Constrained Hybrid Monte Carlo algorithms for gauge-Higgs models

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Abstract

We present the construction of Hybrid Monte Carlo (HMC) algorithms for constrained Hamiltonian systems of gauge-Higgs models in order to measure the constraint effective Higgs potential. In particular we focus on SU(2) Gauge-Higgs Unification models in five dimensions, where the Higgs field is identified with (some of) the five-dimensional components of the gauge field. Previous simulations have identified regions in the Higgs phase of these models which have properties of 4D adjoint or Abelian gauge-Higgs models. We develop new methods to measure constraint effective potentials, using an extension of the so-called Rattle algorithm to general Hamiltonians for constrained systems, which we adapt to the 4D Abelian gauge-Higgs model and the 5D SU(2) gauge theory on the torus and on the orbifold. The derivative of the potential is determined via the expectation value of the Lagrange multiplier for the constraint. To our knowledge, this is the first time this problem has been addressed for theories with gauge fields. The algorithm can also be used in four dimensions to study finite temperature and density transitions via effective Polyakov loop actions.

Keywords: constrained HMC algorithms, constraint effective Higgs potential, Gauge-Higgs Unification in five dimensions, effective Polyakov loop action

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1. INTRODUCTION

The discovery in 2012 of a scalar particle around 125 GeV [1, 2] has all but confirmed the existence of the Higgs mechanism, which renders the Standard Model (SM) of particle physics complete. However, the origin of the potential responsible for Spontaneous Symmetry Breaking (SSB), which leads to the Brout-Englert-Higgs (BEH) mechanism [3, 4] is, as of yet, unknown, and the arbitrary nature of the required fine tuning of parameters, the so-called hierarchy problem, suggests that a more fundamental process is at work.

A class of extensions to the Standard Model aimed at addressing these puzzles by the use of extra dimensions come under the heading of Gauge-Higgs Unification (GHU) [5, 6, 7]. In these models, the Higgs field originates from the extra-dimensional components of the gauge field and gives rise to massive gauge bosons in the regular four dimensions. A particular GHU model in terms of a five-dimensional $SU(2)$ gauge theory where the extra dimension is compactified on an $S^1/Z_2$ orbifold was formulated in [8, 9] in the context of lattice field theory. At the fixed points of the orbifold, the gauge group is broken down to $U(1)$ and the theory exhibits SSB [10, 11] in accordance with Elitzur’s theorem [12], via the spontaneous breaking of the so-called stick symmetry [13, 14], giving rise to the BEH mechanism. This observation was confirmed in [15, 16] via semi-analytic mean-field calculations.

The system has been found to exhibit three phases, see Fig. 1 (left), separated by first order phase transition lines which are characterized by the expectation value of the Polyakov loop in the extra dimension: in the confined (de-confined) phase the Polyakov loop exhibit zero (non-zero) expectation value in every direction. In this context, the de-confined phase is labelled Higgs phase, because it is where the Higgs potential develops SSB, giving rise to non-zero gauge boson masses. The third phase, which is characteristic only of the orbifold geometry, shows confined dynamics in the orbifold’s bulk, and de-confined dynamics on its boundaries; it is, therefore, called hybrid phase. These results, which are favorably pointing towards the suitability of this theory for describing the electro-weak sector of the Standard Model, are reported in [17, 18].

The phase structure is similar to the one of the Abelian gauge-Higgs model, shown in Fig. 1 (right). Moreover on the orbifold boundaries one observes dimensional reduction from five to four dimensions [17], which suggests that there is a localization mechanism for the gauge field. Therefore, we are aiming at the study of the dimensional reduction of the 5D GHU model with torus and orbifold boundary conditions and their connection to the 4D adjoint resp. Abelian-Higgs model by analyzing the effective potentials in the various cases. In particular, we want to see whether the effective potential reproduces the form of the SM potential, i.e.:

$$V_{\text{eff}}(\mathcal{H}) = -\mu^2 \mathcal{H} \mathcal{H}^\dagger + \lambda (\mathcal{H} \mathcal{H}^\dagger)^2,$$

where $\mathcal{H} = (H_0, H^\dagger)$ is the SM Higgs doublet and $\mu^2$ and $\lambda$ are the well-known Higgs mass and Higgs self-coupling parameters. Notice that, in order to have spontaneous symmetry breaking of the electroweak symmetry, the sign in front of $\mu^2$ must be negative and $\lambda$ must be positive to have a well-defined energy minimum, giving the well-known Mexican hat potential. In addition these parameters should reproduce the SM relation $m_H^2 = 4\lambda \nu^2 = 2\mu^2$, where $m_H$ is the Higgs mass and $\nu$ is the vacuum expectation value (vev).

The goal is to measure the so-called constraint effective potential in lattice simulations, which in the infinite volume limit corresponds to the conventional effective potential [19, 20]. Therefore we need to formulate constrained Hamiltonians for the various models, i.e. the energy functional including constraint conditions on the corresponding Higgs fields, and derive constrained equations
1.5 2.0 2.5 3.0

Bulk-driven phase transition
Boundary-driven phase transition
Measured point

Figure 1: (left) From [17]. The phase diagram for $N_5 = 4$ in the region of the Higgs-hybrid phase transition of the 5D orbifold gauge theory (see Sect. 5). The points show the location of a first-order phase transition. The red and blue lines represent the width of the corresponding hystereses, while the dashed orange line represents $\gamma = 1$ ($\beta_4 = \beta_5$). (right) The phase diagram of the Abelian gauge-Higgs model (see Sect. 3) with $\lambda = 1$ showing a similar phase structure. The green and purple curves correspond to different order parameters.

of motion. We discuss the constrained Hybrid Monte Carlo (HMC) algorithm and how to measure the constraint effective potential in Sect. 2. Then we focus on the implementation of the constrained HMC for the 4D Abelian gauge-Higgs model Sect. 3 and the 5D SU(2) gauge theory with torus Sect. 4 and orbifold Sect. 5 boundary conditions, and present constraint effective potentials for all cases. We conclude with final remarks and an outlook to other interesting applications of these constrained algorithms to measure effective potentials, e.g., in finite temperature Quantum Chromodynamics (QCD).

### 2. THE CONSTRAINT EFFECTIVE POTENTIAL

One can calculate the exact effective potential non-perturbatively, using lattice simulations. This was first shown in the pure Higgs theory by Kuti and Shen [21], via simulating the constrained path integral,

$$e^{-\Omega U_{\Omega}(\Phi)} = \int D\phi \delta(\frac{1}{\Omega} \sum_{\mu} H(n_\mu) - \Phi) e^{-S[\phi]}$$

(2.1)

where $n_\mu$ ($\mu = 0, 1, 2, 3$) are the integer coordinates of the points on a lattice with volume $\Omega$ and the average of the Higgs field $H(n_\mu)$, constructed from the field variables $\phi(n_\mu)$, takes a fixed value $\Phi$. During the constrained simulations we measure the derivative of the constraint effective potential $U_{\Omega}$ with respect to the constraint field $\Phi$ and a separate lattice simulation has to be run for every value of $\Phi$. This method is computationally expensive, but determines the effective potential with greater accuracy than fitting a distribution $P(\Phi)$. In the infinite volume limit the constraint potential gives the effective potential $U_{\Omega}(\Phi)$ $\Omega \to \infty \Rightarrow U_{\text{eff}}(\Phi)$ [19, 20]. In order to derive
\[ U_{\Omega}(\Phi) \text{ we rewrite Eq. (2.1) in terms of the constrained Hamiltonian} \]

\[
\hat{H}[\phi, \pi] = H[\phi, \pi] + \lambda^{(1)} \left( \frac{1}{\Omega} \sum_{n_{\mu}} \mathcal{H}(n_{\mu}) - \Phi \right), \quad H[\phi, \pi] = S[\phi] + \frac{1}{2} \sum_{n_{\mu}} \pi^2(n_{\mu}) \tag{2.2}
\]

\[
e^{-\Omega U_{\Omega}(\Phi)} = \int \mathcal{D}\phi \mathcal{D}\pi \mathcal{H}(n_{\mu}) - \Phi e^{-S[\phi]} = \int \mathcal{D}\phi \mathcal{D}\pi e^{-\hat{H}[\phi, \pi]} \tag{2.3}
\]

where the fictitious momentum variables \( \pi(n_{\mu}) \) are introduced and the Lagrange multiplier \( \lambda^{(1)} \) in front of the constraint condition ensures that the Higgs field \( \mathcal{H}(n_{\mu}) \) fluctuates around a fixed average value \( \Phi \). The derivative of Eq. (2.3) with respect to \( \Phi \) yields

\[
-\Omega U_{\Omega}' e^{-\Omega U_{\Omega}} = -\int \mathcal{D}\phi \mathcal{D}\pi \hat{H} e^{-\hat{H}} = \int \mathcal{D}\phi \mathcal{D}\pi \lambda^{(1)} e^{-\hat{H}} \tag{2.4}
\]

\[
\Rightarrow U_{\Omega}'(\Phi) = -\frac{1}{\Omega} \int \mathcal{D}\phi \mathcal{D}\pi \lambda^{(1)} e^{-\hat{H}} e^{-\Omega U_{\Omega}} = -\frac{1}{\Omega} \mathcal{E}^{(1)} \Phi \equiv U_{\Omega,\text{const}}' \tag{2.5}
\]

the derivative of the constraint effective potential \( U_{\Omega}'(\Phi) \equiv U_{\Omega,\text{const}}' \) given by the expectation value of the first Lagrange multiplier during simulations at fixed \( \Phi \) (\( \langle ... \rangle \)).

