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Extending the Worldvolume Hybrid Monte Carlo algorithm to group manifolds†

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The Worldvolume Hybrid Monte Carlo (WV-HMC) method [arXiv:2012.08468] is a reliable and versatile algorithm towards solving the sign problem. This method eliminates the ergodicity problem inherent in methods based on Lefschetz thimbles at low cost. In this talk, in preparation for its application to lattice QCD, we extend the WV-HMC method to the case where the configuration space is a group manifold. The correctness of the algorithm is confirmed for the one-site model with complex coupling or with a topological term.

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1. Introduction

The sign problem has been a major obstacle in first-principle computations of various physical systems. A typical example is Yang-Mills theory with a topological term:

$$S(U) = S_0(U) - i\theta Q(U), \tag{1}$$

where $U = (U_{x,\mu})$ is a link variable, and $S_0(U)$ ($\in \mathbb{R}$) and $Q(U)$ ($\in \mathbb{R}$) are lattice expressions of the Yang-Mills action and the topological charge, respectively:

$$S_0(U) \sim \frac{1}{2g_0^2} \int d^d x \, \mathrm{tr}\, F_{\mu\nu}(x)^2, \tag{2}$$

$$Q(U) \sim \begin{cases} \frac{1}{32\pi^2} \int d^4 x \, \epsilon_{\mu\nu\rho\sigma} \, \mathrm{tr}\, F_{\mu\nu}(x) F_{\rho\sigma}(x) & (d=4) \\ \frac{1}{4\pi} \int d^2 x \, \epsilon_{\mu\nu} \, F_{\mu\nu}(x) & (d=2,\ U(1)). \end{cases} \tag{3}$$

Our concern is to numerically estimate the expectation value of a physical observable $O(U)$ defined by the path integral

$$\langle O \rangle \equiv \frac{\int (dU)\, e^{-S(U)}\, O(U)}{\int (dU)\, e^{-S(U)}}. \tag{4}$$

When $\theta \neq 0$, the action becomes complex, and thus the standard Markov chain Monte Carlo method cannot be adopted directly. The standard workaround for such systems with complex actions is the reweighting method, where $\langle O \rangle$ is estimated as a ratio of reweighted averages,

$$\langle O \rangle = \frac{\int (dU)\, e^{-S_0(U)}\, e^{i\theta Q(U)}\, O(U)}{\int (dU)\, e^{-S_0(U)}\, e^{i\theta Q(U)}} = \frac{\langle e^{i\theta Q(U)}\, O(U) \rangle_{\mathrm{rewt}}}{\langle e^{i\theta Q(U)} \rangle_{\mathrm{rewt}}}. \tag{5}$$

Here, the reweighted average $\langle f(U) \rangle_{\mathrm{rewt}}$ of a function $f(U)$ is defined by

$$\langle f(U) \rangle_{\mathrm{rewt}} \equiv \frac{\int (dU)\, e^{-S_0(U)}\, f(U)}{\int (dU)\, e^{-S_0(U)}}. \tag{6}$$

Since $S_0(U)$ and $Q(U)$ are local functionals, we expect that the numerator and the denominator in Eq. (5) are both exponentially small ($= e^{-O(V)}$) with lattice volume V due to highly oscillatory behaviors of integrands, and thus we need a sample whose size is exponentially large ($N_{\mathrm{conf}} = e^{O(V)}$) in order to reduce statistical errors of $O(1/\sqrt{N_{\mathrm{conf}}})$ relatively smaller than the mean ($= e^{-O(V)}$). This is the sign problem we consider in the present article.

The application of the Lefschetz thimble method [1–4] to Yang-Mills theories was first discussed in a seminal paper by Cristoforetti et al. [2], but it turned out that the original Lefschetz thimble method generally encounters the ergodicity problem [5–8] when the integration surface is deformed largely enough to relax the oscillatory behavior of path integrals. A general solution to this dilemma of the reduction of the sign problem and the appearance of the ergodicity problem was given by the *tempered Lefschetz thimble (TLT) method* [9–13], where the (parallel) tempering algorithm was implemented to the Lefschetz thimble method using the deformation parameter as a tempering parameter. This is the first algorithm that solves the sign and the ergodicity problems simultaneously. The drawback is its high numerical cost of $O(N^3)$ (N: number of degrees of freedom) together with the need to increase the number of replicas to maintain the acceptance in exchanging configurations. This drawback was then resolved in the *Worldvolume Hybrid Monte Carlo (WV-HMC) method* [14–16], where HMC updates are performed on the accumulation of deformed surfaces (*worldvolume*).

