

Extended framework for the hybrid Monte Carlo in lattice gauge theory

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We develop an extended framework for the hybrid Monte Carlo (HMC) algorithm in lattice gauge theory by embedding the $SU(N)$ group into the space of general complex matrices, $M_N(\mathbb{C})$. Auxiliary directions will be completely factorized in the path integral, and the embedding does not alter the expectation values of the original theory. We perform the molecular dynamics updates by using the matrix elements of $W \in M_N(\mathbb{C})$ as the dynamical variables without group theoretic constraints. The framework enables us to introduce nonseparable Hamiltonians for the HMC in lattice gauge theory exactly, whose immediate application includes the Riemannian manifold HMC.

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I. INTRODUCTION

The hybrid Monte Carlo (HMC) algorithm [1] has been widely accepted as an efficient algorithm for lattice QCD. From the early times of its development, strategies for curing critical slowing down have been discussed. The relevance of this issue is becoming increasingly high as the field is now committed to precision calculations using large scale machines.

One of the major promising ideas for critical slowing down is Fourier acceleration [2–4], which introduces a nontrivial kinetic term in the HMC Hamiltonian to align the effective masses for all the Fourier modes. In generalizing the idea to gauge theory, the kernel may be modified to the covariant Laplacian [5,6], making it inevitably dependent on the gauge field, which results in the nonseparable form of the HMC Hamiltonian:

$$H(U, \pi) = \frac{1}{2} \pi_a G_{ab}^{-1}(U) \pi_b + S(U) + \frac{1}{2} \log \det G(U). \quad (1)$$

The degrees of freedom of the kernel matrix $G_{ab}(U)$ can be utilized to accelerate the low modes [7–9], in which context the algorithm is dubbed Riemannian manifold (RM) HMC.

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Despite its physically attractive concept, use of the nonseparable Hamiltonian (1) in gauge theory is not straightforward. Indeed, as was mentioned by Duane and Pendleton in Ref. [6], the discretized molecular dynamics (MD) update generically violates the symplecticity for a nontrivial $G(U)$. The complication is due to the fact that, because the gauge variable is group valued, $U(n, \mu) \in SU(N)$, we need to exponentiate the force vector to update $U(n, \mu)$. Though the continuous Hamiltonian equations preserve the symplectic two-form ω , for a finite time increment, the exponentiation induces nonlinear terms that generically do not cancel in the change of ω (see Appendix B). The present paper is motivated by the recognition that the substantial earlier work of our collaboration developing the RMHMC algorithm for QCD [8–11] relied on an inexact updating algorithm which contained finite step size errors—a problem rectified by the extended algorithm presented here.

This paper aims to extend the framework of the HMC in lattice gauge theory such that nonseparable Hamiltonians can be used exactly without gauge fixing (see Refs. [12,13] for gauge fixing in this context). Since the source of the issue is the constraint $U(n, \mu) \in SU(N)$, we embed $SU(N)$ into the space of complex N by N matrices, $M_N(\mathbb{C})$. The physical $SU(N)$ variables are identified by a polar decomposition. We run the HMC for the two-dimensional $SU(3)$ pure gauge theory to test the embedding framework, in which we take the real and imaginary parts of the matrix elements: $W \equiv (w_{jk}) \in M_N(\mathbb{C})$, $w_{jk} \equiv x_{jk} + iy_{jk}$ as dynamical variables and use the symplectic integrators with the linear form as in unconstrained theories. The exactness of the algorithm is confirmed by comparing the numerical expectation values to the analytical values.

II. ALGORITHM

We use a single group variable to demonstrate the algorithm for simplicity. Due to the tensor product structure of the configuration space, generalization to the lattice gauge system is straightforward.

A. Basic idea

The idea is to allow the dynamical variable in the simulation to deviate from $SU(N)$ into the space of complex matrices, $M_N(\mathbb{C})$ (see Fig. 1). Since $M_N(\mathbb{C})$ is noncompact, we need a systematic way to control the deviation from $SU(N)$ to make the path integral well-defined.

For this purpose, we parametrize the extended variable $W \in M_N(\mathbb{C})$ in the polar decomposition form:

$$W = e^{i\theta} \Phi U, \quad (2)$$

where Φ is a positive $N \times N$ Hermitian matrix and $U \in SU(N)$. The $SU(N)$ part is the physical variable, and the noncompact nature of $M_N(\mathbb{C})$ is fully described by Φ . As an example, we choose the following action for the Φ direction:

$$S_0(\Phi) \equiv \frac{\lambda}{2N} \text{tr}(\Phi - \mathbb{1}_N)^2 - \frac{\kappa}{N} \log \det \Phi \quad (3)$$

with the tunable parameters $\lambda, \kappa > 0$. We do not add an action for the θ direction, though this is in principle possible. The action $S_0(\Phi)$ is chosen such that it prevents Φ from having an excursion to infinity as well as from approaching the singular points, $\det W = 0$, at which the decomposition will be ill-defined.

Note that the value of Φ in the decomposition (2) does not change under right multiplication of a $U(N)$ matrix. This suggests that, for a $U(N)$ -invariant measure (dW), the corresponding decomposition of the integration measure,

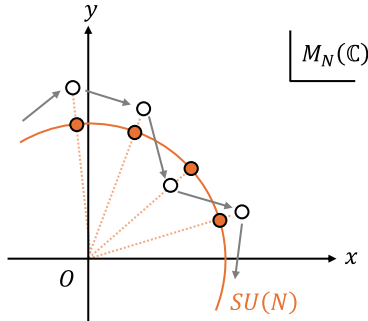


FIG. 1. A schematic sketch of the extended framework. The MD update is performed in the W -space (represented by white circles), and the physical variable U is obtained by using the decomposition (2) as a projective map: $M_N(\mathbb{C}) \rightarrow SU(N)$ (represented by orange, filled circles).

$$(dW) = \sqrt{\det g} d\theta(d\Phi)(dU), \quad (4)$$

has the Jacobian factor $\sqrt{\det g}$ that only depends on Φ . The path integral is then completely factorized into the physical part and the auxiliary part. This factorized structure is reminiscent of the gauge fixing in the path integral. We emphasize, however, that we are enlarging the configuration space for an algorithmic purpose, and not altering the original physical system at all.

