Thermalization algorithms for classical gauge theories

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Abstract

I propose a method, based on a set of Langevin equations, for bringing classical gauge theories to thermal equilibrium while respecting the set of Gauss' constraints *exactly*. The algorithm is described in detail for the SU(2) gauge theory with or without the Higgs doublet. As an example of application, canonical average of the maximal Lyapunov exponent is computed for the SU(2) Yang-Mills theory.

1 Introduction

In studying thermal properties of gauge theories it is useful to consider the classical limit. This is particularly true for classical lattice gauge theories whose numerical simulation is increasingly used as a nonperturbative tool for real-time dynamics of the gauge fields (sphaleron transitions, properties of quark-gluon plasma [2, 3, 4, 5, 6, 8]).

Simulation of a finite-temperature field theory should involve generating the thermal ensemble of field configurations. In case of gauge theories, configurations comprising the ensemble are subject to a set of local Gauss' constraints, whose presence precludes straightforward application of standard importance-sampling methods of ensemble generation in most cases. This work deals with construction and implementation of constraint-respecting thermalization algorithms for a number of physically important classical gauge theories.

So far, three methods have been used to thermalize gauge theories. One method consists of explicitly solving the constraints and applying importance sampling to the remaining gauge-invariant variables [5]. Its practical value is probably limited to simple Abelian models. For more complicated, non-Abelian theories the dynamics in a gauge-invariant language is usually nonlocal and/or suffers from coordinate singularities [16]. The second method handles Gauss' constraints approximately by adding to a Hamiltonian terms which penalize deviations of the static charge density (SCD) from zero [2, 3]. Configurations with large SCD would then be unlikely to appear in a sample generated by an importance sampling procedure. A special cooling procedure is used to remove whatever SCD has nevertheless been generated in the system. This method has its shortcomings too. Large SCD-suppressing terms will dominate the energy functional and slow down the importance sampling. Besides, cooling may lead to deviations from the intended thermal ensemble. Yet another method circumvents the need for preparing initial thermal configurations by employing a self-consistent heat bath interacting with a finite-size system at the boundaries in real time [5, 9]. This method, like the first one, faces technical difficulties when applied to nonabelian theories or in dimensions higher than one.

One would like to have a thermalization algorithm formulated in terms of usual phase-space variables of a gauge theory (*e.g.,* gauge potentials and color electric fields) and accurately maintaining the Gauss' law. It turns out that such a method can in several important cases be based on Langevin equation with a specially designed multiplicative noise term. That Langevin equations with multiplicative noise can be used for thermalization of constrained systems has been known for quite a long time now. This is how unitarity of link variables is maintained in Langevin simulations of Euclidean gauge theories [10]. The unit-magnitude constraint on fields in a sigma model can also be treated this way [10, 11]. In what follows the same idea is employed in order to satisfy the set of Gauss' constraints in a gauge theory. As we shall see, a natural choice of algorithm in this case reflects the fact that Gauss' constraints are first class in Dirac's terminology [14]. For technical reasons, it is convenient to use for our purpose second-order Langevin equations, *i.e.,* of every pair of canonically conjugate phase-space variables only one will

be coupled to a heat bath by adding stochastic terms to its equation of motion [12].

The outlined strategy is discussed in some detail in the sections to follow. In Section 2 I develop a Langevin formalism for Hamiltonian theories with first-class constraints. In Section 3 constraint-respecting coupling to a heat bath is constructed for a number of gauge theories. Based on this construction, a Langevin dynamics is formulated for the SU(2) lattice theory with and without a scalar doublet in Section 4. Section 5 discusses numerical integration of the resulting system of Langevin equations. Application of the Langevin algorithm is illustrated in Section 6 where canonical average of the maximal Lyapunov exponent is computed for the SU(2) Yang-Mills theory. Section 7 contains conclusions and outlook. A brief outline of the ideas presented here was given in Ref. [1].

2 Langevin equations with first-class constraints

In order to present the method in the most general form, I must briefly review the basic phase-space properties of gauge theories. In doing so, I will closely follow Ref. [15]. Let a dynamical system be described by n coordinates q_i and their respective conjugate momenta p_i forming a phase space Γ. Let these variables be subject to m ($m < n$) time-independent first-class constraints

$$C^\alpha(p,q) = 0 \approx \{H, C^\alpha\} \approx \{C^\beta, C^\alpha\},$$

where $H(p,q)$ is the Hamiltonian. The constraint surface $\mathcal{M}$ is a $2n-m$-dimensional subspace of the phase space. The weak equality sign, $\approx$, means, as usual, "equal up to terms vanishing on the constraint surface". A quantity $f(p,q)$ is physically meaningful (observable) if it is gauge-invariant: $\{f, C^\alpha\} \approx 0$. Obviously, the Hamiltonian H is observable. Since any such f is constant along the gauge orbits generated by C^α in $\mathcal{M}$, the physical subspace Γ^* of the phase space is of dimension $2(n-m)$. Since the Poisson bracket of any two observables is again an observable, Γ^* is by itself a phase space with a Poisson bracket $\{\}^*$ defined for observables u and v as

$$\{u,v\}^* \equiv \{u,v\}|_{\mathcal{M}}.$$

It follows that there exists a canonical basis $p_i^*, q_i^*, 1 \le i \le m$ for functions in Γ^* such that

$$\{p_i^*, p_j^*\}^* = \{q_i^*, q_j^*\}^* = 0; \quad \{p_i^*, q_j^*\}^* = \delta_{ij}.$$

All the observables (and H in particular) on $\mathcal{M}$ depend exclusively on $x^* \equiv p^*, q^*$.

Consider now Langevin dynamics in Γ. In its most general form the system of Langevin equations is

$$\dot{x}_i = \{H, x_i\} + D_i(x) + g_i^j(x)\Gamma^j(t)), \tag{1}$$

where I collectively denoted p and q by x. The system (1) is intentionally written as a generalization of Hamiltonian equations of motion: the first term on the r.h.s. describes the canonical evolution, whereas the other two terms arise from interaction

of the dynamical system with a heat bath. The D_i terms are, in general, dissipative. The last term on the r.h.s. is proportional to a white-noise random variable $\Gamma^j(t)$ with average zero and correlation

$$\langle \Gamma^j(t)\Gamma^k(t')\rangle = \delta_{jk}\delta(t-t'). \tag{2}$$

Here and in the following terms of this kind are to be understood in the Stratonovich sense, unless otherwise stated. At the moment, I do not specify the number of independent random variables $\Gamma^j(t)$. Our goal of thermalizing the gauge theory by means of (1) will be achieved if *(a)* it preserves the constraints, *i.e.,* generates a sequence of configurations on $\mathcal{M}$ from an initial condition on $\mathcal{M}$, and *(b)* for a long evolution time generates a sequence of configurations in Γ^* distributed with canonical probability density $\exp(-\beta H(p^*, q^*)$, where β is the inverse temperature. Since Γ^j are random variables independent of x, condition *(a)* requires that

$$g_i^j \partial_i C^\alpha \approx 0. \tag{3}$$

Now I will show that condition *(b)* can be satisfied together with *(a)* for a suitable choice of D_i and g_i^j. In order to arrrive at such an Ansatz, consider first the Fokker-Planck equation [18] for the probability density $W(x,t)$ in the full phase space Γ, which follows from (1)

$$\left[\partial_t + \partial_i\left(\{H, x_i\} + D_i + g_k^j \partial_k g_i^j - \partial_k g_k^j g_i^j\right)\right] W(x,t) = 0 \tag{4}$$

and require that it have $\exp(-\beta H(x))$ as its static solution. To this end it is enough to choose $D_i = g_i^k G^k$, where

$$G^k = \partial_j g_j^k - \beta g_j^k \partial_j H. \tag{5}$$

With this form of D_i (1) is constraint-preserving if (3) holds. Our task is now reduced to finding a correct set of g_j^k which in turn would determine D_i. To further narrow down the search for a suitable g_j^k I require that (1), averaged over realizations of random variables, maps observables to observables. The equation of motion for the average $\langle f(x,t)\rangle \equiv \int d^{2n}x W(x,t) f(x)$ of an observable $f(x)$ is obtained from (4) integrated by parts over the full phase space with boundary terms discarded:

$$\langle \dot{f}\rangle = \langle \{H, f\} + \partial_k\left(g_i^j g_k^j \partial_i f\right) - \beta g_i^j g_k^j \partial_k H \partial_i f\rangle. \tag{6}$$