The main aim of this article is to extend the WV-HMC algorithm to group manifolds. We first prove Cauchy's theorem for group manifolds, then write down the path integral over the worldvolume. The correctness of the algorithm is checked for a simple model, the one-site model.

2. Cauchy's theorem

2.1 Cauchy's theorem for flat spaces

We start with recalling the role of Cauchy's theorem in the Lefschetz thimble method for the flat configuration space $\mathbb{R}^N = \{x = (x^i)\}$, where the expectation value $\langle O \rangle$ takes the form

$$\langle O \rangle \equiv \frac{\int_{\mathbb{R}^N} dx\, e^{-S(x)}\, O(x)}{\int_{\mathbb{R}^N} dx\, e^{-S(x)}}. \tag{7}$$

We first complexify the variable from $x = (x^i) \in \mathbb{R}^N$ to $z = (z^i) \in \mathbb{C}^N = \mathbb{R}^{2N}$, and assume that $e^{-S(z)}$ and $e^{-S(z)}\, O(z)$ are entire functions in $\mathbb{C}^N$. Then, the integration surface $\Sigma_0 = \mathbb{R}^N$ can be continuously deformed to a new surface Σ without changing the values of integrals as long as the boundaries at $|\mathrm{Re}\, z| \to \infty$ are kept fixed:

$$\langle O \rangle = \frac{\int_\Sigma dz\, e^{-S(z)}\, O(z)}{\int_\Sigma dz\, e^{-S(z)}}. \tag{8}$$

In the Lefschetz thimble method, we choose Σ such that $\mathrm{Im}\, S(z)$ is almost constant there in order to reduce the oscillatory behaviors of integrands.

It is Cauchy's theorem that guarantees this invariance of integrals (see Fig. 1):

Theorem 1. *Let $\mathcal{D}$ be a region in $\mathbb{C}^N = \mathbb{R}^{2N}$ and $f(z)$ a holomorphic function on $\mathcal{D}$. Then, the integral I_Σ of $f(z)$ over a real N-dimensional submanifold $\Sigma \subset \mathcal{D}$,*

$$I_\Sigma = \int_\Sigma dz\, f(z) \quad (dz \equiv dz^1 \wedge \cdots \wedge dz^N), \tag{9}$$

depends only on the boundary of Σ.

Proof: We set Σ and Σ' to be (oriented) real N-dimensional submanifolds in $\mathcal{D}$ with a common boundary, and $\mathcal{R}$ a region surrounded by Σ and Σ' (and thus $\partial\mathcal{R} = \Sigma' - \Sigma$). Then, due to Stokes' theorem, we have

$$I_{\Sigma'} - I_\Sigma = \int_{\partial\mathcal{R}} dz\, f(z) = \int_{\mathcal{R}} d[dz f(z)] = (-1)^N \int_{\mathcal{R}} dz \wedge df(z). \tag{10}$$

Here, since $df(z) = dz^i\, (\partial f(z)/\partial z^i) + d\bar{z}^i\, (\partial f(z)/\partial \bar{z}^i) = dz^i\, (\partial f(z)/\partial z^i)$, we have

$$dz \wedge df(z) = \underbrace{(dz^1 \wedge \cdots \wedge dz^N) \wedge dz^i}_{=0} \frac{\partial f(z)}{\partial z^i} = 0, \tag{11}$$

which means that $I_{\Sigma'} - I_\Sigma = 0$.

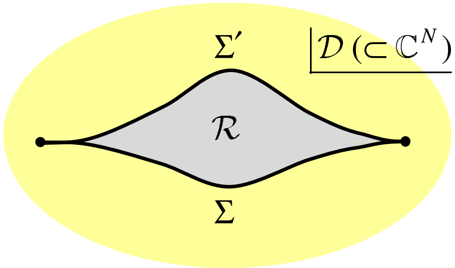

Figure 1: Cauchy's theorem for $\mathbb{C}^N$.