In the following, we formulate the mathematical details of the above outline. The resulting algorithm is simple and is described in Sec. II D.

B. Decomposition along the MD trajectory

We first define a decomposition of W that uniquely determines the gauge field U along the MD trajectory. An important point is that the decomposition is in accord with reversibility, which is necessary for the resulting HMC algorithm to be exact.

As is well known, for an invertible matrix $W \in GL(N, \mathbb{C})$, the polar decomposition

$$W = \Phi \Omega \quad (5)$$

is unique, where Φ is a positive Hermitian matrix and $\Omega \in U(N)$. We assume below that the appearance of the singular points $\det W = 0$ is properly suppressed by an appropriate choice of λ and κ in Eq. (3).

To perform the decomposition of $\Omega \in U(N)$ into $e^{i\theta} \in U(1)$ and $U \in SU(N)$, we need to consider an ambiguity in relation to the center $\mathbb{Z}_N$ of $SU(N)$. Indeed, let us define

$$\theta_0 \equiv \frac{1}{N} \arg \det \Omega, \quad U_0 \equiv e^{-i\theta_0} \Omega, \quad (6)$$

where by the argument of a complex number z we intend an angle $-\pi \leq \arg z < \pi$. Then, all the following pairs (θ_n, U_n) give a consistent decomposition $\Omega = e^{i\theta_n} U_n$:

$$\theta_n \equiv \theta_0 + 2\pi n/N \pmod{2\pi}, \quad U_n \equiv e^{-2\pi i n/N} U_0, \quad (7)$$

where $n = 0, \dots, N-1$. In other words, multiplying U by an element of the center, $e^{2\pi i n/N}$ ($n = 0, \dots, N-1$), can be absorbed into a shift of θ —a shift which corresponds to the ambiguity in the definition of the $\arg$ function in Eq. (6).

We perform the decomposition such that it reduces to a continuous evolution for infinitesimal updates. Suppose we have a configuration W and its decomposition (U, θ, Φ) , and we update W to W' . After obtaining Ω' and Φ' from Eq. (5), we determine U', θ' as

$$\delta\theta \equiv \frac{1}{N} \arg \det[e^{-i\theta} \Omega'], \quad (8)$$

$$\theta' \equiv \theta + \delta\theta \pmod{2\pi, \theta' \in [-\pi, \pi)}, \quad (9)$$

$$U' \equiv e^{-i\theta'} \Omega'. \quad (10)$$

The triplet (U', θ', Φ') is uniquely determined from (U, θ, Φ) in a reversible manner: For a reversed process from W' to W , where W' is decomposed into the triplet (U', θ', Φ') , we obtain the original (U, θ, Φ) through the same decomposition scheme (see Appendix C for the detailed argument for reversibility and exactness of the algorithm).

In the above, we identified the $U(1)$ element of the $U(N)$ group that is proportional to the identity matrix. This corresponds to taking as the $U(1)$ generator $T_0 \propto \mathbb{1}_N$. However, other choices are possible. Indeed, by choosing a $U(1)$ subgroup whose generator is not the identity matrix, we can decompose W into (U, θ, Φ) without ambiguity as is worked out in Appendix D.

C. Path integral in the larger space

We next consider the integration measure for $M_N(\mathbb{C})$ and its decomposition corresponding to Eq. (2). The desired measure can be conveniently defined from the metric tensor $\mathbf{g}$ as

$$\mathbf{g} \equiv \text{tr}[dW dW^\dagger] = \sum_{j,k} [dx_{jk}^2 + dy_{jk}^2], \quad (11)$$

$$(dW) \equiv \prod_{j,k} (dx_{jk} dy_{jk}), \quad (12)$$

where the bilinear form is assumed to be symmetrized.

To discuss the decomposition of (dW) , we prepare the one-form basis for the variables U and Φ . A convenient choice for U is given by the Maurer-Cartan form

$$\Theta \equiv dU U^{-1} \equiv iT_a \Theta_a. \quad (13)$$

Θ_a is dual to the right-invariant derivative D_a :

$$D_a U = iT_a U, \quad dU = \Theta_a D_a U. \quad (14)$$

With the traceless Hermitian generators T_a , we expand the Hermitian matrices as

$$\Phi = \phi_a T_a + \phi_0 \mathbb{1}_N, \quad \text{tr}[T_a T_b] = \delta_{ab}. \quad (15)$$

From the relation

$$dW = ie^{i\theta} \Phi T_a U \Theta_a + ie^{i\theta} \Phi U d\theta + e^{i\theta} T_a U d\phi_a + e^{i\theta} U d\phi_0, \quad (16)$$

the metric tensor can be rewritten accordingly:

$$\begin{aligned} \mathbf{g} = & \text{tr}[T_a T_b \Phi^2] \Theta_a \Theta_b + 2\text{tr}[T_a \Phi^2] \Theta_a d\theta \\ & + \text{tr} \Phi^2 d\theta^2 + d\phi_a^2 + d\phi_0^2. \end{aligned} \quad (17)$$

As advertised, the Jacobian depends only on Φ :

$$(dW) = \sqrt{\det g(\Phi)} d\theta (dU) (d\Phi), \quad (18)$$

where

$$(dU) \equiv \prod_a \Theta_a \quad (19)$$

is the Haar measure, $(d\Phi) \equiv d\phi_0 \prod_a d\phi_a$, and

$$\det g(\Phi) = \det \begin{bmatrix} (1/2) \text{tr}[\{T_a, T_b\} \Phi^2] & \text{tr}[T_b \Phi^2] \\ \text{tr}[T_a \Phi^2] & \text{tr} \Phi^2 \end{bmatrix}. \quad (20)$$