Gauge invariance of $\langle \dot{f}\rangle$ is ensured by choosing

$$g_i^j = M^{jk}(x)\{T^k(x), x_i\}, \tag{7}$$

where T^k is observable and the square matrix $\mathcal{M}M^{jk}$ is such that MM^T is also an observable quantity. Indeed, with this choice the quantity averaged over on the r.h.s. of (6) is

$$\{H, f\} + \{T^k, M^{jk}M^{jl}\{T^l, f\}\} - \beta M^{jk}M^{jl}\{T^k, H\}\{T^l, f\}. \tag{8}$$

In addition, g_i^j as given by (7) satisfies (3). If the initial configuration for (1) lies on $\mathcal{M}$, (8), being an observable, depends exclusively on gauge-invariant canonical variables

x^*. Moreover, Poisson brackets $\{\}$ on Γ can be replaced by their counterparts $\{\}^*$ on Γ^* everywhere in (8). Finally, gauge invariance of (8) allows introduction of a gauge-invariant probability density $W^*(x^*,t)$ on Γ^* such that $\langle f\rangle = \int d^{2(n-m)}x^* W^* f$ for any observable f on $\mathcal{M}$. In view of (6) and (8) W^* satisfies the Fokker-Planck equation

$$\partial_t W^* = \{W^*, H\}^* - \{T^k, M^{jk}M^{jl}(\{T^l, W^*\}^* + \beta W^*\{T^l, H\}^*)\}^*, \tag{9}$$

written entirely in terms of x^*. It is obvious that (9) has $\exp(-\beta H)$, with H restricted to $\mathcal{M}$, as its static solution. In the following I shall reserve the terms "generators" for T^k and "multiplier" for M^{jk}.

Substitution of (7) into (1) gives the equation of motion for an arbitrary variable v:

$$\dot{v} = \{H, v\} + \left(\{T^k, M^{jk}\} - \beta M^{jk}\{T^k, H\} + \Gamma^j\right) M^{jl}\{T^l, v\}. \tag{10}$$

Note that, even though (1) was written in a canonical basis, (10) is basis-independent. This property, familiar from the Hamiltonian equations of motion, is useful whenever the natural choice of independent dynamical variables is not canonical, as is the case for Hamiltonian lattice gauge theories. Another observation is that it is always possible to include in (10) terms with $T^k = C^\alpha$. One one hand, this is allowed because the constraints are themselves first-class quantities. On the other hand, such an inclusion obviously does not change the equations of motion for observables and is therefore a matter of convenience.

There are important special cases of (7). If $M^{jk} = \delta^{jk}$, the r.h.s. of (10) is observable for any observable v and separately for any realization of Γ^j, not only on the average. In this case the stochastic terms in (1,10) may be thought of as arising from interaction of the dynamical system with gauge-invariant degrees of freedom of the heat bath. Some of the examples to follow are of this kind.

The number N of independent random variables Γ^j and the functional form ofT^k, M^{jk} must be specified so as to optimize the convergence of $W^*(x^*,t)$ to $\exp(-\beta H)$. If $N = 2(n-m)$ it is always possible to choose $M^{jk} = \delta^{jk}$, $T^k = x^*_k$ for any canonical basis x^* in Γ^*. With this choice the heat-bath fluctuations described by Γ^j generate the most general variation of variables in Γ^*. The system (1) then becomes a standard system of Langevin equations with additive noise on Γ^*, known to guarantee convergence to the equilibrium distribution. Thus the class of Langevin equations defined by (5) and (7) is rich enough to achieve thermal equilibrium in any gauge theory. Convergent and numerically competitive algorithms are obtained by taking $N = n-m$, $T^k = p^*_k$, *i.e.,* by coupling the heat bath to a single variable in every canonically conjugate pair p^*, q^* [12]. In the following these algorithms are called second order. In the next section I construct Langevin systems of this type for a number of gauge field theories in the continuum. Later on I discuss analogous algorithms for lattice gauge theories.

3 Langevin systems in the continuum

In this Section I study how the general prescription for finding a correct heat bath coupling, as outlined in Section 2, works in a number of gauge theories in the continuum. It is convenient to set, with no loss of generality, $A_0 = 0$. I will assume space dimension 3, which is the case for the most important applications. It is implied that all phase-space variables carry space coordinate labels, omitted here in order to simplify the notation. It should be clear that Langevin systems of equations for a classical field theory in the continuum are formal and cannot be put to immediate use: the Rayleigh-Jeans divergency renders the classical thermal theory in the continuum ill-defined. However, the continuum Langevin systems are useful as a guidance for similar constructions on a lattice.

The simplest example is that of a free electromagnetic field. The Gauss' law involves exclusively the electric fields E_i and reads $\partial_i E_i = 0$. Hence an arbitrary variation of the gauge fields A_i satisfies the Gauss' law. Such an arbitrary variation is generated by $E_k, k = 1, 2, 3$ and can be decomposed into a variation of the physical, transversal part of the gauge potential and a gauge transformation. If $T^k = E_k$, $M^{jk} = \delta^{jk}$ in (10), it is straightforward to verify, by writing (10) for A and E in momentum representation, that the resulting system of equations is indeed second-order for the transversely polarized degrees of freedom.

Next, I discuss the SU(2) Yang-Mills theory. The Gauss' constraints for color gauge fields A_i^α and momenta E_i^α are

$$\partial_i E_i^\alpha - 2\epsilon^{\alpha\beta\gamma} A_i^\beta E_i^\gamma = 0, \tag{11}$$

where α, β, γ are adjoint color labels. For fixed electric fields the most general variation of the gauge fields can be written as

$$\delta A_i^\alpha = S_{ij} E_j^\alpha, \tag{12}$$

where S_{ij} is a (space-dependent) gauge-invariant tensor. Indeed, if the 3×3 matrix E_j^α is invertible, as is the case generically, we find $S_{ij} = \delta A_i^\alpha (E^{-1})_j^\alpha$. For the Gauss' law (11) to hold, however, S_{ij} must be symmetric. Variations of A of this form are generated by the six quantities $T^{[ij]} = E_i^\alpha E_j^\alpha$, where $[ij]$ labels ordered pairs with $1 \le i \le j \le 3$. The variables $T^{[ij]}$ are gauge invariant, generically functionally independent, and commuting with each other. Hence they can be chosen as momentum variables in the observable subspace of the phase space. In fact, it is not difficult to find the corresponding gauge-invariant conjugate variables. To this end the original color electric fields are expressed in terms of $T^{[ij]}$ and three Euler angles θ which parametrize an orthogonal matrix $R^{\alpha a}(\theta)$ transforming E_i^α to some standard form $\mathcal{E}_i^a$. For instance, as pointed out by Goldstone and Jackiw [16], it is possible to require that $\mathcal{E}_i^a$ be a product of an orthogonal matrix by a diagonal one. Then for any $X = T^{[ij]}, \theta_m$