2.2 Cauchy's theorem for group manifolds

Now we consider the case where the configuration space is a group manifold and the expectation value is given by a path integral of the form

$$\langle O\rangle \equiv \frac{\int_G (dU)\, e^{-S(U)}\, O(U)}{\int_G (dU)\, e^{-S(U)}}. \tag{12}$$

Below we construct Cauchy's theorem for group manifolds, which will be used in the next section to define the Lefschetz thimble method (and eventually the WV-HMC method) for group manifolds.

We first recall the definition of the Haar measure (dU) on a compact group $G = \{U\}$. Let $\mathrm{Lie}\,G$ be the Lie algebra of G with a basis $\{T_a\}$ $(a = 1,\dots,N(\equiv \dim G))$ which are taken to be anti-hermitian ($T_a^\dagger = -T_a$) and normalized as $\mathrm{tr}\,T_a T_b = -\delta_{ab}$. We introduce the Maurer-Cartan 1-form by $\theta_0 \equiv dU\,U^{-1} = T_a\,\theta_0^a$ (θ_0^a: real 1-form), and define the metric by

$$ds^2 \equiv \mathrm{tr}\,\theta^\dagger\theta\;(= -\mathrm{tr}\,\theta\theta) = (\theta_0^a)^2, \tag{13}$$

which represents the distance between U, $U + dU \in G$. The last expression indicates that $\{\theta_0^a\}$ are the vielbeins of the metric. The Haar measure (dU) is then defined as the invariant volume element, $(dU) \equiv \theta_0^1 \wedge \cdots \wedge \theta_0^N$ (we ignore the normalization, which is irrelevant in the following discussions). Note that the metric (and thus the Haar measure) is bi-invariant (i.e., both left- and right-invariant).

The complexification $G^{\mathbb{C}}$ of G is defined as follows. We first complexify the linear space $\mathrm{Lie}\,G = \bigoplus_a \mathbb{R}T_a$ to $(\mathrm{Lie}\,G)^{\mathbb{C}} \equiv \bigoplus_a \mathbb{C}T_a$ and introduce the commutator as the natural extension of the original commutator,

$$[X+iY, X'+iY'] \equiv ([X,X'] - [Y,Y']) + i([X,Y'] + [X',Y]) \quad (X,Y,X',Y' \in \mathrm{Lie}\,G). \tag{14}$$

The complexified group $G^{\mathbb{C}}$ is then defined as the set of finite products of the exponentials of elements in $(\mathrm{Lie}\,G)^{\mathbb{C}}$:

$$G^{\mathbb{C}} \equiv \left\{ e^{T_a z^a} e^{T_a z'^a} \cdots e^{T_a z''^a} \,|\, z^a, z'^a, \dots, z''^a \in \mathbb{C} \right\}. \tag{15}$$

Then the following theorem holds (see Fig. 2) [17]:

Theorem 2. *Let $\mathcal{D}$ be a region in $G^{\mathbb{C}}$ and $f(U)$ a holomorphic function on $\mathcal{D}$. Then, the integral I_Σ of $f(U)$ over a real N-dimensional submanifold $\Sigma \subset \mathcal{D}$,*

$$I_\Sigma = \int_\Sigma (dU)_\Sigma\, f(U), \tag{16}$$

depends only on the boundary of Σ*. Here, for* U, $U + dU \in \Sigma$ *we introduce the Maurer-Cartan form on* Σ *as*

$$\theta \equiv dU\,U^{-1} = T_a\,\theta^a, \tag{17}$$

from which the holomorphic N*-form* $(dU)_\Sigma$ *is defined as* $(dU)_\Sigma \equiv \theta^1 \wedge \cdots \wedge \theta^N$.