The simulations now are performed using Hybrid Monte Carlo methods implementing constrained equations of motion (cEOMs) of the form

\[
\dot{\phi}(n_{\mu}) = \frac{\partial \hat{H}}{\partial \pi(n_{\mu})} = \pi(n_{\mu}) \quad \text{and} \quad \dot{\pi}(n_{\mu}) = -\frac{\partial S}{\partial \phi(n_{\mu})} - \frac{\lambda^{(1)}}{\Omega} \frac{\partial \mathcal{H}}{\partial \phi(n_{\mu})}, \tag{2.6}
\]

including a term incorporating the Lagrange multiplier, which has to be evaluated first, before solving the cEOMs. This is done by demanding that the first derivative of the constraint condition with respect to molecular dynamics time, the so-called hidden constraint, vanishes as the constraint is a conserved quantity. In the case of a constraint condition that is linear in the underlying fields, \( \text{i.e.}, \) if the Higgs field \( \mathcal{H}(n_{\mu}) \) is a real, elementary scalar field, the hidden constraint only depends on the momenta \( \pi(n_{\mu}) \) and a standard leap-frog algorithm can be applied. The reason behind that is that leap-frog, as all Runge-Kutta schemes, preserve linear constraints exactly. If the constraint is applied to composite fields however, \( \text{e.g.}, \) \( \mathcal{H}(n_{\mu}) = \phi^{*}(n_{\mu}) \phi(n_{\mu}) \) as in the Abelian gauge-Higgs model, we get additional conditions of the form \( \sum_{n_{\mu}} \phi(n_{\mu}) \phi(n_{\mu}) = \sum_{n_{\mu}} \pi(n_{\mu}) \phi(n_{\mu}) \), depending on \( \pi(n_{\mu}) \) and \( \phi(n_{\mu}) \), which during a standard leap-frog trajectory are never defined at the same integration time and therefore the hidden constraint cannot be evaluated. This is also the case for \( SU(N) \) gauge fields, where the change of the fields in HMC algorithms is not given by an additive but a multiplicative exponential term proportional to the momenta \( \pi(n_{\mu}) \), cf. sections 4 and 5.

In order to implement the constrained equations of motion for these special cases we use an extension of the Newton-Störmer-Verlet-leapfrog method to general Hamiltonians for constrained systems, the so-called Rattle algorithm [22, 23], see also appendix A. These generalized leap-frog algorithms have an additional half integration step to get from \( \pi_{n+1/2} \) to \( \pi_{n+1} \) in order to have the momentum \( \pi \) at the same integration time as the field variable. We use the index \( n \) for the molecular dynamics time steps \( nh \), where \( h \) is the integration step size. This allows us to apply the so-called hidden constraint, which is the first derivative with respect to (integration) time of the constraint condition and involves both field variables and momenta. We successfully implemented the algorithms and numerically tested their time-reversibility and symplecticity. In the following we summarize the new algorithms for the various models with more details in the appendices.
3. 4D ABELIAN GAUGE-HIGGS MODEL

The Abelian gauge-Higgs action is given by

\[
S[U, \phi] = S_g[U] + S_\phi[U, \phi], \quad S_g[U] = \beta \sum_{\mu} \sum_{\mu < \nu} \{1 - \text{Re}U_{\mu\nu}(n_{\mu})\}
\]

\[
S_\phi[U, \phi] = \sum_{n_{\mu}} |\phi(n_{\mu})|^2 - 2\kappa \sum_{\mu} \text{Re} \left\{ \phi^\dagger(n_{\mu})U_{\mu}(n_{\mu})\phi(n_{\mu}) + a\bar{\mu}\right\} + \lambda(|\phi(n_{\mu})|^2 - 1)^2
\]

with \(\beta\) and \(\lambda\) the gauge and quartic couplings, respectively, \(\kappa\) the hopping (mass) parameter, \(\phi = \phi_1 + i\phi_2\) a complex scalar field, \(U_\mu(n_{\mu}) \sim U(1)\) gauge links and \(U_{\mu\nu}(n_{\mu}) = U_\mu(n_{\mu})U_\nu(n_{\mu} + \bar{\mu})U_\mu^\dagger(n_{\mu} + \bar{\nu})U_\nu^\dagger(n_{\mu})\) the standard plaquettes. \(n_{\mu}\) \((\mu = 0, 1, 2, 3)\) are the integer coordinates of the points on the 4D lattice of volume \(\Omega\) and we use a charge parameter \(q = 1\).

In order to respect gauge invariance of the 4D Abelian-Higgs model, the (composite) Higgs field is constructed via \(H(n_{\mu}) = \phi^\dagger(n_{\mu})\phi(n_{\mu})\) and our constraint condition reads

\[
\frac{1}{\Omega} \sum_{n_{\mu}} \phi^\dagger(n_{\mu})\phi(n_{\mu}) = 1, \quad \frac{1}{\Omega} \sum_{n_{\mu}, i=1,2} \phi_i(n_{\mu})^2 = \Phi.
\]

which has to be fulfilled at all times, therefore the field variables \(\phi(n_{\mu})\) have to be initialized with respect to the constraint already. The hidden constraint is given by the first derivative of the constraint condition with respect to integration time, i.e.,

\[
\sum_{n_{\mu}, i=1,2} \phi_i(n_{\mu})\dot{\phi}_i(n_{\mu}) = \sum_{n_{\mu}, i=1,2} \phi_i(n_{\mu})\pi_i(n_{\mu}) = 0,
\]

which has to vanish in order for the constraint condition to be fulfilled at all times. Therefore, when drawing the Gaussian-distributed random conjugate momenta \(\pi^0(n_{\mu})\) we have to ensure that they comply with the hidden constraint Eq. (3.4), which we achieve via orthogonal projection [22]

\[
\pi^0_i(n_{\mu}) = \pi^\prime_i(n_{\mu}) - \frac{\phi_i(n_{\mu})}{\Omega \Phi} \sum_{m_{\mu}, j=1,2} \pi^j(m_{\mu})\phi_j(m_{\mu}).
\]

\(\pi^0_i\) are defined as a linear transformation of \(\{\pi^j_i\}\), and therefore are still normally distributed around zero. The constrained HMC algorithm for the Abelian-Higgs model can be formulated in the following way, using the so-called Rattle algorithm [22, 23] (see appendix A.1 for the derivation)

\[
\pi_{i,n+1/2} = \pi_{i,n} - \frac{h}{2} \left( \frac{\partial S}{\partial \phi_{i,n}} + \frac{2\phi_{i,n}\lambda_{i,n}^{(1)}}{\Omega} \right), \quad \pi_{\mu,n+1/2} = \pi_{\mu,n} - \frac{h}{2} \frac{\partial S}{\partial U_{\mu,n}}
\]

\[
\phi_{i,n+1} = \phi_{i,n} + h\pi_{i,n+1/2}, \quad U_{\mu,n+1} = U_{\mu,n} + hP_{\mu,n+1/2}
\]

\[
\lambda_{i,n}^{(1)} = \frac{\Omega}{h^2} - \sum_{n_{\mu}, i} \phi_{i,n} \frac{\partial S}{2\Phi \partial \phi_{i,n}} \pm \sqrt{\left( \sum_{n_{\mu}, i} \phi_{i,n} \frac{\partial S}{2\Phi \partial \phi_{i,n}} \right)^2 - \frac{\Omega^2}{\Phi} \sum_{n_{\mu}, i} \left( \frac{\pi_{i,n}}{h} - \frac{1}{2} \frac{\partial S}{\partial \phi_{i,n}} \right)^2}.
\]

\[
\pi_{i,n+1} = \pi_{i,n+1/2} - \frac{h}{2} \left( \frac{\partial S}{\partial \phi_{i,n+1}} + \frac{2\phi_{i,n+1}\lambda_{i,n}^{(2)}}{\Omega} \right)
\]

\[
\lambda_{i,n}^{(2)} = \sum_{n_{\mu}, i} \left( \frac{\phi_{i,n+1}\pi_{i,n+1/2}}{h\Phi} - \frac{\phi_{i,n+1}}{2\Phi} \frac{\partial S}{\partial \phi_{i,n+1}} \right)
\]
where $X_{i,n} \equiv X_{i,n}(n_\mu)$ at molecular dynamics (MD) time $nh$ with the (MD) integration step size $h$. The gauge links $U_\mu(n_\mu)$ and corresponding conjugate momenta $P_\mu(n_\mu)$ are updated using the standard leap-frog algorithm. For the Higgs field $\phi(n_\mu)$ and conjugate momenta $\pi(n_\mu)$ the first three (left) equations (3.6a-3.6c) determine $\pi_{n+1/2}$ and $\phi_{n+1}$, such that the constraint is fulfilled at integration step $n+1$. During numerical simulations it turns out that only the $-$ sign in front of the square root fulfills the constraint condition. Equations (3.6d-3.6e) ensure the hidden constraint for fields $\phi_{n+1}$ and momenta $\pi_{n+1}$ at the same integration time, before starting over, i.e., continuing to integration times $n + 3/2$ and $n + 2$ subsequently.

