(D.1)
can be established in a few lines. One first observes that
\[
\frac{1}{2}(M - M^\dagger) = ADA^{-1}, \quad A \in SU(3),
\]  
(D.2)
where $D$ is a diagonal matrix with diagonal elements $\lambda_1, \lambda_2, \lambda_3$. Setting
\[
\bar{\lambda} = \frac{1}{3} \sum_{k=1}^{3} \lambda_k,
\]  
(D.3)
the estimates
\[
\|P\{M\}\|_2 = \max_k |\lambda_k - \bar{\lambda}|
\leq \frac{4}{3} \max |\lambda_k| = \frac{2}{3}\|M - M^\dagger\|_2 \leq \frac{4}{3}\|M\|_2
\]  
(D.4)
then show that the inequality (D.1) holds for all matrices $M$.

An immediate consequence of the bound (D.1) and the Lipschitz bound (B.3) is that
\[
\|P\{A(e^X - e^Y)B\}\|_2 \leq \frac{2}{3}\|X - Y\|_2
\]  
(D.5)
for all $A, B \in SU(3)$ and $X, Y \in su(3)$.

D.2 Solution of eq. (5.1)

For a given link $(x, \mu)$ and any fixed $U'(x, \mu) \in SU(3)$, the function
\[
f(X) = \{[Z(U)](x, \mu)\}_{U(x, \mu) = e^{-\epsilon X} U'(x, \mu)}
\]  
(D.6)
maps $X \in su(3)$ back to $su(3)$. Recalling eq. (5.3), the inequality (D.5) immediately implies that
\[
\|f(X) - f(Y)\|_2 \leq k\|X - Y\|_2, \quad k = 8|\epsilon|.
\]  
(D.7)
The function \( f(X) \) is therefore a strict contraction if the integration step size \( \epsilon \) is in the range (5.5) (which is assumed to be the case from now on).

It is not difficult to prove that strict contractions in a complete metric space have a unique fixed point (see ref. [13], Theorem V.18, for example). In the present case, the fixed point \( X_* \) can be computed by noting that the sequence \( X_0 = 0, X_1, X_2, \ldots \) generated through the recursion \( X_{n+1} = f(X_n) \) satisfies

\[
\|X_n - X_*\|_2 \leq k\|X_{n-1} - X_*\|_2
\]  
(D.8)

and therefore rapidly converges to \( X_* \). The matrix

\[
U(x, \mu) = e^{-\epsilon X_*} U'(x, \mu)
\]  
(D.9)

then provides a solution of eq. (5.1). Moreover, there is no other solution, because the fixed point \( X_* \) of \( f(X) \) is unique.

\section*{D.3 Positivity of the Jacobian}

In order to prove that the determinant of the Jacobian matrix (C.1) is positive at all \( \epsilon \) in the range (5.5), it suffices to show that the matrix has no zero mode, i.e. that

\[
A^{ac} Y^c = 0
\]  
(D.10)

implies \( Y = 0 \). To this end, eq. (D.10) is first written in the form

\[
Y^a = -\epsilon J(X)^{ab} W^b,
\]  
(D.11)

where

\[
X = \epsilon [Z(U)](x, \mu), \quad W^b = [Z_*(U)](x, \mu; x, \mu)^{bc} Y^c.
\]  
(D.12)

Recalling eq. (5.10), the formula

\[
W = \lim_{t \to 0} \frac{1}{t} \left\{ [Z(U)](x, \mu)_{U(x, \mu) - e^{tY} U(x, \mu)} - [Z(U)](x, \mu) \right\}
\]  
(D.13)

may then be derived from which one infers that

\[
\|W\|_2 \leq 8\|Y\|_2.
\]  
(D.14)

The inequality (D.5) has here been used again and also the fact that the norm is a continuous map from \( \mathfrak{su}(3) \) to \( \mathbb{R} \). The combination of eq. (D.11) and the bounds (B.9) and (D.14) now implies \( \|Y\|_2 \leq k\|Y\|_2 \) and thus \( Y = 0 \).
Appendix E. Differentiability of $\tilde{S}_t$

The action $\tilde{S}_t$ solves an elliptic partial differential equation with smooth coefficients and is therefore guaranteed (by elliptic regularity) to be a differentiable function of the gauge field $U$. In this appendix, the simultaneous differentiability in the time $t$ is established by expanding $\tilde{S}_t$ in powers of $t - t_0$ around any fixed time $t_0$. Using Sobolev norms, the expansion can be shown to converge if $t$ is sufficiently close to $t_0$. The pointwise uniform convergence of the series and its derivatives, and therefore the differentiability of $\tilde{S}_t$, then follows from Sobolev’s lemma.

E.1 Sobolev spaces on the field manifold

The definition of the Sobolev spaces on a compact manifold is quite involved and will not be reviewed here. An introduction to the subject and the proof of all statements made in this subsection is given in the first three sections of ref. [8], for example.

Let $C^\infty$ be the space of differentiable functions on the field manifold and $H_k$ the associated Sobolev space of order $k \in \mathbb{Z}$. The latter is the completion of $C^\infty$ with respect to a certain norm $\| \cdot \|_k$. A characteristic feature of these norms is that the bounds

$$\|D\phi\|_k \leq c_k \|\phi\|_{k+p} \quad \text{(E.1)}$$

hold for all $\phi \in C^\infty$ and any differential operator $D$ of order $p$ with smooth coefficients, where the constants $c_k$ depend on $D$ but not on $\phi$. Such differential operators thus extend to bounded linear operators from $H_{k+p}$ to $H_k$. Moreover, $\|\phi\|_k \leq \|\phi\|_l$ if $k < l$ and therefore $H_l \subset H_k$.