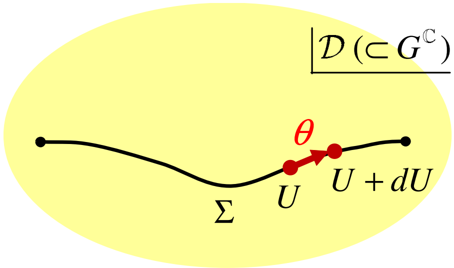

Figure 2: Cauchy's theorem for $G^{\mathbb{C}}$ [17].

Proof: We first notice that the Maurer-Cartan equation $d\theta = \theta \wedge \theta$ can be rewritten as $d\theta^a = (1/2)\,C_{bc}{}^a\,\theta^b \wedge \theta^c$ ($C_{bc}{}^a$ are the structure constants, $[T_b, T_c] = C_{bc}{}^a T_a$), from which follows that $(dU)_\Sigma$ is closed, $d(dU)_\Sigma = 0$. Then, the rest of proof goes in the same way as the flat case.

3. WV-HMC for group manifolds

Denoting the elements on the original integration surface by U_0 ($\in \Sigma_0 \equiv G$), Cauchy's theorem allows us to rewrite the expression (12) to the following form (see Fig. 3):

$$\langle O \rangle = \frac{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}\, O(U)}{\int_\Sigma (dU)_\Sigma\, e^{-S(U)}}. \tag{18}$$

Thus, even when the original path integral on $\Sigma_0 = G$ suffers from the severe sign problem due to the highly oscillatory behavior of $e^{-i\,\mathrm{Im}\,S(U)}$, the situation is expected to be significantly remedied if $\mathrm{Im}\,S(U)$ is almost constant on the new integration surface Σ.

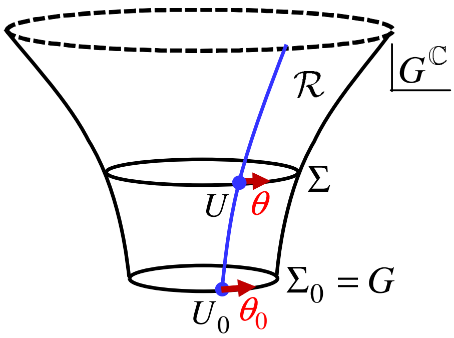

Figure 3: Deformed surface Σ and worldvolume $\mathcal{R}$ in $G^{\mathbb{C}}$ [17].

Such deformation is given by the anti-holomorphic flow equation,

$$\dot{U} = [DS(U)]^\dagger\, U \quad \text{with} \quad U|_{t=0} = U_0, \tag{19}$$

where $Df(U)$ for a holomorphic function $f(U)$ is defined by

$$\delta f(U) \equiv \mathrm{tr}\,[(\delta U\,U^{-1})\,Df(U)]. \tag{20}$$

One can easily see that the real part $\mathrm{Re}\,S(U)$ always increase along the flow except at critical points (where $DS(U)$ vanishes) while $\mathrm{Im}\,S(U)$ is kept constant along the flow from the (in)equality

$$[S(U)]^{\cdot} = \mathrm{tr}\,[(\dot{U}\,U^{-1})DS(U)] = \mathrm{tr}\,[(DS(U))^{\dagger}\,(DS(U))] \geq 0. \tag{21}$$

We are now in a position to rewrite the path integral (18) to the integral over a worldvolume. We first notice that when we set the deformed surface to $\Sigma = \Sigma_t$ (deformed surface at flow time t), the numerator and the denominator are both independent of t due to Cauchy's theorem, so that we can take their averages over t separately with an arbitrary common weight $e^{-W(t)}$:

$$\langle \mathcal{O} \rangle = \frac{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}\, \mathcal{O}(U)}{\int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}} = \frac{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}\, \mathcal{O}(U)}{\int dt\, e^{-W(t)} \int_{\Sigma_t} (dU)_{\Sigma_t}\, e^{-S(U)}}, \tag{22}$$

which can be regarded as a ratio of integrals over the *worldvolume* $\mathcal{R} \equiv \bigcup_t \Sigma_t$.