We check numerically the time reversibility by performing one trajectory with stepsize $+h$ and another one with $-h$, retrieving the initial field and momentum variables. Further, we calculate the Jacobian $J = \frac{\partial(\phi_{n+1}(m_\mu), \pi_{n+1}(m_\mu))}{\partial(\phi_n(m_\mu), \pi_n(m_\mu))}$ numerically, yielding a $(4L^4)^2$ matrix with $\det J = 1$, implying volume preservation. This is just a test of our implementation since the Rattle algorithm ensures these two and other necessary geometric properties, see appendix A.

Using the algorithm we want to measure the derivative of the constraint effective potential $U'_\Omega, \text{const.}(\Phi) = -\frac{1}{\Omega} \langle \lambda^{(1)} \rangle_\Phi$ during Monte Carlo simulations. The numerical observable $\lambda^{(1)}$ however depends on the molecular dynamics integration stepsize $h$, which is not a physical quantity and therefore we want to analyze the continuum limit $h \rightarrow 0$ of this observable by rewriting the square root as a Taylor series

$$\lambda^{(1)} = \frac{1}{2\Phi} \sum_{m_\mu, i} \left( \pi_i^2 - \phi_i \frac{\partial S}{\partial \phi_i} \right) \Rightarrow U'_{\Omega, \text{const.}} \equiv \frac{1}{2\Phi} \sum_{m_\mu, i} \left( \phi_i \frac{\partial S}{\partial \phi_i} - \pi_i^2 \right) \langle \Phi \rangle \quad (3.7)$$

In Fig. 2 (left) we investigate the continuum limit $h \rightarrow 0$ by plotting $U'_{\Omega, \text{const.}}$ for various simulation step sizes $h$, rapidly approaching the continuum value $U'_{\Omega, \text{cont.}}$ at $h = 0$. We conclude that for the purpose of measuring the effective potential an integration step size of $h \leq 0.01$ is sufficient, for simplicity however we use the continuum form anyhow.

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Figure 2: (left) Well defined continuum limit of $U'_{\Omega, \text{const.}}$ (2.5) with respect to step size $h \rightarrow 0$, it agrees with the continuum form $U'_{\Omega, \text{cont.}}$ (3.7) at $h = 0$ for $h \leq 0.01$. (right) Effective potential and derivatives from histogram method and constrained simulations for the Abelian gauge-Higgs model at $\beta = 1.4, \kappa = 0.17, \lambda = 0.15$ on $\Omega = 8^4$ lattices. The potential and its derivative diverge for $\Phi \rightarrow 0$.  

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First results of the effective potential in the Higgs phase are presented in Fig. 2 (right) and Fig. 3 for \( \beta = 1.4, \kappa = 0.17, \lambda = 0.15 \) and \( \beta = 0.6, \kappa = 0.3, \lambda = 1 \) on \( \Omega = 8^4 \) lattices, comparing the derivative of the constraint effective potential \( U'_{\Omega, \text{const.}} \) with the effective potential \( U_{\Omega, \text{hist.}} \) and its derivative obtained from a standard histogram method, \textit{i.e.}, measuring the distribution of the field \( \Phi = \sum_{n_\mu} \phi(n_\mu) \phi(n_\mu) \) in an unconstrained simulation, appropriately binning it in a normalized histogram and taking the logarithm. The unconstrained simulation for the histogram method needs much more statistics than the individual constrained simulations combined to achieve comparable precision, only in the vicinity of the expectation value of the Higgs field \( \Phi_0 = \langle \Phi \rangle \). Note that the latter exactly coincides with the zero crossing of the derivative of the (constraint) effective potential, and we can read off the Higgs mass from the second derivative of the (constraint) effective potential at \( \Phi_0 \). Further notice in the right plot of Fig. 2 that with the new method to measure the derivative of the constraint effective potential, we can access the Higgs potential over the full parameter range \( \Phi \rightarrow 0 \), since only positive values of \( \Phi \) are allowed by definition, see Eq. (3.3).

![Figure 3: Effective potential and derivatives from histogram method and constrained simulations for the Abelian gauge-Higgs model at \( \beta = 0.6, \kappa = 0.3, \lambda = 1 \) (left) and \( \beta = 1.4, \kappa = 0.17, \lambda = 0.15 \) (right, zoom of right plot in Fig. 2) on \( \Omega = 8^4 \) lattices.](image-url)

4. 5D SU(2) GAUGE THEORY ON THE TORUS

The anisotropic Wilson plaquette action for a 5D SU(2) gauge theory with periodic (torus) boundary conditions is given by \([24, 25]\)

\[
S_{\text{W}}^{\text{cor}} = \sum_{n_\mu} \sum_{n_5=0}^{N_5-1} \left[ \frac{\beta_4}{2} \sum_{\mu<\nu} \text{Re Tr}\{1-U_{\mu\nu}(n_\mu, n_5)\} + \frac{\beta_5}{2} \sum_{\mu} \text{Re Tr}\{1-U_{\mu5}(n_\mu, n_5)\} \right],
\]

where \( \beta_4 \) and \( \beta_5 \) are the gauge couplings associated with plaquettes spanning the standard four dimensions \( (U_{\mu\nu}) \) and the fifth dimension \( (U_{\mu5}) \) respectively. The anisotropy is \( \gamma = \sqrt{\beta_5/\beta_4} \) and in the classical limit \( \gamma = a_4/a_5 \), where \( a_4 \) denotes the lattice spacing in the usual four dimensions and \( a_5 \) denotes the lattice spacing in the extra dimension. The theory is defined on the periodic interval \( I = \{n_\mu, 0 \leq n_5 < N_5\} \), where \( (n_\mu, n_5), \mu = 0, 1, 2, 3 \) are the integer coordinates of the points.
The term \( \text{Tr} U \) (4.2c). Hence, only the links in the extra dimension will be affected by the constraint, all other links \( U_\mu(n_\mu, n_5), \mu = 0, 1, 2, 3 \) can be updated using the standard leapfrog method. For the links \( U_5(n_\mu, n_5) \) and momenta \( \pi_5(n_\mu, n_5) \) we apply the Rattle algorithm in appendix A.3 and find

\[
\pi_{n+1/2} = \pi_n - h \left( \frac{\partial S}{\partial U_n} - \frac{\lambda_n^{(1)}}{8\Omega} \text{Tr}[\ldots\sigma_i U_{n_5}] \sigma^i \right) \quad (4.2a)
\]

\[
U_{n+1} = e^{h\pi_{n+1/2}U_n} \quad (4.2b)
\]

\[
0 = \frac{1}{2\Omega} \sum_{n_\mu} \text{Tr} P_{n+1}(n_\mu) - \Phi = \frac{1}{2\Omega} \sum_{n_\mu} \sum_{n_5=0}^{N_5-1} U_{n+1} - \Phi \quad (4.2c)
\]

\[
\pi_{n+1} = \pi_{n+1/2} - \frac{h}{2} \left( \frac{\partial S}{\partial U_{n+1}} - \frac{\lambda_n^{(2)}}{8\Omega} \text{Tr}[\ldots\sigma_i U_{n+1}] \sigma^i \right) \quad (4.2d)
\]

\[
0 = \frac{1}{8\Omega} \sum_{n_\mu, n_5} \text{Tr}[\text{Tr}[\ldots\sigma_i U_{n+1}] \sigma^i \pi_{n+1}] \quad (4.2e)
\]

The term \( \text{Tr}[\ldots\sigma_i U_{n_5}] \sigma^i \) denotes a Polyakov line at \( n_\mu \) with an insertion of \( \sigma_i \) at \( n_5 \), summing over \( i = 1, 2, 3 \) for the three Pauli matrices. The first three equations determine \( (\pi_{n+1/2}, U_{n+1}, \lambda_n^{(1)}) \), whereas the remaining two give \( (\pi_{n+1}, \lambda_n^{(2)}) \).