Collecting the formulas, the path integral in the larger space,

$$Z_{M_N(\mathbb{C})} \equiv \int (dW) e^{-S(U) - S_0(\Phi)}, \quad (21)$$

can be related to the original one:

$$Z_{SU(N)} \equiv \int (dU) e^{-S(U)}, \quad (22)$$

as follows:

$$\begin{aligned} Z_{M_N(\mathbb{C})} &= \int d\theta \int (dU) e^{-S(U)} \int_{\Phi > 0} (d\Phi) \sqrt{\det g(\Phi)} e^{-S_0(\Phi)} \\ &= (2\pi) Z_{SU(N)} \int_{\Phi > 0} (d\Phi) \sqrt{\det g(\Phi)} e^{-S_0(\Phi)}, \end{aligned} \quad (23)$$

where the integration domain $\Phi > 0$ is over positive Hermitian matrices. The factorized Φ integral is well-defined because of the bound

$$\begin{aligned} & \int_{\Phi > 0} (d\Phi) \sqrt{\det g(\Phi)} e^{-S_0(\Phi)} \\ & < \int (d\Phi) e^{-\frac{2}{N} \text{tr}(\Phi^{-1})^2} \sqrt{\det g(\Phi)} |\det \Phi|^{\frac{N}{2}}, \end{aligned} \quad (24)$$

which is a Gaussian integral of a function that has at most a power law increase for large Φ , and thus has a finite value.

The above shows that we can calculate the expectation value of the observable $\mathcal{O}(U)$ directly in the larger path integral as a function of the physical part U . The nontrivial Jacobian factor will automatically drop out in the expectation values, and its precise form is irrelevant for running the simulation.

D. The HMC in the extended space

We now have a path integral (21) over $2N^2$ unconstrained real variables $(w_I) \equiv (x_{jk}, y_{jk})$ with the flat measure (12). We are therefore ready to run the HMC for the flat space to simulate the gauge system.

We write the momentum as p_I conjugate to w_I . The kinetic term of the HMC Hamiltonian can be taken arbitrarily:

$$H(w, p) \equiv \frac{1}{2} p_I K_{IJ}^{-1}(w) p_J + S(U) + S_0(\Phi) + \frac{1}{2} \log \det K(w). \quad (25)$$

With the implicit leapfrog integrator, for example, the entire algorithm will be the following:

- (1) Suppose we have a configuration W .
- (2) Generate p from the Gaussian distribution:

$$P_{\text{init}}(p; w) \propto e^{-\frac{1}{2} p_I K_{IJ}^{-1}(w) p_J}. \quad (26)$$

- (3) Integrate the Hamiltonian equations:

$$p_I^{1/2} = p_I - \frac{\tau}{2} \partial_{w_I} H(w, p^{1/2}), \quad (27)$$

$$w_I^{1/2} = w_I + \frac{\tau}{2} \partial_{p_I} H(w, p^{1/2}), \quad (28)$$

$$w'_I = w_I^{1/2} + \frac{\tau}{2} \partial_{p_I} H(w', p^{1/2}), \quad (29)$$

$$p'_I = p_I^{1/2} - \frac{\tau}{2} \partial_{w_I} H(w', p^{1/2}). \quad (30)$$

- (4) Accept/reject the obtained configuration with the probability:

$$\min(1, e^{-H(w', p') + H(w, p)}). \quad (31)$$

- (5) We add to the ensemble the physical configuration U , calculated from the accepted W , to estimate the expectation values of the observables under the path integral (22).

The symplecticity of the integrator (see Appendix A) implies the conservation of the phase space volume. Together with reversibility, the exactness of the algorithm follows.

Since the action is written in the (U, θ, Φ) -basis while the update is in the W -basis, we need the Jacobian matrix to relate the two in the force calculation. From Eq. (16)

$$\begin{aligned} \begin{bmatrix} dx_{jk} & dy_{jk} \end{bmatrix} &= \begin{bmatrix} \Theta_a & d\theta & d\phi_a & d\phi_0 \end{bmatrix} \begin{bmatrix} -\text{Im}[e^{i\theta}(\Phi T_a U)_{jk}] & \text{Re}[e^{i\theta}(\Phi T_a U)_{jk}] \\ -\text{Im}[e^{i\theta}(\Phi U)_{jk}] & \text{Re}[e^{i\theta}(\Phi U)_{jk}] \\ \text{Re}[e^{i\theta}(T_a U)_{jk}] & \text{Im}[e^{i\theta}(T_a U)_{jk}] \\ \text{Re}[e^{i\theta} U_{jk}] & \text{Im}[e^{i\theta} U_{jk}] \end{bmatrix} \\ &\equiv \begin{bmatrix} \Theta_a & d\theta & d\phi_a & d\phi_0 \end{bmatrix} \times J(U, \theta, \Phi). \end{aligned} \quad (32)$$

The force in the W -basis can be calculated from the (U, θ, Φ) -basis as

$$\begin{bmatrix} \partial_{x_{jk}} H(p, w) \\ \partial_{y_{jk}} H(p, w) \end{bmatrix} = J(U, \theta, \Phi)^{-1} \begin{bmatrix} D_a H(p, w) \\ \partial_\theta H(p, w) \\ \partial_{\phi_a} H(p, w) \\ \partial_{\phi_0} H(p, w) \end{bmatrix}. \quad (33)$$

We comment that, because of the center $\mathbb{Z}_N$, we formally regard the triplet (U, θ, Φ) as a state of the Markov chain, and the global structure of the state space is isomorphic to $GL(N, \mathbb{C}) \times \mathbb{Z}_N$. We emphasize, however, that the center $\mathbb{Z}_N$ does not appear explicitly during the HMC, and we do not need to set up an additional Monte Carlo update for the center. The only occasions that require care are the

initialization of the variables and saving a configuration to a file. To implement a hot start, for example, one can randomly generate W , perform the decomposition into (U_0, θ_0, Φ) by using Eq. (6), and shift (U_0, θ_0) with a randomly chosen $n \in \mathbb{Z}_N$: $(U_0, \theta_0) \rightarrow (U_n, \theta_n)$ as Eq. (7). We associate the triplet (U_n, θ_n, Φ) with the starting configuration W . To store a state of the Markov chain, we save the triplet (U, θ, Φ) , from which the W -variable can be easily reconstructed.

The above argument for the single variable can be readily generalized for the lattice gauge system in arbitrary dimensions. During the simulation, we keep $W(n, \mu)$ and the triplet $(U(n, \mu), \theta(n, \mu), \Phi(n, \mu))$ for all the links (n, μ) . The Jacobian matrix that maps the gradients in the two bases is block-diagonal in the spatial and Lorentz structures. Therefore, we can calculate the force vector for $W(n, \mu)$ by the same formula as Eq. (33) by adding the link labels (n, μ) .