The invariant volume element $|dU|_{\mathcal{R}}$ of $\mathcal{R}$ can be expressed as follows. We first introduce the Maurer-Cartan form on $G^{\mathbb{C}}$ as $\Theta \equiv dUU^{-1}$, and define a metric as $ds^2 \equiv \mathrm{tr}\,\Theta^{\dagger}\Theta$, which represents the distance between U, $U + dU \in G^{\mathbb{C}}$. Note that the metric is only right-invariant with respect to $G^{\mathbb{C}}$ but is still bi-invariant with respect to the original compact group G. Then, the induced metric ds^2_{Σ} on $\Sigma = \Sigma_t$ is given by $ds^2_{\Sigma} \equiv \mathrm{Re}\,\mathrm{tr}\,\theta^{\dagger}\theta$, where $\theta = dUU^{-1}$ is the Maurer-Cartan form on Σ (U, $U + dU \in \Sigma$). Noting that θ^a is linear in θ_0^a of the form $\theta^i = E^i_a\,\theta^a_0$, we can rewrite the induced metric as $ds^2_{\Sigma} = \gamma_{ab}\,\theta^a_0\theta^b_0$ with $\gamma_{ab} = \mathrm{Re}\,\overline{E^i_a}E^i_b$. Then the invariant volume element on Σ_t is given by

$$|dU|_{\Sigma_t} = \sqrt{\gamma}\,(dU_0), \tag{23}$$

with which the invariant volume element on $\mathcal{R}$ is expressed as

$$|dU|_{\mathcal{R}} = \alpha dt\,|dU|_{\Sigma_t} = \alpha\sqrt{\gamma}\,dt\,(dU_0), \tag{24}$$

where αdt is the geodesic distance between Σ_t and Σ_{t+dt} at U (see Fig. 4). Meanwhile, the holomorphic N-form can be written as

$$(dU)_{\Sigma} = \det E\,(dU_0). \tag{25}$$

Thus, we can rewrite the path integral (22) to the form [17]

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)}\, \mathcal{F}(U)\, \mathcal{O}(U)}{\int_{\mathcal{R}} |dU|_{\mathcal{R}}\, e^{-V(U)}\, \mathcal{F}(U)}, \tag{26}$$

where $V(U)$ and $\mathcal{F}(U)$ are the potential and the associated reweighting factor, respectively, that are defined as follows:

$$V(U) \equiv \mathrm{Re}\,S(U) + W(t(U)), \tag{27}$$

$$\mathcal{F}(U) \equiv \frac{dt\,(dU)_{\Sigma_t}}{|dU|_{\mathcal{R}}}\, e^{-i\mathrm{Im}\,S(U)} = \alpha^{-1}\,\frac{\det E}{\sqrt{\gamma}}\, e^{-i\mathrm{Im}\,S(U)}. \tag{28}$$

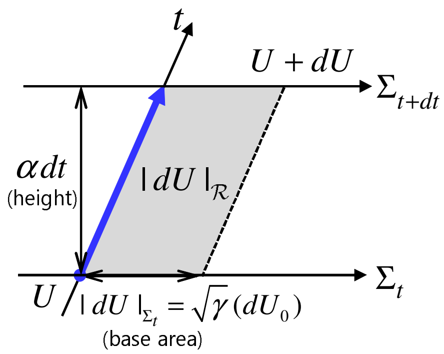

Figure 4: Invariant volume element $|dU|_{\mathcal{R}}$ of worldvolume $\mathcal{R}$ [17].

The path integral (26) can be further rewritten to an integral over a tangent bundle $T\mathcal{R} = \{(U,\pi)\,|\,U \in \mathcal{R},\ \pi \in T_U\mathcal{R}\}$ $(\subset TG^{\mathbb{C}})$ of the form [17]

$$\langle O \rangle = \frac{\int_{T\mathcal{R}} \omega^{N+1} e^{-H(U,\pi)}\, \mathcal{F}(U)\, O(U)}{\int_{T\mathcal{R}} \omega^{N+1} e^{-H(U,\pi)}\, \mathcal{F}(U)}, \tag{29}$$

where the symplectic 2-form ω and the Hamiltonian $H(U,\pi)$ are given, respectively, by

$$\omega = d(\mathrm{Re}\,\mathrm{tr}\,\pi^\dagger\theta), \quad H(U,\pi) = \frac{1}{2}\,\mathrm{tr}\,\pi^\dagger\pi + V(U). \tag{30}$$

Once the last expression (29) is obtained, one can resort to the standard algorithm of WV-HMC [14, 16], which consists of constrained molecular dynamics (RATTLE) [18, 19] in the complexified space ($G^{\mathbb{C}}$ in the current case) satisfying the exact reversibility and the exact volume preservation as well as the approximate conservation of energy to the order of Δs^2 at each molecular dynamics step of step size Δs (as is the case for standard HMC algorithms using leapfrogs). See Ref. [17] for details.