We use a simple Secant method to get \( \lambda_n^{(1)} \) up to machine precision, providing a precise root for the functional given by our constraint condition in Eq. (4.2c)

\[
f(\lambda_n^{(1)}) = \frac{1}{2\Omega} \sum_{n_\mu} \text{Tr} P_{n+1}(n_\mu, \lambda_n^{(1)}) - \Phi = \frac{1}{2\Omega} \sum_{n_\mu} \sum_{n_5=0}^{N_5-1} U_{n+1}(n_\mu, n_5, \lambda_n^{(1)}) - \Phi
\]

with \( U_{n+1}(n_\mu, n_5, \lambda_n^{(1)}) \) given in Eq. (4.2b). We iterate \( \lambda_n^{(1)} = \lambda_n^{(1)} - f(\lambda_n^{(1)}) [\lambda_n^{(1)} - \lambda_n^{(1)}] / [f(\lambda_n^{(1)}) - f(\lambda_n^{(1)} - 1)] \), starting from an approximate solution \( \lambda_{n,0}^{(1)} \) obtained by truncating the exponential in (4.2b) after \( \mathcal{O}(h^2) \)

\[
\frac{\lambda_n^{(1)}}{8\Omega} = \left\{ \sum_{n_\mu, n_5} \left[ \text{Tr}[\ldots \frac{\partial S}{\partial U_{n}(n_\mu, n_5)} U_n(n_\mu, n_5)] - \text{Tr}[\ldots \pi_n^2 U_n(n_\mu, n_5)] \right] - 2 \sum_{n_\mu, n_5, n_5'} \text{Tr}[\ldots \pi_n(n_\mu, n_5) U_n(n_\mu, n_5') \pi_n(n_\mu, m_5) U_n(n_\mu, m_5)] \right\} / \quad (4.3a)
\]

\[
\sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U_n(n_\mu, n_5)] \sigma^i U_n(n_\mu, n_5)]
\]

The iteration stops when \( \lambda_{n,k+1}^{(1)} = \lambda_n^{(1)} \) or \( f(\lambda_n^{(1)}) = f(\lambda_n^{(1)} - 1) \) up to machine precision.

The second Lagrange multiplier is determined as (see appendix A.3 for details)

\[
\frac{\lambda_n^{(2)}}{8\Omega} = \frac{\sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U_{n+1}(n_\mu, n_5)] \text{Tr}[\sigma^i \partial S / \partial U_{n+1}(n_\mu, n_5)] - 2 \sigma^i \pi_{n+1/2}(n_\mu, n_5) / h}{\sum_{n_\mu, n_5} \text{Tr}[\{\text{Tr}[\ldots \sigma_i U_{n+1}(n_\mu, n_5)] \sigma^i\}^2]} \quad (4.4a)
\]
Again, we have to initialize the Polyakov lines to fulfill the constraint condition (4.2c), e.g., with the help of axial gauge, and when drawing the Gaussian-distributed random conjugate momenta $\pi_r(n_\mu, n_5)$ we have to ensure that they comply with the hidden constraint (4.2e), which we achieve via orthogonal projection

$$\pi_0(n_\mu, n_5) = \pi_r(n_\mu, n_5) - \frac{\sum_{n_\mu, n_5} \text{Tr}\{[\sigma_i U(n_\mu, n_5) \ldots] \sigma^i \pi_r(n_\mu, n_5)\}}{\sum_{n_\mu, n_5} \text{Tr}\{(\text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots] \sigma^i)^2\}} \text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots] \sigma^i$$

Fig. 4 shows that the Rattle algorithm for the 5D torus keeps the average Polyakov loop fixed (left plot). The Lagrange multiplier along a trajectory is plotted on the right.

Because of center symmetry, $\langle \text{Tr} P_5 \rangle$ always vanishes in finite volume. Therefore we further investigate the constraint $\frac{1}{4\Omega} \sum_{n_\mu} [\text{Tr} P_5(n_\mu)]^2 = \Phi$ which fixes the Higgs field $\mathcal{H} = \frac{1}{8\Omega} \sum_{n_\mu} \text{Tr}[P_5(n_\mu) - P_5^\dagger(n_\mu)]^2 = \Phi - 1$ of the torus model and is invariant under center symmetry. The algorithm which fulfills the constraint is slightly more complicated than the one above and is formulated in appendix A.4. The implementation is equivalent to the previous cases and therefore we just summarize the important steps:

- initialize the field variables $q$ to fulfill the constraint $g(q) = 0$
- draw (unconstrained) Gaussian distributed random momenta $p$
- project the momenta $p$ to satisfy the hidden constraint $\tilde{g}(q,p)$
- propagate $p$ and $q$ as defined by the Rattle discretization
- accept new fields with probability $r = \min[1, \exp(-\Delta H)]$

With the right tools at hand we now measure the constraint effective potentials $U_\Omega(\Phi)$ via their derivatives $U_\Omega'(\Phi) = -\langle \lambda^{(1)} \rangle / \Omega$ for both cases $\langle \text{Tr} P_5 \rangle / 2$ and $\langle (\text{Tr} P_5)^2 / 4 \rangle$ of the 5D SU(2) gauge theory on the torus. In Fig. 5 we show effective Higgs potentials and their derivatives for the symmetric point $\beta_4 = \beta_5 = 1.66$ on $\Omega = 8^4, N_5 = 4$ lattices. The results of the constrained method
are in good agreement with the histogram potential in the vicinity of the expectation value of the Higgs field. The histogram method is limited to that narrow region, getting narrower the larger the lattice size, while the constraint effective potential can be measured very precisely over the whole parameter range. The unconstrained expectation values of the Higgs field $\Phi_0$ exactly coincide with the zero crossing of the (constraint) effective potentials. $\Phi_0 = \langle \text{Tr} P_5/2 \rangle = \pm 0.282$ is non-zero and we find two degenerate minima of the potential, the derivative of the constraint effective potential accordingly vanishes three times and its (numerical) integral shows the familiar Mexican hat form, which the histogram method cannot reproduce at all because of its limitations in potential width and accuracy. The upper plots in Fig. 6 present effective Higgs potentials for $\beta_4 = 1.0, \beta_5 = 2.8$ on $\Omega = 24 \times 12^3, N_5 = 4$ lattices. This point lies in the so-called compact phase of the theory, where dimensional reduction via compactification is expected. Again we find two degenerate minima of the potential for $\Phi_0 = \langle \text{Tr} P_5/2 \rangle = \pm 0.228$ and the Mexican hat form is reproduced by the constraint effective potential only. The Higgs observable $\langle \text{Tr} P \rangle^2$ only shows
The orbifold theory we consider here is defined in the five-dimensional domain $I = \{n_5, 0 \leq n_5 \leq N_5\}$ with volume $N_5 \times N_5^3 \times N_5$. The anisotropic Wilson gauge action for an SU(2) gauge theory on this orbifold is given by \[ S_{\text{orb}} = \sum_{n_\mu} \left[ \frac{\beta_1}{2} \sum_{n_5=0}^{N_5} \sum_{\mu \leq \nu} w \text{Re} \text{Tr} \{ 1 - U_{\mu \nu}(n_\mu, n_5) \} + \frac{\beta_2}{2} \sum_{n_5=0}^{N_5-1} \sum_{\mu} \text{Re} \text{Tr} \{ 1 - U_{\mu 5}(n_\mu, n_5) \} \right], \] (5.1)
which follows the parametrization of Eq. (4.1). The weight \( w \) is due to the orbifold geometry and takes a value \( w = 1/2 \) for plaquettes \( U_{\mu \nu} \) on the boundaries and it is \( w = 1 \) elsewhere. The boundary links are in the gauge group \( U(1) \) and all other links are in \( SU(2) \). The anisotropy is \( \gamma = \sqrt{\beta_5/\beta_4} \) and in the classical limit \( \gamma = a_4/a_5 \), where \( a_4 \) denotes the lattice spacing in the usual four dimensions and \( a_5 \) denotes the lattice spacing in the extra dimension. The theory is defined on the interval \( I = \{ n_\mu, 0 \leq n_5 \leq N_5 \} \), where \( (n_\mu, n_5) \), \( \mu = 0, 1, 2, 3 \) are the integer coordinates of the points. Given a constrained Hamiltonian for the Polyakov loop

\[
P_5(n_\mu) = \prod_{n_5=0}^{N_5-1} [U_5(n_\mu, n_5)] \sigma_3 \prod_{n_5=N_5-1}^{0} [U_5^\dagger(n_\mu, n_5)] \sigma_3
\]

(5.2)

we solve the constrained equations of motion

\[
\dot{U}_5(n_\mu, n_5) = \pi_5(n_\mu, n_5) U_5(n_\mu, n_5),
\]

\[
\dot{\pi}_5(n_\mu, n_5) = -\frac{\partial S[U_5]}{\partial U_5(n_\mu, n_5)} + \frac{\lambda^{(1)}}{8\Omega} \text{Tr}(...\sigma_i U_5(n_\mu, n_5)... - ...U_5^\dagger(n_\mu, n_5)\sigma_i...)[\sigma_i]
\]