$$P_{X_n} = A_i^\gamma \frac{\partial E_i^\gamma}{\partial X_n} - \epsilon^{\alpha\beta\gamma} \frac{\partial}{\partial X_n} \left(R^{\alpha a}(\theta) \partial_i R^{\beta a}(\theta) E_i^\gamma \right)$$

is the canonically conjugate variable. Corresponding to the described canonical transformation is the generating function

$$\Phi(A,X) = A_i^\gamma E_i^\gamma(X) - \epsilon^{\alpha\beta\gamma} R^{\alpha a}(\theta)\partial_i R^{\beta a}(\theta) E_i^\gamma$$

whose partial derivatives give canonical conjugates of its arguments. Gauge invariance of P_T can be readily verified by performing a gauge transformation

$$A_i^\alpha \to \mathcal{G}^{\alpha\beta} A_i^\beta - \epsilon^{\alpha\beta\gamma}\mathcal{G}^{\gamma\sigma}\partial_i \mathcal{G}^{\beta\sigma}; \quad E_i^\alpha \to \mathcal{G}^{\alpha\beta} E_i^\beta$$

with an orthogonal $\mathcal{G}$. Consequently, the choice of $T^{[ij]} = E_i^\alpha E_j^\alpha$ as generators and $M^{[ij],[kl]} = \delta^{[ij],[kl]}$ as a multiplier results in a second-order Langevin system in the physical subspace of the SU(2) Yang-Mills theory. The system of equations for the standard variables can A, E can be easily derived using (10). It is obvious that the E equations are purely Hamiltonian.

Inclusion of scalar fields in the scheme presents no difficulty. The simplest theory of this kind is scalar electrodynamics. In this case, the Gauss' law is a relation between the electric field and the charge density of the complex scalar field

$$C \equiv \partial_i E_i + i\left(\pi\phi - \phi^*\pi^*\right) = 0, \tag{13}$$

where ϕ and π are scalar field and momentum, respectively. The constraint C generates gauge transformations

$$A_i \to A_i - \partial_i\alpha; \quad \phi \to \phi\exp(-i\alpha); \quad \pi \to \pi\exp(i\alpha),$$

where α is a gauge function. The most general variation of fields consistent with (13) consists of an arbitrary variation of A_i and a change in ϕ proportional to π^*:

$$\delta A_i = V_i; \quad \delta\phi = S\pi^*. \tag{14}$$

These are generated by $E_i, i = 1,2,3$ and $\Pi \equiv \pi^*\pi$,. It is easy to identify the four (per space point) physical degrees of freedom varied by (14). Obviously, one can choose E_i and the magnitude Π of π as gauge-invariant momentum variables. The fifth momentum variable, the phase θ of π, is clearly gauge-dependent. Gauge-invariant canonical partners of E_i and Π follow from the generating function

$$\Phi(A,\phi,E,\Pi,\theta) = E_i A_i + \pi(\Pi,\theta)\phi + \phi^*\pi^*(\Pi,\theta) - E_i\partial_i\theta.$$

These are

$$A_i - \partial_i\theta \quad \text{and} \quad \frac{1}{2\sqrt{\Pi}}\left(\phi\exp(i\theta) + \phi^*\exp(-i\theta)\right),$$

respectively. Choosing E_i, Π as generators and a unit multiplier completes the construction of a second-order system for the scalar electrodynamics.

My final example, the SU(2) theory with a scalar doublet, describes a sector of the Standard Model. The Gauss' law now reads

$$C^\alpha \equiv \partial_i E_i^\alpha - 2\epsilon^{\alpha\beta\gamma} A_i^\beta E_i^\gamma + i(\pi\sigma^\alpha\phi - \phi^*\sigma^\alpha\pi^*) = 0. \tag{15}$$

Here the SU(2) spinors ϕ and π are scalar fields and momenta, σ are Pauli matrices, and the rest of notation is obvious from previous examples.

As before, in order to find a suitable set of generators and multipliers for this system, it is useful first to identify the physical degrees of freedom. To this end, a point transformation of momenta is performed. Introducing $\Pi \equiv \pi\pi^*$, the momentum transformation, possible in the generic case $\Pi \neq 0$, reads

$$\pi = (\sqrt{\Pi}\ \ 0)U^\dagger(\theta); \quad E_i^\alpha = \frac{1}{2}\mathrm{Tr}\left(\sigma^\alpha U(\theta)\mathcal{E}_i^\beta \sigma^\beta U^\dagger(\theta)\right) \equiv R^{\alpha\beta}(\theta)\mathcal{E}_i^\beta,$$

where the Euler angles θ parametrize the unitary matrix U rotating π to a standard form, here chosen to be $(\Pi^{1/2}\ \ 0)$. Matrix R, defined by the last equality, is the orthogonal representation of U. Only θ change under gauge transformations, while Π and the nine $\mathcal{E}$ variables are gauge-invariant. As in the previous examples, the canonical conjugates of Π and $\mathcal{E}$ obtained with the help of a generating function

$$\Phi(A,\phi,\phi^*;\mathcal{E},\Pi,\theta) = A_i^\alpha E_i^\alpha(\mathcal{E},\theta) + \pi(\Pi,\theta)\phi + \phi^*\pi^*(\Pi,\theta) + \frac{i}{2}\mathrm{Tr}\left(\mathcal{E}_i^\alpha \sigma^\alpha U^\dagger(\theta)\partial_i U(\theta)\right) \quad (16)$$

are again gauge invariant. These are

$$\phi_\Pi \equiv (\pi\phi + \phi^*\pi^*)/2\Pi$$

for Π and

$$\mathcal{A}_i^\alpha \equiv \frac{1}{2}\mathrm{Tr}\sigma^\alpha\left(U^\dagger(\theta)A_i^\beta\sigma^\beta U(\theta) + iU^\dagger(\theta)\partial_i U(\theta)\right)$$

for $\mathcal{E}_i$. Thus $\mathcal{E}_i^\alpha, \mathcal{A}_i^\alpha$ and Π, ϕ_Π are the ten pairs of physical variables. It therefore makes sense to choose $\mathcal{E}$ and Π as generators for the second-order Langevin system. In this case, however, a convenient system of equations is obtained by using a nontrivial multiplier $\Pi R^{\beta\gamma}$ for the generators $\mathcal{E}_i^\gamma$. With this choice terms proportional to the noise take especially simple form

$$\Pi\Gamma_j^\gamma R^{\gamma\beta}\{\mathcal{E}_j^\beta, A_i^\alpha\} = \Pi\Gamma_i^\alpha \quad (17)$$

for the gauge potential. For the scalar field the corresponding term is

$$\Pi\Gamma_j^\gamma R^{\gamma\beta}\{\mathcal{E}_j^\beta, \phi\} + \Gamma_\Pi\{\Pi,\phi\}, \quad (18)$$

from which $\mathcal{E}, R, \Pi$ can be readily eliminated in favor of the original variables by noting that an arbitrary variation of the fields can be written as

$$\delta A_i^\alpha = \Pi\Gamma_i^\alpha, \quad \delta\phi = (p + i\Sigma^\alpha\sigma^\alpha)\pi^* \quad (19)$$

with real Γ, p, Σ, provided $|\pi|^2 > 0$ (generic case). Gauss' law (15) is only respected if

$$\Sigma^\alpha = -\epsilon^{\alpha\beta\gamma}\Gamma_i^\beta E_i^\gamma. \quad (20)$$

Since variations (17,18) also respect the constraints, they must be of the form (19,20). Comparing variation of ϕ_Π due to (19) with that due to (18) yields $p = \Gamma_\Pi$. Finally, equality of terms linear in Γ_i^α gives

$$\Pi R^{\beta\gamma}\{\mathcal{E}_i^\gamma, \phi\} = -i\epsilon^{\alpha\beta\gamma}E_i^\gamma\sigma^\alpha\pi^*.$$

4 Lattice Langevin equations: formulation

The next step in our program is space discretization of constraint-preserving thermalization scheme. Langevin equations of motion for lattice gauge theories are constructed, following the analogy with the continuum case. Having in mind applications to electroweak theory and to quark-gluon plasma, I will only write down lattice equations for the two nonabelian theories already considered. The reader should have no difficulty in writing a similar set of equations for the abelian theories.