A fairly concrete description of the Sobolev space $H_k$ can be given when $k$ is even and non-negative. For any $t \in \mathbb{R}$ and $j = 0, 1, 2, \ldots$, another norm $\|\phi\|_{t,j}$ of $\phi \in C^\infty$ may be defined through

$$\|\phi\|_{t,j} = \|\phi\| + \|\mathcal{L}_t^j \phi\|, \quad \text{(E.2)}$$

where $\| \cdot \|$ is the norm associated to the scalar product (4.7). The fact that $\mathcal{L}_t$ is a second-order elliptic differential operator then implies

$$\|\phi\|_{2j} \leq a_{t,j} \|\phi\|_{t,j}, \quad \|\phi\|_{t,j} \leq b_{t,j} \|\phi\|_{2j} \quad \text{(E.3)}$$

for some constants $a_{t,j}, b_{t,j}$. In particular, $H_{2j}$ is the completion of $C^\infty$ with respect to the norm $\| \cdot \|_{t,j}$.
E.2 Properties of the inverse of $L_t$

Let $\mathcal{P}_t$ be the orthogonal projector to the zero mode of $L_t$ in the Hilbert space with scalar product (4.7). Its action on any function $\phi \in C^\infty$ is given by

$$\mathcal{P}_t \phi = (1, \phi)/(1, 1). \quad (E.4)$$

Note that $\mathcal{P}_t$ projects $\phi$ to a constant, but the constant depends on the definition of the scalar product $(\cdot, \cdot)$ and therefore on $t$. The action of the inverse $G_t$ of $L_t$ on $\phi$ is then determined by the equations

$$L_t G_t \phi = (1 - \mathcal{P}_t) \phi, \quad \mathcal{P}_t G_t \phi = 0. \quad (E.5)$$

As already mentioned in subsect. 4.2, the ellipticity of $L_t$ and the absence of further zero modes imply that these equations have, for any fixed $t$, a unique differentiable solution $G_t \phi$. Evidently, $\tilde{S}_t = G_t S$.

Since $L_t$ has a spectral gap in the subspace orthogonal to the zero mode, $G_t$ is a bounded operator with respect to the norm $\| \cdot \|$. As a consequence, there exists a constant $g_t$ such that

$$\| G_t \phi \|_{t,j} \leq g_t \| \phi \|_{t,j-1} \quad (E.6)$$

for all $j = 1, 2, \ldots$ and all $\phi \in C^\infty$. Moreover, recalling the inequalities (E.3), one concludes that

$$\| G_t \phi \|_{2j} \leq g_{t,j} \| \phi \|_{2j-2} \quad (E.7)$$

for some other constants $g_{t,j}$.

E.3 Expansion of $\tilde{S}_t$

For any fixed time $t_0$, the operator $L_t$ may be decomposed according to

$$L_t = L_{t_0} + (t - t_0) L', \quad L' = \sum_{x,\mu} (\partial_{x,\mu}^\alpha S) \partial_{x,\mu}^\alpha. \quad (E.8)$$

Each term in the power series

$$\psi_t = \sum_{n=0}^\infty (t_0 - t)^n (G_{t_0} L')^n G_{t_0} S$$

(E.9)
is then a well-defined differentiable function of both \(t\) and \(U\). Moreover, since

\[
\| \mathcal{G}_{t_0} \mathcal{L}' \phi \|_{2j} \leq g_{t_0,j} \| \mathcal{L}' \phi \|_{2j-2} \leq d_j g_{t_0,j} \| \phi \|_{2j-1} \leq d_j g_{t_0,j} \| \phi \|_{2j},
\]  

(E.10)

all \(j = 1, 2, \ldots\) and some constants \(d_j\), it is clear that the series and all its derivatives with respect to \(t\) converge uniformly in the norm \(\| \cdot \|_{2j}\) if \(t\) is sufficiently close to \(t_0\). Sobolev’s lemma (statement (c) in lemma 1.3.5 of ref. [8]) then implies that the series converges pointwise and uniformly, together with all its derivatives in \(t\) and its derivatives in \(U\) up to some order proportional to \(j\).

If \(t\) is in a neighbourhood of \(t_0\), where the convergence of the series and its derivatives up to order \(l \geq 2\) is guaranteed, the action of the operator \(\mathcal{L}_t\) and the summation may be interchanged and one finds that

\[
\mathcal{L}_t \psi_t = S - \sum_{n=0}^{\infty} (t_0 - t)^n \mathcal{P}_{t_0} (\mathcal{L}' \mathcal{G}_{t_0})^n S = (1 - \mathcal{P}_t) S,
\]  

(E.11)

the second equality being implied by the identities \(\mathcal{P}_t \mathcal{L}_t \psi_t = 0\) and \(\mathcal{P}_t \mathcal{P}_{t_0} = \mathcal{P}_{t_0}\). As a consequence,

\[
(1 - \mathcal{P}_t) \psi_t = \mathcal{G}_t S = \tilde{S}_t,
\]  

(E.12)

which shows that \(\tilde{S}_t\) is, in the specified neighbourhood of \(t_0\), \(l\) times continuously differentiable with respect to \(t\) and \(U\). Since \(t_0\) and \(l\) can be chosen arbitrarily, the simultaneous differentiability of \(\tilde{S}_t\) is thus guaranteed at all times \(t\) and to all orders.

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