(5.3)

using the Rattle algorithm derived in appendix A.5. Like in the torus models, we use a Secant method to determine the first Lagrange multiplier \( \lambda^{(1)} \), starting with an educated guess given by Eq. (A.5.3), and we have to initialize the momenta according to the hidden constraint. The constraint effective potential is measured via its derivative \( U'_{\Omega,\text{const}} = -\langle \lambda^{(1)} \rangle / \Omega \) for the symmetric point \( \beta_4 = \beta_5 = 1.66, \Omega = 8^4, N_5 = 5 \). This point lies in the Higgs phase, where the stick symmetry is broken and we find two degenerate minima of the potential. The left plot is a zoom of the right plot, where we show the full parameter range \(-1 < \text{Tr} P/2 < 1\).
6. CONCLUSIONS AND OUTLOOK

We successfully implemented constrained hybrid Monte Carlo algorithms for the 4D Abelian gauge-Higgs and a 5D $SU(2)$ gauge theory with torus and orbifold boundary conditions which allow us to simulate systems with constraint conditions, which appear as Lagrange multiplier terms in the Hamiltonian. To our knowledge, this is the first time this problem has been solved for theories with gauge fields. In order to solve the constrained equations of motion we use an extension of the Newton-Störmer-Verlet-leapfrog method to general Hamiltonians for constrained systems, the so-called Rattle algorithm. This generalized leap-frog method has an additional half integration step for the conjugate momenta in order to evaluate the so-called hidden constraint, which is the derivative of the constraint condition with respect to molecular dynamics time and in our cases involves both fields and momenta, after a full integration time step, in order to calculate the Lagrange multipliers which ensure that the constraints are fulfilled. The algorithm fulfills all necessary geometrical properties, summarized in appendix A, and we numerically tested the time-reversibility and volume preservation.

We plan to measure the constraint effective potentials on larger lattices and extract the Higgs masses in the different models considered. The latter is given by the second derivative of the constraint effective potential at the vacuum expectation value of the Higgs field and can be compared to the masses measured by different methods, e.g., by fitting two point functions from unconstrained simulations, which will allow us to study renormalization effects of the different mass determinations. Further we can compare the masses measured in the different models and study the compactification and dimensional reduction scenarios of the 5D torus and orbifold models respectively via their connection to the 4D adjoint and Abelian gauge-Higgs model. We can compare with the one-loop effective Higgs potential in the Abelian Higgs [26] and torus [27] models.

Finally, an interesting application of these algorithms are effective Polyakov loop actions in finite temperature QCD. The effective Polyakov loop action (PLA) is the theory which results from integrating out all of the degrees of freedom of the theory, subject to the condition that the Polyakov lines are held fixed. This was studied in the strong coupling expansion [28], but also in full lattice QCD simulations. It was found that this effective theory is more tractable than the underlying lattice gauge theory (LGT) when confronting the sign problem at finite density, for recent advances see [29]. The developed algorithms in this article can be adapted to this problem, where the individual Polyakov lines and not their average over the whole lattice are constrained. This requires Lagrange multiplier terms for each Polyakov line, which appear as a product in the path integral or a sum in the Hamiltonian. There is no additional numerical effort though, instead of summing over the whole lattice to evaluate one Lagrange multiplier, one just calculates the individual factors locally. The extraction of the effective Polyakov loop potential can in principal proceed in a similar way as described in this work, or else by the relative weights approach as presented in [30].

7. ACKNOWLEDGMENTS

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A. The Rattle algorithm for general constrained Hamiltonian systems

The most important numerical method for the solution of constrained Hamiltonian systems, the Rattle algorithm, is an adaptation of the Newton-Störmer-Verlet-leapfrog method that can be interpreted as a partitioned Runge-Kutta method and thus allows the extension to general Hamiltonians, c.f. [22, 23]. We consider mechanical systems with coordinates \( q \) that are subject to constraints \( g(q) = 0 \), and corresponding momenta \( p \). The equations of motion are then given by

\[
\begin{align*}
\dot{p} &= -\nabla_q H(p, q) - \nabla_q g(q) \lambda \\
\dot{q} &= \nabla_p H(p, q), \quad 0 = g(q),
\end{align*}
\]  

(A.0.1)

where the Hamiltonian \( H(p, q) \) is of the form

\[
H(p, q) = \frac{1}{2} p^T M^{-1} p + U(q)
\]  

(A.0.2)

with a positive definite mass matrix \( M \) and a potential \( U(q) \). To compute the Lagrange multiplier \( \lambda \), we differentiate the constraint \( g(q(t)) \) with respect to time, giving the so-called hidden constraint

\[
0 = \nabla_q g(q)^T \nabla_p H(p, q),
\]  

(A.0.3)

which is an invariant of the flow (A.0.1). We choose a step size \( h \) and discretized integration time \( t_n = t_0 + nh \). For initial values \((p_n, q_n) \in M\), i.e., consistent with \( g(q) = 0 \) and (A.0.3), the Rattle method yields an approximation \((p_{n+1}, q_{n+1})\) which is again on the solution manifold \( M \):

\[
\begin{align*}
p_{n+1/2} &= p_n + \frac{h}{2} \left( \nabla_q U(q_n) + \nabla_q g(q_n) \lambda^{(1)}_n \right) \\
q_{n+1} &= q_n + hM^{-1}p_{n+1/2}, \\
0 &= g(q_{n+1}), \\
p_{n+1} &= p_{n+1/2} + \frac{h}{2} \left( \nabla_q U(q_{n+1}) + \nabla_q g(q_{n+1}) \lambda^{(2)}_n \right) \\
0 &= \nabla_q g(q_{n+1})^T M^{-1} p_{n+1}.
\end{align*}
\]  

(A.0.4a-d)

The first three equations determine \((p_{n+1/2}, q_{n+1}, \lambda^{(1)}_n)\), whereas the remaining two give \((p_{n+1}, \lambda^{(2)}_n)\). Note that both Lagrangian multipliers are only intermediate variables and are not transported in the flow \( \Phi_h \). We thus have a numerical flow \( \Phi_h : M \to M \) with the following geometrical properties:

- the Rattle method is time-reversible, i.e., it holds \( \rho \circ \Phi_h \circ \rho \circ \Phi_h = I \) with flipping the momenta denoted by \( \rho(p, q) = (-p, q) \); if symmetry holds, i.e., \( \Phi_h = \Phi^{-1}_h \), this is equivalent to \( \rho \circ \Phi_h = \Phi_{-h} \circ \rho \);
  - symmetry can be checked by exchanging the subscripts \( n \leftrightarrow n + 1 \) and step size \( h \leftrightarrow -h \), which has to leave the method unaltered. In our case, the first equation becomes the forth and vice-versa, if we change the denomination of both Lagrangian multipliers, which are only intermediate variables; the second equation remains unchanged; the nonlinear equations (A.0.4c),(A.0.4e) at time point \( t_n + 1 \) are become those at \( t_n \) (and vice-versa).
  - the condition \( \rho \circ \Phi_h = \Phi_{-h} \circ \rho \) can be easily checked.
ensures long-time energy conservation, to be verified via \( \exp(-\Delta H) = 1 \)
- the Rattle algorithm is symplectic, \( i.e. \), the flow preserves areas in phase space
- \( \det \frac{\partial \Phi_h}{\partial (p,q)} = 1 \), \( i.e. \), the flow preserves the volume in phase space
- conservation of first integrals and preservation of adiabatic invariants
- provides a discrete virial theorem

For more details see \([22, 23]\). Now we summarize the algorithms for the various models\(^1\).

A.1. Rattle algorithm for Abelian gauge-Higgs model

Given a constraint condition for the complex variables \( \phi(n_\mu) \)

\[
\frac{1}{\Omega} \sum_{n_\mu} \phi^\dagger(n_\mu) \phi(n_\mu) = \Phi,
\]

(A.1.1)

the constrained HMC (Rattle) algorithm can be formulated in the following way

\[
\pi_{n+1/2} = \pi_n - \frac{h}{2} \left( \frac{\partial S}{\partial \phi_n} + \frac{2\phi_n \lambda_n^{(1)}}{\Omega} \right)
\]

(A.1.2a)

\[
\phi_{n+1} = \phi_n + h\pi_{n+1/2}
\]

(A.1.2b)

\[
0 = \frac{1}{\Omega} \sum_{n_\mu} \phi^\dagger_{n+1} \phi_{n+1} - \Phi
\]

(A.1.2c)

\[
\pi_{n+1} = \pi_{n+1/2} - \frac{h}{2} \left( \frac{\partial S}{\partial \phi_{n+1}} + \frac{2\phi_{n+1} \lambda_n^{(2)}}{\Omega} \right)
\]

(A.1.2d)

\[
0 = \frac{2}{\Omega} \sum_{n_\mu} \phi_{n+1} \pi_{n+1}
\]

(A.1.2e)