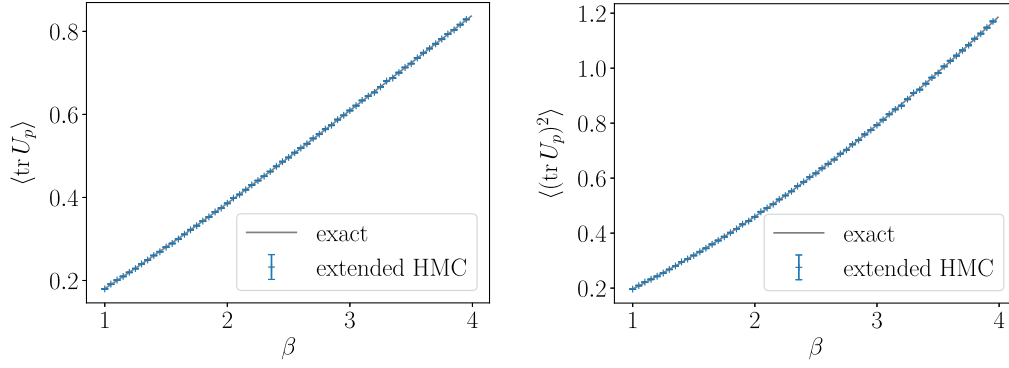


FIG. 2. Expectation values of the plaquette (left) and the plaquette squared (right) calculated with the proposed, extended HMC algorithm.

III. NUMERICAL TEST

To numerically verify the exactness of our algorithm, we perform Monte Carlo calculations for the two-dimensional pure $SU(N=3)$ gauge theory using the Wilson gauge action with $\beta = 1.00, 1.05, \dots, 4.00$. We adopt the trivial kernel $K(w) = \mathbb{1}_{2N^2}$ to test that the HMC gives exact results under the proposed embedding framework, examining it independently from additional complications from implicit iteration.

The lattice is periodic and has the dimension 32×32 . The auxiliary parameters are set to $\lambda = 1$ and $\kappa = 5$. The MD is integrated with the explicit leapfrog. A trajectory of length 1.0 in units of MD time is separated into 10 steps, which gives an acceptance around 0.8. After thermalization from a hot start, we calculate the observables every 10 trajectories. The expectation values are estimated from 1,000 configurations, and the statistical errors are estimated with the jackknife method. Figure 2 shows the expectation values of the plaquette $\langle \text{tr} U_p \rangle$ and the plaquette squared $\langle (\text{tr} U_p)^2 \rangle$. The exact values are calculated from the character expansion. The precision is subpercent level and all the estimates are consistent with the exact value

within 3σ confidence level (see Fig. 3). Good agreement verifies the exactness of the proposed algorithm.

IV. DISCUSSION

In this paper, we develop a framework to extend the HMC in lattice gauge theory by embedding $SU(N)$ into the space of general complex matrices, $M_N(\mathbb{C})$. Our extension not only allows us to use the HMC with nonseparable Hamiltonians but also adds new dimensions to optimize the HMC. For example, let us expand the momentum in the (U, θ, Φ) -basis in terms of the momentum $p \equiv (p_l)$ in the W -basis:

$$(\pi_a, \pi_\theta, \rho_a, \rho_0)^T \equiv J(w) \cdot p. \quad (34)$$

An extension from the RMHMC Hamiltonian (1) is

$$H(w, p) \equiv \frac{1}{2} \pi_a G_{ab}^{-1}(U) \pi_b + \frac{1}{2m_\theta} \pi_\theta^2 + \frac{1}{2m_\rho} \rho_a^2 + \frac{1}{2m_0} \rho_0^2 + S(U) + S_0(\Phi) + \frac{1}{2} \log \det G(U). \quad (35)$$

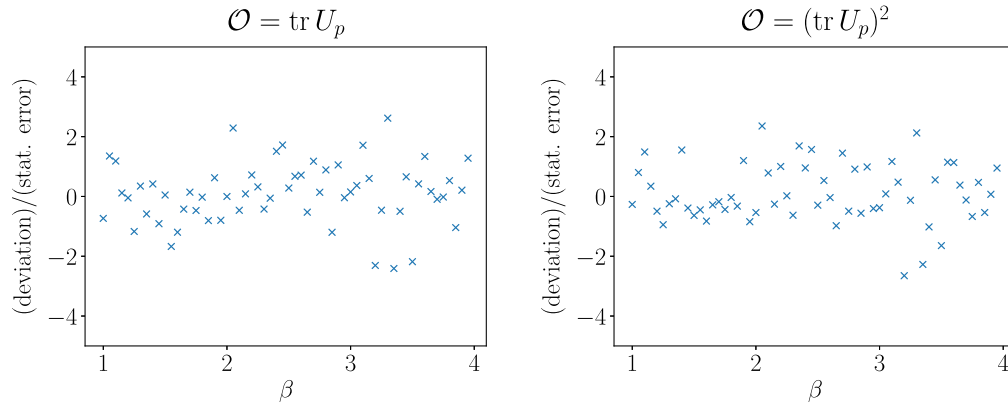


FIG. 3. The deviation of the Monte Carlo estimate $\bar{\mathcal{O}}$ from the exact value $\langle \mathcal{O} \rangle$ in units of the statistical error $\delta \bar{\mathcal{O}}$: $(\bar{\mathcal{O}} - \langle \mathcal{O} \rangle) / \delta \bar{\mathcal{O}}$. In the left panel, $\mathcal{O} = \text{tr} U_p$, and in the right, $\mathcal{O} = (\text{tr} U_p)^2$. The plots show reasonable accuracy for our calculation.