A convenient formalism for Hamiltonian ($A_0 = 0$) lattice gauge theory is that of Kogut and Susskind [17]. The configuration space consists of unitary matrices U_l forming the fundamental representation of the gauge group on every link l of a cubic lattice. In the following I shall use the notation $j, \hat{n}$ for a link along a positive direction $\hat{n}$ originating at site j. Lattice analogs of electric fields are link variables $E_l^{R\alpha}$ generating right covariant derivatives on the group. Poisson brackets obeyed by $E_l^{R\alpha}$ with U_l and among themselves are only nonzero for variables residing on the same link, and then, in the case of SU(2) gauge group

$$\{E_l^{R\alpha}, U_l\} = -iU_l\sigma^\alpha; \quad \{E_l^{R\alpha}, E_l^{R\beta}\} = 2\epsilon^{\alpha\beta\gamma}E_l^{R\gamma}, \tag{21}$$

where σ^α are Pauli matrices. The link variables U_l and $E_l^{R\alpha}$ span the phase space. Alternatively, one could replace $E_l^{R\alpha}$ as independent variables by $E_l^{L\alpha}$, the generators of left covariant derivatives on the group. On every link l the transformation between the two sets of variables reads

$$E_l^{L\alpha}\sigma^\alpha = -E_l^{R\beta}U_l\sigma^\beta U_l^\dagger. \tag{22}$$

As a matter of convention, I choose here $E_l^{R\alpha}$ as independent variables. A useful property is

$$\{E_l^{R\alpha}, E_l^{L\beta}\} = 0. \tag{23}$$

Scalar doublet fields ϕ_j, if added to the theory, are assigned, together with their conjugate momenta π_j, to the sites j of the lattice. Gauge transformations of the variables sharing site j are generated by

$$C_j^\alpha \equiv -\sum_{\hat{n}}\left[E_{j,\hat{n}}^{L\alpha} + E_{j-\hat{n},\hat{n}}^{R\alpha}\right] - i\left(\pi_j\sigma^\alpha\phi_j - \phi_j^*\sigma^\alpha\pi_j^*\right) \tag{24}$$

(the scalar-field terms should be dropped from (24) in case of pure Yang-Mills theory). The set of Gauss' laws is $C_j^\alpha = 0$.

Consider a Langevin system for the Yang-Mills theory first. Proceeding by analogy with the continuum theory, I choose the gauge-invariant generators

$$T^{[\hat{n},\hat{n'}]} = \sqrt{\gamma_E}E_{j,\hat{n}}^{L\alpha}E_{j,\hat{n'}}^{L\alpha}$$

with $1 \le \hat{n} \le \hat{n'} \le 3$, and a unit multiplier. The value of the friction coefficient $\gamma_E > 0$ is arbitrary and can be tuned to optimize the algorithm performance. With the generators and the multiplier chosen, the Langevin system is fully determined by the choice of

a Hamiltonian. The SU(2) Yang-Mills theory on the lattice is usually described by a Kogut-Susskind Hamiltonian

$$H_{YM} = \frac{1}{2}\sum_l E_l^{R\alpha} E_l^{R\alpha} + \sum_{\Box}\left(1 - \frac{1}{2}\mathrm{Tr}U_{\Box}\right). \tag{25}$$

The second term in (25) is the standard plaquette term describing the magnetic part of the energy. The Langevin system can now be written explicitly using (10,21,22,23,25) (the site index j common to all variables is dropped to simplify the notation)

$$\begin{aligned}
\dot{E}^{R\alpha}_{\hat{n}} &= -\frac{i}{2}\mathrm{Tr}\left(\sigma^\alpha U^\dagger_{\hat{n}}\sum_{\Box_{\hat{n}}} U_{\Box_{\hat{n}}}\right); \\
\dot{U}_{\hat{n}} &= -iE^{R\alpha}_{\hat{n}} U_{\hat{n}}\sigma^\alpha - i\sqrt{\gamma_E}\sum_{\hat{n'}}\left(G^{[\hat{n}\hat{n'}]} + \Gamma^{[\hat{n}\hat{n'}]}\right) E^{L\beta}_{\hat{n'}}\sigma^\beta U_{\hat{n}},
\end{aligned} \tag{26}$$

Here $\Gamma^{\hat{n}}, \hat{n'}$ is an independent random variable corresponding to a given combination of a site j and $[\hat{n}\hat{n'}]$,

$$G^{[\hat{n}<\hat{n'}]} \equiv -\frac{i\beta\sqrt{\gamma_E}}{2}\mathrm{Tr}\left(E^{L\alpha}_{\hat{n'}}\sigma^\alpha\sum_{\Box_{\hat{n}}} U_{\Box_{\hat{n}}} + n \leftrightarrow n'\right); \quad G^{mn} = i\frac{i\beta\sqrt{\gamma_E}}{2}\mathrm{Tr}\left(E^{\alpha}_{\hat{n}}\sigma^\alpha\sum_{\Box_{\hat{n}}} U_{\Box_{\hat{n}}}\right), \tag{27}$$

and $\Box_{\hat{n}}$ is any plaquette containing the link $U_{\hat{n}}$. The E^R equation of (26) has no stochastic or dissipative terms because these variables commute with the generators. Note that (26), beside satisfying the Gauss' law, automatically preserves the unitarity of link matrices, as it should.

With the scalar field included, a Langevin system is again constructed by analogy with the continuum case. Gauge invariant generators $\Pi \equiv |\pi|^2$ are introduced through

$$\Pi_j \equiv |\pi_j|^2; \quad \pi_j \equiv \left(\sqrt{\Pi_j}\ 0\right) V_j^\dagger; \quad \mathcal{E}^\alpha_{j,\hat{n}} \equiv -\frac{1}{2}\mathrm{Tr}\left(\sigma^\alpha V_j U_{j,\hat{n}} E^{R\beta}_{j,\hat{n}}\right) \equiv R^{\beta\alpha}_{j,\hat{n}} E^{R\beta}_{j,\hat{n}}.$$