Plugging \( \pi_{n+1/2} \) into \( \phi_{n+1} \) and evaluating the constraint gives \( \lambda_n^{(1)} \):

\[
0 = \sum \left( \frac{\phi_n}{h} + \pi_n - \frac{h}{2} \frac{\partial S}{\partial \phi_n} - \frac{h \phi_n \lambda_n^{(1)}}{\Omega} \right)^2 - \frac{\Omega \Phi}{h^2}
\]

\[
= \sum \frac{\phi_n^2}{h^2} + \sum \pi_n^2 + \sum \frac{h^2}{4} \left( \frac{\partial S}{\partial \phi_n} \right)^2 + \frac{h^2 \lambda_n^{(1)} \lambda_n^{(1)}}{\Omega} + \frac{2h}{\Omega} \sum \phi_n \pi_n - \sum \phi_n \frac{\partial S}{\partial \phi_n}
\]

\[
- 2\lambda_n^{(1)} \sum_{=\Phi} \phi_n \frac{\partial S}{\partial \phi_n} - 2h \lambda_n^{(1)} \sum \phi_n \pi_n + \frac{h^2 \lambda_n^{(1)}}{\Omega} \sum \phi_n \frac{\partial S}{\partial \phi_n} - \frac{\Omega \Phi}{h^2}
\]

\[
= \lambda_n^{(1)} \left( \sum \phi_n \frac{\partial S}{\Phi} - \frac{2\Omega}{h^2} \right) + \frac{\Omega}{\Phi} \sum \left( \frac{\pi_n^2}{h^2} - \phi_n \frac{\partial S}{\Phi} - \pi_n \frac{\partial S}{h \Phi} + \frac{1}{4} \left( \frac{\partial S}{\Phi} \right)^2 \right)
\]

\(^1\)The algorithms for the 5D gauge theories presented in the proceedings \([31]\) differ from the present ones since they were the axial gauge.
Na Higgs-Yukawa theory with

We can use the standard leap-frog algorithm to perform the HMC updates as shown in [33] for to solve for the Lagrange multiplier

\[ \lambda_{n+1}^{(1)} = \frac{\Omega}{\hbar^2} - \sum \phi_n \frac{\partial S}{2\Phi \partial \phi_n} \pm \sqrt{\frac{\Omega^2}{\hbar^2} + \left( \sum \phi_n \frac{\partial S}{2\Phi \partial \phi_n} \right)^2 - \frac{\Omega}{\Phi} \sum \left( \pi_n - \frac{1}{2} \frac{\partial S}{\partial \phi_n} \right)^2} \]

During numerical simulations it turns out that only the \(-\) sign in front of the square root in \(\lambda_{n}^{(1)}\) fulfills the constraint condition. Plugging \(\pi_{n+1}\) into the hidden constraint (A.1.2e) gives

\[ \lambda_{n}^{(2)} = \frac{\omega_{n+1} \pi_n + \pi_n}{2\Phi} \frac{\partial S}{\partial \phi_n} \]

When drawing the Gaussian-distributed random conjugate momenta \(\pi_r(n_{\mu})\) we have to ensure that they comply with the hidden constraint, which we achieve via orthogonal projection

\[ \pi_0(n_{\mu}) = \pi_r(n_{\mu}) - \frac{\phi(n_{\mu})}{\Omega} \sum m_{\mu} \pi_r(m_{\mu}) \phi(m_{\mu}) \]

as can be verified by plugging it back into (A.1.2e).

A.2. Rattle algorithm for Abelian gauge-Higgs model in unitary gauge formulation

Note, we can write the action (3.2) in unitary gauge using the variable transformation proposed in [32] p.322ff, \(\phi(n_{\mu}) = \rho(n_{\mu}) \exp(\varphi(n_{\mu})) \Rightarrow \varphi_1 = \rho \cos \varphi, \varphi_2 = \rho \sin \varphi:\)

\[ S_{\rho}[V_{\mu}, \rho] = \sum_{n_{\mu}} \left[ \rho(n_{\mu})^2 + \lambda(\rho(n_{\mu})^2 - 1)^2 - 2\kappa \rho(n_{\mu}) \text{Re} \sum_{\mu} \rho(n_{\mu} + \hat{\mu}) \text{e}^{-\varphi(n_{\mu} + \hat{\mu})} V_{n_{\mu}}(\rho) \text{e}^{i\varphi(n_{\mu})} \right] \]

with gauge invariant links \(V_{n_{\mu}}(\rho)\). This allows us to rewrite the constrained Hamiltonian as

\[ \tilde{H}[V_{\mu}, \rho] = S_{\rho}[V_{\mu}, \rho] - \ln(\rho) + \frac{1}{2} \sum_{n_{\mu}} \pi(n_{\mu})^2 + \lambda(1) \left( \frac{1}{\Omega} \sum_{n_{\mu}} \rho(n_{\mu}) - \Phi \right) \]

where the \(\ln(\rho)\) term enters from the Jacobian of the variable transformation and plays an important role: for small \(\rho\) we get an diverging contribution to the action which pushes the system away from \(\rho \leq 0\) which would be unphysical. The constrained equations of motion read

\[ \dot{\rho}(n_{\mu}) = \frac{\partial H}{\partial \pi(n_{\mu})} = \pi(n_{\mu}), \quad \dot{\pi}(n_{\mu}) = \frac{\partial H}{\partial \rho(n_{\mu})} = - \frac{\partial S_{\rho}}{\partial \rho(n_{\mu})} + \frac{1}{\rho(n_{\mu})} - \lambda(1) \]

and derivatives of the constraint condition with respect to the molecular dynamics time allow us to solve for the Lagrange multiplier \(\lambda(1)\)

\[ \sum_{n_{\mu}} \dot{\rho}(n_{\mu}) = \sum_{n_{\mu}} \pi(n_{\mu}) = 0 \Rightarrow \sum_{n_{\mu}} \dot{\pi}(n_{\mu}) = 0 \Rightarrow \lambda(1) = \sum_{n_{\mu}} \left( \frac{1}{\rho(n_{\mu})} - \frac{\partial S_{\rho}}{\partial \rho(n_{\mu})} \right) \]

We can use the standard leap-frog algorithm to perform the HMC updates as shown in [33] for a Higgs-Yukawa theory with \(N_f\) fermions. In order to guarantee that the hidden constraint is fulfilled by the algorithm (note that the leap-frog algorithm would yield momenta fulfilling the constraint at the new time point, as it preserves linear constrains only in the momenta exactly), one has to initialize the (random) fictitious momenta \(\pi(n_{\mu})\) in each trajectory accordingly, \(i.e.,\)
with respect to \( \sum_{n_\mu} \pi(n_\mu) = 0 \). During the constrained simulations we measure the derivative of the effective potential \(^2\) \( U_1^{(1)}(\Phi) = -\frac{1}{\Omega} \langle \lambda^{(1)} \rangle = \frac{1}{\Omega} \langle \sum_{n_\mu} \left[ \partial S/\partial \rho(n_\mu) - 1/\rho(n_\mu) \right] \rangle \Phi \), where \( \langle \ldots \rangle_\Phi \) means the expectation value at fixed \( \Phi = \Omega^{-1} \sum_{n_\mu} \rho(n_\mu) \). Results are presented in Fig. 8 in agreement with Fig. 3 with respect to the different constraints.

The constrained HMC (Rattle) algorithm can be formulated in the following way

\[
\frac{1}{2\Omega} \sum_{n_\mu} \Tr \left[ \prod_{n_5=0}^{N_5-1} U_5(n_\mu, n_5) = \Phi \right] \tag{A.3.1}
\]

the constrained HMC (Rattle) algorithm can be formulated in the following way

\[
\begin{align*}
\pi_{n+1/2} &= \pi_n - \frac{\hbar}{2} \left( \frac{\partial S}{\partial U_n} - \frac{\lambda_n^{(1)}}{8\Omega} \Tr[\ldots \sigma_1 U_n \ldots] \sigma^i \right) \\
U_{n+1} &= e^{i\pi_{n+1/2} U_n} \\
0 &= \frac{1}{2\Omega} \sum_{n_\mu} \Tr \left[ \prod_{n_5=0}^{N_5-1} U_{n+1}(n_\mu, n_5) - \Phi \right] \\
\pi_{n+1} &= \pi_{n+1/2} - \frac{\hbar}{2} \left( \frac{\partial S}{\partial U_{n+1}} - \frac{\lambda_{n+1}^{(2)}}{8\Omega} \Tr[\ldots \sigma_1 U_{n+1} \ldots] \sigma^i \right) \\
0 &= \sum_{n_\mu, n_5} \Tr \{(\ldots \sigma_1 U_{n+1}(n_\mu, n_5) \ldots) \sigma^i \pi_{n+1}(n_\mu, n_5)\} 
\end{align*}
\tag{A.3.2}
\]

where \( \Tr[\ldots \sigma_1 U_5(n_\mu, n_5) \ldots] \sigma^i \) is the derivative of the constraint with respect to \( U_5(n_\mu, n_5) \), using

\[
\partial_5 \Tr U_5 \equiv \frac{i}{2} \sigma^a \partial_5 a \Tr U_5 = \frac{i}{2} \sigma^a \lim_{\epsilon \to 0} \frac{\Tr(e^{i\frac{2\pi}{\epsilon} U_5}) - \Tr U_5}{\epsilon} = -\frac{1}{4} \Tr(\sigma_a U_5) \sigma^a
\]