As shown in Appendix E, the continuous Hamiltonian equations for the Hamiltonian (35) reduce to those of the original RMHMC when the evolution is projected onto $SU(N)$. [Of course, if the Hamiltonian in Eq. (35) is to be used in the symplectic finite-time-step update given in Eqs. (27)–(30), the momenta $(\pi_a, \pi_\theta, \rho_a, \rho_0)$ must first be expressed in terms of the p_I using Eq. (34).] However, it is possible in principle to intentionally mix the physical modes π_a with the auxiliary modes π_θ, ρ_a , and ρ_0 by adding off-diagonal terms. It is interesting to consider if the additional degrees of freedom can be utilized to increase the tunneling rate of the topological charge. Machine learning may be especially useful for this purpose (see Refs. [14–19] for gauge invariant neural networks).

Avoiding the singular points, at which $\det W = 0$, is crucial in practice. In the vicinity of the singular points, Φ can take arbitrarily large values, resulting in a slow convergence in the decomposition (2) and a large gradient $\partial S_0(\Phi)$. In this regard, a detailed study of the optimal choice of $S_0(\Phi)$ is important. In our simple choice of the action, Eq. (3), large λ restricts the fluctuation in the non-compact directions to be small, while it can also cause an unbalance between the forces from $S(U)$ and $S_0(\Phi)$. In the RMHMC applications, therefore, it is important to adjust the relative sizes of the canonical masses, m_θ, m_ρ , and m_0 in Eq. (35), at the same time when we engineer the auxiliary action S_0 . It may also be beneficial if we can utilize the multilevel integration scheme [20] by separating the physical and auxiliary actions. We note that the effective action of Φ has a nontrivial contribution from the measure [see Eq. (23)], which can be understood as the potential term for a centrifugal force from the singularity (see Fig. 1). It may be important to design $S_0(\Phi)$ taking this effect into account. In our exploratory runs in four dimensions, we find that using a quartic instead of a quadratic form can increase the efficiency.

Finally, since our goal is to speed up lattice QCD production runs, it is most important to test the algorithm in realistic systems. Though the iterations in the implicit update steps are potentially computationally demanding, it is important to recognize that the increase of the computational cost from these steps is additive to the fermion force calculation in the usual multilevel evolution algorithm [20]. Indeed, we can circumvent reevaluating the fermion force in the implicit iteration by pushing the force terms for the nontrivial kernel $K(w)$ into the lower level where we calculate the gauge force [8,9]. Consequently, the net increase in computational cost can be mild for the dynamical simulations where the cost for the fermion force is substantial. Especially under such circumstances, combining the algorithm with the field transformation [21] may yield further benefit.

Work along these lines is in progress and will be reported elsewhere.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [22,23].

APPENDIX A: COMMENT ON IMPLICIT, SYMPLECTIC INTEGRATORS

The implicit leapfrog integrator, Eqs. (27)–(30), is a symplectic discretization of the Hamiltonian equations

$$\dot{w}_I = \partial_{p_I} H, \quad \dot{p}_I = -\partial_{w_I} H, \quad (\text{A1})$$

which are derived using the symplectic two-form

$$\omega(w, p) \equiv dp_I \wedge dw_I. \quad (\text{A2})$$

Indeed, as one can easily show, for the first pair of the update, ω is preserved:

$$\begin{aligned} \omega(w^{1/2}, p^{1/2}) &= \left(\delta_{IJ} + \frac{\tau}{2} \partial_{p_I} \partial_{w_J} H(w, p^{1/2}) \right) dp_I^{1/2} \wedge dw_J \\ &= \omega(w, p). \end{aligned} \quad (\text{A3})$$

The second pair is determined from the time-reversal symmetry.

This structure may become more transparent by introducing the auxiliary transfer matrices:

$$T^{p, \tau/2} \begin{pmatrix} w \\ p \end{pmatrix} = \begin{pmatrix} w \\ p - \frac{\tau}{2} \partial_w H(w, p) \end{pmatrix}, \quad (\text{A4})$$

$$T^{q, \tau/2} \begin{pmatrix} w \\ p \end{pmatrix} = \begin{pmatrix} w + \frac{\tau}{2} \partial_p H(w, p) \\ p \end{pmatrix}, \quad (\text{A5})$$

which represent explicit steps. The process of incrementing the MD time by τ with the implicit leapfrog can then be

represented as

$$T^{p,\tau/2} \cdot (T^{q,-\tau/2})^{-1} \cdot T^{q,\tau/2} \cdot (T^{p,-\tau/2})^{-1}. \quad (\text{A6})$$

Such a simplified viewpoint enables us to easily write down improved integrators. For example, the Omelyan integrator [24–26] may be written in the nonseparable case as

$$T^{p,\alpha\tau} \cdot (T^{q,-\alpha\tau})^{-1} \cdot T^{q,(1/2-\alpha)\tau} \cdot (T^{p,-(1/2-\alpha)\tau})^{-1} \cdot T^{p,(1/2-\alpha)\tau} \cdot (T^{q,-(1/2-\alpha)\tau})^{-1} \cdot T^{q,\alpha\tau} \cdot (T^{p,-\alpha\tau})^{-1}. \quad (\text{A7})$$

As is well known [27,28], there exists an exactly conserved shadow Hamiltonian $\tilde{H}$ for a given symplectic integrator. For the implicit Omelyan (A7), for example, the shadow Hamiltonian has the formal expansion

$$\begin{aligned} \tilde{H} = H &+ \frac{\tau^2}{12} \left[(6\alpha^2 - 6\alpha + 1) \frac{\partial H}{\partial w_I} \frac{\partial^2 H}{\partial p_I \partial p_J} \frac{\partial H}{\partial w_J} \right. \\ &+ \frac{6\alpha - 1}{2} \frac{\partial H}{\partial p_I} \frac{\partial^2 H}{\partial w_I \partial w_J} \frac{\partial H}{\partial p_J} \\ &\left. + (12\alpha^2 - 6\alpha + 1) \frac{\partial H}{\partial w_I} \frac{\partial^2 H}{\partial p_I \partial w_J} \frac{\partial H}{\partial p_J} \right] + \mathcal{O}(\tau^4). \quad (\text{A8}) \end{aligned}$$

Since we do not know the typical values of the derivatives *a priori*, the parameter α is to be tuned manually for a given system.