The equations take a relatively simple form with multipliers $\sqrt{\gamma}\Pi R^{\beta\alpha}_{j,\hat{n}}$ for $\mathcal{E}^\alpha_{j,\hat{n}}$ and $\sqrt{\gamma_\Pi}$ for Π, where γ and γ_Π are arbitrary positive friction coefficients. With an addidion of the scalar field a representative Hamiltonian is

$$H_H = H_{YM} + \sum_j |\pi_j|^2 + \sum_{j,\hat{n}} |\phi_{j+\hat{n}} - U^\dagger_{j,\hat{n}}\phi_j|^2 + \lambda\sum_j W\left(|\phi_j|^2\right), \tag{28}$$

where W is a local scalar field potential. In the resulting Langevin system the π and E^R equations are simply the Hamiltonian ones, whereas for U and ϕ one obtains

$$\begin{aligned}
\dot{U}_{j,\hat{n}} &= -i\left[E^\alpha_{j,\hat{n}} + \sqrt{\gamma}|\pi_j|^2\left(\Gamma^\alpha_{j,\hat{n}}(t) + G^\alpha_{j,\hat{n}}\right)\right] U_{j,\hat{n}}\sigma^\alpha; \\
\dot{\phi}_j &= \pi^*_j + \sqrt{\gamma_\Pi}\left(\Gamma^\Pi_j + G^\Pi_j\right)\pi^*_j + i\sqrt{\gamma}\epsilon^{\delta\beta\rho}\sum_{\hat{n}} E^\beta_{j,\hat{n}}\left(\Gamma^\rho_{j,\hat{n}} + G^\rho_{j,\hat{n}}\right) U_{j,\hat{n}}\sigma^\delta U^\dagger_{j,\hat{n}}\pi^*_j,
\end{aligned} \tag{29}$$

where, as before, Γ are mutually uncorrelated white noise variables, and

$$\begin{aligned} G^{\alpha}_{j,\hat{n}} &= -i\beta\sqrt{\gamma}\left(\frac{\partial H_H}{\partial U_{j,\hat{n}}}U_{j,\hat{n}}\sigma^{\alpha} + \epsilon^{\alpha\beta\gamma}\frac{\partial H_H}{\partial \phi_j}E^{\beta}_{j,\hat{n}}U_{j,\hat{n}}\sigma^{\gamma}U^{\dagger}_{j,\hat{n}}\pi^{*}_{j}\right) + \text{c.c;} \\ G^{\Pi}_{j} &= -\beta\sqrt{\gamma_{\Pi}}\frac{\partial H_H}{\partial \phi_j}\pi^{*}_{j} + \text{c.c} \end{aligned} \tag{30}$$

(summation over SU(2) spinor and adjoint indices only).

In the continuum theory, discussed in Section 3, the generators commuted among themselves and therefore could be made, by a suitable canonical transformation, canonical physical momenta. As a result, the continuum Langevin systems were second-order systems in the physical subspace. Since the lattice generators do not commute, the lattice Langevin system is not necessarily second-order in this sense. Nevertheless, in the low-temperature regime ($\beta \gg 1$) the continuum Langevin systems are recovered. Indeed, the lattice generators do not commute due to the second relation of (21). However, at low temperature $E^R \sim \beta^{-1/2}$, as can be seen from (25), hence the Poisson bracket of two E^Rs is $\mathcal{O}(\beta^{-1/2})$, much smaller than $\{p, q\} = 1$ for any pair of canonically conjugate p, q. Therefore, at low temperatures both (26) and (29) reduce to second-order Langevin systems in the physical phase space.

5 Lattice Langevin equations: numerical integration

The final step in our construction of thermalization algorithms is finding a suitable numerical integration scheme for a system of stochastic differential equations of the type (10). It is best to use a scheme which respects the Gauss' law. Such a scheme is indeed possible due to the following useful property shared by all the Langevin systems constructed here. Namely, with the conventional choice of variables (space components of the gauge potential and the electric fields) ithe Hamiltonian is a sum of a kinetic term K commuting with all the momentum variables p (of which the lattice color electric fields are a generalization), and a potential term $\mathcal{V}$ commuting with all the coordinates q, with K and $\mathcal{V}$ being *each* gauge-invariant. Moreover, all the proposed generators T^k of (10) commute with all the momenta. As a result, the Gauss' constraints C^{α} are conserved *separately* by the momentum and coordinate equations of motion. This property was used, although not explicitly stated, for purely canonical equations in Ref. [3]. Moreover, since for the noise variables Γ in (26,29) all realizations in time are allowed, it is clear that this property holds if G terms in (26,29) are arbitrary functions of time, not necessarily given by (27) and by (30). We conclude that the Gauss' law holds *exactly* for any combination of (a) integrating exactly the E^R an π equation of motion while keeping U and ϕ fixed, and (b) integrating exactly the U and ϕ equations while keeping E^R, π, and G fixed (the random variables Γ are also kept fixed for the duration of step (b)). The freedom in combining (a) and (b) can be used to optimize accuracy and stability of the algorithm.

Some technical adjustments may have to be made in applying this general idea to a specific gauge theory. Consider first the equation (26) for the SU(2) Yang-Mills theory. For arbitrary Γ and G, the stochastic terms on the r.h.s. involve in a nonlinear fashion all the link variables for links emanating in positive directions from site j. Performing step (b) for such a system of coupled nonlinear equations is a very complex task. If at any step we only allow a single off-diagonal component of the symmetric tensor $\Gamma + G$ to be nonzero, a considerable simplification will follow. Note that the general form of (26) is (no implicit summation over $\hat{n}$ and $\hat{n'}$ in the following)

$$\dot{U}_{\hat{n}} = i \sum_{\hat{n'}} Z_{\hat{n}\hat{n'}} E^L_{\hat{n'}} U_{\hat{n}},$$

where $Z_{\hat{n}\hat{n'}}$, symmetric under exchange of $\hat{n}$ with $\hat{n'}$, is constant for the duration of step (b), and $E^L\hat{n} \equiv E^{L\alpha}\hat{n}\sigma^\alpha$ obeys for fixed E^R an equation of motion

$$\dot{E}^L\hat{n} = i \sum_{\hat{n'}} Z_{\hat{n}\hat{n'}} \left[E^L\hat{n}, E^L_{\hat{n'}} \right],$$

so that $\sum_{\hat{n}} \dot{E}^L\hat{n} = 0$. Consider now a special case where the Z matrix has only one nonzero off-diagonal element, *e.g.*, $Z_{\hat{n}\hat{n}} \equiv Z_{\hat{n}}$, $Z_{\hat{1}\hat{2}} \equiv Z$, $Z_{\hat{1}\hat{3}} = Z_{\hat{2}\hat{3}} = 0$. Then $E^L_{\hat{3}}$, and, equvalently, $E^L_{\hat{1}} + E^L_{\hat{2}}$ are time-independent, and the equations for E^L and for U are easy to solve:

$$\begin{aligned} U_{\hat{1},\hat{2}}(t) &= \exp(-iZ(E^L_{\hat{1}} + E^L_{\hat{2}})t) U_{\hat{1},\hat{2}}(0) \exp(i(Z - Z_{\hat{1},\hat{2}}) E^{R\alpha}_{\hat{1},\hat{2}} \sigma^\alpha t); \\ U_{\hat{3}}(t) &= U_{\hat{3}}(0) \exp(iZ_{\hat{3}} E^{R\alpha}_{\hat{3}} \sigma^\alpha t). \end{aligned}$$

In performing step (b) for the system (29) it helps to note that the third term in the ϕ equation is completely fixed by requiring that it compensates the violation of the Gauss' law generated by the U equation. This suggests the following procedure. First the equations for the link matrices are integrated. Then violation δC^α_j of the Gauss' law at site j, resulting from this change of link matrices alone, is determined. Finally, the Gauss' law is restored by the change in the scalar field:

$$\phi(t) - \phi_j(0) = \left[1 + \sqrt{\gamma_\Pi}(\Gamma^\Pi_j + G^\Pi_j) + \frac{i}{2|\pi_j|^2} \epsilon_{\alpha\beta\gamma} \delta C^\alpha_j \sigma^\alpha \right] \pi^*_j. \tag{31}$$

There is one caveat in this procedure: if $|\pi_j|^2$ is close to zero, divisions by $|\pi_j|^2$ required for the scalar field updates in (31) can be numerically unsafe. At the same time, comparison of (31) with the ϕ equation of (29) shows that $\delta C^\alpha_j / |\pi_j|^2$ approaches a finite value as $|\pi_j|^2 \to 0$. The remedy is therefore to set a minimal value ϵ of $|\pi_j|^2$, and, whenever $|\pi_j|^2 < \epsilon$, replace $\delta C^\alpha_j / |\pi_j|^2$ by an estimate obtained in the following way. First $|\pi_j|^2$ explicitly appearing in the $U_{j,\hat{n}}$ equations of (29) is replaced by ϵ. Next, the $U_{j,\hat{n}}$ equations are integrated in order to find δC^α_j. The estimate is then $\delta C^\alpha_j / \epsilon$. It is not difficult to show that, as a result of this replacement, the Gauss' law is maintained approximately, its violation being at most $\mathcal{O}(\epsilon^2)$, which can be made completely negligible by an appropriate choice of ϵ.