\(^2\)In the proceedings [31] the derivative of the constraint effective potential in the 4D Abelian gauge-Higgs model in unitary gauge was missing a contribution and therefore the result presented in Fig. 1 of the proceedings is inaccurate.
When evaluating the constraint condition for $U_{n+1}$ we truncate the exponential in (A.3.2b)

$$e^{h\pi_{n+1/2}} = 1 + h\pi_n - \frac{h^2}{2} \frac{\partial S}{\partial U_n} + \frac{\lambda_n^{(1)} h^2}{16\Omega} \text{Tr}[\ldots \sigma_i U_n \ldots] \sigma^i + \frac{h^2}{2} \pi_n^2 + O(h^3) \quad (A.3.3)$$

and solve for $\lambda_n^{(1)}$ up to the same order

$$\Phi = \frac{1}{2\Omega} \sum_{n_{\mu}} \text{Tr}[e^{h\pi_{n+1/2}(n_{\mu},0)} U_n(n_{\mu},0) \ldots e^{h\pi_{n+1/2}(n_{\mu},N_5-1)} U_n(n_{\mu},N_5-1)]$$

Again, when drawing the Gaussian-distributed random conjugate momenta $\pi_r(n_{\mu}, n_5)$ we have to ensure that they comply with the hidden constraint, which we achieve by orthogonal projection

$$\pi_0(n_{\mu}, n_5) = \pi_r(n_{\mu}, n_5) - \mu \text{Tr}[\ldots \sigma_i U(n_{\mu}, n_5) \ldots] \sigma^i$$

and solving for $\mu$ by plugging $\pi_0(n_{\mu}, n_5)$ into the hidden constraint (A.3.2e)

$$\mu = \frac{\sum_{n_{\mu}, n_5} \text{Tr}\{\text{Tr}[\ldots \sigma_i U(n_{\mu}, n_5) \ldots] \sigma^i \pi_r(n_{\mu}, n_5)\}}{\sum_{n_{\mu}, n_5} \text{Tr}\{\text{Tr}[\ldots \sigma_i U(n_{\mu}, n_5) \ldots] \sigma^i\}^2}$$
A.4. Rattle algorithm for 5D SU(2) gauge theory on the torus fixing ⟨(Tr P_5)^2⟩

Given a constraint condition for the average of the squared trace of the Polyakov loop \( P_5 \) in the extra dimension constructed from SU(2) link variables \( U_5(n_{\mu}) \)

\[
\frac{1}{4\Omega} \sum_{n_{\mu}} (\text{Tr} P_{n+1})^2 = \frac{1}{4\Omega} \sum_{n_{\mu}} \text{Tr} \left( \prod_{n_5=0}^{N_5-1} U_{n+1}(n_{\mu}, n_5) \right) \text{Tr} \left( \prod_{n_5=0}^{N_5-1} U_{n+1}(n_{\mu}, n_5) \right) = \Phi \tag{A.4.1}
\]

the constrained HMC (Rattle) algorithm can be formulated in the following way

\[
\pi_{n+1/2} = \pi_n - \frac{h}{2} \left( \frac{\partial S}{\partial U_n} - \frac{\lambda_n^{(1)}}{16\Omega} \text{Tr} P_n \text{Tr}[\ldots \sigma_i U_n \ldots] \sigma^i \right) \tag{A.4.2a}
\]

\[
U_{n+1} = e^{h\pi_{n+1/2} U_n} \tag{A.4.2b}
\]

\[
0 = \frac{1}{4\Omega} \sum_{n_{\mu}} \text{Tr} \left( \prod_{n_5=0}^{N_5-1} U_{n+1}(n_{\mu}, n_5) \right) \text{Tr} \left( \prod_{n_5=0}^{N_5-1} U_{n+1}(n_{\mu}, n_5) \right) - \Phi \tag{A.4.2c}
\]

\[
\pi_{n+1} = \pi_{n+1/2} - \frac{h}{2} \left( \frac{\partial S}{\partial U_n} - \frac{\lambda_n^{(2)}}{16\Omega} \text{Tr} P_{n+1} \text{Tr}[\ldots \sigma_i U_{n+1} \ldots] \sigma^i \right) \tag{A.4.2d}
\]

\[
0 = \sum_{n_{\mu}, n_5} \text{Tr} P_{n+1} \text{Tr}[\ldots \sigma_i U_{n+1}(n_{\mu}, n_5) \ldots] \sigma^i \pi_{n+1}(n_{\mu}, n_5) \tag{A.4.2e}
\]

with \( 2\text{Tr} P_5(n_{\mu}) \text{Tr}[\ldots \sigma_i U_5(n_{\mu}, n_5) \ldots] \sigma^i \) the derivative of the constraint with respect to \( U_5(n_{\mu}, n_5) \). Again, we truncate the exponential in (A.4.2b)

\[
e^{h\pi_{n+1/2}} = 1 + h\pi_n - \frac{h^2}{2} \frac{\partial S}{\partial U_n} + \frac{\lambda_n^{(1)} h^2}{32\Omega} \text{Tr} P_n \text{Tr}[\ldots \sigma_i U_n \ldots] \sigma^i + \frac{h^2}{2} \pi_n^2 + O(h^3) \tag{A.4.3}
\]

and plug \( U_{n+1} \) into the constraint condition, solving for \( \lambda_n^{(1)} \) up to the same order

\[
\Phi = \frac{1}{4\Omega} \sum_{n_{\mu}} \left( \text{Tr} \left[ e^{h\pi_{n+1/2}(n_{\mu}, 0)} U_n(n_{\mu}, 0) \ldots e^{h\pi_{n+1/2}(n_{\mu}, N_5-1)} U_n(n_{\mu}, N_5-1) \right] \right)^2
\]

\[
\Phi' = \frac{1}{4\Omega} \sum_{n_{\mu}} \left\{ (\text{Tr} P_n)^2 + 2h \sum_{n_5=0}^{N_5-1} \left( \text{Tr}[\ldots \pi_n U_{n_5} \ldots] - \frac{h}{2} \text{Tr}[\ldots \frac{\partial S}{\partial U_n(n_{\mu}, n_5)} U_n(n_{\mu}, n_5) \ldots] \right) \right. \\
+ \frac{\lambda_n^{(1)} h}{32} \text{Tr} P_n \text{Tr}[\ldots \text{Tr}[\ldots \sigma_i U_n(n_{\mu}, n_5) \ldots] \sigma^i U_n(n_{\mu}, n_5) \ldots] + \frac{h}{2} \text{Tr}[\ldots \pi_n^2(n_{\mu}, n_5) U_n(n_{\mu}, n_5) \ldots] \\
+ h \sum_{m_5 > n_5} \text{Tr}[\ldots \pi_n(n_{\mu}, n_5) U_n(n_{\mu}, n_5) \ldots \pi_n(n_{\mu}, m_5) U_n(n_{\mu}, m_5) \ldots] \right) \text{Tr} P_n(n_{\mu}) \\
+ \left. h^2 \sum_{n_5=0}^{N_5-1} \sum_{m_5=0}^{N_5-1} \text{Tr}[\ldots \pi_n(n_{\mu}, n_5) U_n(n_{\mu}, n_5) \ldots] \text{Tr}[\ldots \pi_n(n_{\mu}, m_5) U_n(n_{\mu}, m_5) \ldots] \right) + O(h^3)
\]

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\[
\frac{\lambda_n^{(1)}}{16\Omega} = \left\{ \sum_{n_\mu} \left[ \text{Tr} P_n(n_\mu) \sum_{n_5} \left( \text{Tr} \left[ \frac{\partial S}{\partial U_n(n_\mu, n_5)} U_n(n_\mu, n_5) \right] - \text{Tr} \left[ \pi_i^2(n_\mu, n_5) U_n(n_\mu, n_5) \right] \right) \right] \right\} \\
- \left( 2 \sum_{m_5 > n_5} \text{Tr} \left[ \pi_i(n_\mu, n_5) U_n(n_\mu, n_5) \right] \pi_i(n_\mu, m_5) U_n(n_\mu, m_5) \right) \\
- \left( \sum_{n_5} \sum_{m_5} \text{Tr} \left[ \pi_i(n_\mu, n_5) U_n(n_\mu, n_5) \right] \text{Tr} \left[ \pi_i(n_\mu, m_5) U_n(n_\mu, m_5) \right] \right) \\
/ \sum_{n_\mu, n_5} \left( \text{Tr} P_n(n_\mu) \right)^2 \text{Tr} \left\{ \left( \text{Tr} \left[ \pi_i U_n(n_\mu, n_5) \right] \right) \pi_i^2 \right\} + O(h^3)
\]