APPENDIX B: COMPLICATIONS OF NONSEPARABLE HAMILTONIANS FOR GROUP VARIABLES

With the symplectic form for the $SU(N)$ variable [29]

$$\omega_{SU(N)}(U, \pi) \equiv d(\pi_a \Theta_a), \quad (\text{B1})$$

the continuous Hamiltonian equations can be written down as

$$\dot{U}U^{-1} = iT_a \partial_{\pi_a} H, \quad (\text{B2})$$

$$\dot{\pi}_a = -D_a H - \pi_c f_{abc} \partial_{\pi_b} H, \quad (\text{B3})$$

under which $\dot{H} = 0$ and $\dot{\omega} = 0$. Note here that Θ is not closed, and thus

$$d\Theta_a = -\frac{1}{2} f_{bcd} \Theta_b \wedge \Theta_c, \quad (\text{B4})$$

where $[T_a, T_b] \equiv if_{abc} T_c$.

The problem for the case of a nonseparable Hamiltonian (1) arises for gauge theory when we discretize the Hamiltonian equations (B2) and (B3). As a simple example, let us consider applying the implicit leapfrog as follows:

$$\pi_a^{1/2} = \pi_a - \frac{\tau}{2} \{D_a H(U, \pi^{1/2}) + \pi_c^{1/2} f_{abc} \partial_{\pi_b} H(U, \pi^{1/2})\}, \quad (\text{B5})$$

$$U^{1/2} = \exp \left[\frac{i\tau}{2} T_a \partial_{\pi_a} H(U, \pi^{1/2}) \right] U, \quad (\text{B6})$$

$$U' = \exp \left[\frac{i\tau}{2} T_a \partial_{\pi_a} H(U', \pi^{1/2}) \right] U^{1/2}, \quad (\text{B7})$$

$$\pi'_a = \pi_a^{1/2} - \frac{\tau}{2} \{D_a H(U', \pi^{1/2}) + \pi_c^{1/2} f_{abc} \partial_{\pi_b} H(U', \pi^{1/2})\}. \quad (\text{B8})$$

To see the nonpreservation of ω , we write the differential of the exponential map as

$$iT_b A(X)_{ba} \equiv \partial_{X_a} e^{iX_c T_c} \cdot e^{-iX_c T_c}, \quad (\text{B9})$$

or equivalently

$$\begin{aligned} A(X) &= \frac{\exp(iX_c F_c) - \mathbb{1}_{N^2-1}}{iX_c F_c} \\ &= \sum_{k=0}^{\infty} \frac{1}{(k+1)!} (iX_c F_c)^k, \quad (\text{B10}) \end{aligned}$$

where $(F_c)_{ab} \equiv if_{acb}$. We have for the second step, Eq. (B6),

$$\Theta_b^{1/2} = \exp(iX_c F_c)_{ba} \Theta_a + A(X)_{ba} dX_a, \quad (\text{B11})$$

where $X_a \equiv \frac{\tau}{2} \partial_{\pi_a} H(U, \pi^{1/2})$. The exponentiation resulted in the nonlinear factors $\exp(iX_c F_c)$ and $A(X)$.

Note that for a trivial kernel, $G = \mathbb{1}_{N^2-1}$, we have $X = (\tau/2)\pi^{1/2}$. Because of the antisymmetry of f_{abc} , the nonlinearity drops out in this case when they are contracted with $\pi^{1/2}$: $X_b \exp(iX_c F_c)_{ba} = X_a$ and $X_b A(X)_{ba} = X_a$. As a result, the symplectic form is preserved at each step: $\omega_{SU(N)}(U^{1/2}, \pi^{1/2}) = \omega_{SU(N)}(U, \pi^{1/2}) = \omega_{SU(N)}(U, \pi)$. On the other hand, for a nonseparable Hamiltonian, the preservation of $\omega_{SU(N)}$ is designed to hold for the paired update of the first two steps [see Eq. (A3)]. Because of the complicated form of X , the nonlinear terms do not simplify as in the former case, and there are no counterterms from the first step that cancel them. Therefore, the naive application of the implicit leapfrog to a nonseparable Hamiltonian in gauge theory generically violates symplecticity.

To overcome the issue, one may consider introducing coordinate systems instead of working in the invariant bases $\{\Theta_a\}$, $\{D_a\}$. This turns out, however, not to be straightforward. For simplicity, let us take $SU(N=2) \simeq S^3$ as an example. One may divide S^3 into two hyper-

hemispherical patches and introduce exponential coordinates $q_{N/S}$ around the pole points $U_{N/S}$ (where N/S is an abbreviation for North/South):

$$U = \exp[iq_{N/S}^a T_a] U_{N/S}. \quad (\text{B12})$$

By defining the momentum p_a conjugate to q^a (N/S labels are suppressed),

$$p_a \equiv \pi_b A(q)_{ba}, \quad (\text{B13})$$

the symplectic form (B1) will have a flat form:

$$\omega_{SU(N)} = dp_a \wedge dq^a. \quad (\text{B14})$$

We can therefore apply the implicit, symplectic integrators for the unconstrained variables in a given patch by taking (q, p) as the phase space variables.

The complication arises when the trajectory steps over the boundary between the patches. Note that preserving the symplecticity and the conservation of H can be dealt with straightforwardly because we know the transformation laws for (q^a, p_a) from Eqs. (B12) and (B13). However, it is difficult to determine which coordinate system to use in a reversible way. In fact, for a finite τ , the force vector differs depending on the choice of the coordinates. Accordingly, tedious exception handling occurs for the cases where the update steps over the boundary with the initially chosen coordinate system but does not for the reversed sequence. For a nontrivial kernel G , the change of coordinates on one link affects the determination for the other links, giving rise to a global optimization problem. We did not pursue this direction since it was already difficult to maintain reversibility for a small-size system in a systematic way.