Steps (a) and (b) must be combined in a suitable fashion to form an accurate and stable integration algorithm. A simple scheme accurate to the order 3/2 in the time step Δ is as follows. Initially ($t = 0$) a set of random variables Γ is generated. These remain constant for the duration of the step. The integration step is schematically represented as

1. $E^R(0), \pi(0) \to E^R\left(\frac{\Delta}{2}\right), \pi\left(\frac{\Delta}{2}\right)$ for fixed $U(0), \phi(0)$;
2. $U(0), \phi(0) \to U\left(\frac{\Delta}{2}\right), \phi\left(\frac{\Delta}{2}\right)$ for fixed $E^R\left(\frac{\Delta}{2}\right), \pi\left(\frac{\Delta}{2}\right), G(0)$;
3. $U(0), \phi(0) \to U(\Delta), \phi(\Delta)$ for fixed $E^R\left(\frac{\Delta}{2}\right), \pi\left(\frac{\Delta}{2}\right), G\left(\frac{\Delta}{2}\right)$;
4. $E^R\left(\frac{\Delta}{2}\right), \pi\left(\frac{\Delta}{2}\right) \to E^R(\Delta), \pi(\Delta)$ for fixed $U(\Delta), \phi(\Delta)$.

Here the $\to$ symbol denotes exact integration. All the color and space indices have been dropped in order to simplify the notation. For a pure Yang-Mills theory the ϕ and π variables should be omitted. Note that this scheme is a generalization of the simplest leapfrog algorithm to which it reduces in the absence of stochastic terms (item 2 above then becomes obsolete). If not for the Γ terms present in the stochastic equations the algorithm would have an $\mathcal{O}(\Delta^3)$ error per step, similar to the simplest leapfrog. However, the noise terms Γ must be implemented as random variables having average 0 and variance $2/\Delta$ in order to approximate (2). The error per step is therefore $\mathcal{O}(\Delta^{3/2})$.

Numerical tests, conducted at high ($\beta = 2$) and low ($\beta = 12$) temperatures, confirm that the algorithms in question indeed achieve the correct thermalization while maintaining the Gauss' law with high accuracy. The tests were performed on 12^3 lattices with algorithm parameters $\gamma_E = 0.05$, $\Delta = 0.01$ for the Yang-Mills theory and $\gamma = 0.04$, $\gamma_\Pi = 0.2$, $\Delta = 0.005$ in presence of the scalar field. The scalar potential was $\lambda(|\phi|^2 - v^2)^2$, *i.e.,* H_H corresponded to the bosonic SU(2) sector of the Standard Model. The algorithm was tested with $\lambda = 0.5$, setting unit Higgs to vector boson mass ratio, and $v^2 = 0.05$, corresponding to the Higgs inverse mass of about 4.5 lattice spacings.

Figure 1 illustartes the thermalization process for the SU(2) Yang-Mills theory described by (25). The initial configuration had zero electric fields and the energy far below the average one for the assigned inverse temperature $\beta = 12$. The system then rapidly reached thermal equilibrium. An extremely small static color charge per site generated by the algorithm is entirely due to a limited computer accuracy and does not depend on the time step. On a Cray-C90 processor with single-precision arithmetic the magnitude of the spurious static charge was less than 4×10^{-12} per site at the end of evolution shown in Figure 1. Similar negligible amounts of constraint violation were observed in tests of the Langevin system (29) with the scalar field.

Several criteria were used to judge how close the algorithms come to generating canonical distributions for the two theories in question. In one instance, the thermal average of an observable is known analytically. Namely, the radial component of the scalar field momentum, $2\mathrm{Re}\pi\phi/|\phi|$ appears in H_H quadratically and can be chosen as

system	size	β	initial	final
H_{YM}	2×2	12	0.7519(4)	0.7521(4)
H_{YM}	3×3	12	0.584(1)	0.584(1)
H_{YM}	4×4	12	0.436(2)	0.436(2)
H_{YM}	5×5	12	0.316(2)	0.318(2)
H_{YM}	1×2	2	0.1046(5)	0.1049(5)
H_{YM}	2×2	2	0.0450(8)	0.0450(7)
H_{YM}	2×3	2	0.0046(5)	0.0051(5)
H_H	2×2	12	0.7501(4)	0.7507(5)
H_H	3×3	12	0.580(1)	0.581(1)
H_H	4×4	12	0.432(2)	0.433(2)
H_H	5×5	12	0.312(2)	0.312(2)
H_H	1×2	2	0.1052(5)	0.1046(5)
H_H	2×2	2	0.0448(8)	0.0452(7)
H_H	2×3	2	0.0041(5)	0.0047(5)

Table 1: Summary of measured canonical averages for spatial Wilson loops of various sizes at the beginning (initial) and at the end (final) of a Hamiltonian trajectory 50 time units long.

an independent physical canonical variable. Hence the average radial kinetic energy per lattice site should be $1/2\beta$. This exact result was indeed found within margins of the measurement error in both low and high temperature regimes, with a 0.2% accuracy.

Unfortunately, I am not aware of other observables with exactly known thermal averages. For some quantities, however, perturbative estimates should be reliable at low temperatures, opening another possibility of comparison with numerical experiment. In particular, since the low-temperature system is only weakly nonlinear, the average energy per degree of freedom should be close to the equipartition value $1/\beta$. At $\beta = 12$ the measured average energy per degree of freedom is $1.0091(7)/\beta$ for the Yang-Mills theory and $1.0053(7)/\beta$ with the scalar fields.

Finally, the equilibrium statistical weight, $\exp(-\beta H)$, being a function of the energy only, is conserved by the Hamiltonian evolution. This property is used for the following consistency test of the algorithms. An initial thermal configuration is subject to the Hamiltonian evolution, and observables are measured at the beginning and at the end of the Hamiltonian trajectory. For any observable, the two sets of measurements should yield the same average if the generated distribution is indeed canonical. This test was conducted for a number of observables of the Yang-Mills theory, namely, the color electric energy density, the topological charge density, and spatial Wilson loops of various sizes. With the scalar field included, the radial kinetic energy density, the Bricmont-Fröhlich correlation function [19] at various distances, and the "string bit" $\phi_j^* U_{j,\hat{n}} \phi_{j+\hat{n}} / (|\phi_j^*||\phi_{j+\hat{n}}|)^{1/2}$ were added to this list. All the measurements show that the generated distributions are close to the canonical ones. As an example, Table 1 summarizes the results for the spatial Wilson loops.