4. Numerical test: one-site model

As a numerical test of the algorithm, we consider the one-site model defined by the action

$$\begin{aligned} S(U) &\equiv \beta e(U) - i\theta q(U) \\ &\equiv -\frac{\beta}{4}\,\mathrm{tr}\,(U + U^{-1}) - \frac{\theta}{4\pi}\,\mathrm{tr}\,(U - U^{-1}). \end{aligned} \tag{31}$$

4.1 $G = SU(2)$ with pure imaginary coupling

We consider $G = SU(2)$ with $\beta \in i\,\mathbb{R}$ and $\theta = 0$. The analytic result is $\langle e \rangle = -I_2(\beta)/I_1(\beta)$, where I_k $(k = 1, 2)$ are the modified Bessel functions of the first kind. Figure 5 shows that the obtained results are in good agreement with analytic values.

4.2 $G = U(2)$ with a topological term

We consider $G = U(2)$ with $\beta,\ \theta \in \mathbb{R}$. The analytic result is $\langle q \rangle = (i\theta/2\pi^2\zeta^2)\, I_1^2(\zeta)/[I_0^2(\zeta) - I_1^2(\zeta)]$ with $\zeta = (1/2)\sqrt{\beta^2 - (\theta/\pi)^2}$. Note that $U(2)$ is *not* a simple product $SU(2)\times U(1)$ (actually

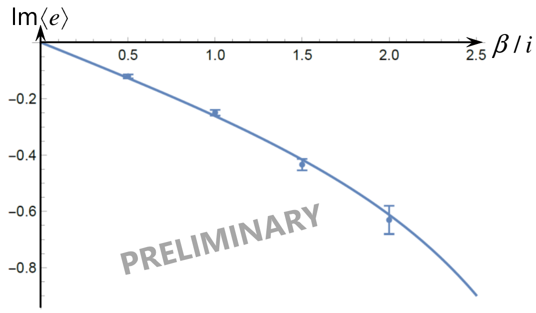

Figure 5: Values of Im $\langle e \rangle$ for various $\beta \in i\,\mathbb{R}$.

$U(2) = SU(2) \times U(1)/\mathbb{Z}_2$), and thus contributions to the topological term are not the same as those from pure $U(1)$ subgroup although $SU(2)$ elements do not affect the topological term due to G-parity. Figure 6 shows the results for $\beta = 0.5$ and $\theta = n\pi$ ($n = 1, \ldots, 5$). We again see good agreement with analytic values.

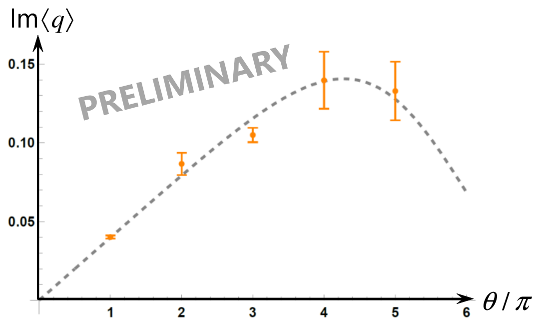

Figure 6: Values of Im $\langle q \rangle$ for various θ with $\beta = 0.5$.

5. Conclusion and outlook

We have shown that WV-HMC algorithm can be extended to group manifolds [17]. The key ingredient of the construction is again Cauchy's theorem, which allows the introduction of the worldvolume for a given group manifold and a given complex action. We have confirmed the correctness of the algorithm by performing numerical simulations for the one-site model.

The application of the present formalism to lattice gauge theories is straightforward, on which we are working now. The result on pure Yang-Mills theory with finite θ will be reported elsewhere.

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