APPENDIX C: MORE ON THE EXACTNESS OF THE ALGORITHM

In this appendix, we elaborate on reversibility for the decomposition scheme developed in Sec. II B. Since the main concern will be in relation to the center ambiguity, we demonstrate the reversibility first for the update in the $U(1)$ direction and drop the Φ -dependence:

$$\Omega' \equiv e^{i\delta\omega} \Omega. \quad (\text{C1})$$

According to Eq. (8), we calculate

$$\delta\theta = \frac{1}{N} \arg e^{iN\delta\omega} = \frac{1}{N} [N\delta\omega], \quad (\text{C2})$$

where $[\theta]$ is the projection of the angular variable θ onto the range $[-\pi, \pi]$. We obtain

$$U' = e^{i(\delta\omega - \delta\theta)} U = e^{i(\delta\omega - \frac{1}{N}[N\delta\omega])} U. \quad (\text{C3})$$

The map is manifestly reversible, except for the case with $[N\delta\omega] = -\pi$ to be dealt with later, because the reverse process corresponds to switching the sign of $\delta\omega$, for which Eq. (C3) still applies with the negative sign, correctly reproducing (U, θ) from (U', θ') . A general update of Ω can be given by a left multiplication of an $SU(N)$ matrix in Eq. (C1), which does not change the conclusion.

Given that our decomposition scheme provides a reversible update, the HMC remains exact. In fact, as mentioned in Sec. II D, a state of the Markov chain can be labeled as (W, n) [$W \in GL(N, \mathbb{C}), n \in \mathbb{Z}_N$]. Note, however, that the volume element in the W -space does not depend on n for the same W . The leapfrog integrators in the W -space guarantee the volume preservation for the extended phase space measure $(dW)(dp)$ thanks to the functional form of the force vector, irrespective of n that the updated configuration will be labeled by. The reversibility and the volume preservation then guarantee the exactness of the algorithm.

The exceptional case with $[N\delta\omega] = -\pi$ is measure zero, and thus it does not affect the algorithm under perfect real arithmetic. Nevertheless, it may be of academic interest to show that the algorithm is exact even when the exceptional case is taken into account by using the skew detailed balance [30]. Let us write the transition probability from the state (U, θ, Φ) to (U', θ', Φ') as $P(U', \theta', \pi' | U, \theta, \Phi)$, in which the range of the angular variable is $[-\pi, \pi]$. We further introduce the transition probability $P_R(U', \theta', \Phi' | U, \theta, \Phi)$ that represents the same algorithm except that the range of the angular variable is replaced by $(-\pi, \pi]$. Note that P_R serves as the reverse algorithm of P including the exceptional case by accommodating the edge value with the different sign. We then see that they satisfy the skew detailed balance relation

$$\begin{aligned} & P(U', \theta', \Phi' | U, \theta, \Phi) e^{-S(U) - S_0(\Phi)} \\ &= P_R(U, \theta, \Phi | U', \theta', \Phi') e^{-S(U') - S_0(\Phi')}, \end{aligned} \quad (\text{C4})$$

which shows that the Boltzmann factor is the fixed point of the transition matrix P as we see by integrating over the triplet (U, θ, Φ) . The algorithm is therefore exact.

We finally comment on the discontinuous jump of (U', θ') at $\delta\omega = \pi/N$ which we encounter when we continuously increase $\delta\omega$ in Eq. (C2). Such a jump generically implies a significant deviation from the continuous time trajectory, leading to a violation of the energy conservation. While the actual probability of encountering the discontinuity can be system-dependent, we can argue that it only happens when the acceptance rate would be low in the first place due to the appearance of the large force F . In fact, for the worst case where F is aligned with the $U(1)$

direction, a nontrivial jump occurs when we have the force with a sizable magnitude for the single link variable $\tau F \sim O(1/N)$, where τF should usually be suppressed by a rational order of the volume. At least for small N , such a sizable update would mean a mistuning of τ that leads to a small acceptance rate. Conversely, in practical calculations with large volumes, the discontinuous jump rarely occurs and hardly affects the acceptance rate. We emphasize that the algorithm is exact even with the discontinuous jumps as discussed in the first half of the appendix.

APPENDIX D: ALTERNATIVE DECOMPOSITION WITHOUT THE $\mathbb{Z}_N$ AMBIGUITY

In this appendix, we consider an alternative decomposition:

$$J(U, \theta, \Phi) = \begin{bmatrix} -\text{Im}[\Phi \exp(i\theta T_0) T_a U]_{jk} & \text{Re}[\Phi \exp(i\theta T_0) T_a U]_{jk} \\ -\text{Im}[e^{i\theta} (\Phi T_0 U)_{jk}] & \text{Re}[e^{i\theta} (\Phi T_0 U)_{jk}] \\ \text{Re}[T_a \exp(i\theta T_0) U]_{jk} & \text{Im}[T_a \exp(i\theta T_0) U]_{jk} \\ \text{Re}[\exp(i\theta T_0) U]_{jk} & \text{Im}[\exp(i\theta T_0) U]_{jk} \end{bmatrix}. \quad (\text{D3})$$

Compared to Eq. (7), with this decomposition, (U, θ) can simply be given from Ω by Eq. (D2) and there are no multiple solutions with θ in the range $-\pi \leq \theta < \pi$. The removal of the $\mathbb{Z}_N$ ambiguity can be understood as a breaking of the connection between the elements of the center $\mathbb{Z}_N$ and the angle θ . Specifically, a right multiplication of $\exp(i\theta T_0)$ by an element of $\mathbb{Z}_N$, $e^{2\pi i n/N} \mathbb{1}_N$, cannot be absorbed by a shift of θ .

With the decomposition given in the main text, the $\mathbb{Z}_N$ ambiguity demands special care when W is treated independently from the variables (U, θ, Φ) . This includes when we perform a hot start and when we save a configuration in terms of the W variable (see Sec. II D). The removal of the $\mathbb{Z}_N$ ambiguity simplifies the algorithm in this regard.

We provide an implementation of the algorithm with the decomposition (D1) in the GRID PYTHON TOOLKIT (GPT) [23], which uses Grid [31,32] for performance portability.

APPENDIX E: REDUCED HAMILTONIAN EQUATIONS

In this appendix, we derive the reduced Hamiltonian equations in the variables (U, θ, Φ) in the continuous time limit.

It is convenient to write the decomposed bases collectively as

$$W = \Phi \exp(i\theta T_0) U, \quad T_0 \equiv \text{diag}(1, 0, \dots, 0), \quad (\text{D1})$$

and show that the $\mathbb{Z}_N$ ambiguity mentioned in Sec. II B can be removed. The argument holds for any Hermitian matrix T_0 with the same eigenvalues and their geometric multiplicity as those of the T_0 defined by Eq. (D1).