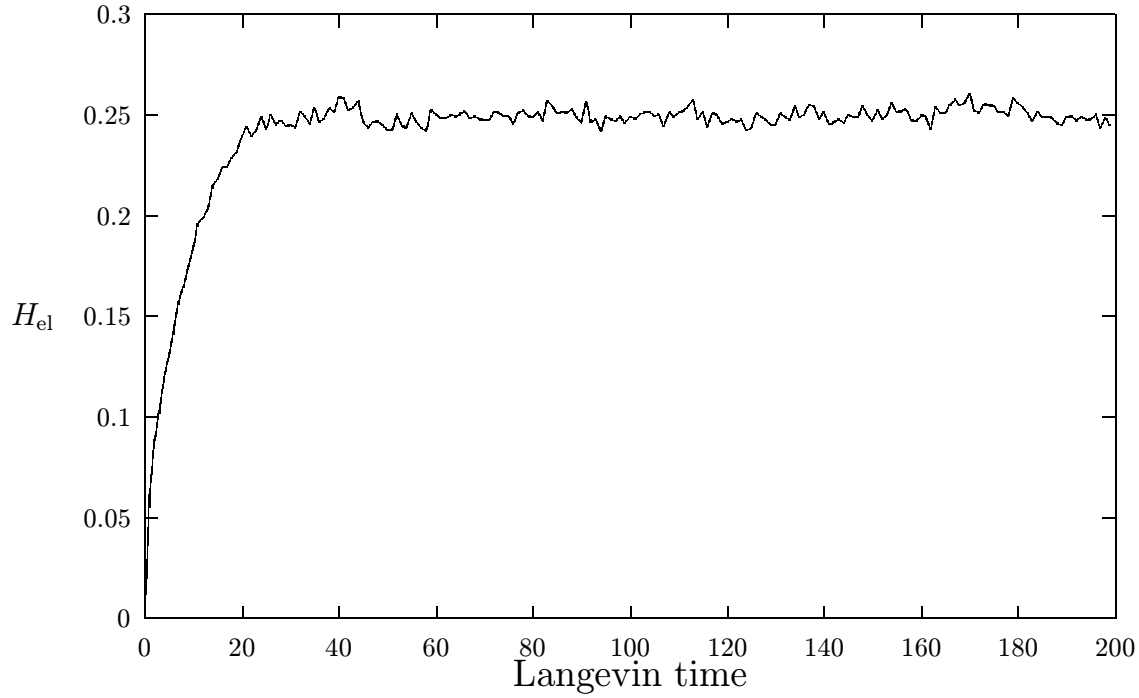

Figure 1: Langevin time history of the color electric energy per site for the SU(2) Yang-Mills theory on a 12^3 lattice. The algorithm time step was 0.01. Initial configuration had energy small compared to the average one for the inverse temperature $\beta = 12$.

6 Application: maximal Lyapunov exponent of the SU(2) Yang-Mills theory

As pointed out in the Introduction, lattice theories in the classical approximation are especially valuable in dealing with dynamical properties at finite temperature since in this case the arsenal of nonperturbative tools applicable to a full quantum theory is extremely scarce. Lyapunov exponents of a gauge theory belong to this category. According to recent numerical work [6], the maximal Lyapunov exponents $\lambda_{\rm max}$ of the classical SU(2) and SU(3) lattice gauge theories are approximately independent of the lattice spacing and proportional to the average energy per degree of freedom in a range of values of the latter. This approximate scaling property of $\lambda_{\rm max}$ was suggested based on a set of initial configurations with zero electric energy and the values of link matrices randomly chosen from a closed vicinity of identity. Here I use the thermalization algorithm for the SU(2) Yang-Mills theory described by (25) to compute $\langle\lambda_{\rm max}\rangle$, the *canonical ensemble* average of $\lambda_{\rm max}$ (notation $\langle\rangle$ is used for canonical averages in the following). Taking this average allows to directly establish a relation between the maximal Lyapunov exponent and the temperature and to study deviations of $\langle\lambda_{\rm max}\rangle$ from the scaling prediction of Ref. [6] as compared to the statistical error of $\langle\lambda_{\rm max}\rangle$.

The procedure used for measuring $\lambda_{\rm max}$ was as follows. A sample of phase-space configurations corresponding to an inverse temperature β was generated. Each member

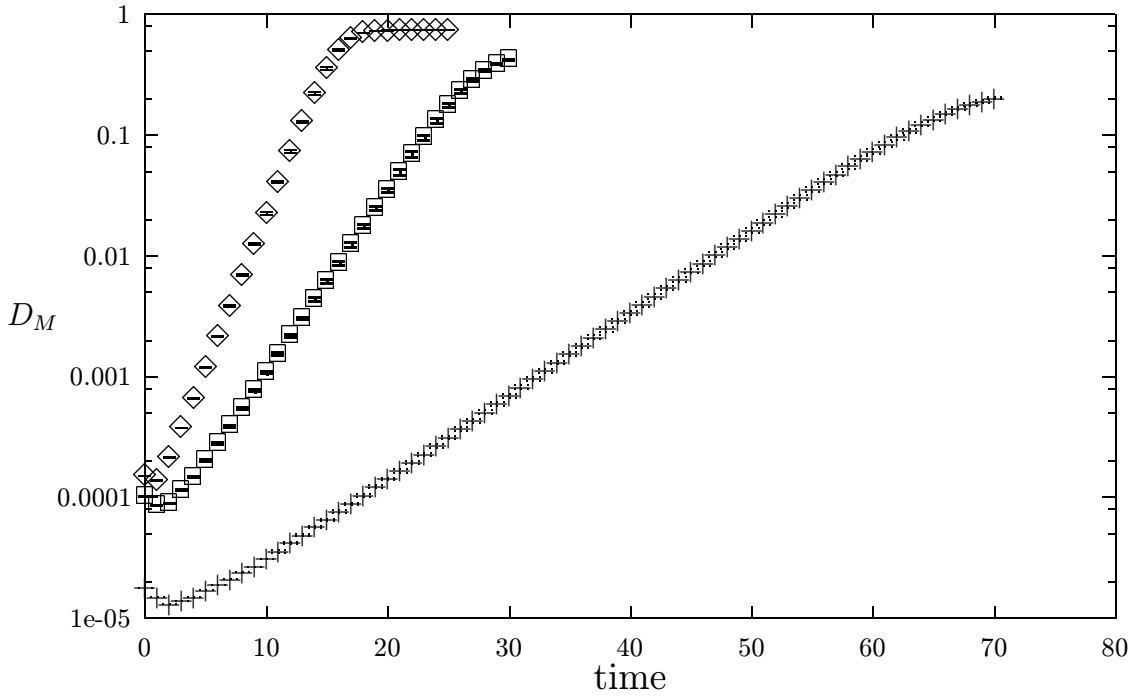

Figure 2: Distance D_M between two diverging trajectories as a function of time for $\beta = 2.5$ (diamonds), $\beta = 4$ (squares), and $\beta = 7.5$ (pluses) on a 12^3 lattice. The error bars are smaller than the plotting symbols

of the sample served as a reference initial configuration. A neighboring configuration was then generated by applying the algorithm briefly (in terms of Langevin time) to a reference one. Every such pair of nearby initial configurations was let evolve according to the Hamiltonian equations of motion, and the distances between the two configurations, defined as

$$D_E \equiv \sum_l |E_l^\alpha E_l^\alpha - E'^\alpha_l E'^\alpha_l|; \quad D_M \equiv \sum_\Box |\mathrm{Tr}U_\Box - \mathrm{Tr}U'_\Box|,$$

[6], were monitored (the unprimed and primed variables correspond to the reference and the neighboring configuration, respectively). A Langevin trajectory between two consecutive Hamiltonian ones was long enough to eliminate autocorrelations of $\langle D_{E,M}(t)\rangle$ within the sample. The measurements were performed for inverse temperatures $2 \leq \beta \leq 10$. A 20^3 lattice was used for $\beta \geq 5$, and a 12^3 lattice for higher temperatures; this size reduction had no measurable effect on $\langle \lambda_{\max}\rangle$ already at $\beta = 4$. The Hamiltonian time step was small enough to ensure conservation of energy to six significant digits. For every value of the temperature 25 Hamiltonian trajectories were performed.