We use a Secant method to get the Lagrange multiplier with machine precision. Plugging \(\pi_{n+1}\) (A.4.2d) into the hidden constraint (A.4.2e) gives \(\lambda_n^{(2)}\):

\[
\frac{\lambda_n^{(2)}}{16\Omega} = \sum_{n_\mu, n_5} \left( \text{Tr} P_n(n_\mu) \text{Tr} \left[ \pi_i U_{n+1}(n_\mu, n_5) \right] \sigma_i \sigma^i \text{Tr} P_{n+1}(n_\mu, n_5) \right) \\
- 2 \text{Tr} P_n(n_\mu) \text{Tr} \left[ \pi_i U_{n+1}(n_\mu, n_5) \right] \sigma_i \pi_{n+1/2} U(n_\mu, n_5) / h \right) / \sum_{n_\mu, n_5} \left( \text{Tr} P_n(n_\mu) \right)^2 \text{Tr} \left\{ \left( \text{Tr} \left[ \pi_i U_{n+1}(n_\mu, n_5) \right] \right) \pi_i^2 \right\}
\]

Again, when drawing the Gaussian-distributed random conjugate momenta \(\pi_i(n_\mu, n_5)\) we have to ensure that they comply with the hidden constraint, which we achieve by the orthogonal projection

\[
\pi_0(n_\mu, n_5) = \pi_r(n_\mu, n_5) - \mu \text{Tr} P \text{Tr} \left[ \pi_i U(n_\mu, n_5) \right] \sigma_i
\]

and solving for \(\mu\) by plugging \(\pi_0(n_\mu, n_5)\) into the hidden constraint (A.4.2e)

\[
\mu = \frac{\sum_{n_\mu, n_5} \text{Tr} \left[ \pi_i U(n_\mu, n_5) \right]}{\sum_{n_\mu, n_5} \text{Tr} \left[ \text{Tr} P \text{Tr} \left[ \pi_i U(n_\mu, n_5) \right] \pi_i^2 \right]}
\]

A.5. Rattle algorithm for the 5D orbifold gauge-Higgs model fixing (TrP)

Given a constraint condition for the SU(2) link variables \(U_5(n_\mu)\) in the fifth dimension

\[
\frac{1}{20} \sum_{n_\mu, n_5} \prod_{n_5=0}^{N_5-1} [U_5(n_\mu, n_5)] \sigma_3 \prod_{n_5=0}^{N_5-1} [U_5^\dag(n_\mu, n_5)] \sigma_3 = \Phi
\]  

(A.5.1)
the constrained HMC (Rattle) algorithm can be formulated in the following way

$$
\pi_{n+1/2} = \pi_n - \frac{h}{2} \left( \frac{\partial S}{\partial U_n} - \frac{\lambda^{(1)}_n}{8\Omega} \text{Tr}[\ldots \sigma_i U_n \ldots - \ldots U^\dagger_n \sigma_i \ldots] \sigma^i \right) \tag{A.5.2a}
$$

$$
U_{n+1} = e^{h\pi_{n+1/2}} U_n, \quad U^\dagger_{n+1} = U_n e^{-h\pi_{n+1/2}} \tag{A.5.2b}
$$

$$
0 = \frac{1}{2\Omega} \sum_{n_5} \text{Tr} \left[ \prod_{n_5=1}^{N_5-1} [U_{n+1}(n_\mu, n_5)] \sigma_3 \prod_{n_5=N_5-1}^0 [U^\dagger_{n+1}(n_\mu, n_5)] \sigma_3 - \Phi \right] \tag{A.5.2c}
$$

$$
\pi_{n+1} = \pi_{n+1/2} - \frac{h}{2} \left( \frac{\partial S}{\partial U_{n+1}} - \frac{\lambda^{(2)}_n}{8\Omega} \text{Tr}[\ldots \sigma_i U_{n+1} \ldots - \ldots U^\dagger_{n+1} \sigma_i \ldots] \sigma^i \right) \tag{A.5.2d}
$$

$$
0 = \frac{1}{2\Omega} \sum_{n_\mu, n_5} \text{Tr} \left[ \text{Tr}[\ldots \sigma_i U_{n+1} \ldots - \ldots U^\dagger_{n+1} \sigma_i \ldots] \sigma^i \pi_{n+1}(n_\mu, n_5) \right] \tag{A.5.2e}
$$

The first three lines determine \((\pi_{n+1/2}, U_{n+1}, \lambda^{(1)}_n)\), whereas the remaining two give \((\pi_{n+1}, \lambda^{(2)}_n)\).

Again, we truncate the exponential in \((A.5.2b)\)

$$
e^{h\pi_{n+1/2}} = 1 + h\pi_n - \frac{h^2}{2} \frac{\partial S}{\partial U_n} \left[ \frac{h^2 \lambda}{16\Omega} \text{Tr}[\ldots \sigma_i U_n \ldots - \ldots U^\dagger_n \sigma_i \ldots] \sigma^i + \frac{h^2}{2} \pi_n^2 + O(h^3) \right]
$$

$$
e^{-h\pi_{n+1/2}} = 1 - h\pi_n - \frac{h^2}{2} \frac{\partial S}{\partial U_n} \left[ -\frac{h^2 \lambda}{16\Omega} \text{Tr}[\ldots \sigma_i U_n \ldots - \ldots U^\dagger_n \sigma_i \ldots] \sigma^i + \frac{h^2}{2} \pi_n^2 + O(h^3) \right]
$$

and solve the constraint \((A.5.2c)\) for the first Lagrange multipliers

$$
\frac{\lambda^{(1)}_n}{8\Omega} = \left\{ \sum_{n_\mu, n_5} \left( \text{Tr}[\ldots \frac{\partial S}{\partial U_n(n_\mu, n_5)} U_n(n_\mu, n_5) \ldots - \ldots U^\dagger_n(n_\mu, n_5) \frac{\partial S}{\partial U_n(n_\mu, n_5)} \ldots] - \text{Tr}[\ldots \pi^2_n(n_\mu, n_5) U_n(n_\mu, n_5) \ldots + \ldots U^\dagger_n(n_\mu, n_5) \pi^2_n(n_\mu, n_5) \ldots] - \sum_{m_5} \text{Tr}[\ldots \pi_n(n_\mu, n_5) U_n(n_\mu, n_5) \ldots - \ldots U^\dagger_n(n_\mu, n_5) \pi_n(n_\mu, m_5 > n_5) U_n(n_\mu, m_5 > n_5) \ldots - \ldots \pi_n(n_\mu, n_5) U_n(n_\mu, m_5 > n_5) \ldots] \right) / \right\} \tag{A.5.3}
$$

We use a Secant method to get the Lagrange multiplier with machine precision. Plugging \(\pi_{n+1}\) \((A.5.2d)\) into the hidden constraint \((A.5.2e)\) gives \(\lambda^{(2)}_n\):

$$
\frac{\lambda^{(2)}_n}{8\Omega} = \sum_{n_\mu, n_5} \left( \text{Tr}[\ldots \sigma_i U_n \ldots - \ldots U^\dagger_n \sigma_i \ldots] \sigma^i \text{Tr}[\ldots \sigma_i U_{n+1} \ldots - \ldots U^\dagger_{n+1} \sigma_i \ldots] \sigma^i \right) / h \tag{A.5.4}
$$

$$
-2\text{Tr}[\ldots \sigma_i U_n \ldots - \ldots U^\dagger_n \sigma_i \ldots] \sigma^i \pi_{n+1/2}(n_\mu, n_5) / h \right) / \right\} \tag{A.5.4}
$$

$$
\sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U_{n+1} \ldots - \ldots U^\dagger_{n+1} \sigma_i \ldots] \sigma^i \pi_{n+1/2}(n_\mu, n_5)]^2 \right) \right) / h \right) / \right\}
$$

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We initialize momenta $\pi_0$ from Gaussian-random distributed $\pi_r$ via orthogonal projection

$$
\pi_0(n_\mu, n_5) = \pi_r(n_\mu, n_5) - \mu \text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots - U(n_\mu, n_5)^\dagger \sigma_i \ldots] \sigma^i \\
0 = \frac{1}{8D} \sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots - U(n_\mu, n_5)^\dagger \sigma_i \ldots] \sigma^i \pi_0(n_\mu, n_5) \\
\Rightarrow \mu = \frac{\sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots - U(n_\mu, n_5)^\dagger \sigma_i \ldots] \sigma^i \pi_r(n_\mu, n_5)}{\sum_{n_\mu, n_5} \text{Tr}[\ldots \sigma_i U(n_\mu, n_5) \ldots - U(n_\mu, n_5)^\dagger \sigma_i \ldots] \sigma^i]^2}
$$

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