As in the main text, we first perform the polar decomposition (5) to obtain Ω and Φ . We then set θ and U as

$$\theta \equiv \arg \det \Omega, \quad U \equiv \exp(-i\theta T_0) \Omega. \quad (\text{D2})$$

The Jacobian matrix $J(U, \theta, \Phi)$ will be modified as

$$(\Theta^A) \equiv (\Theta_a, d\theta, d\phi_a, d\phi_0), \quad (\text{E1})$$

$$(D_A) \equiv (D_a, \partial_\theta, \partial_{\phi_a}, \partial_{\phi_0}). \quad (\text{E2})$$

We distinguish the upper and lower indices in the extended bases. The relation between the Jacobian matrix and the metric tensor (11) is

$$dw^I = \Theta^A J_A^I(w), \quad \mathbf{g} = g_{AB}(w) \Theta^A \Theta^B \quad (\text{E3})$$

with

$$g_{AB}(w) \equiv \delta_{IJ} J_A^I(w) J_B^J(w). \quad (\text{E4})$$

Defining the pairing between a tangent vector (or simply a differential operator) D and a one-form df ,

$$\langle D, df \rangle \equiv Df, \quad (\text{E5})$$

we find $\langle D_A, \Theta^B \rangle = \delta_A^B$. In particular,

$$\langle D_a, \Theta_b \rangle = -i \text{tr}[T_b D_a U U^{-1}] = \delta_{ab}, \quad (\text{E6})$$

$$\langle \partial_{\phi_a}, d\phi_b \rangle = \partial_{\phi_a} \phi_b = \delta_{ab}, \quad (\text{E7})$$

where we used $\Theta_a = -i \text{tr}[T_a dU U^{-1}]$.

We first note that, for an $SU(N)$ variable, the Hamiltonian equations with the symplectic form (B1) can be written as¹

$$\left\langle \frac{d}{dt}, \Theta_a \right\rangle = \partial_{\pi_a} H, \quad (\text{E12})$$

$$\frac{d\pi_a}{dt} = -D_a H - \pi_c f_{abc} \partial_{\pi_b} H, \quad (\text{E13})$$

where t is the MD time. Equation (E12) is equivalent to Eq. (B2) because

$$iT_a \left\langle \frac{d}{dt}, \Theta_a \right\rangle = \left\langle \frac{d}{dt}, \Theta \right\rangle = \dot{U} U^{-1} = iT_a \partial_{\pi_a} H, \quad (\text{E14})$$

where $\dot{U} \equiv dU/dt$.

Next, in the extended system, we have the symplectic form

$$\omega = dp_I \wedge dw^I = d(\pi_A \Theta^A), \quad (\text{E15})$$

¹In general, given a basis of the tangent space of the phase space, $\{D_\mu\}$, and the dual basis $\{\Theta^\mu\}$, we have the Hamiltonian vector field (see, e.g., Ref. [28]):

$$\text{where} \quad \frac{d}{dt} \equiv \omega^{\mu\nu} (D_\nu H) D_\mu, \quad (\text{E8})$$

$$\omega \equiv \frac{1}{2} \omega_{\mu\nu} \Theta^\mu \wedge \Theta^\nu, \quad (\omega^{\mu\nu}) \equiv (\omega_{\mu\nu})^{-1}, \quad (\text{E9})$$

and $\omega_{\mu\nu} = -\omega_{\nu\mu}$. For $\omega = \omega_{SU(N)}$, with $\{D_\mu\} = \{D_a, \partial_{\pi_a}\}$ and $\{\Theta^\mu\} = \{\Theta_a, d\pi_a\}$, Eqs. (E12) and (E13) can be derived by noting that:

$$(\omega_{\mu\nu}) = \begin{pmatrix} -\pi_c f_{abc} & -\delta_{ab} \\ \delta_{ab} & 0 \end{pmatrix}, \quad (\text{E10})$$

$$(\omega^{\mu\nu}) = \begin{pmatrix} 0 & \delta_{ab} \\ -\delta_{ab} & -\pi_c f_{abc} \end{pmatrix}, \quad (\text{E11})$$

where

$$\pi_A \equiv J_A^I(w) p_I. \quad (\text{E16})$$

As in Sec. IV, we write $(\pi_A) = (\pi_a, \pi_\theta, \rho_a, \rho_0)^T$. The Hamiltonian equations can be written in two different ways:

$$\frac{dw^I}{dt} = \partial_{p_I} H, \quad \frac{dp_I}{dt} = -\partial_{w^I} H, \quad (\text{E17})$$

which are in the canonical form, and

$$\left\langle \frac{d}{dt}, \Theta^A \right\rangle = \partial_{\pi_A} H, \quad (\text{E18})$$

$$\frac{d\pi_A}{dt} = -D_A H - \pi_C f_{AB}^C \partial_{\pi_B} H, \quad (\text{E19})$$

analogously to Eqs. (E12) and (E13), where

$$d\Theta^A \equiv -(1/2) \Theta^B \wedge \Theta^C f_{BC}^A. \quad (\text{E20})$$

The continuous time limit of the MD update described by Eqs. (27)–(30) is Eq. (E17). Its equivalent description in the (U, θ, Φ) -basis is, therefore, Eqs. (E18) and (E19). Note that Θ^A are closed forms except for Θ_a . Accordingly, the structure constants f_{AB}^C are only nontrivial within the $SU(N)$ sector, and they reduce to f_{abc} in this sector. For a block-diagonal kernel $K(w)$ as given in Eq. (35), the time evolution of the (U, θ, Φ) variables factorize in Eqs. (E18) and (E19). We thus see that the reduced Hamiltonian equations for the physical variable U are exactly Eqs. (E12) and (E13). One can further derive the reduced equations for θ , ϕ_a , and ϕ_0 , which have the canonical form. For example,

$$\frac{d\phi_a}{dt} = \partial_{\rho_a} H, \quad \frac{d\rho_a}{dt} = -\partial_{\phi_a} H. \quad (\text{E21})$$

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