As functions of time, $\langle D_{E,M}(t)\rangle$ both exhibit transient effects early on, then grow exponentially, and, finally, saturate (Figure 2). The maximal Lyapunov exponent $\lambda_{\max}$ is defined as the rate of the exponential growth of $D_{E,M}(t)$. A fit of $D_{E,M}(t)$ to an exponential function of time yields $\langle \lambda_{\max}\rangle$. Within the measurement errors the values of $\langle \lambda_{\max}\rangle$, determined from both definitions of distance, coincide. Measurements in Ref. [6]

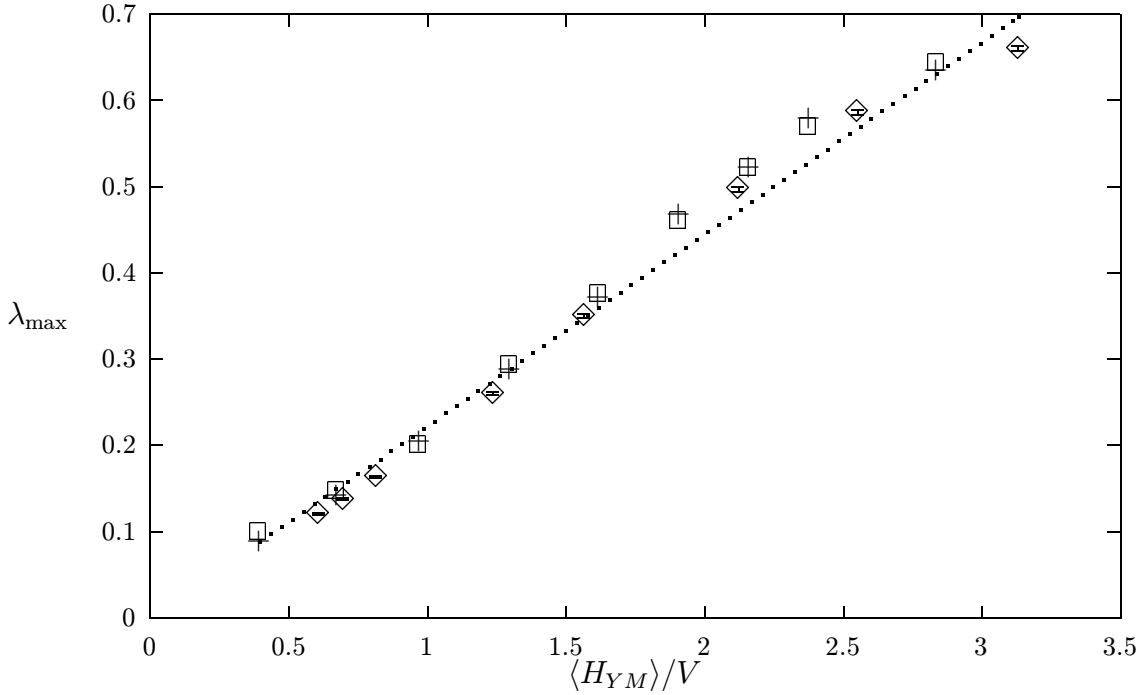

Figure 3: Maximal Lyapunov exponent $\lambda_{\max}$ as a function of average energy per site. Diamonds with the error bars smaller than plotting symbols are canonical averages of the present work. Pluses and squares are single-trajectory results of Ref. [6]. The dotted line is a linear fit through the origin.

β	volume	$\langle H_{YM}\rangle$/volume	$\langle\lambda_{\max}\rangle$
2	12^3	3.130	0.659 ± 0.002
2.5	12^3	2.551	0.586 ± 0.002
3	12^3	2.120	0.497 ± 0.004
4	12^3	1.566	0.350 ± 0.003
5	20^3	1.238	0.260 ± 0.002
7.5	20^3	0.8149	0.163 ± 0.001
8.75	20^3	0.6956	0.137 ± 0.001
10	12^3	0.6072	0.115 ± 0.002
10	20^3	0.6074	0.120 ± 0.001

Table 2: Summary of measured canonical averages of $\lambda_{\max}$.

suggested scaling of $\langle\lambda_{\max}\rangle$ with the average energy per site:

$$\langle\lambda_{\max}\rangle/\langle H_{YM}\rangle = \kappa. \tag{32}$$

According to Ref. [6] $\kappa \approx 2/9$ in the units of energy and time used in this work. The best linear fit through the origin for the data in Figure 3 is indeed very close to 2/9. However, the goodness of fit is very poor since, as Table 2 shows, statistically significant deviations from (32) are as large as 10%. Hence the estimate of κ in the range of temperatures considered may not be reliable. It is obvious from dimensional considerations that any deviation from scaling $\langle\lambda_{\max}\rangle \propto T$ implies dependence of $\langle\lambda_{\max}\rangle$ on the lattice spacing. Lattice artifacts tend to increase with the temperature due to the compact form of the lattice magnetic term (*cf* (25)). Thus, in order to safely establish the value of κ, $\lambda_{\max}$ should be measured at temperatures $T < 0.1$. Larger lattice sizes may be required in order to control finite size effects, clearly visible already at $T = 0.1$. An accurate knowledge of κ through a low-temperature measurement is necessary in order to test the relation of $\langle\lambda_{\max}\rangle$ to the plasmon damping rate as suggested in Ref. [7].

7 Concluding remarks

Methods presented in this work enable one to accurately bring a variety of classical lattice gauge theories to thermal equilibrium while respecting the local charge conservation. Due to their local nature, these methods easily lend themselves to vector and parallel computer implementations[1]. The algorithms can be applied to the study of real-time properties of high-temperature gauge theories, where the classical approach is by far the simplest if not the only one available. There is a growing body of evidence that some interesting nonperturbative quantities can be reliably determined by classical real-time simulations and are not plagued by ultraviolet divergencies inherent in classical thermodynamics. The examples include approximate scaling of thermalization rate in

[1]The codes are available upon request from the author

(3+1)-dimensional Yang-Mills theories discussed in the previous section, as well as numerical evidence for the existence of continuum limit of fermion-number violation rate in (1+1)-dimensional Abelian Higgs model [2, 5, 4]. More recently, the SU(2) Yang-Mills thermalization algorithm described here was applied to determine the baryon-number violation rate in the Standard model at temperatures well above the electroweak phase transition [8]. The results show the existence of continuum limit for the rate and its sensitivity to long-range properties of the theory [2].

It is possible to generalize the method to other gauge theories, most notably to the physically important SU(3) Yang-Mills theory. Again, the algorithm construction begins with finding a suitable set of gauge-invariant generators. A candidate generator set is

$$T^{[ij]} \equiv E_i^\alpha E_j^\alpha; \quad T^{[ijk]} \equiv d^{\alpha\beta\gamma} E_i^\alpha E_j^\beta E_k^\gamma,$$

where E are the color electric fields, d are the symmetric SU(3) constants, and $i \leq j \leq k$. Gauge invariance of T can be explicitly verified, they commute with each other, and their number is 16, the number of the physical degrees of freedom. A lattice algorithm can be developed along these lines.

Finally, it should be noted that this work has concentrated on constructing the algorithms and verifying their validity, rather than on tuning the algorithm performance. The latter is postponed to subsequent work. For the most obvious and important applications of the algorithms, however, namely, real-time studies of gauge theories, generation of initial thermal configurations typically consumes little time compared to canonical real-time evolution. With this kind of application in mind, the algorithm optimization can only lead to modest gains in computing time.

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